



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 09:58 am BST

PDB ID : 2O5J
Title : Crystal structure of the T. thermophilus RNAP polymerase elongation complex with the NTP substrate analog
Authors : Vassilyev, D.G.; Vassilyeva, M.N.
Deposited on : 2006-12-06
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

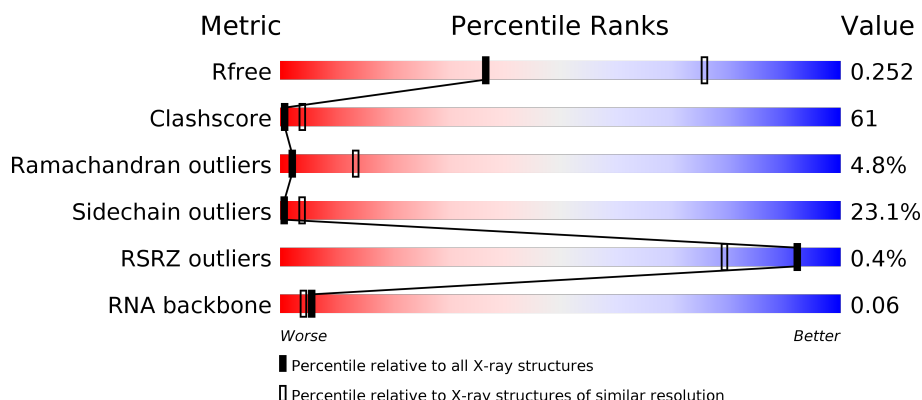
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	G	23	<div> <div>17%</div> <div>57%</div> <div>22%</div> <div>.</div> </div>
1	X	23	<div> <div>17%</div> <div>61%</div> <div>13%</div> <div>9%</div> </div>
2	H	16	<div> <div>19%</div> <div>81%</div> </div>
2	Y	16	<div> <div>31%</div> <div>69%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	14	<div><div></div><div>21%64%7%7%</div></div>
3	Z	14	<div><div></div><div>29%64%7%</div></div>
4	A	315	<div><div></div><div>21%42%10%27%</div></div>
4	B	315	<div><div>%</div><div></div><div>22%40%11%27%</div></div>
4	K	315	<div><div></div><div>23%42%8%27%</div></div>
4	L	315	<div><div></div><div>18%42%13%27%</div></div>
5	C	1119	<div><div></div><div>23%57%19%.</div></div>
5	M	1119	<div><div>%</div><div></div><div>23%58%18%. .</div></div>
6	D	1524	<div><div></div><div>21%47%14%.17%</div></div>
6	N	1524	<div><div></div><div>22%47%14%.17%</div></div>
7	E	99	<div><div></div><div>22%49%23%. .</div></div>
7	O	99	<div><div></div><div>20%59%16%. .</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 51213 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a DNA chain called 5'-D(P*CP*CP*CP*TP*GP*TP*CP*TP*GP*GP*CP*GP*TP*TP*CP*GP*CP*GP*CP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	23	Total	C	N	O	P	0	0	0
			467	220	80	144	23			
1	X	23	Total	C	N	O	P	0	0	0
			467	220	80	144	23			

- Molecule 2 is a RNA chain called 5'-R(P*GP*AP*GP*UP*CP*UP*GP*CP*GP*GP*CP*GP*CP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	16	Total	C	N	O	P	0	0	0
			347	153	64	114	16			
2	Y	16	Total	C	N	O	P	0	0	0
			347	153	64	114	16			

- Molecule 3 is a DNA chain called 5'-D(*AP*AP*CP*GP*CP*CP*AP*GP*AP*CP*AP*GP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	13	Total	C	N	O	P	0	0	0
			270	126	57	74	13			
3	Z	13	Total	C	N	O	P	0	0	0
			270	126	57	74	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase alpha chain.

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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is a protein called DNA-directed RNA polymerase beta chain.

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

- Molecule 6 is a protein called DNA-directed RNA polymerase beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	1264	Total	C	N	O	S	0	0	0
			9960	6302	1773	1852	33			
6	N	1264	Total	C	N	O	S	0	0	0
			9960	6302	1773	1852	33			

- Molecule 7 is a protein called DNA-directed RNA polymerase omega chain.

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

- Molecule 8 is ZINC ION (three-letter code: 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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

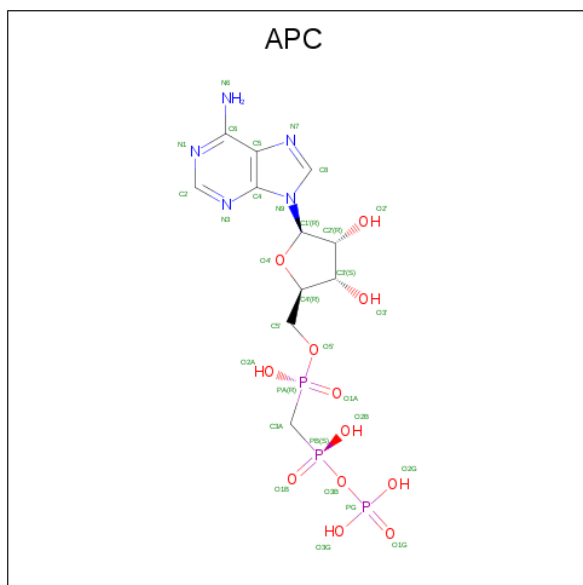
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Mg	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	N	2	Total	Mg	0	0
			2	2		

- Molecule 10 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	106	Total 106	O 106	0	0
11	B	82	Total 82	O 82	0	0
11	C	482	Total 482	O 482	0	0
11	D	506	Total 506	O 506	0	0
11	E	60	Total 60	O 60	0	0
11	K	86	Total 86	O 86	0	0
11	L	104	Total 104	O 104	0	0
11	M	483	Total 483	O 483	0	0
11	N	491	Total 491	O 491	0	0
11	O	39	Total 39	O 39	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: 5'-D(P*CP*CP*CP*TP*GP*TP*CP*TP*GP*GP*CP*GP*TP*TP*CP*GP*CP*GP*CP*GP*CP*CP*G)-3'

Chain G: 



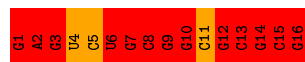
- Molecule 1: 5'-D(P*CP*CP*CP*TP*GP*TP*CP*TP*GP*GP*CP*GP*TP*TP*CP*GP*CP*GP*CP*GP*CP*CP*G)-3'

Chain X: 



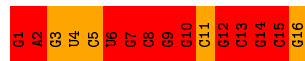
- Molecule 2: 5'-R(P*GP*AP*GP*UP*CP*UP*GP*CP*GP*GP*CP*GP*CP*GP*CP*G)-3',

Chain H: 

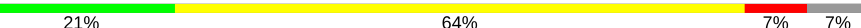


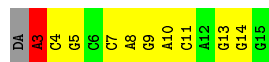
- Molecule 2: 5'-R(P*GP*AP*GP*UP*CP*UP*GP*CP*GP*GP*CP*GP*CP*GP*CP*G)-3',

Chain Y: 



- Molecule 3: 5'-D(*AP*AP*CP*GP*CP*CP*AP*GP*AP*CP*AP*GP*GP*G)-3'

Chain I: 

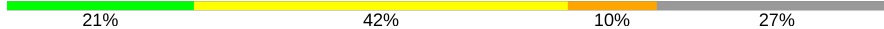


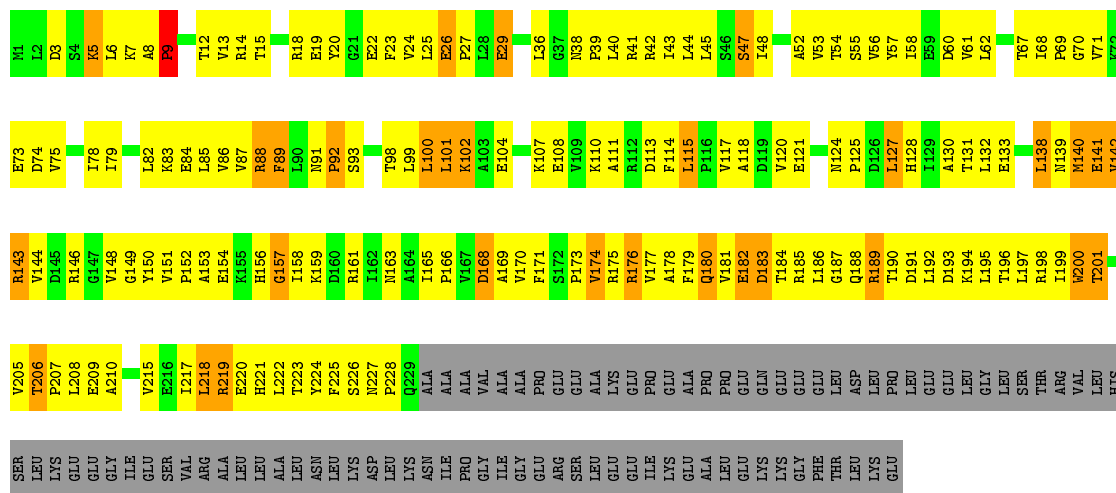
- Molecule 3: 5'-D(*AP*AP*CP*GP*CP*CP*AP*GP*AP*CP*AP*GP*GP*G)-3'

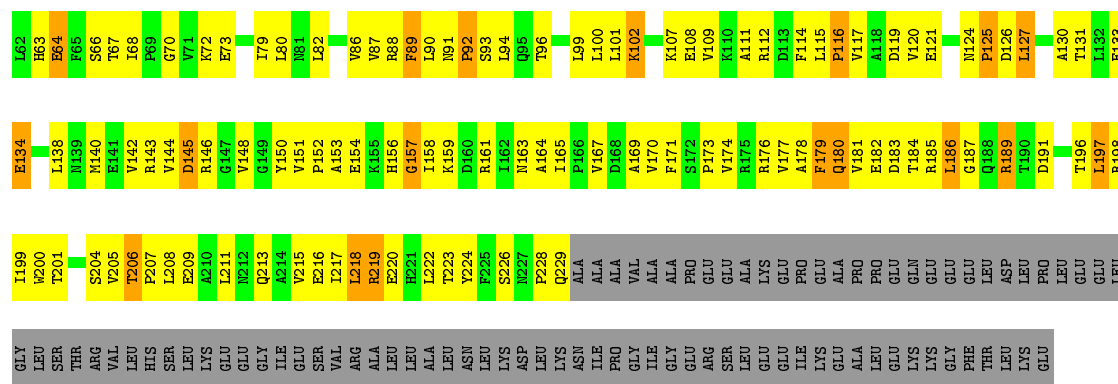
Chain Z: 



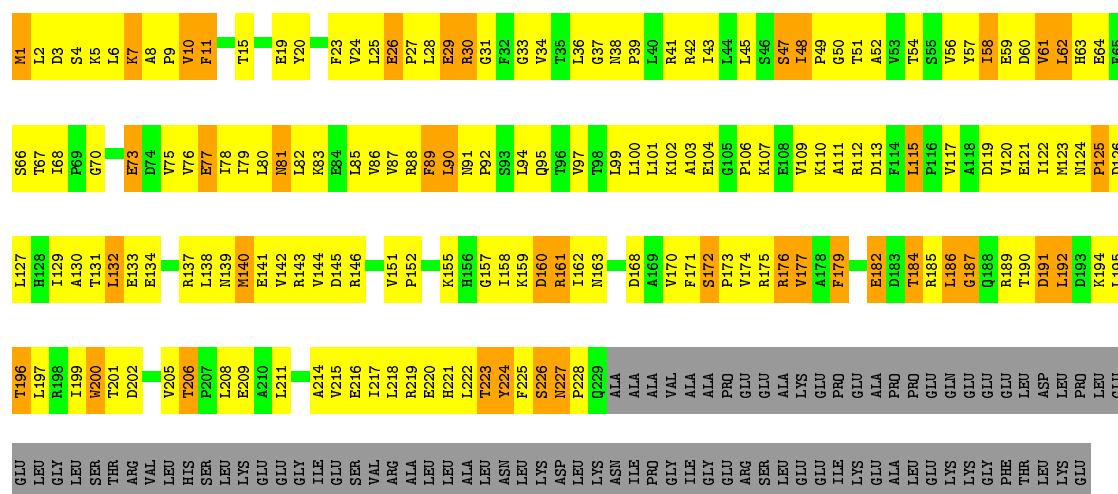
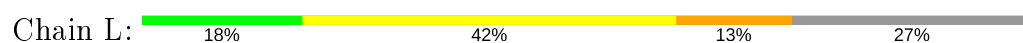
• Molecule 4: DNA-directed RNA polymerase alpha chain

Chain A: 

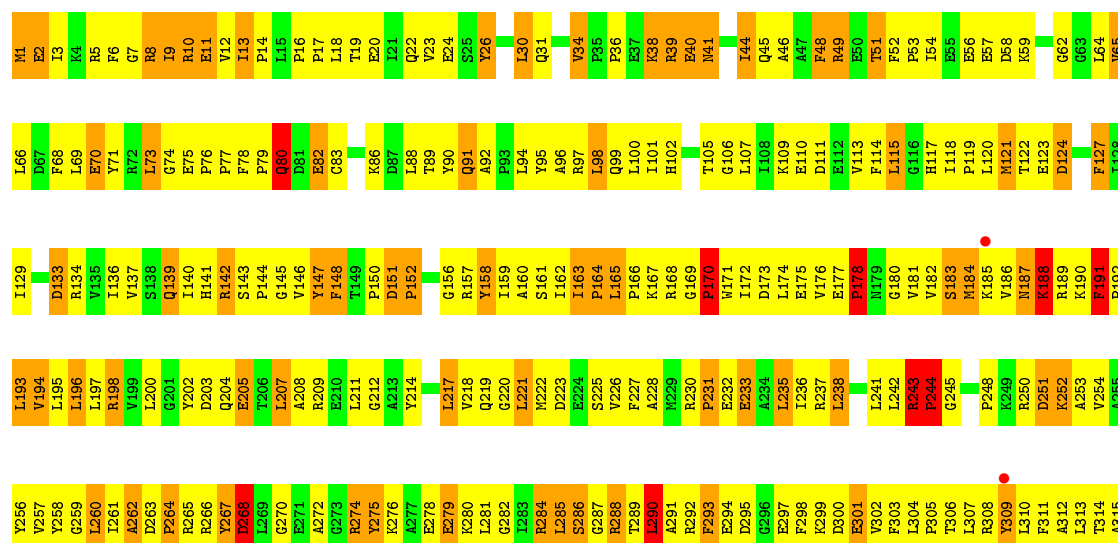




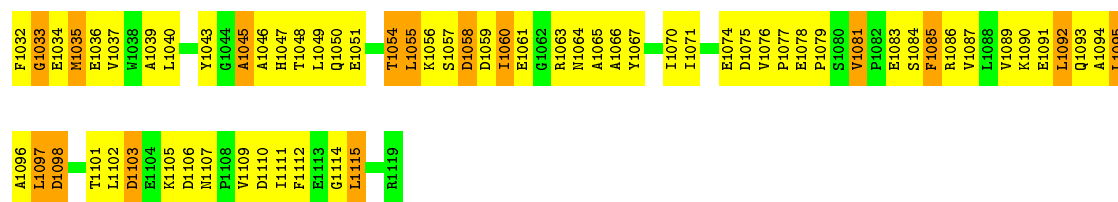
• Molecule 4: DNA-directed RNA polymerase alpha chain



• Molecule 5: DNA-directed RNA polymerase beta chain

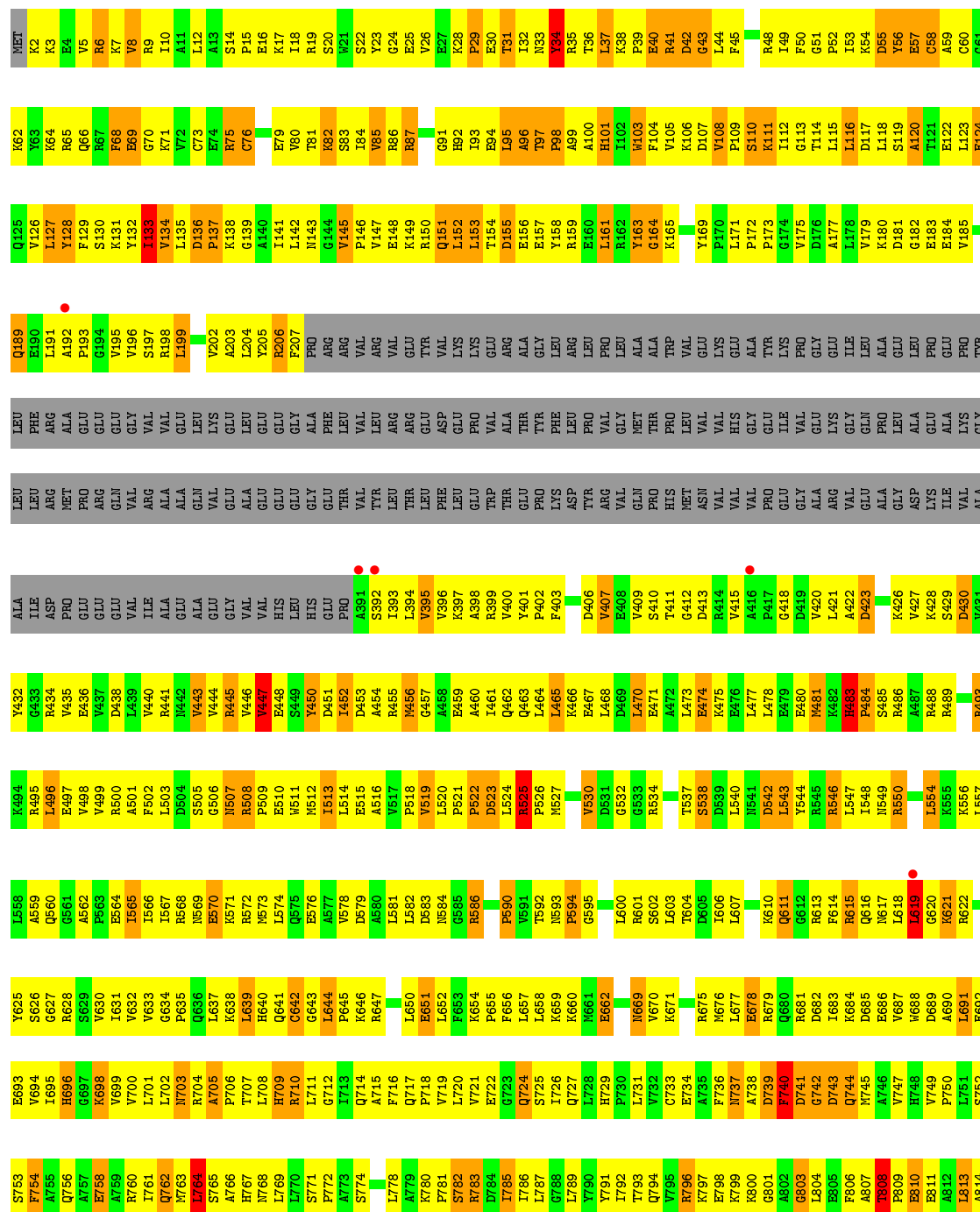


K971	V972	V973	L974	V975	D976	G977	R978	T979	G980	A981	P982	L983	E984	G985	P986	L987	V988	V989	G990	Q991	M992	F993	L994	M995	K996	L997	M998	H999	M1000	V1001	E1002	D1003	K1004	M1005	H1006	A1007	R1008	S1009	T1010	G1011	P1012	Y1013	S1014	L1015	I1016	T1017	Q1018	Q1019	P1020	L1021	G1022	G1023	A1025	L1026	F1027	Q1030	R1031	
L839	A840	M841	R842	H843	G844	K845	K846	G847	V848	V849	K850	K851	L852	T853	L854	V855	E856	D857	M858	P859	H860	L861	P862	D863	D864	T865	P866	V867	D868	V869	L870	L871	M872	L873	L874	G875	V876	P877	S878	R879	M880	N881	L882	G883	Q884	L885	L886	E887	T888	H889	L892	A893	G894	L897	G898	Q899	Q900	
Y901	I902	S903	P904	I905	F906	D907	K908	A909	R910	E911	P912	K913	I914	K915	R916	V917	L918	E919	Q920	F926	I927	G927	K928	L929	A930	K931	E932	V933	D937	K938	R939	D940	P941	L942	V943	R946	A947	E948	K949	V953	T954	P955	G956	T958	P959	E960	E961	Q962	L963	L966	P967	L968	Q969	Q1030	R1031			
S776	I777	G778	F779	E780	K781	A782	R783	D784	K785	V786	D787	K788	S789	L790	R791	V792	P793	P794	G798	I799	L800	L801	R802	T803	R804	T805	L806	R807	V808	G809	D810	P811	G812	R813	L814	E815	L816	P817	G818	V819	R820	E821	V822	R823	R824	V827	R828	Q829	K830	R831	K832	L833	Q834	V835	G836	D837	R838	
L839	A840	M841	R842	H843	G844	K845	K846	G847	V848	V849	K850	K851	L852	T853	L854	V855	E856	D857	M858	P859	H860	L861	P862	D863	D864	T865	P866	V867	D868	V869	L870	L871	M872	L873	L874	G875	V876	P877	S878	R879	M880	N881	L882	G883	Q884	L885	L886	E887	T888	H889	L892	A893	G894	L897	G898	Q899	Q900	
Y901	I902	S903	P904	I905	F906	D907	K908	A909	R910	E911	P912	K913	I914	K915	R916	V917	L918	E919	Q920	F926	I927	G927	K928	L929	A930	K931	E932	V933	D937	K938	R939	D940	P941	L942	V943	R946	A947	E948	K949	V953	T954	P955	G956	T958	P959	E960	E961	Q962	L963	L966	P967	L968	Q969	Q1030	R1031			
E711	A712	R713	D714	K715	T716	L717	A718	P719	D720	K721	I726	P727	R728	L729	M730	S731	G732	A733	L734	R735	D736	L737	R738	T739	E740	G741	V742	V743	R744	I745	E748	V749	K750	E751	G752	D753	I754	L755	V756	G757	E758	T759	K762	G763	E764	S765	E766	V767	T701	P768	S702	I703	P704	R705	E706	L774	R775	
Q647	R648	V649	E650	K651	V652	G652	D653	L654	L655	D656	G658	P659	A660	S661	E662	M663	G664	F665	L666	A667	L668	G669	Q670	M671	V672	L673	V674	G675	I676	M677	P678	F679	D680	F684	E685	D686	A687	L688	V689	I690	S691	E692	E693	L694	L695	K696	R697	A698	Q699	Y700	T701	S702	I703	P704	R705	E706	L774	R775
G582	L583	E584	E585	K586	V587	V588	R589	A593	A594	E595	L596	E597	E598	E599	D600	G601	E602	V603	A604	K605	V606	D607	M608	V609	L610	I611	V612	G613	V614	R615	E616	D617	G618	R619	L620	V621	E622	Y623	P624	L625	L626	R627	F628	Y629	R630	S631	M632	Q633	L637	R640	P641	R642	V643	V644	V645	G646		
V518	G519	T520	P521	V522	L523	V524	V525	A526	S527	E528	V529	E530	F531	M532	D533	G534	R535	P536	K537	Q538	V539	F540	S541	V542	M543	L546	I547	P548	F549	L550	E551	H552	D553	D554	R557	M560	G561	M564	Q565	T566	Q567	A568	V569	P570	L571	I572	R573	A574	Q575	E576	A577	P578	V579	M580	T581			
I452	T453	S454	L455	A456	A457	A458	A459	R460	V461	D462	E463	E464	L465	F466	G467	R468	T469	P470	Y471	R472	R473	A474	V475	V478	T479	T480	V483	V484	Y485	M486	A488	T489	E490	R493	Y494	T495	I496	A497	Q498	P502	L503	M506	R507	I508	A509	A510	E511	R512	V513	V514	A515	R516	R517					
P318	G319	H320	E321	V322	D323	D324	L325	D326	H327	L328	G329	R330	R331	R332	R333	R334	T335	G336	G337	E338	L339	M340	T341	D342	Q343	F344	R345	I346	G347	L348	R349	L350	L351	A352	R353	G354	V355	R358	M359	L360	M361	G362	S363	E364	D365	R367	L367	T368	P369	A370	G371	R372	L373	G374	S375	R376	P377	L378
A381	L382	R383	E384	F385	D386	S387	R388	S392	G393	E394	K395	D396	E397	T398	L399	G400	L401	S402	L403	R404	R405	T406	D407	Q408	F409	I410	S411	A412	L413	G414	P415	L418	T419	R422	A423	G424	D425	V426	V427	V430	H431	R432	T433	H434	Y435	G436	R437	L438	C439	P440	V441	E442	T443	P444				
I452	T453	S454	L455	A456	A457	A458	A459	R460	V461	D462	E463	E464	L465	F466	G467	R468	T469	P470	Y471	R472	R473	A474	V475	V478	T479	T480	V483	V484	Y485	M486	A488	T489	E490	R493	Y494	T495	I496	A497	Q498	P502	L503	M506	R507	I508	A509	A510	E511	R512	V513	V514	A515	R516	R517					



• Molecule 6: DNA-directed RNA polymerase beta' chain

Chain D: 21% 47% 14% 17%





L127	K62	MET
L128	V63	K2
F129	K64	K3
S130	R65	E4
K131	Q66	V5
Y132	R67	R6
I133	F68	K7
V134	E69	V8
D135	G73	R9
L136	E74	I10
P137	R75	A11
K138	R76	L12
G139	C76	A13
A140	G77	S14
I141	V78	P15
L142	E79	E16
H143	V80	K17
G144	T81	I18
V145	T84	R19
P146	R85	S20
V147	R86	W21
A148	S87	S22
K149	R88	Y23
R150	T88	G24
Q151	R89	E25
L152	G90	V26
S153	G91	E27
T154	H92	K28
D155	I93	P29
E156	E94	E30
E157	L95	T31
V158	A96	I32
E159	T97	N33
E160	P98	V34
L161	H101	R35
R162	I102	L36
V163	W103	L37
G164	F104	K38
K165	V105	P39
Q166	K106	E40
E167	D107	R41
T168	V108	D42
V169	P109	G43
P170	S110	L44
L171	K111	F45
P172	I112	D46
V175	L115	E47
D176	L116	R48
L178	D117	F50
V179	L118	Q51
K180	S119	P62
D181	A120	T53
G182	T121	K54
E183	E122	D65
V184	L123	E56
E185	E124	B57
L186	Q125	C58
L187	V126	Q61

Y1145	G1081	L1020	D952	I1885	R818	A755	E693	S629	I566	L503	V443	GLU	PRO	GLU	GLU	A192
G1146	A1082	Y1021	D953	V886	G819	Q756	V694	V630	I567	G506	V444	GLU	ARG	GLU	GLU	P193
R1147	D1083	Y1022	A954	A987	A954	A757	I695	I631	R568	R507	R445	GLU	GLN	GLU	GLY	G194
V1148	T1084	M1023	V955	E888	V821	E758	H696	V632	I569	R507	V446	VAL	VAL	VAL	VAL	V195
L1149	A1085	A1025	I956	A889	A823	A759	A899	V633	R508	R508	V447	VAL	ARG	VAL	VAL	R198
A1150	L1086	Q1024	P957	V890	L423	R760	A822	G634	K571	P509	E448	ALA	ALA	ALA	ALA	L199
R1151	R1087	S1026	R558	E993	R824	I761	V700	P835	R572	E510	S449	GLU	ALA	GLU	GLU	
E1152	T1088	G1027	E959	E893	A825	Q762	L701	Q636	H573	N511	R450	LEU	GLN	LEU	LEU	
V1153	A1089	A1028	R960	R994	P826	M763	L702	L637	H574	N512	R451	LYS	VAL	LYS	LYS	V202
E1154	D1090	R1029	K961	V895	I827	L764	N703	R638	Q575	I513	R452	GLU	GLU	GLU	GLU	A203
V1155	S1091	G1030	Q962	A996	R328	S765	R704	L639	E576	I514	R453	LEU	ALA	LEU	LEU	L204
L1156	G1092	M1031	V963	H997	V629		A705	H640	A577	E515	R454	GLU	GLU	GLU	GLU	Y205
G1157	Y1083	Q1032	L964	E993	A830	N768	P706	G641	H578	A516	R455	HIS	GLU	GLU	GLU	R206
V1158	L1094	Q1033	E965	L999	G831	L769	T707	G642	H579	N517	R456	LEU	GLU	GLY	GLY	F207
R1159	T1095	Q1034	R966	I900	R832	L770	L708	R832	A580	P518	G457	HIS	GLY	ALA	ALA	PRO
L1160	R1096	I1035	A967	Q901	E833	S771	H709	I644	I581	V519	A458	GLU	GLU	PHE	PHE	ARG
E1161	K1097	L1036	D968	R1092	T834	P772	R710	P645	L582	L520	E459	LEU	THR	LEU	LEU	ARG
E1162	R1098	Q1037	R969	D903	S835	A773	L711	R646	D583	P521	A460	VAL	VAL	VAL	VAL	VAL
G1163	V1099	L1038	K970	V904	V836	S774	G712	R647	H584	P522	I461	LEU	TYR	LEU	ARG	ARG
R1164	D1100	C1039	L971	P905	G837	G776	P718	R654	H585	D523	Q482	LEU	TYR	LEU	ARG	GLU
V1165	V1101	G1040	L972	Q906	R838	E776	T714	R656	H586	I524	Q483	ARG	THR	ARG	GLU	GLU
S1166	T1102	R1041	Q973	E907	L839	P777	A715	L652	H587	R525	I464	LEU	THR	ARG	GLU	GLU
S1167		R1042	I974	K908	R340	L778	F716	P526	H588	P526	I465	PHE	ASP	GLU	GLY	TYR
M1168		G1043	E975		V841	A779	Q717	R653	A589	N527	R466	LEU	GLU	GLU	LYS	LYS
D1169	V1106	L1044	Q976	I911		K780	P718	R654	P590	V528	E467	PRO	GLU	PRO	GLU	GLU
D1170	V1107	M1045	A977	K912	A844	P781	V719	P655	P594	N529	L488	TRP	TRP	VAL	VAL	GLU
V1171	R1108	Q1046		D913	R846	S782	L720	P656	P594	N530	D469	THR	THR	ALA	ALA	ARG
	E1109	K1047	P982	R914	R846	R783	V721	L657	G595	D531	L470	GLU	GLU	THR	THR	ALA
L1174	A1110	P1048	L983	V915	D847	D784	E722	R658	S596	G532	F402	PRO	PRO	GLY	GLY	GLY
	D1111	S1049	T984	V916	E848	K659	G723	R659	D597	G533	A472	LYS	LYS	PHE	PHE	LEU
A1177	G1112	G1050	D985	Q917	E848	L786	Q724	R660	H598	R534	L473	ASP	ASP	LEU	LEU	ARG
A1178	I1113	E1051	E886	A918	L851	L787	S725	R661	P599		E474	TYR	TYR	PRO	LEU	LEU
E1179	T1114	T1052	E987	F919	A852	G788	I726	R666	L600	S538	R476	VAL	ARG	VAL	PRO	PRO
	N1116	F1053	R988	R921	V853	L789	Q727	A667	R601	D539	L477	GLY	GLN	GLY	LEU	LEU
Q1184	N1117	E1054	R990	L922		Y791	Y790	L667	S602	L540	E478	MET	PRO	GLY	ALA	ALA
E1185	I1118	V1055	G990	G923	I857	I792	H729	P668	L603	N541	E479	THR	HIS	PRO	TRP	TRP
V1186	S1119	V1057	Q901	R924	V858	T793	P730	N669	T604	D542	E480	VAL	ASN	LEU	VAL	VAL
P1187	V1120	R1058	L993	N924	D859	Q794	V732	H671	L606	L543	R481	VAL	ASN	VAL	GLU	GLU
V1188	P1121	S1059	Q994	K926	L860	R796	C733	A672	L607	R544	R482	VAL	VAL	VAL	LYS	LYS
R1189	L1122	L1060	L995		Q861	K797	E734	A673	R545	R546	R483	VAL	VAL	HIS	GLU	GLU
S1190	F1123	F1061	N996	R929	V863	K797	A735	R674	K610	L547	P484	VAL	VAL	GLY	ALA	ALA
P1191	Q1124	R1062	T987	L930	V864	E798	F736	R675	Q611	L547	S485	PRO	PRO	GLY	TYR	TYR
L1192	P1125	E1063	E998			K799	N737	R676	H612	I548	R486	GLY	GLY	ILE	ILE	LYS
T1193		G1064	T999	L934	V868	K900	A738	L677	R613	N549	A487	VAL	GLY	VAL	VAL	PRO
G1194	V1128	L1065	E1000	K935			D739	B678	F614	R550	R488	ALA	ALA	GLY	GLY	GLY
Q1195	T1129	T1066	E1001	Y936	K871	G803	F740	B678	R615	N551	R489	ARG	ARG	LYS	LYS	GLU
T1196	R1130	V1067	K1002	Y937	R872	L804	D741	R679	Q616	N552	A490	VAL	VAL	GLY	GLY	GLU
R1197		L1068	V1003	G938	L873	E805	G742	Q680	H617	R553	K491	GLY	GLY	GLN	GLN	LEU
Y1198	L1134	E1069	F1007	F939	G874	F806	D743	D882	L618	L564	R492	ALA	ALA	PRO	ALA	ALA
G1199	R1135	Y1070	V1007		T875	A807	Q744	L683	L619		R493	GLY	GLY	LEU	LEU	GLU
V1200	K1136	F1071	F1008	T943	S876	T808	H745	R684	G620	I557	R494	ASP	ASP	ALA	ALA	LEU
C1201	R1137	K1009	T944	T944	P877	P909	A746	D685	R621	L558	R495	LYS	LYS	GLU	GLU	PRO
A1138	A1138	S1073	N1010	S945	G878	E810	V747	E586	R622	A559	R496	ILE	ILE	ALA	ALA	GLU
K1203	L1139	S1074	G946	G946	R879	R679	H748	V687	V623	O560	E497	VAL	VAL	LYS	LYS	PRO
C1204	I1140	H1075	I947	I947	T880	L813	V749	R688	D624	G561	V498	ALA	ALA	GLY	GLY	TYR
Y1205	E1141		T948	T948	L881	A814	P750	P689	V625	H562	V499	ALA	ALA	LEU	LEU	LEU
G1206	A1142	R1078	P1016	I949	P882	A815	L751	A690	S626	P563	R500	ILE	ILE	LEU	LEU	PHE
Y1207	G1143	K1079	F1017	G950	A883	H616	L691	L691	G627	E564	R441	ASP	ASP	ARG	ARG	ARG
D1208	L1144	G1080		I951	R884	E817	F754	B692	R628	I565	F502	ALA	ALA	MET	MET	ALA



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	152.34Å 152.34Å 524.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 38.29 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.3 (40.00-3.00) 83.5 (38.29-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.257 0.227 , 0.252	Depositor DCC
R_{free} test set	11219 reflections (5.70%)	wwPDB-VP
Wilson B-factor (Å ²)	64.2	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 136.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.146 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	51213	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: APC, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	G	1.04	1/520 (0.2%)	1.12	1/798 (0.1%)
1	X	1.12	2/520 (0.4%)	1.14	1/798 (0.1%)
2	H	1.39	3/387 (0.8%)	2.45	39/601 (6.5%)
2	Y	1.36	3/387 (0.8%)	2.44	33/601 (5.5%)
3	I	0.72	0/304	0.92	1/467 (0.2%)
3	Z	0.73	0/304	0.91	0/467
4	A	0.69	0/1838	0.76	0/2498
4	B	0.76	0/1838	0.76	2/2498 (0.1%)
4	K	0.73	0/1838	0.82	3/2498 (0.1%)
4	L	0.73	0/1838	0.78	4/2498 (0.2%)
5	C	0.79	1/8997 (0.0%)	0.89	17/12164 (0.1%)
5	M	0.78	1/8997 (0.0%)	0.90	17/12164 (0.1%)
6	D	0.79	1/10128 (0.0%)	0.91	18/13681 (0.1%)
6	N	0.79	2/10128 (0.0%)	0.89	22/13681 (0.2%)
7	E	0.83	1/784 (0.1%)	1.07	3/1057 (0.3%)
7	O	0.78	1/784 (0.1%)	1.07	3/1057 (0.3%)
All	All	0.80	16/49592 (0.0%)	0.95	164/67528 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	6
1	X	0	5
2	H	0	2
2	Y	0	1
3	I	0	1
All	All	0	15

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	G	OP3-P	10.56	1.73	1.61
1	G	1	DC	OP3-P	-7.74	1.51	1.61
1	X	1	DC	OP3-P	-7.13	1.52	1.61
7	E	94	PRO	N-CA	6.34	1.58	1.47
5	C	439	CYS	CB-SG	-6.08	1.72	1.82
7	O	94	PRO	N-CA	6.07	1.57	1.47
2	Y	7	G	C5-C6	-6.04	1.36	1.42
6	N	1039	CYS	CB-SG	-5.96	1.72	1.81
6	D	1101	VAL	CB-CG2	-5.49	1.41	1.52
2	Y	1	G	OP3-P	5.44	1.67	1.61
2	Y	2	A	O3'-P	-5.32	1.54	1.61
5	M	422	ARG	CG-CD	5.29	1.65	1.51
2	H	9	G	C5-C6	-5.22	1.37	1.42
2	H	2	A	C3'-O3'	-5.17	1.34	1.42
6	N	103	TRP	CB-CG	-5.10	1.41	1.50
1	X	13	DT	O3'-P	5.04	1.67	1.61

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	2	A	N9-C1'-C2'	-18.09	90.48	114.00
5	M	409	ARG	NE-CZ-NH1	15.09	127.85	120.30
2	Y	7	G	N9-C1'-C2'	-12.29	98.02	114.00
7	E	94	PRO	CA-N-CD	-11.28	95.71	111.50
2	H	1	G	N9-C1'-C2'	11.20	128.56	114.00
7	O	94	PRO	CA-N-CD	-11.13	95.92	111.50
2	H	7	G	N9-C1'-C2'	-11.00	99.70	114.00
5	M	409	ARG	NE-CZ-NH2	-9.94	115.33	120.30
2	H	2	A	N9-C1'-C2'	-9.73	101.29	112.00
2	H	2	A	P-O3'-C3'	-9.28	108.56	119.70
7	O	94	PRO	N-CA-C	9.25	136.15	112.10
7	E	94	PRO	N-CA-C	9.02	135.55	112.10
2	H	9	G	O4'-C1'-N9	9.00	115.40	108.20
2	Y	2	A	O4'-C1'-N9	-8.97	101.03	108.20
2	Y	14	G	O4'-C1'-N9	8.84	115.27	108.20
2	Y	4	U	O4'-C1'-N1	8.73	115.18	108.20
2	Y	9	G	O4'-C1'-N9	8.71	115.17	108.20
5	C	409	ARG	NE-CZ-NH1	8.58	124.59	120.30
2	H	4	U	O4'-C1'-N1	8.56	115.05	108.20
6	N	1389	LEU	CA-CB-CG	8.45	134.74	115.30
2	H	6	U	O4'-C1'-N1	8.40	114.92	108.20
4	K	197	LEU	CA-CB-CG	8.16	134.07	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	243	ARG	C-N-CD	-8.15	102.66	120.60
2	Y	14	G	N9-C1'-C2'	-8.15	103.03	112.00
2	Y	5	C	O4'-C1'-N1	8.11	114.69	108.20
2	H	5	C	O4'-C1'-N1	8.05	114.64	108.20
2	Y	9	G	C5'-C4'-O4'	-7.86	99.66	109.10
2	H	14	G	O4'-C1'-N9	7.86	114.49	108.20
2	H	13	C	N1-C1'-C2'	-7.86	103.36	112.00
2	H	1	G	O4'-C1'-N9	-7.78	101.98	108.20
2	H	9	G	C5'-C4'-O4'	-7.76	99.79	109.10
2	Y	6	U	O4'-C1'-N1	7.69	114.35	108.20
2	Y	9	G	N9-C1'-C2'	-7.67	103.56	112.00
2	H	12	G	O4'-C1'-N9	7.67	114.34	108.20
2	H	14	G	N9-C1'-C2'	-7.52	103.73	112.00
5	M	98	LEU	CA-CB-CG	7.48	132.49	115.30
6	N	1429	LEU	CA-CB-CG	7.42	132.35	115.30
5	M	243	ARG	C-N-CD	-7.36	104.41	120.60
5	C	409	ARG	NE-CZ-NH2	-7.30	116.65	120.30
2	Y	3	G	OP1-P-OP2	-7.28	108.68	119.60
2	H	9	G	N9-C1'-C2'	-7.26	104.01	112.00
2	Y	14	G	O5'-P-OP2	7.21	119.35	110.70
2	Y	12	G	O4'-C1'-N9	7.18	113.95	108.20
6	N	1244	GLY	N-CA-C	7.15	130.97	113.10
6	D	1244	GLY	N-CA-C	7.14	130.96	113.10
6	N	1244	GLY	CA-C-N	7.05	130.29	116.20
6	D	133	ILE	CA-C-N	-7.03	101.73	117.20
5	M	861	LEU	CA-CB-CG	7.02	131.45	115.30
2	H	8	C	O4'-C1'-N1	6.99	113.79	108.20
2	Y	3	G	O4'-C1'-N9	-6.85	102.72	108.20
2	Y	12	G	N9-C1'-C2'	-6.84	104.48	112.00
2	Y	2	A	OP1-P-OP2	-6.83	109.35	119.60
6	D	1244	GLY	CA-C-N	6.80	129.81	116.20
6	D	133	ILE	C-N-CA	6.79	138.68	121.70
5	M	422	ARG	NE-CZ-NH1	6.74	123.67	120.30
6	D	1243	THR	CA-C-N	6.71	129.63	116.20
4	K	218	LEU	CA-CB-CG	6.71	130.74	115.30
6	D	1096	ARG	NE-CZ-NH2	-6.65	116.97	120.30
2	H	12	G	N9-C1'-C2'	-6.58	104.76	112.00
2	Y	1	G	OP1-P-OP2	-6.48	109.87	119.60
2	H	1	G	OP1-P-OP2	-6.47	109.90	119.60
6	N	1243	THR	CA-C-N	6.46	129.12	116.20
2	Y	2	A	C3'-C2'-C1'	-6.45	96.34	101.50
2	H	10	G	O4'-C1'-N9	6.44	113.35	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	207	LEU	CA-CB-CG	6.41	130.04	115.30
4	B	90	LEU	CA-CB-CG	6.41	130.03	115.30
2	H	2	A	OP1-P-OP2	-6.39	110.02	119.60
2	H	13	C	O4'-C1'-N1	6.36	113.29	108.20
2	Y	13	C	N1-C1'-C2'	-6.34	105.03	112.00
2	Y	8	C	O4'-C1'-N1	6.33	113.26	108.20
2	H	10	G	N9-C1'-C2'	-6.29	105.08	112.00
5	M	207	LEU	CA-CB-CG	6.28	129.75	115.30
2	H	3	G	OP1-P-OP2	-6.28	110.18	119.60
6	D	153	LEU	CA-CB-CG	6.24	129.64	115.30
2	H	2	A	N9-C4-C5	6.18	108.27	105.80
2	H	2	A	C4'-C3'-C2'	6.17	108.77	102.60
2	H	14	G	O5'-P-OP2	6.16	118.09	110.70
2	H	7	G	C4'-C3'-O3'	6.13	125.26	113.00
4	L	90	LEU	CA-CB-CG	6.13	129.39	115.30
6	N	1243	THR	C-N-CA	-6.13	109.44	122.30
2	Y	13	C	O4'-C1'-N1	6.08	113.07	108.20
2	H	11	C	N1-C1'-C2'	-6.08	105.32	112.00
6	N	450	TYR	CA-C-N	-6.04	103.91	117.20
6	D	1429	LEU	CA-CB-CG	5.98	129.06	115.30
2	H	6	U	C3'-C2'-C1'	5.95	106.26	101.50
2	H	11	C	O4'-C1'-N1	5.94	112.95	108.20
2	Y	16	G	O4'-C1'-N9	5.91	112.93	108.20
2	H	15	C	O4'-C1'-N1	5.91	112.92	108.20
2	Y	7	G	C4'-C3'-O3'	5.90	124.81	113.00
6	N	394	LEU	CA-CB-CG	5.90	128.88	115.30
2	Y	6	U	C3'-C2'-C1'	5.89	106.21	101.50
2	H	2	A	C8-N9-C4	-5.87	103.45	105.80
6	D	1363	LEU	CA-CB-CG	5.83	128.71	115.30
2	Y	11	C	O4'-C1'-N1	5.82	112.86	108.20
6	D	1109	GLU	CA-C-N	-5.81	104.43	117.20
6	D	1243	THR	C-N-CA	-5.79	110.14	122.30
6	N	1109	GLU	CA-C-N	-5.78	104.49	117.20
5	C	58	ASP	C-N-CA	5.76	136.09	121.70
6	N	153	LEU	CA-CB-CG	5.75	128.52	115.30
2	Y	10	G	O4'-C1'-N9	5.73	112.79	108.20
5	M	58	ASP	C-N-CA	5.73	136.04	121.70
1	G	18	DG	N9-C1'-C2'	-5.73	101.72	112.60
6	D	1109	GLU	C-N-CA	5.70	135.96	121.70
5	M	304	LEU	CA-CB-CG	5.66	128.31	115.30
2	H	7	G	O4'-C1'-N9	5.64	112.72	108.20
2	Y	11	C	N1-C1'-C2'	-5.63	105.81	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	450	TYR	CA-CB-CG	-5.61	102.75	113.40
6	N	488	ARG	NE-CZ-NH1	5.59	123.09	120.30
4	K	186	LEU	CA-CB-CG	5.58	128.15	115.30
4	L	115	LEU	CA-CB-CG	5.58	128.13	115.30
2	H	1	G	C4'-C3'-C2'	5.57	108.17	102.60
6	N	450	TYR	CA-CB-CG	-5.54	102.88	113.40
5	M	424	GLY	N-CA-C	5.53	126.93	113.10
2	Y	10	G	N9-C1'-C2'	-5.51	105.94	112.00
5	C	422	ARG	NE-CZ-NH1	5.50	123.05	120.30
6	N	619	LEU	CA-CB-CG	5.49	127.92	115.30
2	H	2	A	P-O5'-C5'	-5.48	112.13	120.90
2	Y	1	G	C2'-C3'-O3'	-5.48	97.45	109.50
6	N	1109	GLU	C-N-CA	5.48	135.39	121.70
6	D	619	LEU	CA-CB-CG	5.46	127.86	115.30
6	N	1244	GLY	CA-C-O	-5.46	110.78	120.60
2	Y	7	G	O4'-C1'-N9	5.44	112.56	108.20
5	C	165	LEU	C-N-CD	-5.44	108.63	120.60
5	C	600	ASP	CB-CG-OD1	-5.40	113.44	118.30
4	L	186	LEU	CA-CB-CG	-5.40	102.88	115.30
6	D	764	LEU	CA-CB-CG	5.40	127.71	115.30
5	M	165	LEU	C-N-CD	-5.38	108.75	120.60
1	X	18	DG	N9-C1'-C2'	-5.36	102.42	112.60
5	C	30	LEU	CA-CB-CG	5.36	127.63	115.30
6	D	1101	VAL	CB-CA-C	-5.36	101.23	111.40
4	L	192	LEU	CA-CB-CG	5.34	127.59	115.30
5	C	600	ASP	CB-CG-OD2	5.34	123.11	118.30
5	C	728	HIS	CA-C-N	5.29	128.84	117.20
6	N	488	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	H	16	G	O4'-C1'-N9	5.27	112.41	108.20
5	M	285	LEU	CA-CB-CG	5.26	127.39	115.30
5	M	728	HIS	CA-C-N	5.25	128.75	117.20
5	M	409	ARG	CA-CB-CG	5.25	124.94	113.40
5	M	409	ARG	CD-NE-CZ	5.22	130.91	123.60
5	M	728	HIS	C-N-CA	-5.21	108.69	121.70
3	I	3	DA	OP1-P-OP2	-5.20	111.80	119.60
5	C	858	MET	CB-CG-SD	-5.20	96.81	112.40
5	C	244	PRO	CA-N-CD	-5.19	104.24	111.50
5	C	191	PHE	C-N-CA	-5.17	100.27	122.00
6	N	621	LYS	CA-C-N	5.16	128.54	117.20
6	N	813	LEU	CA-CB-CG	5.15	127.15	115.30
2	H	16	G	C5'-C4'-O4'	-5.15	102.92	109.10
6	D	813	LEU	CA-CB-CG	5.14	127.13	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	50	THR	C-N-CA	5.14	134.56	121.70
5	C	165	LEU	C-N-CA	5.13	143.56	122.00
6	N	1201	CYS	CA-CB-SG	-5.13	104.76	114.00
5	C	328	LEU	CA-CB-CG	-5.11	103.55	115.30
2	Y	15	C	O4'-C1'-N1	5.10	112.28	108.20
5	M	997	LEU	CB-CG-CD2	-5.10	102.34	111.00
2	H	12	G	C4'-C3'-C2'	5.09	107.69	102.60
7	O	50	THR	C-N-CA	5.09	134.43	121.70
2	H	2	A	C3'-C2'-C1'	-5.09	97.43	101.50
6	N	1112	CYS	CA-CB-SG	5.08	123.14	114.00
2	Y	12	G	C4'-C3'-C2'	5.06	107.66	102.60
5	C	728	HIS	C-N-CA	-5.05	109.07	121.70
4	B	115	LEU	CA-CB-CG	5.04	126.90	115.30
6	D	1244	GLY	CA-C-O	-5.04	111.52	120.60
6	N	1039	CYS	CA-CB-SG	-5.03	104.95	114.00
6	N	496	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	13	DT	Sidechain
1	G	15	DC	Sidechain
1	G	16	DG	Sidechain
1	G	17	DC	Sidechain
1	G	18	DG	Sidechain
1	G	19	DC	Sidechain
2	H	14	G	Sidechain
2	H	16	G	Sidechain
3	I	3	DA	Sidechain
1	X	13	DT	Sidechain
1	X	15	DC	Sidechain
1	X	16	DG	Sidechain
1	X	17	DC	Sidechain
1	X	18	DG	Sidechain
2	Y	14	G	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	467	0	259	43	0
1	X	467	0	259	43	0
2	H	347	0	174	58	0
2	Y	347	0	174	81	0
3	I	270	0	144	14	0
3	Z	270	0	144	12	0
4	A	1806	0	1861	169	0
4	B	1806	0	1861	174	0
4	K	1806	0	1861	182	0
4	L	1806	0	1861	199	0
5	C	8829	0	8933	1208	0
5	M	8829	0	8933	1204	0
6	D	9960	0	10183	1379	0
6	N	9960	0	10183	1351	0
7	E	770	0	784	108	0
7	O	770	0	784	101	0
8	D	2	0	0	0	0
8	N	2	0	0	0	0
9	D	2	0	0	0	0
9	N	2	0	0	0	0
10	D	31	0	14	2	0
10	N	31	0	14	2	0
11	A	106	0	0	16	0
11	B	82	0	0	21	0
11	C	482	0	0	120	0
11	D	506	0	0	138	0
11	E	60	0	0	6	0
11	G	32	0	0	3	0
11	H	37	0	0	3	0
11	I	22	0	0	3	0
11	K	86	0	0	19	0
11	L	104	0	0	23	0
11	M	483	0	0	129	0
11	N	491	0	0	115	0
11	O	39	0	0	6	0
11	X	43	0	0	4	0
11	Y	30	0	0	6	0
11	Z	30	0	0	4	0
All	All	51213	0	48426	5871	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 (5871) 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)
2:Y:7:G:N1	5:M:1014:SER:HA	1.62	1.13
2:Y:16:G:H21	6:N:705:ALA:HB1	1.11	1.12
6:N:18:ILE:HG23	6:N:518:PRO:HG3	1.33	1.10
5:C:409:ARG:HA	5:C:454:SER:HA	1.27	1.10
6:N:1189:ARG:HB3	6:N:1204:CYS:HA	1.34	1.09
6:D:695:ILE:HD11	6:D:718:PRO:HB2	1.31	1.08
4:K:112:ARG:HE	4:K:125:PRO:HB2	1.15	1.07
6:D:908:LYS:HB2	6:D:1027:GLY:HA3	1.39	1.04
4:B:59:GLU:HB2	4:B:137:ARG:HH12	1.20	1.04
6:N:1220:ALA:HB1	6:N:1223:ILE:HD13	1.39	1.03
6:D:783:ARG:HA	6:D:1028:ALA:HA	1.40	1.03
6:N:1335:LEU:HD23	6:N:1344:VAL:HG22	1.39	1.03
6:D:161:LEU:HD21	6:D:452:ILE:HG21	1.38	1.02
5:C:305:PRO:HG3	5:C:308:ARG:HH22	1.22	1.02
5:C:752:GLY:H	5:C:792:VAL:HB	1.25	1.01
6:D:798:GLU:HB2	6:D:828:LYS:HE3	1.43	1.01
5:M:695:LEU:HD21	5:M:832:LYS:HD3	1.43	1.01
5:C:433:THR:HG21	5:C:488:ALA:HB1	1.42	1.01
5:M:946:ARG:HB3	5:M:946:ARG:HH11	1.22	1.01
6:N:180:LYS:HG2	6:N:183:GLU:HB2	1.42	1.01
2:Y:2:A:H3'	2:Y:2:A:C8	1.94	1.00
5:M:905:ILE:HD12	5:M:905:ILE:H	1.27	1.00
6:N:633:VAL:HG22	6:N:635:PRO:HD3	1.43	1.00
4:L:179:PHE:HB3	4:L:197:LEU:HD12	1.44	0.99
2:Y:7:G:H1	5:M:1014:SER:HA	0.85	0.99
6:D:637:LEU:HD21	6:D:642:CYS:HA	1.45	0.99
6:N:783:ARG:HA	6:N:1028:ALA:HA	1.41	0.98
6:N:1379:VAL:HG12	6:N:1419:PRO:HA	1.40	0.98
2:Y:7:G:H21	5:M:1021:LEU:HB2	1.27	0.98
6:N:95:LEU:HD11	6:N:517:VAL:HG23	1.46	0.97
5:C:578:VAL:HG13	5:C:671:ASN:HB3	1.46	0.97
6:N:1042:ARG:HH21	6:N:1073:SER:HB3	1.28	0.97
6:D:1183:ILE:HG22	6:N:561:GLY:HA2	1.47	0.97
2:Y:7:G:H1	5:M:1014:SER:CA	1.79	0.96
4:A:85:LEU:HA	4:A:124:ASN:HD22	1.28	0.96
6:D:1109:GLU:HG2	6:D:1201:CYS:HA	1.44	0.96
6:D:1112:CYS:HB2	6:D:1195:GLN:HG2	1.45	0.96
5:M:333:ILE:H	5:M:465:GLY:HA3	1.31	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:579:VAL:HG11	5:C:887:GLU:HG3	1.47	0.96
6:N:996:TRP:HA	6:N:999:THR:HG22	1.46	0.96
7:O:45:ARG:HG2	7:O:46:PRO:HD2	1.47	0.96
6:D:455:ARG:HB2	6:D:460:ALA:HA	1.47	0.95
5:M:110:GLU:HG3	5:M:369:PRO:HB3	1.44	0.95
6:N:543:LEU:HD22	6:N:580:ALA:HB1	1.47	0.95
6:N:921:ARG:HH11	6:N:921:ARG:HB3	1.29	0.95
6:N:972:LEU:HG	6:N:976:GLN:HE22	1.31	0.95
5:C:636:ALA:HB3	5:C:703:ILE:HD13	1.46	0.95
4:L:89:PHE:HB3	4:L:94:LEU:HD13	1.47	0.94
6:N:1144:LEU:HD12	6:N:1171:VAL:HG13	1.48	0.94
5:M:478:VAL:HG13	5:M:506:ASN:HB3	1.48	0.94
5:M:120:LEU:HD22	5:M:121:MET:H	1.32	0.94
4:B:64:GLU:HB2	4:B:165:ILE:HG21	1.48	0.94
6:N:1109:GLU:HG2	6:N:1201:CYS:HA	1.48	0.94
5:M:157:ARG:HD3	5:M:314:THR:HB	1.49	0.93
6:N:793:THR:HB	6:N:879:ARG:HD3	1.49	0.93
6:D:136:ASP:HB3	6:D:137:PRO:HD3	1.51	0.93
5:M:304:LEU:HD23	5:M:305:PRO:HD3	1.47	0.93
5:C:39:ARG:H	5:C:39:ARG:HD2	1.31	0.93
5:M:183:SER:HB2	5:M:190:LYS:HG2	1.48	0.93
5:M:939:ARG:HB3	5:M:982:PRO:HG3	1.47	0.93
6:N:1487:VAL:HG11	6:N:1492:LEU:HD23	1.50	0.93
2:Y:12:G:H8	2:Y:12:G:H5'	1.32	0.93
5:C:36:PRO:HG2	5:C:70:GLU:HB3	1.50	0.93
5:M:395:LYS:HE2	5:M:403:SER:HB2	1.49	0.93
5:M:857:ASP:HB2	5:M:978:ARG:HG2	1.49	0.93
4:B:18:ARG:HH12	4:B:123:MET:HE1	1.33	0.93
2:Y:2:A:H5''	6:N:671:LYS:HZ1	1.31	0.92
1:X:18:DG:H2''	1:X:19:DC:H5'	1.51	0.92
6:D:1223:ILE:HG22	6:D:1227:GLN:HE21	1.33	0.92
5:M:313:LEU:HD13	5:M:321:GLU:HB2	1.50	0.92
1:X:14:DT:H5''	6:N:1089:ALA:HA	1.48	0.92
4:B:97:VAL:HG11	4:B:120:VAL:HG21	1.52	0.92
6:D:143:ASN:HD21	6:D:145:VAL:HG12	1.32	0.92
6:N:133:ILE:HD12	6:N:153:LEU:HD13	1.50	0.91
5:M:1097:LEU:H	5:M:1097:LEU:HD22	1.33	0.91
5:M:197:LEU:HD13	5:M:207:LEU:HD11	1.52	0.91
5:C:313:LEU:HB2	11:C:1168:HOH:O	1.70	0.91
11:B:374:HOH:O	6:D:847:ASP:HB3	1.69	0.91
5:C:673:LEU:HD22	5:C:867:VAL:HA	1.52	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:6:U:H2'	2:H:7:G:C8	2.06	0.90
2:Y:2:A:C3'	2:Y:2:A:C8	2.51	0.90
2:Y:8:C:O2'	2:Y:9:G:H5'	1.71	0.90
6:D:785:ILE:HD12	6:D:785:ILE:H	1.34	0.90
6:D:1253:THR:O	6:D:1257:PRO:HD2	1.71	0.90
2:H:13:C:H4'	5:C:409:ARG:HH22	1.37	0.90
6:D:145:VAL:HG22	6:D:146:PRO:HD2	1.53	0.90
6:N:52:PRO:HD2	6:N:85:VAL:HG21	1.52	0.90
6:N:890:VAL:HG12	6:N:926:LYS:HD2	1.54	0.90
2:H:12:G:H5'	2:H:12:G:H8	1.38	0.89
5:M:170:PRO:HB3	5:M:186:VAL:HG12	1.52	0.89
5:M:536:PRO:HD2	5:M:537:LYS:HZ2	1.37	0.89
2:Y:6:U:H2'	2:Y:7:G:C8	2.07	0.89
4:L:87:VAL:HG21	4:L:144:VAL:HG11	1.53	0.89
6:N:507:ASN:HD22	6:N:507:ASN:H	1.16	0.89
6:D:785:ILE:HG22	6:D:789:LEU:HD11	1.53	0.89
5:C:1049:LEU:HD23	6:D:1472:ILE:HD12	1.55	0.89
5:C:176:VAL:HG12	5:C:182:VAL:HG13	1.54	0.89
5:C:260:LEU:HB2	5:C:291:ALA:HB1	1.55	0.89
6:N:206:ARG:HG2	6:N:394:LEU:HD22	1.55	0.89
6:D:613:ARG:NH1	6:D:616:GLN:HG2	1.88	0.88
5:M:755:LEU:HD21	5:M:792:VAL:HG22	1.52	0.88
5:C:305:PRO:HG3	5:C:308:ARG:NH2	1.88	0.88
6:D:206:ARG:HG2	6:D:394:LEU:HD22	1.52	0.88
5:M:578:VAL:HG11	5:M:991:GLN:HB3	1.56	0.88
6:D:1468:LEU:HD22	6:D:1470:ARG:HB2	1.52	0.88
5:M:39:ARG:HD2	5:M:39:ARG:H	1.34	0.88
2:Y:14:G:O2'	2:Y:15:C:H5'	1.73	0.88
2:H:14:G:O2'	2:H:15:C:H5'	1.72	0.88
5:M:739:GLU:HG3	5:M:742:VAL:HB	1.52	0.88
6:N:1121:PRO:HD2	6:N:1346:ARG:HH21	1.35	0.88
5:C:148:PHE:HE2	5:C:281:LEU:HD13	1.39	0.88
6:D:204:LEU:HD21	6:D:400:VAL:HB	1.53	0.88
5:C:759:THR:HB	5:C:785:VAL:HG11	1.56	0.88
2:H:8:C:O2'	2:H:9:G:H5'	1.71	0.88
5:M:537:LYS:H	5:M:537:LYS:HD2	1.38	0.88
6:N:1253:THR:O	6:N:1257:PRO:HD2	1.74	0.88
1:X:15:DC:H4'	5:M:1035:MET:SD	2.13	0.87
6:N:786:ILE:HG21	6:N:1027:GLY:H	1.37	0.87
6:N:394:LEU:HD11	6:N:445:ARG:NH1	1.90	0.87
6:D:708:LEU:HB3	6:D:1231:GLU:HB2	1.55	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:1258:ARG:HH12	6:N:1268:PRO:HB3	1.40	0.87
6:D:786:ILE:HG22	6:D:1026:SER:HB3	1.55	0.87
4:L:59:GLU:HB2	4:L:137:ARG:HH12	1.39	0.87
5:C:1055:LEU:HD22	5:C:1066:ALA:HB2	1.54	0.87
5:M:64:LEU:HB2	5:M:359:MET:SD	2.14	0.87
4:K:117:VAL:HB	4:K:120:VAL:HG12	1.57	0.87
4:B:82:LEU:HA	4:B:85:LEU:HD12	1.57	0.87
5:C:342:ASP:HA	5:C:345:ARG:HD2	1.55	0.87
1:G:18:DG:H2''	1:G:19:DC:H5'	1.57	0.86
5:M:700:TYR:HB3	5:M:833:LEU:HD13	1.55	0.86
6:N:1124:GLN:HE21	6:N:1135:ARG:HA	1.37	0.86
6:N:87:ARG:HB3	6:N:523:ASP:HB3	1.57	0.86
5:C:578:VAL:HG11	5:C:991:GLN:HB3	1.57	0.86
4:B:56:VAL:HG13	4:B:142:VAL:HG12	1.55	0.86
5:C:721:ARG:HG2	5:C:820:ARG:HH22	1.41	0.86
1:G:22:DC:H4'	5:C:388:ARG:HD2	1.56	0.86
2:Y:7:G:H21	5:M:1021:LEU:CB	1.87	0.86
6:N:501:ALA:HB1	6:N:1453:ALA:HB2	1.58	0.86
5:C:573:ARG:HB2	5:C:573:ARG:HH11	1.39	0.86
6:N:1492:LEU:HB3	6:N:1493:LYS:HE2	1.57	0.86
4:A:178:ALA:HB3	4:A:198:ARG:HG3	1.58	0.86
5:C:192:PRO:HD2	5:C:195:LEU:HB2	1.55	0.86
4:L:102:LYS:NZ	4:L:137:ARG:HG2	1.91	0.86
4:B:103:ALA:HB1	4:B:107:LYS:HD3	1.57	0.86
6:D:484:PRO:HB3	6:D:488:ARG:HE	1.38	0.85
4:A:54:THR:HG22	4:A:158:ILE:HG13	1.56	0.85
6:D:1144:LEU:HD11	6:D:1186:VAL:HG21	1.56	0.85
5:M:345:ARG:HA	5:M:348:LEU:HD12	1.57	0.85
5:M:810:ASP:HB3	5:M:813:VAL:HG12	1.57	0.85
2:Y:12:G:C8	2:Y:12:G:H5'	2.11	0.85
5:C:478:VAL:HG13	5:C:506:ASN:HB3	1.56	0.85
6:D:462:GLN:HG3	6:D:513:ILE:HD13	1.59	0.85
2:Y:16:G:N2	6:N:705:ALA:HB1	1.90	0.85
6:N:1036:ARG:NH2	6:N:1042:ARG:HA	1.92	0.85
6:N:1223:ILE:H	6:N:1223:ILE:HD12	1.41	0.85
2:Y:13:C:H4'	5:M:409:ARG:HH22	1.41	0.85
5:C:174:LEU:HD22	5:C:307:LEU:HB2	1.57	0.85
6:N:897:TRP:HA	6:N:900:ILE:HG12	1.58	0.85
5:C:587:VAL:HG11	5:C:666:LEU:HD22	1.56	0.85
6:D:526:PRO:O	6:D:537:THR:HA	1.77	0.85
2:Y:2:A:H5''	6:N:671:LYS:NZ	1.90	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:87:VAL:HG21	4:B:144:VAL:HG11	1.59	0.84
5:C:144:PRO:HG2	5:C:265:ARG:HH21	1.41	0.84
5:C:197:LEU:HD13	5:C:207:LEU:HD11	1.57	0.84
5:M:675:ALA:HB2	5:M:867:VAL:HG11	1.55	0.84
5:M:953:VAL:HG13	5:M:966:LEU:HD13	1.58	0.84
6:D:24:GLY:HA3	6:D:49:ILE:HG12	1.57	0.84
5:M:36:PRO:HG2	5:M:70:GLU:HB3	1.60	0.84
6:N:1259:VAL:HG11	6:N:1356:TYR:OH	1.77	0.84
5:C:409:ARG:HA	5:C:454:SER:CA	2.07	0.84
5:M:141:HIS:HB3	5:M:418:LEU:HD23	1.57	0.84
5:M:5:ARG:HE	5:M:8:ARG:HH22	1.24	0.84
5:C:857:ASP:HB3	5:C:978:ARG:HG2	1.60	0.84
5:C:687:ALA:HB2	6:D:740:PHE:HB2	1.59	0.84
6:D:1271:LYS:NZ	6:D:1331:ASP:HB3	1.92	0.84
6:N:86:ARG:O	6:N:522:PRO:HD2	1.77	0.84
4:L:1:MET:HG2	4:L:5:LYS:HB3	1.58	0.84
5:M:160:ALA:HB2	11:M:1183:HOH:O	1.78	0.84
5:M:467:ILE:HA	11:M:1287:HOH:O	1.76	0.84
5:M:675:ALA:HA	5:M:989:VAL:HG12	1.58	0.84
6:D:486:ARG:HA	6:D:489:ARG:HD3	1.60	0.83
4:K:34:VAL:HB	5:M:939:ARG:NH1	1.93	0.83
5:C:1031:ARG:HA	6:D:621:LYS:O	1.76	0.83
5:M:595:LEU:HG	5:M:655:LEU:HD12	1.59	0.83
4:B:94:LEU:HD11	4:B:119:ASP:HB2	1.59	0.83
6:D:1144:LEU:HB3	6:D:1166:LEU:HD11	1.58	0.83
6:D:853:VAL:HG22	6:D:858:VAL:HG23	1.60	0.83
5:M:436:GLY:HA2	5:M:538:GLN:O	1.79	0.83
4:L:102:LYS:HD3	4:L:139:ASN:HB2	1.59	0.83
5:C:326:ASP:HB3	5:C:431:HIS:HB2	1.60	0.83
6:D:8:VAL:HG23	6:D:1457:ASP:HB3	1.59	0.83
6:D:28:LYS:HB2	6:D:41:ARG:HH11	1.43	0.83
2:H:14:G:H4'	5:C:567:GLN:HE22	1.44	0.83
5:C:987:ILE:HG23	6:D:948:THR:HG21	1.60	0.83
6:N:111:LYS:HE2	6:N:1452:ILE:HD13	1.60	0.83
5:M:1065:ALA:HB1	5:M:1077:PRO:HG2	1.59	0.83
5:C:751:PRO:HG3	5:C:796:GLU:HA	1.58	0.83
6:D:396:VAL:HG12	6:D:447:VAL:HA	1.61	0.83
6:N:1205:TYR:HD2	6:N:1215:VAL:HG21	1.43	0.83
2:Y:5:C:H2'	2:Y:6:U:C6	2.13	0.83
6:D:1228:SER:O	6:D:1232:PRO:HD2	1.78	0.83
5:C:478:VAL:HA	5:C:506:ASN:O	1.79	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:12:VAL:HG12	5:M:534:VAL:HG13	1.61	0.82
6:D:521:PRO:HG2	6:D:524:LEU:HD22	1.59	0.82
6:N:119:SER:H	6:N:123:LEU:HD22	1.44	0.82
6:D:1389:LEU:HG	6:D:1390:LEU:H	1.44	0.82
5:C:34:VAL:HB	5:C:38:LYS:HG3	1.60	0.82
6:D:1481:VAL:HG11	7:E:18:ARG:HA	1.59	0.82
6:N:172:PRO:HG3	11:N:9050:HOH:O	1.79	0.82
5:C:512:ARG:HB3	5:C:523:ILE:HD11	1.61	0.82
6:D:1046:GLN:HA	6:D:1052:THR:HA	1.61	0.82
6:D:141:ILE:HD11	6:D:165:LYS:HZ1	1.43	0.82
6:D:455:ARG:CB	6:D:460:ALA:HA	2.09	0.82
7:O:41:GLU:HA	7:O:45:ARG:HG3	1.62	0.82
5:M:732:ALA:HA	5:M:735:ARG:HH21	1.45	0.82
6:D:119:SER:H	6:D:123:LEU:HD22	1.42	0.82
6:D:1449:GLU:HA	6:D:1452:ILE:HD12	1.60	0.82
6:D:434:ARG:H	6:D:447:VAL:HG22	1.42	0.82
5:C:953:VAL:HG13	5:C:966:LEU:HD13	1.60	0.82
6:D:123:LEU:HD11	6:D:152:LEU:HD22	1.61	0.82
4:L:25:LEU:HD23	4:L:28:LEU:HD21	1.62	0.82
5:M:715:THR:HB	5:M:717:LEU:HG	1.60	0.82
5:M:405:ARG:HH22	5:M:566:THR:HG21	1.45	0.82
5:M:701:THR:HG22	5:M:832:LYS:HG2	1.62	0.82
6:N:540:LEU:H	6:N:540:LEU:HD12	1.44	0.82
4:A:117:VAL:HB	4:A:120:VAL:HG12	1.59	0.81
5:C:146:VAL:HG11	5:C:306:THR:HB	1.62	0.81
2:H:12:G:H5'	2:H:12:G:C8	2.14	0.81
7:O:18:ARG:HD3	7:O:75:PHE:HE1	1.44	0.81
4:B:85:LEU:HG	4:B:127:LEU:HD23	1.62	0.81
6:D:1464:GLU:HB3	11:D:8024:HOH:O	1.80	0.81
6:D:81:THR:HG22	6:D:82:LYS:H	1.45	0.81
6:N:543:LEU:HD13	6:N:581:LEU:HA	1.59	0.81
6:D:616:GLN:HE22	6:D:621:LYS:HG2	1.44	0.81
6:N:1108:ARG:HH11	6:N:1108:ARG:HB2	1.45	0.81
5:C:343:GLN:HA	5:C:343:GLN:HE21	1.45	0.81
6:D:618:LEU:HD11	6:D:1463:LYS:HE2	1.62	0.81
2:H:5:C:H2'	2:H:6:U:C6	2.14	0.81
5:M:435:TYR:HE1	5:M:539:VAL:HG22	1.44	0.81
6:N:1046:GLN:HA	6:N:1052:THR:HA	1.62	0.81
4:B:59:GLU:HG3	4:B:139:ASN:ND2	1.94	0.81
6:D:1376:MET:SD	6:D:1421:LEU:HD13	2.20	0.81
6:D:799:LYS:HB3	6:D:826:PRO:HG2	1.63	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:111:ALA:HB2	4:A:127:LEU:HD23	1.63	0.81
5:C:408:ARG:HG3	5:C:455:LEU:HG	1.62	0.81
5:C:708:TYR:HB2	5:C:825:VAL:HG23	1.62	0.81
5:M:139:GLN:O	5:M:333:ILE:HA	1.81	0.81
6:N:119:SER:HB2	6:N:123:LEU:HB2	1.62	0.81
4:A:58:ILE:HB	4:A:61:VAL:HB	1.63	0.81
5:M:110:GLU:H	5:M:368:THR:HG21	1.45	0.81
5:M:442:GLU:HG2	5:M:454:SER:HB2	1.63	0.81
6:N:400:VAL:HG22	6:N:443:VAL:HG21	1.61	0.81
6:D:793:THR:HG21	6:D:906:GLN:HG2	1.63	0.81
5:M:239:PHE:HE1	5:M:254:VAL:HB	1.44	0.81
5:M:478:VAL:HA	5:M:506:ASN:O	1.81	0.81
6:D:1205:TYR:HD2	6:D:1215:VAL:HG21	1.44	0.81
7:E:47:LYS:HB2	7:E:52:GLU:OE2	1.79	0.81
1:X:13:DT:H5"	6:N:1093:TYR:CE2	2.15	0.81
2:H:13:C:H4'	5:C:409:ARG:NH2	1.96	0.81
6:D:1262:LEU:HD21	6:D:1351:GLU:HG3	1.63	0.80
6:D:772:PRO:HB3	6:D:1224:VAL:HG13	1.61	0.80
5:M:677:MET:HE1	5:M:679:PHE:HD1	1.46	0.80
5:M:585:GLU:HG2	5:M:589:ARG:HH12	1.47	0.80
6:N:73:CYS:HB3	6:N:76:CYS:O	1.82	0.80
5:C:5:ARG:HE	5:C:8:ARG:HH12	1.30	0.80
6:D:1220:ALA:HB1	6:D:1223:ILE:HD12	1.63	0.80
6:D:616:GLN:NE2	6:D:621:LYS:HG2	1.96	0.80
6:N:610:LYS:O	6:N:615:ARG:HD3	1.81	0.80
4:L:97:VAL:HG11	4:L:120:VAL:HG21	1.62	0.80
7:O:40:LEU:HB3	7:O:72:ARG:HH21	1.45	0.80
5:C:703:ILE:HD12	5:C:703:ILE:H	1.46	0.80
6:N:785:ILE:HG12	6:N:935:LYS:HA	1.62	0.80
7:E:13:VAL:HG21	7:E:19:LEU:HB2	1.63	0.80
5:M:736:ASP:HA	5:M:744:ARG:NH1	1.96	0.80
6:N:156:GLU:O	6:N:159:ARG:HG2	1.82	0.80
5:C:677:MET:SD	5:C:987:ILE:HG21	2.22	0.80
5:C:949:LYS:HD3	6:D:796:ARG:HH22	1.44	0.80
6:N:520:LEU:HD12	6:N:521:PRO:HD2	1.64	0.80
5:M:1056:LYS:O	6:N:624:ASP:HB2	1.81	0.80
4:A:206:THR:HG22	4:A:209:GLU:HG3	1.62	0.79
6:D:1196:THR:HG23	11:D:8314:HOH:O	1.82	0.79
6:D:740:PHE:HB3	11:D:8291:HOH:O	1.82	0.79
6:N:481:MET:SD	6:N:1388:ARG:HB3	2.22	0.79
6:D:1153:VAL:HG13	6:N:561:GLY:HA3	1.63	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:7:G:N2	5:M:1021:LEU:HB2	1.96	0.79
1:G:17:DC:H2"	1:G:18:DG:H5'	1.62	0.79
5:M:1055:LEU:HD22	5:M:1066:ALA:HB2	1.64	0.79
5:M:65:VAL:HB	5:M:101:ILE:HB	1.63	0.79
5:M:854:PRO:HB2	5:M:856:GLU:HG3	1.64	0.79
5:M:915:LYS:HA	11:M:1454:HOH:O	1.83	0.79
5:M:1109:VAL:HG22	6:N:3:LYS:HE3	1.62	0.79
6:N:96:ALA:HB3	6:N:554:LEU:HD23	1.64	0.79
5:C:1017:THR:OG1	5:C:1019:GLN:HG2	1.83	0.79
5:C:139:GLN:HG2	5:C:334:ARG:HB2	1.65	0.79
6:D:1393:GLN:CD	6:D:1394:VAL:H	1.85	0.79
6:D:899:LEU:HD13	6:D:914:LEU:HD21	1.62	0.79
5:M:260:LEU:HB2	5:M:291:ALA:HB1	1.64	0.79
5:M:462:ASP:HB3	5:M:468:ARG:HD2	1.65	0.79
5:M:762:LYS:HD2	5:M:786:LYS:HG3	1.65	0.79
4:B:1:MET:HG2	4:B:5:LYS:HB3	1.65	0.79
5:C:710:ILE:HB	5:C:790:LEU:HD22	1.65	0.79
5:M:597:ALA:HB2	5:M:655:LEU:HD21	1.63	0.79
5:M:732:ALA:HB2	11:M:1476:HOH:O	1.82	0.79
4:L:62:LEU:H	4:L:62:LEU:HD12	1.45	0.79
6:D:1003:VAL:O	6:D:1007:VAL:HG23	1.83	0.79
6:D:1495:ILE:HG12	7:E:80:VAL:HG11	1.63	0.79
5:M:292:ARG:HD2	5:M:299:LYS:HZ3	1.47	0.79
4:K:31:GLY:HA3	4:L:42:ARG:HH21	1.49	0.78
6:N:1459:LEU:HB3	6:N:1465:ASN:HD21	1.47	0.78
6:N:796:ARG:HE	6:N:828:LYS:HZ3	1.30	0.78
5:C:140:ILE:HG22	5:C:333:ILE:HG13	1.64	0.78
5:C:356:ARG:HA	11:C:1191:HOH:O	1.82	0.78
6:D:550:ARG:HA	6:D:550:ARG:HE	1.45	0.78
6:N:887:ALA:HB1	6:N:893:GLU:HG3	1.66	0.78
5:M:141:HIS:O	5:M:331:ARG:HA	1.84	0.78
5:M:66:LEU:HD22	5:M:372:LEU:HD23	1.66	0.78
5:M:1034:GLU:HB3	6:N:619:LEU:HD22	1.65	0.78
5:C:2:GLU:HG3	5:C:899:GLN:HB3	1.64	0.78
6:D:771:SER:HB3	6:D:778:LEU:HD13	1.65	0.78
6:D:782:SER:H	6:D:785:ILE:HD13	1.48	0.78
4:K:87:VAL:HG21	4:K:144:VAL:HG11	1.66	0.78
5:M:360:LEU:HD23	11:M:1129:HOH:O	1.84	0.78
5:M:769:PRO:HD2	6:N:65:ARG:CZ	2.12	0.78
6:N:1204:CYS:HB3	11:N:9238:HOH:O	1.82	0.78
6:N:810:GLU:O	6:N:813:LEU:HG	1.84	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:671:ASN:HD22	5:M:671:ASN:N	1.81	0.78
6:N:1036:ARG:HH21	6:N:1042:ARG:HA	1.48	0.78
2:Y:9:G:H2'	2:Y:10:G:C8	2.17	0.78
2:Y:16:G:H21	6:N:705:ALA:CB	1.95	0.78
4:L:85:LEU:HA	4:L:124:ASN:HD22	1.48	0.78
5:M:151:ASP:HB2	5:M:157:ARG:O	1.83	0.78
5:C:625:LEU:HA	5:C:639:GLN:HE21	1.47	0.78
5:C:748:GLU:HB2	5:C:799:ILE:HD12	1.64	0.78
6:D:127:LEU:HD12	6:D:128:TYR:H	1.49	0.78
6:N:1045:MET:HE2	6:N:1073:SER:HB3	1.63	0.78
5:M:1090:LYS:HD2	6:N:90:MET:HG3	1.66	0.78
4:A:87:VAL:HG21	4:A:144:VAL:HG11	1.65	0.78
5:C:198:ARG:HD2	5:C:204:GLN:HE21	1.47	0.78
5:C:752:GLY:N	5:C:792:VAL:HB	1.99	0.77
6:D:1099:VAL:HA	11:D:8257:HOH:O	1.84	0.77
5:M:12:VAL:HB	5:M:472:ARG:CZ	2.15	0.77
5:M:468:ARG:HH21	5:M:487:THR:H	1.32	0.77
6:N:774:SER:HB3	6:N:1362:LYS:O	1.84	0.77
5:M:1050:GLN:HE22	6:N:1471:LEU:N	1.82	0.77
4:A:43:ILE:HG13	4:A:218:LEU:HD12	1.65	0.77
5:C:10:ARG:HA	5:C:10:ARG:HH11	1.47	0.77
5:C:308:ARG:HG2	11:C:1224:HOH:O	1.84	0.77
5:C:577:PRO:HD2	5:C:580:MET:SD	2.24	0.77
5:C:684:PHE:H	5:C:687:ALA:HB3	1.49	0.77
4:L:179:PHE:HB2	4:L:195:LEU:HD11	1.66	0.77
5:M:413:LEU:H	5:M:413:LEU:HD12	1.48	0.77
5:M:684:PHE:H	5:M:687:ALA:HB3	1.48	0.77
2:Y:12:G:H2'	2:Y:13:C:C6	2.20	0.77
4:L:24:VAL:HG13	4:L:196:THR:HG22	1.66	0.77
5:M:516:ARG:HD2	5:M:521:PRO:HA	1.66	0.77
6:N:394:LEU:HD21	6:N:445:ARG:NH2	1.99	0.77
5:C:979:THR:HG23	5:C:981:GLU:H	1.48	0.77
5:C:687:ALA:HB1	11:C:1474:HOH:O	1.83	0.77
5:C:1082:PRO:HG2	6:D:1469:GLY:HA3	1.66	0.77
5:M:905:ILE:H	5:M:905:ILE:CD1	1.96	0.77
5:C:958:THR:HG23	5:C:961:GLU:HB2	1.67	0.77
5:M:64:LEU:HD22	5:M:359:MET:HG3	1.66	0.77
6:N:1266:ARG:HG2	6:N:1267:ARG:H	1.50	0.77
6:N:684:LYS:HB2	6:N:686:GLU:HG3	1.66	0.77
5:C:328:LEU:HB2	5:C:433:THR:HB	1.66	0.77
6:D:699:VAL:H	6:D:756:GLN:NE2	1.83	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:1426:LYS:HA	6:N:1429:LEU:HD13	1.66	0.77
5:C:139:GLN:HE21	5:C:334:ARG:HD3	1.49	0.77
5:C:433:THR:HG22	5:C:437:ARG:NH1	1.99	0.77
6:D:774:SER:HB3	6:D:1362:LYS:O	1.84	0.77
6:D:785:ILE:HG13	6:D:939:PHE:CE2	2.19	0.77
5:M:516:ARG:NE	6:N:1068:LEU:HD13	1.99	0.77
5:M:938:LYS:HB2	5:M:938:LYS:HZ2	1.50	0.77
6:N:397:LYS:O	6:N:448:GLU:HB2	1.84	0.77
5:M:511:GLU:O	5:M:526:PRO:HD3	1.84	0.77
5:M:758:ARG:CZ	5:M:788:THR:HB	2.14	0.77
6:D:136:ASP:CB	6:D:455:ARG:HE	1.99	0.77
6:D:9:ARG:HA	6:D:1455:LYS:O	1.84	0.77
6:D:897:TRP:HA	6:D:900:ILE:HG12	1.65	0.77
6:N:554:LEU:HD13	6:N:570:GLU:HG2	1.67	0.76
5:C:1083:GLU:HG2	5:C:1086:ARG:HH21	1.48	0.76
6:N:1459:LEU:HB3	6:N:1465:ASN:ND2	2.00	0.76
5:C:431:HIS:CD2	5:C:433:THR:H	2.03	0.76
6:D:908:LYS:CB	6:D:1027:GLY:HA3	2.15	0.76
6:N:1003:VAL:O	6:N:1007:VAL:HG23	1.85	0.76
5:C:874:LEU:O	5:C:877:PRO:HD2	1.86	0.76
6:D:1087:ARG:HG3	6:D:1237:THR:HG21	1.67	0.76
6:D:202:VAL:HB	6:D:398:ALA:O	1.86	0.76
6:D:710:ARG:HG2	6:D:772:PRO:HG2	1.68	0.76
5:M:1032:PHE:O	5:M:1036:GLU:HB2	1.86	0.76
6:N:895:VAL:HG11	6:N:922:LEU:HD21	1.65	0.76
6:D:28:LYS:HG3	6:D:29:PRO:HD2	1.68	0.76
5:M:244:PRO:HD2	5:M:245:GLY:H	1.50	0.76
5:M:5:ARG:NE	5:M:8:ARG:HH12	1.83	0.76
6:N:1390:LEU:HD21	11:N:9287:HOH:O	1.86	0.76
11:M:1524:HOH:O	6:N:616:GLN:HA	1.84	0.76
6:D:1271:LYS:HZ2	6:D:1331:ASP:HB3	1.48	0.76
5:C:1032:PHE:O	5:C:1036:GLU:HB2	1.85	0.76
5:M:998:TYR:HE2	5:M:1000:MET:HG3	1.49	0.76
6:N:486:ARG:HA	6:N:489:ARG:HG2	1.68	0.76
6:N:1481:VAL:HG11	7:O:18:ARG:HA	1.68	0.76
5:C:614:ARG:HG3	5:C:620:LEU:HD22	1.68	0.76
6:N:1108:ARG:NH1	6:N:1108:ARG:HB2	2.01	0.76
6:N:1394:VAL:HB	6:N:1397:LYS:HB2	1.68	0.76
4:A:222:LEU:HD21	4:B:218:LEU:HB3	1.68	0.75
4:A:75:VAL:HA	4:A:78:ILE:HD12	1.68	0.75
6:D:131:LYS:HG3	6:D:568:ARG:HG2	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:53:ILE:HD12	6:D:86:ARG:HH22	1.51	0.75
6:D:554:LEU:HD21	6:D:571:LYS:HE2	1.66	0.75
6:D:25:GLU:HG3	6:D:93:ILE:HA	1.66	0.75
6:D:455:ARG:O	6:D:460:ALA:HB2	1.87	0.75
6:D:73:CYS:HB3	6:D:76:CYS:O	1.87	0.75
6:N:122:GLU:O	6:N:126:VAL:HG23	1.84	0.75
6:N:399:ARG:HB2	6:N:401:TYR:CZ	2.21	0.75
6:N:47:GLU:HA	11:N:9490:HOH:O	1.85	0.75
5:C:1016:ILE:HD13	5:C:1016:ILE:H	1.50	0.75
5:M:312:ALA:HB1	5:M:318:PRO:HG2	1.67	0.75
4:B:52:ALA:HB2	4:B:170:VAL:O	1.86	0.75
6:D:1103:HIS:CD2	6:D:1463:LYS:H	2.05	0.75
5:M:997:LEU:HD21	11:M:1517:HOH:O	1.87	0.75
6:N:136:ASP:HB3	6:N:137:PRO:HD3	1.67	0.75
5:C:1031:ARG:HE	6:D:621:LYS:HB3	1.50	0.75
5:M:626:ARG:HH12	5:M:637:LEU:HB2	1.51	0.75
1:X:17:DC:H2''	1:X:18:DG:H5'	1.66	0.75
5:M:331:ARG:HH21	5:M:427:VAL:HG13	1.51	0.75
5:M:378:LEU:HG	5:M:382:ILE:HD11	1.69	0.75
5:M:758:ARG:HB3	5:M:788:THR:O	1.87	0.75
6:N:603:LEU:O	6:N:606:ILE:HG22	1.87	0.75
5:C:650:ARG:HG3	5:C:653:ASP:HB2	1.67	0.75
4:L:162:ILE:HA	11:L:316:HOH:O	1.86	0.75
5:M:150:PRO:HA	5:M:158:TYR:HB3	1.69	0.75
6:N:496:LEU:HD12	6:N:500:ARG:HG2	1.69	0.75
6:N:764:LEU:HD12	6:N:765:SER:H	1.52	0.75
4:B:152:PRO:HB2	4:B:155:LYS:HD2	1.69	0.75
6:D:139:GLY:O	6:D:147:VAL:HB	1.87	0.75
6:N:133:ILE:HG12	6:N:456:MET:HE2	1.68	0.75
6:D:1149:LEU:HD12	6:D:1161:GLU:O	1.87	0.75
6:D:148:GLU:HB3	6:D:151:GLN:HB2	1.69	0.75
6:D:651:GLU:HA	6:D:654:LYS:NZ	2.02	0.75
6:N:29:PRO:HD3	6:N:548:ILE:HG21	1.68	0.75
4:B:211:LEU:O	4:B:215:VAL:HG13	1.86	0.74
5:C:169:GLY:HA3	5:C:263:ASP:HB3	1.69	0.74
2:H:12:G:H2'	2:H:13:C:C6	2.22	0.74
6:N:853:VAL:HG22	6:N:858:VAL:HG23	1.69	0.74
4:B:41:ARG:HD2	4:B:177:VAL:HG23	1.69	0.74
1:X:13:DT:H5''	6:N:1093:TYR:HE2	1.51	0.74
6:N:1155:VAL:HA	11:N:9051:HOH:O	1.88	0.74
6:N:1448:THR:O	6:N:1452:ILE:HD12	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:141:HIS:HB3	5:C:418:LEU:HD23	1.67	0.74
5:C:904:PRO:HD2	5:C:908:GLY:HA2	1.67	0.74
2:Y:2:A:H8	2:Y:2:A:H3'	1.48	0.74
4:A:57:TYR:HB3	4:A:141:GLU:HG3	1.67	0.74
6:D:1195:GLN:HG3	6:D:1196:THR:N	2.02	0.74
5:M:1092:LEU:HA	5:M:1095:LEU:HD12	1.68	0.74
6:N:1228:SER:O	6:N:1232:PRO:HD2	1.88	0.74
6:N:139:GLY:O	6:N:147:VAL:HB	1.86	0.74
5:C:186:VAL:HG23	5:C:187:ASN:H	1.51	0.74
5:C:1034:GLU:HB3	6:D:619:LEU:HD22	1.67	0.74
2:H:9:G:H2'	2:H:10:G:C8	2.21	0.74
5:M:443:THR:HG21	6:N:1078:ARG:HE	1.52	0.74
2:Y:10:G:H1'	11:Y:1398:HOH:O	1.86	0.74
2:Y:10:G:H2'	2:Y:11:C:C6	2.23	0.74
5:C:943:VAL:HG11	5:C:973:VAL:HG21	1.70	0.74
5:M:433:THR:HG21	5:M:488:ALA:HB1	1.70	0.74
5:M:807:ARG:H	5:M:807:ARG:HE	1.36	0.74
5:M:5:ARG:HB2	5:M:8:ARG:HH22	1.51	0.74
6:N:1424:VAL:HG13	6:N:1425:THR:H	1.50	0.74
5:C:328:LEU:H	5:C:433:THR:CB	1.99	0.74
5:C:437:ARG:HE	5:C:469:THR:HB	1.52	0.74
5:C:872:ASN:HD21	5:C:874:LEU:HD13	1.51	0.74
6:D:581:LEU:HG	6:D:582:LEU:HG	1.68	0.74
5:M:781:LYS:HD3	5:M:781:LYS:H	1.51	0.74
6:N:409:VAL:HG21	6:N:421:LEU:HD23	1.67	0.74
5:M:673:LEU:HD22	5:M:867:VAL:HA	1.69	0.74
5:C:959:PRO:HB2	11:C:1203:HOH:O	1.85	0.74
6:N:972:LEU:HG	6:N:976:GLN:NE2	2.03	0.74
4:B:59:GLU:HB2	4:B:137:ARG:NH1	1.99	0.74
6:D:65:ARG:HG3	6:D:66:GLN:H	1.53	0.74
6:D:806:PHE:CE1	6:D:813:LEU:HB3	2.23	0.74
5:M:68:PHE:HZ	5:M:71:TYR:HD2	1.36	0.74
6:N:204:LEU:HD13	6:N:445:ARG:NE	2.03	0.74
6:N:786:ILE:HG21	6:N:1027:GLY:N	2.01	0.74
4:K:39:PRO:HG3	11:L:348:HOH:O	1.86	0.73
6:N:1093:TYR:O	6:N:1097:LYS:HG2	1.88	0.73
5:M:1034:GLU:N	6:N:619:LEU:HB3	2.03	0.73
6:D:1098:LEU:HD23	6:D:1226:ALA:HA	1.70	0.73
5:C:1042:ALA:HA	6:D:1220:ALA:HB3	1.68	0.73
6:N:166:GLN:HG3	6:N:447:VAL:HB	1.71	0.73
4:A:194:LYS:HG3	11:A:338:HOH:O	1.86	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:603:LEU:O	6:D:606:ILE:HG22	1.88	0.73
11:D:8449:HOH:O	7:E:28:GLN:HG3	1.88	0.73
5:M:546:LEU:HD12	5:M:565:GLN:HE22	1.50	0.73
6:N:1166:LEU:HD23	6:N:1166:LEU:H	1.53	0.73
5:M:1005:MET:HB2	6:N:648:MET:CE	2.18	0.73
4:A:82:LEU:HD22	4:A:142:VAL:HG11	1.69	0.73
11:A:325:HOH:O	4:B:215:VAL:HG21	1.89	0.73
7:E:54:LEU:HG	7:E:58:PRO:HG2	1.71	0.73
5:C:668:LEU:HD13	5:C:995:MET:SD	2.29	0.73
5:C:722:ILE:HD12	5:C:823:VAL:HG21	1.69	0.73
6:D:483:HIS:HB2	6:D:484:PRO:HD3	1.68	0.73
6:N:1481:VAL:HG13	7:O:18:ARG:HE	1.53	0.73
6:N:959:GLU:HB2	6:N:963:TYR:CE1	2.24	0.73
5:C:810:ASP:HB3	5:C:813:VAL:HG12	1.70	0.73
6:D:1105:ILE:HD12	6:D:1373:ARG:HH21	1.52	0.73
6:D:171:LEU:HD21	6:D:192:ALA:CB	2.18	0.73
4:L:59:GLU:HB2	4:L:137:ARG:NH1	2.03	0.73
5:M:671:ASN:HA	11:M:1511:HOH:O	1.88	0.73
5:C:881:ASN:O	5:C:884:GLN:HG3	1.89	0.73
5:C:946:ARG:HB3	5:C:946:ARG:HH11	1.52	0.73
5:C:516:ARG:NE	6:D:1068:LEU:HD13	2.03	0.73
5:M:290:LEU:HD22	5:M:302:VAL:HG11	1.70	0.73
5:M:52:PHE:CD2	5:M:68:PHE:HB2	2.24	0.73
6:N:541:ASN:O	6:N:545:ARG:HG3	1.89	0.73
5:C:1035:MET:HA	5:C:1038:TRP:CE3	2.24	0.73
5:C:263:ASP:HB2	5:C:264:PRO:HD3	1.69	0.73
5:C:837:ASP:HA	5:C:999:HIS:HE1	1.52	0.73
6:D:1231:GLU:CD	6:D:1232:PRO:HD3	2.09	0.73
6:D:1462:LEU:HD21	6:D:1474:ALA:HB3	1.71	0.73
6:D:171:LEU:HD23	6:D:172:PRO:HD2	1.69	0.73
5:M:758:ARG:NH2	5:M:788:THR:HB	2.04	0.73
6:N:989:TYR:O	6:N:993:LEU:HG	1.87	0.73
6:D:834:THR:HG22	6:D:838:ARG:HH11	1.53	0.73
5:M:132:ALA:HB1	5:M:632:ASN:HD21	1.54	0.73
5:C:479:VAL:HG11	5:C:503:LEU:HD11	1.71	0.73
6:D:1083:ASP:O	6:D:1087:ARG:HG2	1.89	0.73
4:K:189:ARG:HH12	4:L:155:LYS:HE3	1.54	0.73
4:L:218:LEU:O	4:L:222:LEU:HG	1.88	0.73
5:M:313:LEU:HD23	11:M:1189:HOH:O	1.89	0.73
4:K:42:ARG:HH11	5:M:978:ARG:HA	1.53	0.73
6:N:1166:LEU:HD12	6:N:1171:VAL:HG22	1.71	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:48:MET:HB2	7:O:54:LEU:HB2	1.70	0.73
7:E:76:GLY:HA3	7:E:79:LEU:HD13	1.69	0.72
5:M:554:ASP:CB	5:M:880:MET:HB2	2.19	0.72
5:M:872:ASN:HD21	5:M:874:LEU:HB2	1.53	0.72
5:C:1095:LEU:HD23	6:D:582:LEU:HD22	1.71	0.72
5:M:756:VAL:O	5:M:789:SER:HB3	1.89	0.72
6:N:643:GLY:HA3	6:N:727:GLN:HB2	1.70	0.72
2:Y:6:U:H2'	2:Y:7:G:N7	2.03	0.72
5:C:768:THR:HB	5:C:771:GLU:HB3	1.72	0.72
5:M:578:VAL:HG23	5:M:579:VAL:HG12	1.71	0.72
5:C:312:ALA:HB1	5:C:318:PRO:HG2	1.70	0.72
5:C:710:ILE:HD12	5:C:790:LEU:HB2	1.70	0.72
5:C:850:ALA:HB2	11:C:1474:HOH:O	1.88	0.72
6:D:486:ARG:HA	6:D:489:ARG:CD	2.19	0.72
2:H:10:G:H2'	2:H:11:C:C6	2.25	0.72
2:Y:13:C:H4'	5:M:409:ARG:NH2	2.05	0.72
6:D:153:LEU:HD11	6:D:158:TYR:HB2	1.72	0.72
6:D:25:GLU:HA	6:D:92:HIS:O	1.89	0.72
6:D:394:LEU:O	6:D:396:VAL:HG23	1.88	0.72
6:D:68:PHE:HB2	11:D:8148:HOH:O	1.89	0.72
6:N:929:ARG:NH1	6:N:929:ARG:HB2	2.05	0.72
6:N:95:LEU:H	6:N:95:LEU:HD12	1.54	0.72
4:B:79:ILE:HA	4:B:82:LEU:HD12	1.70	0.72
5:C:677:MET:HB3	5:C:987:ILE:HD13	1.71	0.72
6:D:1465:ASN:HD21	6:D:1470:ARG:HE	1.36	0.72
5:M:412:ALA:HB1	5:M:419:THR:HG21	1.71	0.72
6:N:116:LEU:HD13	6:N:118:LEU:HD11	1.71	0.72
4:A:226:SER:O	4:A:228:PRO:HD3	1.90	0.72
4:B:218:LEU:O	4:B:222:LEU:HG	1.89	0.72
5:C:464:LEU:HD21	11:C:1308:HOH:O	1.89	0.72
6:N:951:ILE:HG23	6:N:1062:ARG:HE	1.55	0.72
7:O:54:LEU:O	7:O:54:LEU:HD23	1.90	0.72
7:O:46:PRO:HG3	7:O:66:LYS:HD3	1.70	0.72
4:B:186:LEU:HD21	11:B:367:HOH:O	1.87	0.72
6:D:53:ILE:HD12	6:D:86:ARG:NH2	2.04	0.72
4:K:189:ARG:NH1	4:L:155:LYS:HE3	2.04	0.72
6:N:493:ARG:HG2	6:N:1390:LEU:HB2	1.71	0.72
6:D:30:GLU:HB3	6:D:40:GLU:HG2	1.71	0.72
5:C:689:VAL:HB	5:C:870:ILE:HG13	1.71	0.72
6:D:122:GLU:O	6:D:126:VAL:HG23	1.90	0.72
6:D:810:GLU:O	6:D:813:LEU:HG	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:608:GLY:C	5:M:609:ASN:HD22	1.94	0.72
4:K:38:ASN:HB2	5:M:980:GLY:HA3	1.71	0.72
6:N:1205:TYR:CD2	6:N:1215:VAL:HG21	2.25	0.72
6:N:179:VAL:HG13	6:N:183:GLU:HB3	1.72	0.72
4:A:61:VAL:HG23	11:A:319:HOH:O	1.90	0.71
6:D:677:LEU:HD23	6:D:683:ILE:HG13	1.72	0.71
4:K:89:PHE:HD1	4:K:120:VAL:HG23	1.54	0.71
5:M:1060:ILE:HG22	11:M:1405:HOH:O	1.90	0.71
6:N:421:LEU:HD22	6:N:444:VAL:HG11	1.69	0.71
5:C:158:TYR:HD1	5:C:314:THR:HG22	1.54	0.71
5:C:409:ARG:CA	5:C:454:SER:HA	2.16	0.71
5:C:861:LEU:HA	5:C:974:LEU:HD12	1.72	0.71
6:N:133:ILE:HG21	6:N:454:ALA:HB1	1.71	0.71
4:A:179:PHE:HB2	4:A:195:LEU:HD11	1.71	0.71
5:C:129:ILE:HD13	5:C:134:ARG:HB2	1.73	0.71
5:C:436:GLY:O	5:C:459:ALA:HB2	1.90	0.71
5:C:675:ALA:HB2	5:C:867:VAL:HG11	1.71	0.71
6:D:409:VAL:HG23	6:D:421:LEU:HA	1.71	0.71
6:D:646:LYS:HG3	6:D:720:LEU:HD23	1.70	0.71
4:K:153:ALA:HA	4:K:156:HIS:CE1	2.26	0.71
5:M:270:GLY:O	5:M:274:ARG:HB3	1.89	0.71
5:M:704:HIS:O	5:M:828:ALA:HA	1.90	0.71
5:M:874:LEU:HA	6:N:1023:MET:SD	2.31	0.71
5:C:143:SER:HB2	5:C:276:LYS:HZ3	1.55	0.71
5:C:1031:ARG:NE	6:D:621:LYS:HB3	2.06	0.71
4:K:56:VAL:HG22	4:K:142:VAL:HG12	1.70	0.71
5:M:1090:LYS:HE3	5:M:1112:PHE:HE1	1.55	0.71
5:M:1101:THR:HG21	5:M:1111:ILE:HG23	1.71	0.71
5:M:34:VAL:HB	5:M:38:LYS:HG3	1.71	0.71
6:N:1042:ARG:NH2	6:N:1073:SER:HB3	2.05	0.71
6:N:1136:LYS:HB2	6:N:1139:ASP:OD2	1.90	0.71
5:C:355:VAL:HA	5:C:358:ARG:HD3	1.72	0.71
5:C:950:LEU:HB3	5:C:952:LEU:HD23	1.72	0.71
6:D:119:SER:HB2	6:D:123:LEU:HB2	1.72	0.71
5:M:554:ASP:HB2	5:M:880:MET:HB2	1.71	0.71
6:N:145:VAL:HG22	6:N:146:PRO:HD2	1.71	0.71
6:N:792:ILE:HD11	6:N:878:GLY:O	1.91	0.71
6:N:921:ARG:NH1	6:N:921:ARG:HB3	2.05	0.71
5:C:142:ARG:HB3	5:C:142:ARG:HH11	1.55	0.71
5:C:804:VAL:HG11	5:C:824:ARG:HH21	1.56	0.71
5:C:675:ALA:HA	5:C:989:VAL:HG13	1.71	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1037:GLN:HG2	6:D:1042:ARG:HB3	1.73	0.71
6:D:185:VAL:HG11	6:D:191:LEU:HD21	1.72	0.71
6:D:421:LEU:HB2	6:D:427:VAL:HG12	1.72	0.71
6:N:521:PRO:HG2	6:N:524:LEU:HD22	1.72	0.71
11:M:1216:HOH:O	6:N:950:GLY:HA3	1.91	0.71
5:C:675:ALA:HB1	5:C:677:MET:SD	2.31	0.71
5:C:837:ASP:HA	5:C:999:HIS:CE1	2.25	0.71
6:D:615:ARG:NH2	6:D:1096:ARG:NH1	2.39	0.71
5:M:1115:LEU:HG	6:N:85:VAL:HG12	1.72	0.71
5:M:376:ARG:HG2	11:M:1395:HOH:O	1.90	0.71
5:M:546:LEU:HD21	11:M:1376:HOH:O	1.90	0.71
6:D:83:SER:O	6:D:86:ARG:HB3	1.90	0.71
5:M:325:ILE:HD11	11:M:1567:HOH:O	1.91	0.71
5:M:584:GLU:CD	5:M:584:GLU:H	1.95	0.71
4:K:178:ALA:HB2	5:M:864:GLY:H	1.55	0.71
6:N:1146:GLY:HA3	6:N:1207:TYR:HB2	1.71	0.71
6:N:50:PHE:CG	6:N:522:PRO:HD3	2.26	0.71
5:M:1019:GLN:NE2	6:N:616:GLN:HE22	1.88	0.71
6:D:1160:LEU:HD11	6:D:1174:LEU:HD21	1.71	0.71
6:D:1332:PRO:HG3	6:D:1347:TYR:HE2	1.54	0.71
6:D:486:ARG:HA	6:D:489:ARG:HG2	1.73	0.71
4:K:178:ALA:HB3	4:K:198:ARG:HG3	1.72	0.71
4:L:89:PHE:HB3	4:L:94:LEU:CD1	2.21	0.71
6:D:1087:ARG:HH21	6:D:1253:THR:HG22	1.56	0.70
6:D:1383:ASP:HB2	6:D:1416:ALA:HB3	1.71	0.70
6:D:1481:VAL:HG22	7:E:18:ARG:HE	1.56	0.70
5:M:609:ASN:HD22	5:M:609:ASN:N	1.86	0.70
6:N:1033:GLN:HE21	6:N:1036:ARG:NH1	1.88	0.70
6:N:1094:LEU:HB2	6:N:1260:ILE:HD11	1.72	0.70
6:N:502:PHE:CE1	6:N:509:PRO:HB3	2.26	0.70
5:C:1046:ALA:HA	6:D:1472:ILE:HG13	1.72	0.70
2:H:12:G:H1'	5:C:393:GLN:HG2	1.73	0.70
6:D:1093:TYR:O	6:D:1097:LYS:HG2	1.91	0.70
4:K:220:GLU:O	4:K:223:THR:HG22	1.89	0.70
6:N:1168:MET:HE3	6:N:1171:VAL:HB	1.72	0.70
6:N:1406:ARG:HG3	6:N:1412:LYS:HG2	1.72	0.70
1:G:13:DT:H5"	6:D:1093:TYR:CE2	2.26	0.70
4:L:102:LYS:HE3	4:L:104:GLU:HG3	1.73	0.70
5:M:1031:ARG:HA	6:N:621:LYS:O	1.92	0.70
5:C:502:PRO:HB2	5:C:509:ALA:HB3	1.73	0.70
5:C:1007:ALA:HB1	6:D:652:LEU:HD13	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:507:ASN:H	6:N:507:ASN:ND2	1.90	0.70
6:N:78:VAL:HG12	6:N:80:VAL:HG22	1.74	0.70
5:C:1017:THR:HB	6:D:613:ARG:HH22	1.56	0.70
6:D:403:PHE:HB2	6:D:423:ASP:OD1	1.91	0.70
2:H:6:U:H2'	2:H:7:G:N7	2.05	0.70
5:M:108:ILE:HB	5:M:368:THR:OG1	1.91	0.70
5:C:1085:PHE:O	5:C:1089:VAL:HG23	1.91	0.70
6:D:177:ALA:HB3	6:D:205:TYR:OH	1.90	0.70
6:D:150:ARG:HH22	6:D:473:LEU:HD21	1.57	0.70
5:M:433:THR:HG22	5:M:437:ARG:HH11	1.56	0.70
6:N:434:ARG:HB3	6:N:434:ARG:NH1	2.07	0.70
2:Y:2:A:OP2	6:N:671:LYS:NZ	2.25	0.70
6:N:786:ILE:HG22	6:N:1026:SER:HB3	1.73	0.70
5:C:244:PRO:HB3	11:C:1256:HOH:O	1.92	0.70
6:D:1090:ASP:HA	6:D:1093:TYR:HB2	1.72	0.70
6:D:1098:LEU:HD21	6:D:1229:ILE:HD12	1.73	0.70
6:D:179:VAL:HG13	6:D:183:GLU:HB3	1.74	0.70
4:K:48:ILE:HB	11:K:973:HOH:O	1.90	0.70
5:M:745:ILE:HD12	5:M:745:ILE:H	1.57	0.70
5:C:144:PRO:HG2	5:C:265:ARG:NH2	2.06	0.70
5:C:673:LEU:HB3	5:C:868:ASP:OD1	1.92	0.70
6:D:1209:LEU:HD23	6:D:1210:SER:N	2.06	0.70
6:D:1496:GLU:HA	6:D:1499:ARG:NE	2.06	0.70
6:D:117:ASP:H	6:D:150:ARG:NH1	1.90	0.70
6:D:117:ASP:HB2	6:D:495:ARG:NH2	2.07	0.70
4:K:88:ARG:O	4:K:121:GLU:HG2	1.91	0.70
5:M:806:LEU:HD11	5:M:824:ARG:NH2	2.06	0.70
6:N:565:ILE:H	6:N:565:ILE:HD12	1.56	0.70
4:A:227:ASN:O	4:B:11:PHE:HB3	1.91	0.70
5:C:762:LYS:HD3	5:C:784:ASP:O	1.90	0.70
6:D:1005:GLN:HA	6:D:1005:GLN:HE21	1.57	0.70
6:D:496:LEU:O	6:D:500:ARG:HG2	1.92	0.70
6:D:584:ASN:OD1	6:D:590:PRO:HD2	1.91	0.70
5:M:39:ARG:HD2	5:M:39:ARG:N	2.05	0.70
6:N:1042:ARG:O	6:N:1057:VAL:HB	1.92	0.70
2:Y:9:G:H2'	2:Y:10:G:H8	1.56	0.70
4:B:38:ASN:HB3	4:B:39:PRO:HD3	1.74	0.70
6:D:1086:LEU:HD12	11:D:8404:HOH:O	1.91	0.70
6:D:119:SER:HB2	6:D:123:LEU:H	1.57	0.70
4:L:110:LYS:HD3	4:L:126:ASP:HA	1.74	0.70
6:N:871:LYS:HB3	6:N:873:LEU:HD21	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:874:LEU:HD12	5:C:874:LEU:H	1.56	0.69
6:N:462:GLN:HB2	6:N:513:ILE:HD13	1.74	0.69
7:O:54:LEU:HA	7:O:58:PRO:HG2	1.74	0.69
4:B:89:PHE:HB3	4:B:94:LEU:HD12	1.74	0.69
5:C:841:ASN:H	5:C:841:ASN:HD22	1.38	0.69
6:D:105:VAL:HG21	6:D:128:TYR:HE1	1.57	0.69
6:N:760:ARG:HH11	7:O:61:VAL:HG23	1.57	0.69
4:A:56:VAL:HG22	4:A:142:VAL:HG13	1.73	0.69
5:C:547:ILE:HG21	5:C:550:LEU:HD13	1.74	0.69
5:C:886:LEU:HD13	6:D:951:ILE:HG13	1.73	0.69
6:D:546:ARG:HA	11:D:8178:HOH:O	1.91	0.69
6:D:684:LYS:HB3	6:D:686:GLU:HG3	1.72	0.69
5:M:242:LEU:HD13	11:M:1532:HOH:O	1.92	0.69
5:C:159:ILE:HG13	11:C:1362:HOH:O	1.93	0.69
5:C:689:VAL:HG12	5:C:690:ILE:H	1.56	0.69
6:D:38:LYS:HG2	6:D:39:PRO:HD2	1.73	0.69
6:D:786:ILE:HD13	6:D:908:LYS:HB2	1.75	0.69
5:M:872:ASN:ND2	5:M:874:LEU:HB2	2.06	0.69
6:D:1147:ARG:HB3	6:D:1188:VAL:HG21	1.73	0.69
6:D:1192:LEU:HB3	6:D:1345:GLU:OE2	1.92	0.69
6:D:136:ASP:HB2	6:D:455:ARG:HE	1.57	0.69
6:D:1395:LEU:HD23	6:D:1396:GLU:N	2.08	0.69
6:D:141:ILE:HD11	6:D:165:LYS:NZ	2.08	0.69
6:D:756:GLN:HG3	6:D:760:ARG:HH11	1.57	0.69
5:M:333:ILE:N	5:M:465:GLY:HA3	2.05	0.69
5:M:877:PRO:HG2	6:N:1023:MET:SD	2.31	0.69
6:N:41:ARG:HD3	6:N:42:ASP:H	1.57	0.69
6:N:554:LEU:HD21	6:N:571:LYS:HD3	1.75	0.69
7:O:31:LEU:HD21	7:O:60:ALA:HB2	1.73	0.69
5:C:265:ARG:HH11	5:C:267:TYR:HB3	1.55	0.69
5:C:341:THR:HA	11:C:1289:HOH:O	1.91	0.69
5:C:457:ALA:HB3	5:C:538:GLN:HA	1.74	0.69
5:C:69:LEU:HB2	5:C:97:ARG:HB2	1.73	0.69
5:C:1100:GLN:HE21	5:C:1100:GLN:HA	1.57	0.69
5:C:872:ASN:HD21	5:C:874:LEU:CD1	2.04	0.69
6:D:1059:SER:HA	11:D:8349:HOH:O	1.93	0.69
6:D:741:ASP:O	6:D:743:ASP:N	2.25	0.69
6:D:957:PRO:HA	11:D:8083:HOH:O	1.91	0.69
5:M:838:LYS:HG2	11:M:1491:HOH:O	1.93	0.69
5:M:853:LEU:HD23	5:M:858:MET:HB3	1.74	0.69
6:N:130:SER:HB3	6:N:132:TYR:HE1	1.57	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:197:LEU:HG	4:A:199:ILE:HD11	1.75	0.69
5:C:134:ARG:HH21	5:C:392:SER:HB2	1.56	0.69
5:C:431:HIS:HD2	5:C:433:THR:H	1.41	0.69
5:C:578:VAL:HG23	5:C:579:VAL:HG12	1.74	0.69
6:D:95:LEU:HD21	6:D:574:LEU:HD21	1.73	0.69
5:M:689:VAL:HG12	5:M:690:ILE:H	1.57	0.69
5:C:511:GLU:O	5:C:526:PRO:HD3	1.93	0.69
6:D:399:ARG:HH11	6:D:430:ASP:HB2	1.57	0.69
6:D:656:PHE:HB3	6:D:694:VAL:HG11	1.73	0.69
7:E:41:GLU:OE1	7:E:42:PRO:HD3	1.93	0.69
4:L:52:ALA:HB2	4:L:170:VAL:O	1.92	0.69
6:N:1124:GLN:HB3	6:N:1135:ARG:HD3	1.74	0.69
6:N:54:LYS:HD2	6:N:55:ASP:H	1.58	0.69
6:N:586:ARG:NH2	6:N:1444:THR:HG21	2.07	0.69
6:N:889:ALA:HB3	6:N:930:LEU:HD12	1.74	0.69
4:B:64:GLU:HA	4:B:165:ILE:HD13	1.75	0.69
6:D:1403:LEU:HD23	6:D:1407:LEU:HD13	1.74	0.69
5:C:1034:GLU:H	6:D:619:LEU:HD13	1.58	0.69
6:D:644:LEU:HD23	6:D:718:PRO:HB3	1.73	0.69
2:H:8:C:H5"	11:H:37:HOH:O	1.93	0.69
5:M:580:MET:SD	5:M:584:GLU:HG3	2.33	0.69
5:M:881:ASN:O	5:M:884:GLN:HG3	1.91	0.69
5:C:411:SER:HA	5:C:451:LEU:O	1.93	0.69
5:C:31:GLN:HB3	5:C:71:TYR:OH	1.92	0.69
6:D:554:LEU:HD11	6:D:571:LYS:HD3	1.75	0.69
11:B:374:HOH:O	6:D:851:LEU:HD21	1.93	0.69
5:M:331:ARG:NH2	5:M:427:VAL:HG13	2.07	0.69
5:M:405:ARG:HH22	5:M:566:THR:CG2	2.05	0.69
1:X:17:DC:H5"	5:M:1030:GLN:HE21	1.58	0.69
5:C:182:VAL:HG21	5:C:220:GLY:O	1.93	0.68
6:D:1046:GLN:HG2	6:D:1052:THR:HG22	1.74	0.68
6:D:10:ILE:HB	6:D:1451:ALA:HA	1.73	0.68
6:D:634:GLY:HA2	6:D:727:GLN:HE21	1.57	0.68
6:D:781:PRO:HG2	6:D:911:LEU:HD23	1.75	0.68
5:M:904:PRO:HD2	5:M:908:GLY:HA2	1.75	0.68
6:N:489:ARG:NH2	6:N:1389:LEU:HD21	2.07	0.68
6:N:834:THR:HG22	6:N:838:ARG:HH11	1.58	0.68
5:C:405:ARG:HG3	5:C:442:GLU:OE1	1.93	0.68
5:C:946:ARG:HH22	6:D:861:GLN:HE22	1.40	0.68
4:K:94:LEU:HD21	4:K:119:ASP:HB3	1.74	0.68
5:M:252:LYS:NZ	5:M:296:GLY:HA3	2.08	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:148:PHE:HZ	5:M:281:LEU:HD13	1.57	0.68
5:M:479:VAL:HG11	5:M:503:LEU:HD11	1.75	0.68
4:B:197:LEU:HD21	4:B:199:ILE:HD11	1.74	0.68
6:D:1399:ASP:O	6:D:1403:LEU:HB2	1.93	0.68
6:D:524:LEU:O	6:D:526:PRO:HD3	1.92	0.68
1:G:14:DT:H5'	1:G:14:DT:H6	1.59	0.68
4:L:61:VAL:HG21	4:L:75:VAL:HG21	1.75	0.68
5:M:333:ILE:H	5:M:465:GLY:CA	2.05	0.68
6:N:1492:LEU:HD12	6:N:1493:LYS:NZ	2.09	0.68
6:N:807:ALA:HB2	6:N:833:GLU:OE1	1.93	0.68
4:B:59:GLU:CB	4:B:137:ARG:HH12	2.03	0.68
5:C:158:TYR:O	5:C:310:LEU:HD11	1.93	0.68
6:D:1109:GLU:HG2	6:D:1201:CYS:CA	2.20	0.68
6:D:1196:THR:HG22	11:D:8501:HOH:O	1.94	0.68
6:D:1380:GLU:HG3	6:D:1420:LEU:HD12	1.74	0.68
6:D:868:TYR:HB2	6:D:873:LEU:HD12	1.76	0.68
5:M:343:GLN:HG2	5:M:385:PHE:HB2	1.75	0.68
5:C:5:ARG:CZ	5:C:8:ARG:HH22	2.06	0.68
6:D:964:LEU:HD21	6:D:1058:ARG:HE	1.57	0.68
6:D:409:VAL:CG2	6:D:421:LEU:HA	2.24	0.68
6:D:526:PRO:HA	11:D:8171:HOH:O	1.93	0.68
6:D:800:LYS:HE3	6:D:804:LEU:HD22	1.74	0.68
6:D:98:PRO:HB3	11:D:8058:HOH:O	1.93	0.68
5:M:305:PRO:HG3	5:M:308:ARG:HH22	1.59	0.68
6:N:1161:GLU:HG2	6:N:1164:ARG:HB2	1.74	0.68
6:D:22:SER:HB2	6:D:92:HIS:HB3	1.76	0.68
6:D:988:ARG:O	6:D:992:ILE:HG13	1.94	0.68
4:K:58:ILE:HG21	4:K:68:ILE:HD11	1.75	0.68
6:N:1191:PRO:HG2	6:N:1370:ILE:HD13	1.74	0.68
5:C:435:TYR:HE1	5:C:539:VAL:HG22	1.58	0.68
6:D:1223:ILE:CG2	6:D:1227:GLN:HE21	2.06	0.68
6:D:1252:ILE:HG13	6:D:1253:THR:H	1.59	0.68
6:D:1197:ARG:HB3	6:D:1396:GLU:HG3	1.74	0.68
6:D:650:LEU:HD23	6:D:691:LEU:HD23	1.75	0.68
5:M:874:LEU:O	5:M:877:PRO:HD2	1.93	0.68
6:N:119:SER:HB2	6:N:123:LEU:H	1.59	0.68
6:N:394:LEU:O	6:N:396:VAL:HG23	1.94	0.68
6:N:879:ARG:HH21	6:N:904:VAL:N	1.90	0.68
6:D:455:ARG:HB3	6:D:459:GLU:HG2	1.76	0.68
6:D:984:THR:HG22	6:D:987:GLU:HG3	1.76	0.68
5:M:244:PRO:HG2	5:M:246:ASP:OD2	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:510:ALA:HB3	5:M:513:VAL:HG23	1.76	0.68
5:M:536:PRO:HD2	5:M:537:LYS:NZ	2.08	0.68
6:N:1111:ASP:CG	6:N:1203:LYS:HG3	2.14	0.68
4:B:85:LEU:HA	4:B:124:ASN:HD22	1.57	0.68
5:C:408:ARG:HG2	5:C:454:SER:HB3	1.74	0.68
6:D:1032:PRO:HB2	11:D:8254:HOH:O	1.93	0.68
6:N:526:PRO:O	6:N:537:THR:HA	1.94	0.68
5:M:292:ARG:HD2	5:M:299:LYS:NZ	2.08	0.68
5:M:516:ARG:NH1	5:M:521:PRO:HB3	2.09	0.68
7:O:51:LEU:HD23	7:O:52:GLU:H	1.59	0.68
5:C:709:GLU:HG3	5:C:824:ARG:HG2	1.76	0.67
5:M:495:THR:H	5:M:530:GLU:CD	1.96	0.67
5:M:768:THR:HB	5:M:771:GLU:HB3	1.75	0.67
6:N:546:ARG:NH1	6:N:546:ARG:HB3	2.08	0.67
5:C:106:GLY:O	5:C:107:LEU:HD23	1.94	0.67
5:C:610:ARG:HD3	5:C:622:GLU:OE2	1.94	0.67
6:D:1252:ILE:HG13	6:D:1253:THR:N	2.09	0.67
6:D:29:PRO:CG	6:D:549:ASN:HD21	2.07	0.67
6:D:782:SER:N	6:D:785:ILE:HD13	2.08	0.67
2:H:8:C:HO2'	2:H:9:G:H5'	1.58	0.67
4:L:206:THR:HG22	4:L:209:GLU:H	1.59	0.67
5:M:1111:ILE:HG13	5:M:1112:PHE:H	1.57	0.67
5:M:438:ILE:HD11	5:M:467:ILE:HD12	1.75	0.67
5:M:762:LYS:HD3	5:M:784:ASP:O	1.94	0.67
5:M:432:ARG:HH22	6:N:1047:LYS:HD3	1.59	0.67
6:N:402:PRO:HG2	11:N:9030:HOH:O	1.93	0.67
5:C:1:MET:HG2	5:C:900:ARG:HH22	1.60	0.67
5:C:762:LYS:HD2	5:C:786:LYS:HB2	1.75	0.67
5:M:1034:GLU:HB3	6:N:619:LEU:HD13	1.75	0.67
6:N:1412:LYS:O	6:N:1414:PRO:HD3	1.93	0.67
6:N:637:LEU:HD11	6:N:641:GLN:C	2.15	0.67
2:Y:11:C:H2'	2:Y:12:G:C8	2.30	0.67
5:C:1050:GLN:HE22	6:D:1471:LEU:HB2	1.59	0.67
5:C:433:THR:HG22	5:C:437:ARG:HH11	1.58	0.67
5:C:630:ARG:HA	5:C:705:ILE:HD13	1.77	0.67
6:D:786:ILE:HG21	6:D:1027:GLY:H	1.58	0.67
6:D:1101:VAL:CG2	6:D:1424:VAL:HG23	2.23	0.67
6:D:952:ASP:HA	6:D:1062:ARG:HH21	1.60	0.67
6:N:1124:GLN:NE2	6:N:1135:ARG:HA	2.10	0.67
6:N:1434:TRP:CZ3	6:N:1457:ASP:HB2	2.29	0.67
6:N:524:LEU:O	6:N:526:PRO:HD3	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:814:ALA:O	6:N:818:ARG:HG3	1.95	0.67
5:C:909:ALA:HB1	5:C:914:ILE:HD11	1.76	0.67
6:D:455:ARG:HB2	6:D:460:ALA:CA	2.25	0.67
6:D:610:LYS:O	6:D:615:ARG:HD3	1.93	0.67
6:D:654:LYS:HB3	6:D:655:PRO:HD3	1.77	0.67
5:M:549:PHE:CD1	5:M:886:LEU:HD23	2.30	0.67
6:N:483:HIS:HB2	6:N:484:PRO:HD3	1.76	0.67
4:B:58:ILE:HB	4:B:61:VAL:HB	1.76	0.67
5:C:235:LEU:HD21	11:C:1313:HOH:O	1.93	0.67
5:C:898:GLY:HA2	11:C:1408:HOH:O	1.94	0.67
5:M:805:ARG:HD3	5:M:823:VAL:HG22	1.75	0.67
6:N:131:LYS:HD3	6:N:456:MET:SD	2.35	0.67
6:N:520:LEU:HD21	6:N:524:LEU:HD23	1.76	0.67
5:M:252:LYS:HA	11:M:1276:HOH:O	1.95	0.67
6:N:1201:CYS:SG	6:N:1204:CYS:HB2	2.35	0.67
6:N:394:LEU:HD21	6:N:445:ARG:HH22	1.58	0.67
4:B:206:THR:HG22	4:B:209:GLU:H	1.59	0.67
5:C:443:THR:HG22	5:C:453:THR:HB	1.77	0.67
6:D:134:VAL:HB	6:D:464:LEU:HD11	1.75	0.67
6:D:1393:GLN:OE1	6:D:1394:VAL:HG23	1.95	0.67
6:D:396:VAL:O	6:D:398:ALA:N	2.25	0.67
6:D:715:ALA:HB3	6:D:764:LEU:HA	1.76	0.67
5:M:1115:LEU:HB3	6:N:89:ARG:NH1	2.10	0.67
6:N:908:LYS:HB2	6:N:1027:GLY:HA3	1.76	0.67
6:N:971:LEU:O	6:N:975:GLU:HG2	1.94	0.67
5:C:872:ASN:HD22	5:C:872:ASN:C	1.99	0.67
6:D:101:HIS:HD1	6:D:103:TRP:HB2	1.59	0.67
6:D:1498:ALA:HB2	7:E:88:GLU:OE1	1.95	0.67
4:K:1:MET:SD	4:K:5:LYS:HB3	2.35	0.67
5:M:971:LYS:HA	5:M:988:VAL:HA	1.76	0.67
6:N:1340:GLY:O	6:N:1344:VAL:HG23	1.94	0.67
6:N:1480:PHE:HB2	11:N:9408:HOH:O	1.94	0.67
6:D:1465:ASN:ND2	6:D:1470:ARG:HB3	2.09	0.67
1:G:17:DC:H4'	6:D:628:ARG:CZ	2.25	0.67
6:D:963:TYR:CE2	6:D:1002:LYS:HB3	2.29	0.67
6:D:1485:GLN:HE21	7:E:78:ASN:HA	1.60	0.67
5:M:399:ASN:OD1	5:M:401:LEU:HB3	1.95	0.67
5:M:552:HIS:CD2	5:M:886:LEU:HD22	2.30	0.67
6:N:1267:ARG:HG3	6:N:1271:LYS:HZ3	1.59	0.67
1:G:18:DG:O3'	5:C:1001:VAL:HB	1.94	0.66
5:C:244:PRO:HG3	11:C:1490:HOH:O	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:518:LYS:O	5:C:520:GLU:HG2	1.95	0.66
5:C:5:ARG:NE	5:C:8:ARG:HH22	1.93	0.66
5:C:884:GLN:HB3	5:C:992:MET:HE1	1.75	0.66
6:D:786:ILE:HG21	6:D:1027:GLY:N	2.10	0.66
6:D:1252:ILE:O	6:D:1256:LEU:HD12	1.95	0.66
6:D:127:LEU:HD12	6:D:128:TYR:N	2.10	0.66
6:D:396:VAL:HG12	6:D:398:ALA:HB2	1.77	0.66
6:D:434:ARG:N	6:D:447:VAL:HG22	2.09	0.66
6:D:584:ASN:HB2	6:D:602:SER:HB3	1.78	0.66
6:D:38:LYS:NZ	6:D:59:ALA:HB1	2.09	0.66
2:H:11:C:H2'	2:H:12:G:C8	2.29	0.66
5:M:473:ARG:HA	5:M:531:PHE:HD1	1.60	0.66
6:N:1346:ARG:HD3	11:N:9293:HOH:O	1.95	0.66
4:A:79:ILE:HA	4:A:82:LEU:HD12	1.77	0.66
5:C:270:GLY:O	5:C:274:ARG:HB3	1.96	0.66
6:D:716:PHE:CE1	6:D:765:SER:HB3	2.30	0.66
6:D:977:ALA:HB1	6:D:983:LEU:HD21	1.77	0.66
1:G:14:DT:H2''	1:G:15:DC:H5'	1.76	0.66
4:K:150:TYR:HE2	4:K:152:PRO:HG3	1.60	0.66
5:M:433:THR:HG22	5:M:437:ARG:NH1	2.10	0.66
5:M:45:GLN:HB2	5:M:71:TYR:CE2	2.31	0.66
5:M:561:GLY:O	5:M:564:MET:HG3	1.95	0.66
6:N:1121:PRO:HD2	6:N:1346:ARG:NH2	2.09	0.66
5:M:764:GLU:HB2	6:N:54:LYS:HD3	1.77	0.66
5:C:1103:ASP:HB3	5:C:1105:LYS:HZ1	1.59	0.66
5:C:435:TYR:CE1	5:C:539:VAL:HG22	2.31	0.66
5:C:494:TYR:HB3	11:C:1172:HOH:O	1.96	0.66
6:D:480:GLU:O	6:D:484:PRO:HD2	1.96	0.66
5:M:251:ASP:HB3	5:M:252:LYS:HD2	1.78	0.66
5:M:953:VAL:HB	5:M:962:GLN:NE2	2.10	0.66
6:N:1000:THR:O	6:N:1003:VAL:HG12	1.95	0.66
6:N:119:SER:H	6:N:123:LEU:CD2	2.07	0.66
5:C:315:ALA:HB3	11:C:1454:HOH:O	1.94	0.66
5:C:313:LEU:HB2	5:C:321:GLU:HG3	1.76	0.66
5:M:102:HIS:HB2	5:M:106:GLY:O	1.95	0.66
5:M:288:ARG:HG3	11:M:1542:HOH:O	1.94	0.66
5:M:841:ASN:ND2	5:M:844:GLY:H	1.93	0.66
6:N:1266:ARG:HG2	6:N:1267:ARG:N	2.10	0.66
6:N:800:LYS:NZ	6:N:804:LEU:HD13	2.11	0.66
6:N:813:LEU:O	6:N:817:GLU:HB2	1.96	0.66
5:C:516:ARG:HD2	5:C:521:PRO:HA	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:52:PRO:HG2	6:D:80:VAL:HG13	1.76	0.66
6:N:1111:ASP:HB2	6:N:1203:LYS:HZ1	1.60	0.66
6:N:900:ILE:HG22	6:N:914:LEU:HD11	1.75	0.66
5:C:151:ASP:HB2	5:C:157:ARG:O	1.95	0.66
5:C:987:ILE:HG13	11:C:1149:HOH:O	1.94	0.66
5:C:1118:LYS:HA	6:D:23:TYR:OH	1.95	0.66
4:K:31:GLY:HA3	4:L:42:ARG:NH2	2.09	0.66
4:L:56:VAL:HG13	4:L:142:VAL:HG12	1.78	0.66
5:M:129:ILE:HG12	5:M:386:PHE:O	1.95	0.66
5:M:861:LEU:HD13	5:M:865:THR:CG2	2.25	0.66
6:N:1106:VAL:HG11	6:N:1474:ALA:HB1	1.78	0.66
6:N:796:ARG:NE	6:N:828:LYS:HZ3	1.94	0.66
4:A:14:ARG:HH22	4:A:24:VAL:HG23	1.61	0.66
4:B:125:PRO:HD2	11:B:346:HOH:O	1.94	0.66
5:C:629:TYR:HA	11:C:1337:HOH:O	1.96	0.66
6:D:1462:LEU:HD22	6:D:1472:ILE:HG22	1.77	0.66
5:C:1091:GLU:OE1	6:D:613:ARG:HG2	1.96	0.66
6:D:691:LEU:O	6:D:695:ILE:HG22	1.95	0.66
5:M:689:VAL:HG12	5:M:690:ILE:N	2.11	0.66
5:M:443:THR:HG21	6:N:1078:ARG:NE	2.10	0.66
6:N:1111:ASP:HB2	6:N:1203:LYS:NZ	2.11	0.66
5:C:236:ILE:HG13	11:C:1121:HOH:O	1.96	0.66
5:C:244:PRO:HD2	5:C:245:GLY:H	1.60	0.66
5:C:678:PRO:HD2	11:D:8199:HOH:O	1.95	0.66
6:D:879:ARG:HH21	6:D:903:ASP:HA	1.60	0.66
4:K:124:ASN:HD22	4:K:127:LEU:HD22	1.60	0.66
5:M:473:ARG:HA	5:M:531:PHE:CD1	2.30	0.66
5:M:810:ASP:OD2	5:M:815:LEU:HD22	1.96	0.66
6:N:396:VAL:HG12	6:N:447:VAL:HA	1.76	0.66
6:N:542:ASP:HA	6:N:545:ARG:HE	1.60	0.66
7:O:45:ARG:HG2	7:O:46:PRO:CD	2.24	0.66
5:C:516:ARG:HE	6:D:1068:LEU:HD13	1.60	0.66
5:C:597:ALA:HB2	5:C:655:LEU:HD21	1.78	0.66
5:C:755:LEU:HD21	5:C:792:VAL:HG22	1.75	0.66
5:C:838:LYS:HG3	5:C:997:LEU:HB2	1.78	0.66
6:D:1252:ILE:HA	11:D:8219:HOH:O	1.96	0.66
6:D:1396:GLU:HA	6:D:1399:ASP:OD2	1.96	0.66
6:D:466:LYS:HA	11:D:8320:HOH:O	1.95	0.66
6:D:568:ARG:O	6:D:572:ARG:HG3	1.96	0.66
2:H:6:U:H5'	11:H:45:HOH:O	1.94	0.66
4:L:221:HIS:HB3	11:L:365:HOH:O	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:267:TYR:HB2	5:M:272:ALA:HB1	1.78	0.66
5:M:979:THR:HG23	5:M:981:GLU:H	1.60	0.66
6:N:1044:LEU:HD22	6:N:1052:THR:HG22	1.76	0.66
4:A:117:VAL:HB	4:A:120:VAL:CG1	2.26	0.66
5:C:69:LEU:HD13	5:C:109:LYS:HE3	1.78	0.66
5:C:12:VAL:HG13	5:C:13:ILE:HG12	1.78	0.66
6:D:1089:ALA:HB3	11:D:8250:HOH:O	1.95	0.66
6:D:1189:ARG:HB3	6:D:1204:CYS:HA	1.78	0.66
6:D:481:MET:HE2	6:D:493:ARG:HB2	1.76	0.66
5:M:861:LEU:HD23	5:M:863:ASP:H	1.61	0.66
5:M:553:ASP:HA	5:M:881:ASN:HA	1.78	0.66
5:M:928:LYS:NZ	5:M:932:GLU:HG3	2.10	0.66
6:N:1151:ARG:HG2	6:N:1187:PRO:HB2	1.77	0.66
6:N:468:LEU:HB3	11:N:9068:HOH:O	1.96	0.66
6:N:618:LEU:HB3	6:N:619:LEU:HD23	1.78	0.66
5:C:83:CYS:HA	5:C:88:LEU:HB2	1.78	0.65
6:D:1329:ALA:O	6:D:1330:ILE:HD12	1.96	0.65
6:D:890:VAL:HG11	6:D:922:LEU:HD13	1.78	0.65
4:K:198:ARG:HH22	5:M:932:GLU:HB3	1.61	0.65
5:M:200:LEU:HD13	5:M:300:ASP:CG	2.16	0.65
5:M:502:PRO:HB2	5:M:509:ALA:HB3	1.77	0.65
5:M:690:ILE:CD1	5:M:833:LEU:HD23	2.26	0.65
6:N:413:ASP:O	6:N:435:VAL:HG23	1.96	0.65
6:N:553:ARG:O	6:N:557:LEU:HG	1.96	0.65
7:O:27:ALA:HB2	7:O:61:VAL:HG12	1.77	0.65
5:C:608:GLY:C	5:C:609:ASN:HD22	1.99	0.65
5:C:676:ILE:CG2	5:C:988:VAL:HG13	2.27	0.65
6:D:761:ILE:HG23	7:E:6:ILE:HD11	1.78	0.65
5:M:98:LEU:HD13	5:M:110:GLU:O	1.95	0.65
6:N:1148:VAL:HB	6:N:1203:LYS:O	1.96	0.65
6:N:1342:GLU:HA	11:N:9208:HOH:O	1.96	0.65
6:N:769:LEU:HD12	6:N:770:LEU:HG	1.77	0.65
6:N:917:GLN:O	6:N:921:ARG:HG2	1.96	0.65
5:C:1067:TYR:O	5:C:1071:ILE:HG12	1.96	0.65
5:C:194:VAL:HA	5:C:197:LEU:HD12	1.78	0.65
5:C:52:PHE:CD2	5:C:68:PHE:HB2	2.31	0.65
5:C:937:ASP:HB2	5:C:940:GLU:HG3	1.78	0.65
6:D:796:ARG:HH21	6:D:828:LYS:HE2	1.61	0.65
5:M:689:VAL:HB	5:M:870:ILE:HG13	1.78	0.65
5:M:911:GLU:O	5:M:915:LYS:HG2	1.96	0.65
6:N:788:GLY:O	6:N:792:ILE:HG22	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:213:GLN:O	4:B:217:ILE:HD13	1.96	0.65
6:D:879:ARG:HG3	6:D:879:ARG:HH11	1.60	0.65
6:D:1476:THR:HG23	7:E:21:VAL:HG22	1.77	0.65
1:G:17:DC:O3'	6:D:628:ARG:NH2	2.29	0.65
5:M:129:ILE:HD13	5:M:134:ARG:HB2	1.78	0.65
6:N:150:ARG:HG3	11:N:9044:HOH:O	1.96	0.65
6:N:960:LYS:HB3	11:N:9374:HOH:O	1.96	0.65
11:M:1409:HOH:O	7:O:31:LEU:HD13	1.96	0.65
5:C:22:GLN:HE22	5:C:407:LYS:HG2	1.59	0.65
4:L:102:LYS:HB2	4:L:139:ASN:OD1	1.96	0.65
6:N:1112:CYS:HB2	6:N:1195:GLN:HG2	1.78	0.65
6:N:1437:ALA:O	6:N:1446:VAL:HG21	1.95	0.65
6:N:660:LYS:HD2	6:N:694:VAL:HG22	1.78	0.65
6:N:1490:LYS:HE2	7:O:93:TYR:OH	1.96	0.65
6:D:1231:GLU:HG2	6:D:1235:GLN:CD	2.16	0.65
6:N:1174:LEU:HD22	6:N:1183:ILE:HD13	1.79	0.65
6:N:778:LEU:HA	6:N:780:LYS:HE2	1.78	0.65
4:A:197:LEU:HD23	4:A:197:LEU:H	1.62	0.65
5:C:274:ARG:HG3	5:C:285:LEU:HD22	1.79	0.65
5:C:837:ASP:O	5:C:848:VAL:HG13	1.96	0.65
5:C:841:ASN:N	5:C:841:ASN:HD22	1.91	0.65
5:C:971:LYS:HA	5:C:988:VAL:HA	1.79	0.65
4:K:112:ARG:NE	4:K:125:PRO:HB2	2.00	0.65
5:M:305:PRO:HG3	5:M:308:ARG:NH2	2.12	0.65
5:M:808:ARG:NH2	5:M:820:ARG:HH21	1.95	0.65
5:M:705:ILE:HA	5:M:827:VAL:O	1.97	0.65
6:N:132:TYR:HA	11:N:9432:HOH:O	1.96	0.65
6:N:421:LEU:HB2	6:N:427:VAL:HG12	1.79	0.65
6:N:661:MET:HA	6:N:666:ILE:HD12	1.79	0.65
2:Y:10:G:O2'	2:Y:11:C:H5'	1.96	0.65
4:B:137:ARG:NH1	4:B:139:ASN:HB3	2.11	0.65
5:C:17:PRO:HB2	5:C:20:GLU:HB2	1.77	0.65
5:C:328:LEU:H	5:C:433:THR:HB	1.61	0.65
6:D:131:LYS:HA	6:D:456:MET:HB2	1.77	0.65
6:D:133:ILE:O	6:D:152:LEU:HB2	1.97	0.65
6:D:996:TRP:O	6:D:1000:THR:HG22	1.96	0.65
2:H:12:G:O2'	2:H:13:C:H5'	1.97	0.65
5:M:435:TYR:CE1	5:M:539:VAL:HG22	2.29	0.65
5:M:937:ASP:HB3	5:M:940:GLU:H	1.62	0.65
6:N:637:LEU:HD21	6:N:642:CYS:HA	1.79	0.65
6:N:754:PHE:CE2	6:N:1476:THR:HG21	2.32	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:54:THR:HG22	4:B:158:ILE:HG13	1.78	0.65
5:C:1060:ILE:HG23	5:C:1061:GLU:H	1.62	0.65
6:D:50:PHE:HB3	6:D:522:PRO:HG3	1.79	0.65
4:K:27:PRO:HG2	4:K:186:LEU:HD13	1.77	0.65
6:N:74:GLU:HB3	6:N:75:ARG:NH2	2.12	0.65
6:N:876:SER:O	6:N:880:ILE:HG12	1.97	0.65
7:O:28:GLN:HB3	7:O:32:ARG:HH22	1.61	0.65
1:G:16:DG:OP1	5:C:1031:ARG:HD3	1.95	0.65
5:C:290:LEU:HD22	5:C:302:VAL:HG11	1.79	0.65
6:D:1084:THR:OG1	6:D:1238:MET:HA	1.96	0.65
6:D:822:ALA:HB1	11:D:8089:HOH:O	1.97	0.65
7:E:27:ALA:HB2	7:E:61:VAL:HG12	1.79	0.65
5:M:1056:LYS:HB3	6:N:624:ASP:H	1.60	0.65
6:N:131:LYS:HG2	6:N:568:ARG:HG2	1.79	0.65
6:N:948:THR:HB	11:N:9020:HOH:O	1.97	0.65
6:D:882:PHE:HA	6:D:885:ILE:HD12	1.79	0.64
6:D:895:VAL:O	6:D:899:LEU:HG	1.97	0.64
5:M:442:GLU:HG2	5:M:454:SER:CB	2.26	0.64
6:N:1147:ARG:HB3	6:N:1188:VAL:HG21	1.79	0.64
5:C:343:GLN:HA	5:C:343:GLN:NE2	2.11	0.64
5:C:689:VAL:HG12	5:C:690:ILE:N	2.12	0.64
5:M:166:PRO:HG3	11:M:1337:HOH:O	1.97	0.64
5:M:158:TYR:CE1	5:M:313:LEU:HG	2.33	0.64
4:B:25:LEU:O	4:B:28:LEU:HD21	1.97	0.64
5:C:158:TYR:CD1	5:C:313:LEU:HG	2.32	0.64
5:C:525:SER:HB2	5:C:527:GLU:HG3	1.79	0.64
5:C:470:PRO:HB2	5:C:534:VAL:HG21	1.78	0.64
6:D:141:ILE:HD13	6:D:450:TYR:HB3	1.79	0.64
6:D:1101:VAL:HG21	6:D:1424:VAL:HG23	1.78	0.64
6:D:484:PRO:CB	6:D:488:ARG:HE	2.07	0.64
7:E:48:MET:HB2	7:E:54:LEU:HD12	1.80	0.64
2:H:10:G:O2'	2:H:11:C:H5'	1.97	0.64
4:K:52:ALA:HA	11:K:1094:HOH:O	1.96	0.64
5:M:462:ASP:CG	5:M:463:GLU:H	2.01	0.64
5:M:771:GLU:HG3	11:M:1181:HOH:O	1.96	0.64
6:N:996:TRP:O	6:N:1000:THR:HG22	1.96	0.64
6:N:1087:ARG:HB3	6:N:1256:LEU:HD22	1.79	0.64
6:N:762:GLN:HA	11:N:9032:HOH:O	1.97	0.64
6:N:793:THR:HB	6:N:879:ARG:CD	2.25	0.64
4:A:48:ILE:HD12	4:A:174:VAL:HG21	1.78	0.64
5:C:146:VAL:HG22	5:C:162:ILE:HG23	1.77	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:609:ASN:N	5:C:609:ASN:HD22	1.94	0.64
6:D:119:SER:OG	6:D:123:LEU:HD13	1.96	0.64
6:D:402:PRO:HA	6:D:443:VAL:HG23	1.80	0.64
6:D:792:ILE:HG23	6:D:793:THR:HG23	1.79	0.64
6:D:804:LEU:HB2	6:D:830:ALA:O	1.98	0.64
6:D:1209:LEU:HD21	7:E:16:LYS:NZ	2.12	0.64
4:K:30:ARG:HH22	5:M:938:LYS:HD2	1.63	0.64
5:M:140:ILE:HA	5:M:332:ARG:O	1.97	0.64
5:M:542:VAL:HG23	11:M:1602:HOH:O	1.96	0.64
4:A:12:THR:OG1	4:A:24:VAL:HB	1.97	0.64
4:A:71:VAL:HG22	4:A:132:LEU:HG	1.78	0.64
4:A:36:LEU:O	4:A:40:LEU:HG	1.97	0.64
4:B:59:GLU:HG3	4:B:139:ASN:HD22	1.61	0.64
4:L:138:LEU:HD12	11:L:362:HOH:O	1.98	0.64
4:L:177:VAL:HG12	4:L:199:ILE:HG12	1.79	0.64
5:M:362:GLY:HA3	5:M:367:LEU:HD23	1.78	0.64
5:M:29:ALA:O	5:M:44:ILE:HG12	1.96	0.64
5:M:836:GLY:HA3	6:N:724:GLN:NE2	2.12	0.64
6:N:15:PRO:HA	6:N:18:ILE:HG12	1.79	0.64
6:N:396:VAL:HG12	6:N:398:ALA:HB2	1.80	0.64
6:N:786:ILE:HD13	6:N:1027:GLY:HA3	1.78	0.64
3:Z:8:DA:H1'	3:Z:9:DG:H5'	1.79	0.64
4:B:212:ASN:O	4:B:215:VAL:HG22	1.97	0.64
5:C:124:ASP:OD2	5:C:592:LEU:HB2	1.97	0.64
5:C:204:GLN:OE1	5:C:221:LEU:HD12	1.97	0.64
11:A:362:HOH:O	5:C:832:LYS:HD2	1.98	0.64
6:D:104:PHE:HB3	6:D:512:MET:SD	2.38	0.64
6:D:613:ARG:HH12	6:D:616:GLN:HG2	1.62	0.64
6:D:813:LEU:HD21	11:D:8233:HOH:O	1.97	0.64
6:D:823:LEU:O	6:D:823:LEU:HD23	1.98	0.64
2:H:9:G:O2'	2:H:10:G:H5'	1.97	0.64
5:M:684:PHE:CD2	5:M:685:GLU:HG2	2.33	0.64
6:N:1422:MET:SD	6:N:1426:LYS:HB3	2.37	0.64
7:O:47:LYS:HA	7:O:54:LEU:HB3	1.80	0.64
5:C:1105:LYS:NZ	5:C:1107:ASN:HD22	1.96	0.64
5:C:839:LEU:HD22	5:C:996:LYS:HA	1.80	0.64
6:D:71:LYS:NZ	6:D:71:LYS:HB2	2.12	0.64
6:D:973:GLN:HB3	11:D:8398:HOH:O	1.96	0.64
4:L:59:GLU:HG3	4:L:137:ARG:HH22	1.63	0.64
5:M:265:ARG:NH2	5:M:332:ARG:HH22	1.95	0.64
6:N:554:LEU:O	6:N:558:LEU:HG	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:91:GLY:O	6:N:519:VAL:N	2.21	0.64
6:D:1087:ARG:HD2	6:D:1256:LEU:HD13	1.78	0.64
6:D:1471:LEU:HD23	11:D:8477:HOH:O	1.98	0.64
6:D:860:LEU:HD23	6:D:877:PRO:HB2	1.79	0.64
6:D:1485:GLN:NE2	7:E:79:LEU:H	1.96	0.64
5:M:100:LEU:HD23	5:M:368:THR:HA	1.80	0.64
6:N:1380:GLU:HG3	6:N:1381:VAL:N	2.13	0.64
6:N:1415:VAL:HB	11:N:9268:HOH:O	1.96	0.64
6:N:17:LYS:HA	6:N:20:SER:HB3	1.80	0.64
6:N:41:ARG:HD3	6:N:42:ASP:N	2.13	0.64
6:N:679:ARG:HB2	6:N:682:ASP:OD2	1.98	0.64
5:C:18:LEU:HD12	5:C:18:LEU:H	1.61	0.64
5:C:194:VAL:HG21	5:C:221:LEU:O	1.97	0.64
5:C:872:ASN:HD22	5:C:873:PRO:N	1.95	0.64
6:D:1044:LEU:HD21	6:D:1053:PHE:O	1.98	0.64
6:D:496:LEU:HD21	6:D:1388:ARG:HG3	1.79	0.64
6:D:18:ILE:HG23	6:D:518:PRO:HG3	1.80	0.64
5:M:1005:MET:HB2	6:N:648:MET:HE1	1.78	0.64
5:M:170:PRO:HG2	11:M:1194:HOH:O	1.98	0.64
5:M:410:ILE:HD11	5:M:455:LEU:HB3	1.79	0.64
5:M:9:ILE:HG21	11:M:1490:HOH:O	1.98	0.64
6:N:29:PRO:HG3	6:N:549:ASN:HD21	1.61	0.64
5:C:9:ILE:HG13	5:C:907:ASP:OD2	1.98	0.64
6:D:136:ASP:CG	6:D:463:GLN:HB3	2.18	0.64
6:D:486:ARG:HA	6:D:489:ARG:CG	2.28	0.64
5:M:314:THR:HG21	11:M:1381:HOH:O	1.97	0.64
5:M:342:ASP:O	5:M:345:ARG:HG2	1.98	0.64
5:M:906:PHE:CD1	6:N:1067:VAL:HG22	2.33	0.64
6:N:1353:GLN:HB3	6:N:1357:ARG:NE	2.12	0.64
4:A:206:THR:HG22	4:A:209:GLU:H	1.63	0.63
5:C:688:ILE:HG21	5:C:871:LEU:HD23	1.80	0.63
6:D:637:LEU:HB2	11:D:8105:HOH:O	1.98	0.63
2:H:11:C:H2'	2:H:12:G:H8	1.63	0.63
4:K:117:VAL:HB	4:K:120:VAL:CG1	2.26	0.63
4:K:226:SER:O	4:K:228:PRO:HD3	1.97	0.63
4:L:175:ARG:O	6:N:851:LEU:HD11	1.98	0.63
5:M:598:GLU:O	5:M:651:LYS:HG3	1.98	0.63
6:N:1491:THR:O	6:N:1495:ILE:HD13	1.98	0.63
6:N:792:ILE:HD13	6:N:793:THR:HG22	1.80	0.63
4:B:42:ARG:HA	4:B:42:ARG:NH1	2.13	0.63
5:C:694:LEU:HD21	5:C:868:ASP:HB3	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1169:ASP:O	6:D:1173:LEU:HD13	1.98	0.63
6:D:440:VAL:HB	6:D:441:ARG:HH21	1.61	0.63
5:M:83:CYS:HA	5:M:88:LEU:HB2	1.78	0.63
6:N:1462:LEU:HD22	6:N:1472:ILE:HG22	1.79	0.63
6:N:887:ALA:HB1	6:N:893:GLU:CG	2.27	0.63
6:N:971:LEU:HA	6:N:974:ILE:HD12	1.80	0.63
5:C:1031:ARG:NH2	6:D:621:LYS:HG3	2.13	0.63
5:C:174:LEU:HB3	5:C:307:LEU:HD13	1.79	0.63
5:C:265:ARG:HB3	5:C:267:TYR:CD2	2.34	0.63
6:D:1119:SER:HA	6:D:1186:VAL:O	1.99	0.63
4:K:156:HIS:CD2	4:K:158:ILE:HG12	2.34	0.63
5:M:861:LEU:HD13	5:M:865:THR:HG23	1.79	0.63
6:N:474:GLU:O	6:N:478:LEU:HG	1.98	0.63
7:O:41:GLU:HB2	7:O:45:ARG:CZ	2.27	0.63
6:N:760:ARG:HH11	7:O:61:VAL:CG2	2.11	0.63
5:C:284:ARG:HG3	5:C:285:LEU:H	1.64	0.63
5:C:631:SER:HB3	5:C:637:LEU:HD11	1.79	0.63
6:D:1412:LYS:O	6:D:1414:PRO:HD3	1.99	0.63
6:D:610:LYS:HA	6:D:615:ARG:HD3	1.80	0.63
6:D:632:VAL:HG22	11:D:8291:HOH:O	1.99	0.63
6:D:705:ALA:HB3	6:D:706:PRO:HD3	1.80	0.63
5:M:395:LYS:HD3	5:M:397:GLU:OE2	1.99	0.63
5:M:549:PHE:CD2	5:M:886:LEU:HB3	2.33	0.63
6:N:806:PHE:CE1	6:N:813:LEU:HB3	2.34	0.63
6:N:799:LYS:O	6:N:826:PRO:HD2	1.98	0.63
5:C:143:SER:CB	5:C:276:LYS:HZ3	2.10	0.63
5:C:874:LEU:HG	6:D:1023:MET:SD	2.39	0.63
6:D:1185:GLU:HG2	6:N:559:ALA:HB1	1.80	0.63
5:M:352:ALA:HA	5:M:355:VAL:HG12	1.80	0.63
6:N:1109:GLU:OE1	6:N:1201:CYS:HB2	1.98	0.63
6:N:1402:ALA:HA	11:N:9043:HOH:O	1.98	0.63
6:N:654:LYS:O	6:N:658:LEU:HG	1.98	0.63
5:M:729:LEU:HD13	6:N:675:ARG:CZ	2.29	0.63
6:N:98:PRO:HA	11:N:9070:HOH:O	1.97	0.63
1:X:17:DC:H5''	5:M:1030:GLN:NE2	2.14	0.63
2:Y:12:G:H2'	2:Y:13:C:H6	1.64	0.63
2:Y:12:G:O2'	2:Y:13:C:H5'	1.98	0.63
2:Y:7:G:H2'	2:Y:7:G:N3	2.12	0.63
5:C:100:LEU:HD22	5:C:372:LEU:HD22	1.81	0.63
5:C:410:ILE:HG21	5:C:438:ILE:HD11	1.79	0.63
5:C:437:ARG:HB3	5:C:467:ILE:HB	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:805:ARG:HD3	5:C:807:ARG:HG3	1.81	0.63
6:D:1047:LYS:HG2	6:D:1053:PHE:CZ	2.33	0.63
6:D:657:LEU:HD22	6:D:691:LEU:HD23	1.81	0.63
6:D:82:LYS:HB3	6:D:84:ILE:HG12	1.79	0.63
5:M:146:VAL:HG12	5:M:162:ILE:HG12	1.81	0.63
5:M:759:THR:HB	5:M:785:VAL:CG1	2.28	0.63
5:M:1005:MET:HE1	6:N:724:GLN:HA	1.81	0.63
4:B:123:MET:C	4:B:125:PRO:HD3	2.19	0.63
5:C:157:ARG:HG3	5:C:314:THR:CG2	2.29	0.63
5:C:408:ARG:HG3	5:C:455:LEU:H	1.64	0.63
5:C:600:ASP:OD1	5:C:651:LYS:N	2.32	0.63
5:C:906:PHE:CE1	6:D:1067:VAL:HA	2.34	0.63
6:D:119:SER:H	6:D:123:LEU:CD2	2.11	0.63
6:D:704:ARG:HD3	6:D:738:ALA:HB2	1.79	0.63
7:E:54:LEU:HG	7:E:58:PRO:CG	2.28	0.63
5:M:432:ARG:HG3	11:M:1314:HOH:O	1.99	0.63
5:M:650:ARG:HG3	5:M:653:ASP:HB2	1.81	0.63
4:A:220:GLU:O	4:A:223:THR:HG22	1.99	0.63
5:C:276:LYS:HG2	5:C:280:LYS:NZ	2.14	0.63
5:C:279:GLU:HG3	5:C:280:LYS:HG3	1.79	0.63
5:C:672:VAL:HG12	5:C:699:PHE:CE1	2.34	0.63
5:C:690:ILE:CD1	5:C:833:LEU:HD23	2.29	0.63
5:C:670:GLN:NE2	5:C:699:PHE:O	2.30	0.63
6:D:614:PHE:CZ	6:D:1438:ALA:HB1	2.34	0.63
4:K:12:THR:OG1	4:K:24:VAL:HB	1.99	0.63
5:M:176:VAL:HG12	5:M:182:VAL:HG12	1.80	0.63
5:M:693:GLU:HA	5:M:696:LYS:HD2	1.80	0.63
6:N:1049:SER:O	6:N:1079:LYS:HE3	1.98	0.63
6:N:675:ARG:HA	6:N:678:GLU:HG2	1.80	0.63
6:N:696:HIS:HD2	7:O:59:ASN:HB2	1.64	0.63
5:C:410:ILE:HD12	5:C:438:ILE:CG1	2.29	0.63
5:C:327:HIS:HA	5:C:433:THR:OG1	1.98	0.63
5:C:441:VAL:HG13	5:C:559:LEU:HA	1.81	0.63
6:D:753:SER:HB2	11:D:8449:HOH:O	1.98	0.63
6:D:793:THR:O	6:D:879:ARG:HD3	1.99	0.63
7:E:48:MET:N	7:E:54:LEU:HB2	2.14	0.63
5:M:290:LEU:HD23	5:M:290:LEU:H	1.64	0.63
5:C:1033:GLY:O	5:C:1037:VAL:HG23	1.97	0.62
5:C:10:ARG:NH1	5:C:10:ARG:HA	2.12	0.62
5:C:98:LEU:O	5:C:109:LYS:HD2	1.99	0.62
2:H:4:U:H2'	2:H:5:C:C6	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:8:DA:H1'	3:I:9:DG:H5'	1.81	0.62
5:M:580:MET:HB3	5:M:584:GLU:OE1	1.99	0.62
6:N:131:LYS:HE2	6:N:564:GLU:OE1	1.98	0.62
6:N:1440:PHE:HB3	11:N:9289:HOH:O	1.99	0.62
5:C:218:VAL:HA	5:C:221:LEU:HD23	1.81	0.62
5:C:710:ILE:HD12	5:C:790:LEU:HD13	1.81	0.62
5:C:882:LEU:HD23	5:C:885:ILE:HB	1.81	0.62
6:D:1267:ARG:HH11	6:D:1267:ARG:HB2	1.64	0.62
6:D:1364:HIS:ND1	6:D:1366:LYS:HG3	2.14	0.62
6:D:455:ARG:CZ	6:D:463:GLN:HG3	2.29	0.62
6:D:891:GLU:HB2	11:D:8407:HOH:O	1.98	0.62
7:E:70:THR:HB	7:E:72:ARG:HG2	1.81	0.62
2:H:6:U:C2'	2:H:7:G:C8	2.82	0.62
5:M:304:LEU:HG	5:M:308:ARG:HH21	1.64	0.62
6:N:165:LYS:HA	6:N:199:LEU:HD22	1.81	0.62
1:X:14:DT:H3'	6:N:610:LYS:NZ	2.14	0.62
4:B:20:TYR:OH	4:B:198:ARG:HD2	1.98	0.62
5:C:1037:VAL:O	5:C:1041:GLU:HG3	1.99	0.62
5:C:750:LYS:HD3	6:D:681:ARG:HD3	1.81	0.62
5:C:775:ARG:HD2	5:C:782:ALA:HB3	1.80	0.62
5:C:840:ALA:HB2	5:C:846:LYS:HG3	1.79	0.62
6:D:1437:ALA:O	6:D:1446:VAL:HG21	1.99	0.62
6:D:143:ASN:ND2	6:D:145:VAL:HG12	2.10	0.62
6:D:175:VAL:HG11	11:D:8081:HOH:O	1.99	0.62
6:D:1029:ARG:HH22	10:D:3999:APC:PG	2.22	0.62
5:M:44:ILE:HG23	5:M:344:PHE:HE1	1.64	0.62
5:M:576:ALA:HB3	5:M:900:ARG:NH1	2.13	0.62
4:K:180:GLN:HE22	5:M:937:ASP:HA	1.65	0.62
5:M:906:PHE:CE1	6:N:1067:VAL:HA	2.35	0.62
6:N:1219:GLU:HG2	6:N:1221:VAL:HG23	1.81	0.62
6:N:95:LEU:HB2	11:N:9070:HOH:O	1.99	0.62
5:C:720:GLU:HG2	5:C:760:SER:HB3	1.82	0.62
6:D:1000:THR:O	6:D:1003:VAL:HG12	1.99	0.62
6:D:574:LEU:O	6:D:578:VAL:HG23	1.98	0.62
7:E:54:LEU:O	7:E:54:LEU:HD23	2.00	0.62
2:H:9:G:H2'	2:H:10:G:H8	1.63	0.62
4:L:211:LEU:O	4:L:215:VAL:HG13	2.00	0.62
5:M:1098:ASP:HB2	6:N:21:TRP:HZ2	1.64	0.62
5:M:307:LEU:HG	5:M:311:PHE:CE2	2.34	0.62
5:M:468:ARG:HE	5:M:487:THR:N	1.98	0.62
5:M:807:ARG:H	5:M:807:ARG:NE	1.96	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:1051:GLU:HG3	6:N:1051:GLU:O	2.00	0.62
6:N:895:VAL:O	6:N:899:LEU:HG	2.00	0.62
5:C:144:PRO:HA	5:C:163:ILE:HD11	1.81	0.62
6:D:1083:ASP:OD1	6:D:1252:ILE:HD12	2.00	0.62
6:D:138:LYS:HD3	11:D:8147:HOH:O	2.00	0.62
6:D:660:LYS:HD2	6:D:694:VAL:HG22	1.80	0.62
6:D:853:VAL:HG11	6:D:860:LEU:HG	1.81	0.62
5:M:135:VAL:HG11	5:M:407:LYS:HA	1.81	0.62
5:M:537:LYS:HE3	5:M:905:ILE:HD13	1.81	0.62
5:M:759:THR:HA	5:M:786:LYS:O	2.00	0.62
6:N:1125:PRO:HB3	6:N:1130:ARG:HH22	1.64	0.62
6:N:172:PRO:HG2	6:N:175:VAL:HG21	1.82	0.62
5:C:573:ARG:HB2	5:C:573:ARG:NH1	2.13	0.62
5:C:798:GLY:H	5:C:827:VAL:CG1	2.13	0.62
6:D:396:VAL:C	6:D:398:ALA:H	2.03	0.62
6:D:398:ALA:HB1	6:D:446:VAL:H	1.64	0.62
6:D:1495:ILE:HG21	7:E:80:VAL:HG13	1.82	0.62
4:L:58:ILE:CG2	4:L:61:VAL:HB	2.29	0.62
5:M:1090:LYS:HG2	5:M:1112:PHE:HZ	1.65	0.62
6:N:130:SER:HB3	6:N:132:TYR:CE1	2.34	0.62
6:N:1424:VAL:HG13	6:N:1425:THR:N	2.14	0.62
6:N:166:GLN:CG	6:N:396:VAL:HG13	2.29	0.62
6:N:764:LEU:HD12	6:N:765:SER:N	2.14	0.62
7:O:41:GLU:HG2	7:O:42:PRO:HD3	1.82	0.62
1:X:20:DG:H3'	11:X:610:HOH:O	2.00	0.62
2:Y:6:U:C2'	2:Y:7:G:C8	2.82	0.62
5:C:162:ILE:HD11	5:C:306:THR:HG21	1.82	0.62
5:C:329:GLY:N	5:C:488:ALA:HB3	2.13	0.62
5:C:410:ILE:O	5:C:452:ILE:HA	1.99	0.62
5:C:436:GLY:HA2	5:C:538:GLN:O	1.99	0.62
6:D:792:ILE:O	6:D:878:GLY:HA3	1.99	0.62
5:M:1087:VAL:HG23	6:N:524:LEU:HD11	1.80	0.62
5:M:120:LEU:HD22	5:M:121:MET:N	2.11	0.62
5:M:273:GLY:HA2	5:M:276:LYS:HE3	1.80	0.62
5:M:457:ALA:HB3	5:M:538:GLN:HA	1.80	0.62
5:M:587:VAL:HG12	5:M:588:VAL:N	2.13	0.62
6:N:1146:GLY:O	6:N:1207:TYR:HB2	2.00	0.62
1:X:14:DT:H2''	1:X:15:DC:H5'	1.80	0.62
2:Y:1:G:O6	5:M:773:LEU:HD12	2.00	0.62
5:C:554:ASP:HB2	6:D:1061:PHE:HE2	1.65	0.62
5:C:674:VAL:HG23	5:C:869:VAL:HG13	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:702:SER:HB3	5:C:996:LYS:HZ2	1.63	0.62
5:M:113:VAL:HG11	5:M:373:VAL:CG1	2.30	0.62
5:M:194:VAL:HA	5:M:197:LEU:HD12	1.82	0.62
5:M:194:VAL:HG11	5:M:221:LEU:O	2.00	0.62
6:N:741:ASP:O	6:N:743:ASP:N	2.29	0.62
5:C:862:PRO:HD2	5:C:925:TYR:OH	2.00	0.62
6:D:81:THR:HG22	6:D:82:LYS:N	2.14	0.62
2:Y:7:G:C2	5:M:1014:SER:HA	2.33	0.62
6:N:471:GLU:O	6:N:474:GLU:HB3	2.00	0.62
6:N:490:ALA:O	6:N:493:ARG:HG3	1.99	0.62
6:N:639:LEU:HB3	11:N:9466:HOH:O	1.98	0.62
11:N:9137:HOH:O	7:O:17:TYR:HB2	1.99	0.62
7:O:86:GLN:O	7:O:90:GLU:HG3	2.00	0.62
5:C:830:LYS:HD3	5:C:832:LYS:HE2	1.82	0.62
4:L:102:LYS:HZ1	4:L:137:ARG:HG2	1.64	0.62
5:M:629:TYR:HB3	11:M:1373:HOH:O	1.99	0.62
6:N:1121:PRO:HD3	6:N:1346:ARG:HE	1.63	0.62
2:Y:10:G:H2'	2:Y:11:C:H6	1.64	0.62
4:B:78:ILE:O	4:B:82:LEU:HG	2.00	0.61
5:C:101:ILE:HG23	5:C:107:LEU:HD22	1.82	0.61
6:D:550:ARG:HE	6:D:550:ARG:CA	2.11	0.61
4:K:58:ILE:HB	4:K:61:VAL:HB	1.82	0.61
5:M:23:VAL:HA	5:M:121:MET:HE1	1.81	0.61
5:M:265:ARG:HB3	5:M:267:TYR:CE2	2.35	0.61
5:M:928:LYS:HZ2	5:M:932:GLU:HG3	1.65	0.61
6:N:41:ARG:HD3	6:N:42:ASP:HB2	1.80	0.61
6:N:626:SER:HB2	6:N:748:HIS:CE1	2.34	0.61
6:N:902:LEU:HD23	6:N:902:LEU:H	1.65	0.61
4:B:102:LYS:NZ	4:B:139:ASN:HB2	2.14	0.61
5:C:343:GLN:HB2	5:C:385:PHE:CE2	2.34	0.61
5:M:1030:GLN:NE2	6:N:628:ARG:HD3	2.15	0.61
5:M:198:ARG:NH1	5:M:231:PRO:HG3	2.15	0.61
6:N:1036:ARG:HB3	6:N:1036:ARG:NH1	2.15	0.61
6:N:583:ASP:OD2	6:N:604:THR:HG21	1.99	0.61
5:C:456:ALA:HB1	5:C:538:GLN:O	1.99	0.61
6:D:440:VAL:HB	6:D:441:ARG:HE	1.63	0.61
6:D:544:TYR:O	6:D:548:ILE:HG12	2.00	0.61
6:D:762:GLN:HB2	7:E:16:LYS:HE2	1.82	0.61
5:M:83:CYS:HG	5:M:90:TYR:HD2	1.47	0.61
4:A:41:ARG:O	4:A:45:LEU:HD13	2.00	0.61
5:C:436:GLY:HA3	5:C:538:GLN:OE1	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:7:GLY:C	5:C:8:ARG:HD2	2.20	0.61
6:D:101:HIS:ND1	6:D:103:TRP:HB2	2.15	0.61
6:D:559:ALA:HB2	11:D:8141:HOH:O	1.98	0.61
6:D:707:THR:HG23	6:D:712:GLY:HA3	1.81	0.61
5:M:30:LEU:HA	5:M:44:ILE:HG12	1.80	0.61
11:M:1524:HOH:O	6:N:621:LYS:HE3	2.00	0.61
4:B:47:SER:OG	4:B:48:ILE:HD12	1.99	0.61
5:C:1076:VAL:HG21	11:D:8371:HOH:O	1.99	0.61
5:C:400:PRO:HG2	5:C:593:ALA:HB2	1.82	0.61
5:C:672:VAL:HG12	5:C:699:PHE:HE1	1.65	0.61
6:D:1219:GLU:HA	7:E:17:TYR:HE2	1.65	0.61
6:D:1267:ARG:HH11	6:D:1267:ARG:CB	2.13	0.61
6:D:1101:VAL:HG13	6:D:1427:SER:OG	2.00	0.61
6:D:135:LEU:HA	6:D:453:ASP:O	2.01	0.61
6:D:677:LEU:HD21	6:D:687:VAL:HG11	1.81	0.61
2:H:13:C:H2'	2:H:14:G:H8	1.65	0.61
5:M:909:ALA:HB1	5:M:914:ILE:HD11	1.81	0.61
4:A:181:VAL:HG11	11:A:382:HOH:O	2.01	0.61
4:A:182:GLU:O	4:A:194:LYS:HB3	2.00	0.61
5:C:464:LEU:O	5:C:466:PHE:N	2.34	0.61
5:C:79:PRO:HG2	5:C:82:GLU:HB2	1.80	0.61
6:D:10:ILE:HD12	6:D:1450:ALA:HB3	1.82	0.61
6:D:1493:LYS:O	6:D:1497:GLU:HG2	2.01	0.61
4:K:90:LEU:HB2	4:K:119:ASP:OD2	2.01	0.61
5:M:759:THR:HB	5:M:785:VAL:CG2	2.31	0.61
6:N:584:ASN:ND2	6:N:590:PRO:HD2	2.16	0.61
4:B:133:GLU:HA	4:B:133:GLU:OE1	2.00	0.61
5:C:857:ASP:CB	5:C:978:ARG:HG2	2.31	0.61
5:C:99:GLN:HB3	5:C:109:LYS:HD3	1.81	0.61
6:D:724:GLN:HG3	6:D:725:SER:N	2.14	0.61
6:D:955:VAL:HG11	6:D:1015:TYR:HE2	1.66	0.61
4:L:78:ILE:O	4:L:82:LEU:HG	2.00	0.61
5:M:110:GLU:N	5:M:368:THR:HG21	2.14	0.61
2:Y:4:U:H2'	2:Y:5:C:C6	2.36	0.61
5:C:198:ARG:HD2	5:C:204:GLN:NE2	2.15	0.61
5:C:398:THR:HG21	5:C:567:GLN:HA	1.83	0.61
6:D:123:LEU:HG	6:D:152:LEU:HD13	1.82	0.61
6:D:1346:ARG:HH12	6:D:1349:VAL:HG11	1.66	0.61
5:M:408:ARG:NE	5:M:455:LEU:HD11	2.15	0.61
5:M:694:LEU:HD21	5:M:868:ASP:HB3	1.83	0.61
6:N:50:PHE:CD2	6:N:522:PRO:HD3	2.36	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:9036:HOH:O	7:O:89:MET:HE1	1.99	0.61
5:C:1060:ILE:HG22	5:C:1086:ARG:NH2	2.15	0.61
5:C:318:PRO:HD2	5:C:321:GLU:OE1	2.01	0.61
5:C:431:HIS:CG	5:C:432:ARG:N	2.69	0.61
5:C:988:VAL:HG23	11:C:1330:HOH:O	2.00	0.61
6:D:393:ILE:HD13	11:D:8118:HOH:O	2.01	0.61
6:D:615:ARG:HH22	6:D:1096:ARG:HD2	1.64	0.61
6:D:633:VAL:HB	6:D:740:PHE:CE1	2.36	0.61
5:M:232:GLU:HB3	11:M:1516:HOH:O	1.99	0.61
5:M:113:VAL:HG11	5:M:373:VAL:HG11	1.81	0.61
5:M:524:VAL:CG1	5:M:528:GLU:HB2	2.31	0.61
5:M:676:ILE:CG2	5:M:988:VAL:HG13	2.31	0.61
6:N:135:LEU:HA	6:N:453:ASP:O	2.01	0.61
6:N:1105:ILE:HD11	6:N:1374:GLN:OE1	2.01	0.61
6:N:507:ASN:HD22	6:N:507:ASN:N	1.90	0.61
4:A:39:PRO:O	4:A:43:ILE:HG12	1.99	0.61
5:C:267:TYR:HB2	5:C:272:ALA:HB1	1.82	0.61
5:C:252:LYS:HB3	5:C:298:PHE:HZ	1.65	0.61
5:C:578:VAL:HG21	5:C:991:GLN:O	2.01	0.61
5:C:911:GLU:O	5:C:915:LYS:HG2	2.00	0.61
6:D:19:ARG:HH21	6:D:516:ALA:HB2	1.64	0.61
2:H:12:G:H2'	2:H:13:C:H6	1.66	0.61
5:M:554:ASP:HB3	5:M:880:MET:O	2.01	0.61
5:M:816:LYS:HB2	5:M:819:VAL:HG21	1.83	0.61
4:K:41:ARG:HH21	5:M:977:GLY:HA2	1.65	0.61
5:M:983:ILE:HG21	5:M:987:ILE:HD12	1.80	0.61
7:O:30:LEU:O	7:O:35:PHE:HA	2.01	0.61
4:A:124:ASN:ND2	4:A:127:LEU:HD22	2.16	0.60
4:A:225:PHE:CE1	4:B:40:LEU:HD11	2.35	0.60
6:D:153:LEU:CD1	6:D:158:TYR:HB2	2.31	0.60
6:D:8:VAL:HB	6:D:1434:TRP:CH2	2.36	0.60
5:M:464:LEU:O	5:M:466:PHE:N	2.33	0.60
6:N:619:LEU:HD12	6:N:621:LYS:HZ3	1.66	0.60
6:N:780:LYS:HD3	6:N:912:LYS:HE3	1.82	0.60
4:B:115:LEU:HB3	11:B:371:HOH:O	2.01	0.60
5:C:597:ALA:HA	5:C:655:LEU:HD11	1.83	0.60
5:C:626:ARG:H	5:C:639:GLN:NE2	1.98	0.60
6:D:1166:LEU:HD23	6:D:1166:LEU:H	1.65	0.60
6:D:873:LEU:HD11	11:D:8072:HOH:O	2.01	0.60
6:N:1045:MET:HG3	6:N:1073:SER:OG	2.00	0.60
6:N:1145:TYR:O	6:N:1147:ARG:HG2	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:1243:THR:HG22	11:N:9395:HOH:O	2.01	0.60
6:N:1350:GLU:O	6:N:1354:LYS:HG2	2.02	0.60
6:N:489:ARG:CZ	6:N:1389:LEU:HD21	2.31	0.60
6:N:699:VAL:HG22	6:N:756:GLN:HE22	1.64	0.60
5:C:136:ILE:HG21	5:C:336:VAL:HG13	1.81	0.60
5:C:806:LEU:HD13	5:C:813:VAL:HG21	1.83	0.60
5:C:798:GLY:H	5:C:827:VAL:HG11	1.66	0.60
5:C:881:ASN:HD22	5:C:881:ASN:N	1.99	0.60
6:D:136:ASP:CB	6:D:137:PRO:HD3	2.30	0.60
6:D:592:THR:N	6:D:600:LEU:HD11	2.16	0.60
2:H:1:G:N2	5:C:770:GLU:HB3	2.17	0.60
4:K:111:ALA:HB2	4:K:127:LEU:HD23	1.82	0.60
4:K:209:GLU:HB3	11:K:1765:HOH:O	2.00	0.60
5:M:537:LYS:N	5:M:537:LYS:HD2	2.12	0.60
6:N:1007:VAL:HG12	6:N:1011:PHE:CE2	2.35	0.60
6:N:1109:GLU:HG2	6:N:1201:CYS:CA	2.29	0.60
6:N:1268:PRO:HD2	6:N:1271:LYS:NZ	2.15	0.60
6:N:804:LEU:HB2	6:N:830:ALA:O	2.02	0.60
2:Y:13:C:H2'	2:Y:14:G:H8	1.64	0.60
4:A:85:LEU:HA	4:A:124:ASN:ND2	2.08	0.60
5:C:575:GLN:HB2	5:C:670:GLN:OE1	2.02	0.60
5:C:56:GLU:HB3	5:C:64:LEU:HD23	1.82	0.60
6:D:1216:SER:HB3	7:E:16:LYS:H	1.67	0.60
6:D:754:PHE:CD1	7:E:24:ALA:HB1	2.36	0.60
4:K:42:ARG:NH2	4:L:34:VAL:HB	2.15	0.60
6:N:118:LEU:HD13	6:N:124:GLU:OE2	2.01	0.60
11:N:9248:HOH:O	7:O:16:LYS:HB2	2.02	0.60
5:C:627:ARG:O	5:C:638:ASP:HB2	2.00	0.60
5:C:86:LYS:HB3	11:C:1560:HOH:O	2.02	0.60
5:C:764:GLU:HG3	6:D:54:LYS:NZ	2.15	0.60
6:D:853:VAL:HG13	6:D:858:VAL:O	2.01	0.60
4:K:112:ARG:HE	4:K:125:PRO:CB	2.03	0.60
5:M:110:GLU:H	5:M:368:THR:CG2	2.12	0.60
5:M:751:PRO:HA	5:M:792:VAL:HB	1.83	0.60
5:M:805:ARG:HG2	5:M:823:VAL:HG13	1.84	0.60
6:N:1228:SER:HB2	11:N:9308:HOH:O	2.00	0.60
5:M:1007:ALA:HB1	6:N:652:LEU:HD13	1.84	0.60
6:N:929:ARG:HB2	6:N:929:ARG:HH11	1.65	0.60
6:D:1371:VAL:HG12	6:D:1375:MET:CE	2.32	0.60
6:D:28:LYS:HA	11:D:8201:HOH:O	2.01	0.60
6:D:480:GLU:HB2	11:D:8139:HOH:O	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:764:LEU:HD11	6:D:766:ALA:HB3	1.84	0.60
6:D:829:VAL:HA	11:D:8279:HOH:O	2.01	0.60
7:E:54:LEU:HA	7:E:58:PRO:HG2	1.83	0.60
5:M:671:ASN:N	5:M:671:ASN:ND2	2.50	0.60
6:N:1109:GLU:CD	6:N:1202:GLN:H	2.03	0.60
6:N:1438:ALA:N	6:N:1446:VAL:HG11	2.16	0.60
5:C:326:ASP:HB2	5:C:431:HIS:ND1	2.17	0.60
5:C:65:VAL:HG23	5:C:101:ILE:HB	1.83	0.60
5:C:660:ALA:HB1	5:C:667:ALA:O	2.02	0.60
6:D:1042:ARG:HH21	6:D:1061:PHE:HZ	1.50	0.60
6:D:952:ASP:HA	6:D:1062:ARG:NH2	2.16	0.60
6:D:1336:LEU:HD11	6:D:1341:PRO:HG3	1.82	0.60
6:D:1263:PHE:HB3	6:D:1424:VAL:HG11	1.83	0.60
6:D:762:GLN:HE22	7:E:20:THR:CG2	2.15	0.60
5:M:759:THR:HG21	5:M:783:ARG:HH21	1.67	0.60
6:N:1438:ALA:O	6:N:1443:THR:HG22	2.01	0.60
6:N:399:ARG:HE	6:N:431:VAL:HG23	1.65	0.60
5:C:19:THR:O	5:C:23:VAL:HG23	2.01	0.60
5:C:573:ARG:CG	5:C:670:GLN:HE22	2.14	0.60
5:C:859:PRO:HB3	5:C:974:LEU:HD23	1.83	0.60
5:C:910:LYS:HB2	11:C:1325:HOH:O	2.01	0.60
5:C:943:VAL:HG11	5:C:973:VAL:CG2	2.31	0.60
6:D:109:PRO:O	6:D:111:LYS:HD3	2.01	0.60
6:D:127:LEU:HD22	6:D:460:ALA:CB	2.32	0.60
6:D:54:LYS:HD2	6:D:55:ASP:H	1.66	0.60
6:D:896:ALA:HB2	11:D:8341:HOH:O	2.02	0.60
5:M:1033:GLY:O	5:M:1037:VAL:HG23	2.02	0.60
5:M:52:PHE:CG	5:M:68:PHE:HB2	2.36	0.60
5:M:637:LEU:HD22	5:M:659:PRO:HG2	1.83	0.60
6:N:522:PRO:O	6:N:525:ARG:HD3	2.02	0.60
6:N:29:PRO:HD3	6:N:548:ILE:CG2	2.32	0.60
5:C:843:HIS:HA	11:C:1257:HOH:O	2.01	0.60
6:D:119:SER:CB	6:D:123:LEU:HD13	2.31	0.60
6:D:1495:ILE:HG22	6:D:1499:ARG:HH21	1.66	0.60
6:D:8:VAL:HB	6:D:1434:TRP:HH2	1.67	0.60
6:D:963:TYR:CD2	6:D:1002:LYS:HB3	2.37	0.60
1:G:18:DG:H2''	1:G:19:DC:C5'	2.32	0.60
5:M:267:TYR:HB2	5:M:272:ALA:CB	2.32	0.60
6:N:398:ALA:HB2	6:N:447:VAL:HA	1.82	0.60
6:N:610:LYS:HA	11:N:9272:HOH:O	2.01	0.60
6:D:1205:TYR:CD2	6:D:1215:VAL:HG21	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1255:GLY:O	6:D:1259:VAL:HG23	2.02	0.60
6:D:1376:MET:HE3	6:D:1421:LEU:HB2	1.83	0.60
6:D:521:PRO:CG	6:D:524:LEU:HD22	2.29	0.60
5:C:1099:VAL:HA	6:D:9:ARG:O	2.02	0.60
5:M:143:SER:C	5:M:276:LYS:HZ3	2.05	0.60
5:M:144:PRO:HG3	5:M:265:ARG:NH1	2.16	0.60
6:N:1267:ARG:HG3	6:N:1271:LYS:NZ	2.17	0.60
6:N:633:VAL:HG22	6:N:635:PRO:CD	2.25	0.60
6:N:76:CYS:HB3	11:N:9086:HOH:O	2.01	0.60
4:A:83:LYS:NZ	4:A:168:ASP:HB2	2.17	0.59
5:C:45:GLN:HG2	5:C:49:ARG:CZ	2.32	0.59
5:C:461:VAL:HG12	11:C:1351:HOH:O	2.02	0.59
5:C:721:ARG:HG3	5:C:820:ARG:HH12	1.66	0.59
6:D:116:LEU:CD2	6:D:150:ARG:HD3	2.32	0.59
6:D:1259:VAL:HG11	6:D:1356:TYR:OH	2.02	0.59
6:D:1485:GLN:NE2	7:E:78:ASN:HA	2.17	0.59
4:K:151:VAL:HB	4:K:169:ALA:HB3	1.84	0.59
5:M:127:PHE:HB3	11:M:1483:HOH:O	2.01	0.59
5:M:409:ARG:HA	5:M:454:SER:HA	1.84	0.59
6:N:1192:LEU:HD13	6:N:1345:GLU:HG2	1.83	0.59
6:N:185:VAL:HG21	6:N:203:ALA:HB2	1.84	0.59
5:M:1005:MET:CE	6:N:724:GLN:HA	2.32	0.59
4:A:159:LYS:NZ	4:A:166:PRO:HD3	2.17	0.59
5:C:218:VAL:HG22	5:C:221:LEU:HD21	1.84	0.59
5:C:148:PHE:CE2	5:C:281:LEU:HD13	2.28	0.59
6:D:456:MET:HG2	6:D:459:GLU:OE1	2.02	0.59
6:D:970:LYS:HD3	6:D:995:LEU:HD13	1.84	0.59
6:N:1106:VAL:HG11	6:N:1474:ALA:CB	2.31	0.59
6:N:478:LEU:HD23	6:N:496:LEU:HD21	1.84	0.59
6:N:477:LEU:HD11	6:N:495:ARG:HD3	1.84	0.59
6:N:495:ARG:O	6:N:499:VAL:HG23	2.02	0.59
6:N:761:ILE:HB	7:O:20:THR:HG23	1.83	0.59
4:A:8:ALA:HB1	4:B:224:TYR:HE1	1.65	0.59
5:C:26:TYR:HD2	5:C:121:MET:HB2	1.66	0.59
6:D:1080:GLY:O	6:D:1083:ASP:HB3	2.02	0.59
6:D:1231:GLU:O	6:D:1235:GLN:HG3	2.02	0.59
6:D:1335:LEU:HD23	6:D:1344:VAL:HG22	1.84	0.59
6:D:436:GLU:CD	6:D:445:ARG:HG3	2.22	0.59
6:D:99:ALA:O	6:D:514:LEU:N	2.33	0.59
2:H:7:G:N3	2:H:7:G:H2'	2.17	0.59
4:K:89:PHE:HB3	4:K:94:LEU:HD13	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:876:VAL:HG13	5:M:881:ASN:ND2	2.16	0.59
6:N:1268:PRO:HD2	6:N:1271:LYS:HZ2	1.67	0.59
6:N:480:GLU:O	6:N:484:PRO:HD2	2.02	0.59
5:C:252:LYS:HB3	5:C:298:PHE:CZ	2.38	0.59
5:C:583:LEU:HB3	11:C:1190:HOH:O	2.01	0.59
6:D:1438:ALA:N	6:D:1446:VAL:HG11	2.17	0.59
4:K:67:THR:CG2	5:M:609:ASN:HD21	2.15	0.59
5:M:1051:GLU:OE1	5:M:1056:LYS:HE2	2.03	0.59
5:M:149:THR:HG21	11:M:1567:HOH:O	2.01	0.59
5:M:18:LEU:H	5:M:18:LEU:HD12	1.67	0.59
4:K:133:GLU:OE1	5:M:605:LYS:HB3	2.02	0.59
6:N:794:GLN:HG2	6:N:1017:PHE:CZ	2.38	0.59
6:N:1375:MET:HB3	6:N:1422:MET:O	2.02	0.59
6:N:161:LEU:O	6:N:161:LEU:HD23	2.03	0.59
6:N:23:TYR:O	6:N:49:ILE:HG23	2.01	0.59
5:M:1056:LYS:HD3	6:N:625:TYR:HD1	1.67	0.59
6:N:966:GLU:HA	6:N:969:ARG:NH2	2.18	0.59
6:N:983:LEU:HD13	6:N:991:GLN:OE1	2.02	0.59
4:A:89:PHE:CZ	4:A:146:ARG:HB2	2.37	0.59
4:A:38:ASN:HB3	4:A:39:PRO:HD3	1.85	0.59
5:C:318:PRO:HG3	11:C:1342:HOH:O	2.01	0.59
5:C:352:ALA:HA	5:C:355:VAL:HG12	1.85	0.59
5:C:73:LEU:HD22	5:C:94:LEU:HD13	1.84	0.59
6:D:135:LEU:H	6:D:135:LEU:HD12	1.67	0.59
6:D:172:PRO:HG2	6:D:175:VAL:HG21	1.84	0.59
6:D:769:LEU:HD12	6:D:919:PHE:HE1	1.68	0.59
6:D:803:GLY:HA3	11:D:8427:HOH:O	2.00	0.59
4:K:209:GLU:O	4:K:213:GLN:HG3	2.02	0.59
4:K:31:GLY:CA	4:L:42:ARG:HH21	2.15	0.59
4:L:68:ILE:HD13	11:L:362:HOH:O	2.01	0.59
6:N:1209:LEU:HD23	6:N:1210:SER:H	1.66	0.59
6:N:1412:LYS:HD2	6:N:1414:PRO:HG3	1.83	0.59
6:N:615:ARG:HG3	6:N:619:LEU:HD21	1.84	0.59
2:Y:6:U:H1'	11:Y:2617:HOH:O	2.03	0.59
4:A:91:ASN:OD1	4:A:92:PRO:HD2	2.03	0.59
6:D:1209:LEU:HD23	6:D:1210:SER:H	1.65	0.59
4:K:79:ILE:HA	4:K:82:LEU:HD12	1.84	0.59
5:M:468:ARG:HH21	5:M:487:THR:N	2.00	0.59
5:M:854:PRO:HB2	5:M:856:GLU:CG	2.32	0.59
6:N:1389:LEU:HG	6:N:1390:LEU:HG	1.84	0.59
6:N:156:GLU:HB2	6:N:157:GLU:OE1	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:54:THR:HB	4:A:143:ARG:HG2	1.85	0.59
5:C:260:LEU:HD22	11:C:1406:HOH:O	2.00	0.59
5:C:274:ARG:HB2	5:C:285:LEU:HD13	1.85	0.59
5:C:516:ARG:NH1	5:C:521:PRO:HB3	2.17	0.59
5:C:627:ARG:HG3	5:C:628:PHE:H	1.67	0.59
5:C:835:VAL:HG12	11:C:1129:HOH:O	2.03	0.59
6:D:106:LYS:HG2	11:D:8237:HOH:O	2.01	0.59
6:N:1009:LYS:HG2	11:N:9338:HOH:O	2.03	0.59
6:N:1059:SER:OG	6:N:1065:LEU:HD12	2.03	0.59
5:C:193:LEU:HD21	11:C:1142:HOH:O	2.02	0.59
5:C:692:GLU:HG2	5:C:696:LYS:HE2	1.83	0.59
6:D:1465:ASN:HD21	6:D:1470:ARG:HB3	1.68	0.59
4:K:5:LYS:HE3	4:K:5:LYS:HA	1.85	0.59
5:M:1055:LEU:CD2	5:M:1066:ALA:HB2	2.31	0.59
5:M:119:PRO:HG2	5:M:386:PHE:CG	2.37	0.59
5:M:575:GLN:HB2	5:M:670:GLN:HG2	1.85	0.59
6:N:787:LEU:HD13	6:N:1023:MET:HA	1.84	0.59
6:N:422:ALA:HA	11:N:9357:HOH:O	2.01	0.59
6:N:455:ARG:HB3	6:N:460:ALA:HA	1.83	0.59
6:N:481:MET:CE	6:N:493:ARG:HA	2.32	0.59
6:N:584:ASN:OD1	6:N:590:PRO:HD2	2.03	0.59
6:D:1440:PHE:CG	6:D:1441:GLN:N	2.71	0.59
6:D:161:LEU:CD2	6:D:452:ILE:HD13	2.33	0.59
6:D:462:GLN:O	6:D:466:LYS:HE3	2.03	0.59
6:D:93:ILE:HG13	6:D:519:VAL:HG22	1.85	0.59
7:E:17:TYR:O	7:E:21:VAL:HG23	2.03	0.59
4:A:225:PHE:HE1	4:B:40:LEU:HD11	1.68	0.59
4:B:94:LEU:HD11	4:B:119:ASP:CB	2.32	0.59
5:C:492:ASP:CG	5:C:518:LYS:HB3	2.24	0.59
5:C:833:LEU:HD21	5:C:839:LEU:HD11	1.84	0.59
4:L:94:LEU:HD11	4:L:119:ASP:CB	2.33	0.59
4:K:224:TYR:HB3	4:L:9:PRO:HB2	1.83	0.59
5:M:1000:MET:HB3	5:M:1002:GLU:HG2	1.84	0.59
5:M:1081:VAL:HG23	5:M:1086:ARG:HH21	1.67	0.59
5:M:140:ILE:HB	5:M:331:ARG:HG2	1.83	0.59
5:M:498:GLN:HA	5:M:533:ASP:OD2	2.03	0.59
6:N:396:VAL:O	6:N:398:ALA:N	2.31	0.59
6:N:86:ARG:HD3	6:N:523:ASP:OD2	2.02	0.59
6:N:860:LEU:HD23	6:N:877:PRO:HB2	1.85	0.59
6:N:970:LYS:HA	6:N:973:GLN:CD	2.23	0.59
5:C:218:VAL:HG22	5:C:221:LEU:CD2	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:342:ASP:O	5:C:346:VAL:HG23	2.03	0.58
5:C:488:ALA:HA	11:C:1287:HOH:O	2.02	0.58
5:C:48:PHE:O	5:C:52:PHE:HB2	2.02	0.58
6:D:401:TYR:CZ	6:D:429:SER:HA	2.38	0.58
6:D:582:LEU:HA	6:D:603:LEU:HD12	1.85	0.58
6:D:799:LYS:O	6:D:826:PRO:HD2	2.02	0.58
1:G:2:DC:H2''	1:G:3:DC:C6	2.38	0.58
4:L:173:PRO:HB2	11:L:366:HOH:O	2.02	0.58
5:M:755:LEU:HD12	5:M:790:LEU:HG	1.85	0.58
6:N:191:LEU:HB3	6:N:393:ILE:HD12	1.85	0.58
2:Y:11:C:O2'	2:Y:12:G:H5''	2.02	0.58
4:A:54:THR:CG2	4:A:158:ILE:HG13	2.30	0.58
4:A:5:LYS:HE3	4:A:5:LYS:HA	1.84	0.58
4:B:20:TYR:HE2	4:B:198:ARG:HB3	1.68	0.58
5:C:1009:SER:HB2	6:D:651:GLU:O	2.03	0.58
5:C:913:GLU:O	5:C:917:LEU:HG	2.03	0.58
5:C:983:ILE:HG21	5:C:987:ILE:HD11	1.85	0.58
6:D:693:GLU:HA	11:D:8294:HOH:O	2.03	0.58
6:D:918:ALA:O	6:D:922:LEU:HG	2.02	0.58
2:H:9:G:C8	2:H:9:G:H5'	2.38	0.58
4:L:174:VAL:HG23	11:L:366:HOH:O	2.02	0.58
5:M:701:THR:HG21	5:M:830:LYS:HE2	1.84	0.58
5:M:946:ARG:CB	5:M:946:ARG:HH11	2.08	0.58
6:N:464:LEU:O	6:N:468:LEU:HG	2.02	0.58
6:N:567:ILE:O	6:N:571:LYS:HG2	2.03	0.58
6:N:728:LEU:HD21	6:N:733:CYS:SG	2.43	0.58
7:O:18:ARG:HD3	7:O:75:PHE:CE1	2.33	0.58
1:X:18:DG:H5'	1:X:18:DG:H8	1.68	0.58
4:B:99:LEU:HB3	4:B:114:PHE:CD2	2.38	0.58
5:C:398:THR:HA	11:C:1367:HOH:O	2.03	0.58
6:D:1236:LEU:CD1	6:D:1359:GLN:HB3	2.33	0.58
6:D:752:SER:HB2	11:D:8371:HOH:O	2.03	0.58
6:D:835:SER:N	6:D:838:ARG:HD3	2.18	0.58
5:M:861:LEU:HA	5:M:974:LEU:HD12	1.85	0.58
6:N:15:PRO:O	6:N:18:ILE:HB	2.03	0.58
6:N:815:ALA:HA	6:N:818:ARG:HD2	1.84	0.58
7:O:48:MET:N	7:O:54:LEU:HB2	2.18	0.58
7:O:40:LEU:CB	7:O:72:ARG:HH21	2.15	0.58
2:Y:8:C:HO2'	2:Y:9:G:H5'	1.66	0.58
4:A:44:LEU:O	4:A:174:VAL:HG21	2.04	0.58
6:D:1084:THR:HB	6:D:1241:PHE:CD2	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1238:MET:HG3	11:D:8018:HOH:O	2.03	0.58
6:D:124:GLU:O	6:D:127:LEU:HD12	2.02	0.58
5:M:102:HIS:NE2	5:M:365:ASP:HA	2.18	0.58
5:M:252:LYS:HZ3	5:M:296:GLY:HA3	1.69	0.58
2:Y:13:C:C4'	5:M:409:ARG:HH22	2.13	0.58
6:N:1146:GLY:CA	6:N:1207:TYR:HB2	2.33	0.58
6:N:522:PRO:HG2	6:N:523:ASP:H	1.68	0.58
6:N:695:ILE:HD11	6:N:718:PRO:HB2	1.84	0.58
4:A:9:PRO:HB3	4:A:25:LEU:HG	1.84	0.58
6:D:957:PRO:HG2	6:D:1007:VAL:HG22	1.85	0.58
6:D:101:HIS:O	6:D:105:VAL:HG23	2.02	0.58
6:D:23:TYR:O	6:D:49:ILE:HG23	2.03	0.58
4:L:59:GLU:CB	4:L:137:ARG:HH22	2.16	0.58
5:M:497:ALA:HA	5:M:515:ALA:HA	1.85	0.58
6:N:1112:CYS:HB2	6:N:1195:GLN:CG	2.34	0.58
6:N:711:LEU:HD21	6:N:768:ASN:CB	2.33	0.58
6:N:962:GLN:HG2	6:N:966:GLU:OE1	2.03	0.58
6:N:989:TYR:HA	6:N:992:ILE:HD12	1.83	0.58
5:C:1100:GLN:HA	5:C:1100:GLN:NE2	2.18	0.58
6:D:426:LYS:HE3	6:D:427:VAL:HG23	1.85	0.58
6:D:50:PHE:CD2	6:D:522:PRO:HD3	2.38	0.58
7:E:48:MET:HG2	7:E:49:GLN:H	1.69	0.58
5:M:938:LYS:HB2	5:M:938:LYS:NZ	2.18	0.58
5:M:99:GLN:HG2	5:M:109:LYS:HG3	1.85	0.58
6:N:136:ASP:CB	6:N:137:PRO:HD3	2.33	0.58
4:B:177:VAL:HG12	4:B:199:ILE:HG23	1.86	0.58
5:C:1014:SER:HB2	5:C:1017:THR:HG23	1.85	0.58
5:C:211:LEU:CD1	5:C:308:ARG:HA	2.34	0.58
5:C:548:PRO:HD3	5:C:842:ARG:HD2	1.86	0.58
5:C:580:MET:SD	5:C:584:GLU:HG3	2.44	0.58
5:C:712:ALA:O	5:C:820:ARG:HB3	2.04	0.58
5:C:841:ASN:H	5:C:841:ASN:ND2	2.02	0.58
6:D:1271:LYS:HZ1	6:D:1331:ASP:HB3	1.69	0.58
1:G:6:DT:H2''	1:G:7:DC:C6	2.39	0.58
5:M:347:GLY:HA2	11:M:1457:HOH:O	2.02	0.58
5:M:831:ARG:HA	11:M:1437:HOH:O	2.04	0.58
5:M:841:ASN:HD21	5:M:844:GLY:H	1.51	0.58
6:N:1486:VAL:HG23	11:N:9307:HOH:O	2.03	0.58
6:N:584:ASN:HD21	6:N:589:ALA:HA	1.67	0.58
5:C:573:ARG:HB3	11:C:1209:HOH:O	2.03	0.58
5:C:693:GLU:OE1	5:C:696:LYS:HD2	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:871:LYS:HE2	6:D:873:LEU:HD21	1.86	0.58
7:E:26:ARG:O	7:E:30:LEU:HD12	2.04	0.58
5:M:34:VAL:HG12	11:M:1176:HOH:O	2.04	0.58
5:M:54:ILE:CG2	5:M:66:LEU:HB3	2.34	0.58
5:M:549:PHE:HB3	5:M:552:HIS:HD2	1.67	0.58
5:M:701:THR:CG2	5:M:832:LYS:HG2	2.32	0.58
6:N:996:TRP:HA	6:N:999:THR:CG2	2.25	0.58
4:B:54:THR:CG2	4:B:158:ILE:HG13	2.33	0.58
5:C:358:ARG:HH22	5:C:373:VAL:C	2.06	0.58
6:D:1017:PHE:HE1	11:D:8095:HOH:O	1.87	0.58
6:D:1373:ARG:HE	6:D:1374:GLN:NE2	2.02	0.58
6:D:206:ARG:HB3	6:D:206:ARG:HH11	1.68	0.58
6:D:465:LEU:HD22	6:D:510:GLU:HA	1.86	0.58
4:K:211:LEU:O	4:K:215:VAL:HG23	2.04	0.58
5:M:1094:ALA:HA	6:N:90:MET:HE1	1.86	0.58
5:M:91:GLN:CD	5:M:383:ARG:HH22	2.08	0.58
5:M:431:HIS:H	5:M:434:HIS:CE1	2.22	0.58
5:M:444:PRO:HD2	5:M:452:ILE:O	2.04	0.58
5:M:874:LEU:HD12	5:M:874:LEU:H	1.69	0.58
6:N:1081:GLY:O	6:N:1084:THR:HG22	2.04	0.58
6:N:1119:SER:O	6:N:1121:PRO:HD3	2.04	0.58
6:N:134:VAL:HG12	6:N:152:LEU:HD22	1.86	0.58
5:M:1056:LYS:HD3	6:N:751:LEU:HD11	1.86	0.58
6:N:966:GLU:HA	6:N:969:ARG:HH22	1.67	0.58
2:Y:13:C:H2'	2:Y:14:G:C8	2.39	0.58
4:B:99:LEU:HG	11:B:336:HOH:O	2.03	0.58
5:C:775:ARG:NH1	5:C:782:ALA:HB1	2.18	0.58
6:D:116:LEU:HD22	6:D:118:LEU:HD21	1.86	0.58
3:I:7:DC:H5"	6:D:1264:GLU:OE2	2.04	0.58
6:D:182:GLY:HA3	6:D:400:VAL:HG11	1.85	0.58
6:D:396:VAL:C	6:D:398:ALA:N	2.56	0.58
6:D:616:GLN:HG3	11:D:8092:HOH:O	2.03	0.58
6:D:786:ILE:HD11	6:D:908:LYS:HD3	1.85	0.58
5:M:310:LEU:HB2	11:M:1183:HOH:O	2.03	0.58
5:M:452:ILE:HD12	5:M:452:ILE:H	1.69	0.58
5:M:464:LEU:HB2	11:M:1525:HOH:O	2.03	0.58
5:M:549:PHE:HB3	5:M:552:HIS:CD2	2.39	0.58
6:N:161:LEU:HD21	11:N:9092:HOH:O	2.02	0.58
6:N:930:LEU:O	6:N:934:LEU:HG	2.04	0.58
6:N:970:LYS:HG3	6:N:973:GLN:OE1	2.04	0.58
5:C:1101:THR:OG1	6:D:5:VAL:HG12	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:211:LEU:HD11	5:C:308:ARG:HA	1.86	0.57
5:C:495:THR:HG23	11:C:1226:HOH:O	2.03	0.57
5:C:626:ARG:H	5:C:639:GLN:HE21	1.50	0.57
5:C:959:PRO:HG2	11:C:1413:HOH:O	2.03	0.57
6:D:1171:VAL:O	6:D:1175:ILE:HG13	2.04	0.57
6:D:810:GLU:HB3	11:D:8233:HOH:O	2.03	0.57
6:D:890:VAL:HG23	11:D:8341:HOH:O	2.03	0.57
5:M:1030:GLN:HB2	6:N:626:SER:OG	2.04	0.57
5:M:1032:PHE:O	5:M:1033:GLY:O	2.21	0.57
5:M:134:ARG:HH11	5:M:392:SER:CB	2.17	0.57
5:M:470:PRO:HD3	5:M:485:TYR:CE2	2.39	0.57
5:M:546:LEU:CD1	5:M:565:GLN:HE22	2.17	0.57
5:M:715:THR:HG21	11:M:1222:HOH:O	2.03	0.57
5:M:875:GLY:O	5:M:879:ARG:HD2	2.03	0.57
6:N:1397:LYS:HE3	6:N:1432:LYS:HD2	1.85	0.57
1:X:6:DT:H2'	1:X:7:DC:C6	2.39	0.57
5:C:573:ARG:HB3	5:C:670:GLN:HE22	1.69	0.57
6:D:30:GLU:HB3	6:D:40:GLU:CB	2.34	0.57
6:D:400:VAL:HG22	6:D:443:VAL:HG21	1.85	0.57
5:M:535:SER:HB3	5:M:537:LYS:NZ	2.19	0.57
6:N:149:LYS:HD2	6:N:150:ARG:H	1.69	0.57
6:N:677:LEU:HD23	6:N:683:ILE:HG13	1.86	0.57
6:N:62:LYS:HG3	6:N:75:ARG:NH1	2.19	0.57
7:O:32:ARG:HB2	7:O:32:ARG:CZ	2.34	0.57
5:C:264:PRO:HG3	11:C:1383:HOH:O	2.04	0.57
5:C:577:PRO:HB3	5:C:842:ARG:NH2	2.18	0.57
5:C:99:GLN:HB3	5:C:109:LYS:CD	2.34	0.57
6:D:1418:LYS:HD3	6:D:1419:PRO:HD2	1.85	0.57
6:D:30:GLU:HB3	6:D:40:GLU:CG	2.34	0.57
6:D:444:VAL:HB	11:D:8164:HOH:O	2.04	0.57
6:D:614:PHE:CE2	6:D:1438:ALA:HB1	2.39	0.57
6:D:959:GLU:CD	6:D:959:GLU:H	2.04	0.57
2:H:10:G:H2'	2:H:11:C:H6	1.66	0.57
2:H:13:C:H2'	2:H:14:G:C8	2.39	0.57
4:K:145:ASP:HB3	11:K:1799:HOH:O	2.03	0.57
4:K:49:PRO:HB3	4:K:148:VAL:HG22	1.86	0.57
4:K:42:ARG:HH21	4:L:31:GLY:C	2.08	0.57
4:L:123:MET:C	4:L:125:PRO:HD3	2.24	0.57
5:M:205:GLU:HA	5:M:209:ARG:NH1	2.20	0.57
11:Y:1707:HOH:O	5:M:777:ILE:HG21	2.03	0.57
5:M:79:PRO:HG2	5:M:82:GLU:HB2	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:399:ARG:HE	6:N:431:VAL:CG2	2.18	0.57
6:N:510:GLU:HB2	6:N:511:TRP:CZ3	2.39	0.57
6:N:637:LEU:HD11	6:N:641:GLN:HB2	1.86	0.57
7:O:33:HIS:HB2	7:O:37:ASN:ND2	2.18	0.57
2:Y:14:G:H4'	11:Y:1734:HOH:O	2.03	0.57
5:C:1030:GLN:NE2	6:D:628:ARG:HD3	2.20	0.57
6:D:155:ASP:O	6:D:159:ARG:HG3	2.04	0.57
6:D:793:THR:HG21	6:D:906:GLN:CG	2.33	0.57
4:L:58:ILE:HG21	4:L:68:ILE:HD11	1.85	0.57
5:M:1031:ARG:HG3	6:N:621:LYS:HB3	1.86	0.57
6:N:394:LEU:HG	6:N:396:VAL:HG23	1.85	0.57
5:C:468:ARG:HE	5:C:487:THR:N	2.02	0.57
5:C:584:GLU:H	5:C:584:GLU:CD	2.07	0.57
6:D:501:ALA:HB1	6:D:1453:ALA:HB2	1.87	0.57
6:D:525:ARG:HB2	6:D:538:SER:HB3	1.86	0.57
4:B:170:VAL:HG11	6:D:848:GLU:OE1	2.04	0.57
6:D:879:ARG:HG3	6:D:879:ARG:NH1	2.17	0.57
5:M:166:PRO:HB3	11:M:1157:HOH:O	2.03	0.57
5:M:452:ILE:N	5:M:452:ILE:HD12	2.19	0.57
5:M:841:ASN:HD22	5:M:841:ASN:C	2.07	0.57
4:K:181:VAL:HG21	5:M:939:ARG:HH11	1.70	0.57
5:M:975:TYR:HE1	11:M:1220:HOH:O	1.86	0.57
6:N:28:LYS:HG3	6:N:29:PRO:HD2	1.87	0.57
2:Y:9:G:O2'	2:Y:10:G:H5'	2.04	0.57
4:A:43:ILE:HG13	4:A:218:LEU:CD1	2.33	0.57
1:G:20:DG:H4'	5:C:394:PHE:CE1	2.39	0.57
6:D:772:PRO:HB3	6:D:1224:VAL:CG1	2.34	0.57
5:M:205:GLU:HA	5:M:209:ARG:CZ	2.34	0.57
6:N:1083:ASP:O	6:N:1087:ARG:HG2	2.05	0.57
6:N:1191:PRO:HG3	11:N:9238:HOH:O	2.03	0.57
6:N:1336:LEU:HA	6:N:1344:VAL:CG2	2.34	0.57
6:N:583:ASP:CG	6:N:586:ARG:HG3	2.25	0.57
6:N:758:GLU:HA	7:O:20:THR:HG21	1.86	0.57
4:A:100:LEU:HD22	4:A:102:LYS:HE2	1.87	0.57
4:A:221:HIS:HB3	4:B:36:LEU:HD21	1.86	0.57
4:B:85:LEU:HG	4:B:127:LEU:CD2	2.32	0.57
5:C:971:LYS:HD2	5:C:986:PRO:HG2	1.87	0.57
6:D:1020:LEU:HD21	6:D:1038:LEU:HD12	1.86	0.57
1:G:13:DT:H5"	6:D:1093:TYR:HE2	1.68	0.57
6:D:1103:HIS:CD2	6:D:1463:LYS:HB2	2.40	0.57
6:D:1263:PHE:HE2	6:D:1371:VAL:HG11	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:214:ALA:O	4:L:217:ILE:HG22	2.04	0.57
5:M:567:GLN:O	5:M:997:LEU:HD12	2.05	0.57
6:N:1129:THR:HG23	6:N:1130:ARG:H	1.69	0.57
6:N:139:GLY:HA2	6:N:451:ASP:O	2.05	0.57
2:Y:11:C:H2'	2:Y:12:G:H8	1.66	0.57
4:A:68:ILE:HD12	4:A:68:ILE:H	1.69	0.57
5:C:188:LYS:HD3	11:C:1301:HOH:O	2.03	0.57
5:C:834:GLN:HB2	11:C:1129:HOH:O	2.04	0.57
6:D:1224:VAL:HA	6:D:1227:GLN:OE1	2.05	0.57
6:D:1335:LEU:HD22	6:D:1344:VAL:HG13	1.86	0.57
6:D:1332:PRO:HG3	6:D:1347:TYR:CE2	2.37	0.57
6:D:1216:SER:CB	7:E:16:LYS:H	2.18	0.57
6:D:1485:GLN:HE21	7:E:79:LEU:H	1.51	0.57
4:K:138:LEU:HD11	4:K:140:MET:SD	2.44	0.57
4:L:124:ASN:OD1	4:L:127:LEU:HB2	2.05	0.57
5:M:1046:ALA:HB2	11:N:9022:HOH:O	2.03	0.57
5:M:121:MET:HE3	5:M:125:GLY:HA2	1.87	0.57
5:M:208:ALA:HB3	5:M:209:ARG:HH21	1.70	0.57
5:M:693:GLU:HA	5:M:696:LYS:CD	2.34	0.57
6:N:1023:MET:O	6:N:1028:ALA:HB3	2.05	0.57
5:M:498:GLN:OE1	6:N:1067:VAL:HB	2.05	0.57
6:N:1153:VAL:HG12	6:N:1155:VAL:HG13	1.86	0.57
5:C:1049:LEU:HD11	5:C:1053:LEU:HD11	1.87	0.57
5:C:1103:ASP:OD1	6:D:3:LYS:HD3	2.05	0.57
5:C:1105:LYS:HZ3	5:C:1107:ASN:HB2	1.70	0.57
5:C:192:PRO:HD2	5:C:195:LEU:CB	2.32	0.57
5:C:144:PRO:CG	5:C:265:ARG:HH21	2.13	0.57
5:C:472:ARG:HG3	5:C:534:VAL:HG22	1.85	0.57
1:X:19:DC:H5"	5:M:1001:VAL:HB	1.87	0.57
5:M:162:ILE:O	5:M:164:PRO:HD3	2.05	0.57
5:M:691:SER:OG	5:M:694:LEU:HG	2.04	0.57
6:N:434:ARG:HH11	6:N:434:ARG:HB3	1.70	0.57
4:B:88:ARG:HG3	11:B:365:HOH:O	2.04	0.57
5:C:51:THR:OG1	5:C:348:LEU:HG	2.05	0.57
5:C:531:PHE:HB2	11:C:1172:HOH:O	2.05	0.57
5:C:975:TYR:HA	5:C:982:PRO:HA	1.86	0.57
6:D:1406:ARG:HD2	6:D:1412:LYS:HZ3	1.70	0.57
6:D:455:ARG:C	6:D:460:ALA:HB2	2.25	0.57
6:D:65:ARG:CG	6:D:66:GLN:H	2.18	0.57
6:D:657:LEU:HD22	6:D:691:LEU:CD2	2.35	0.57
4:K:42:ARG:CZ	4:L:34:VAL:HB	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:79:ILE:HA	4:L:82:LEU:HD12	1.87	0.57
5:M:1085:PHE:O	5:M:1089:VAL:HG23	2.05	0.57
5:M:174:LEU:HD22	5:M:307:LEU:HD13	1.87	0.57
5:M:400:PRO:HG2	5:M:593:ALA:HB2	1.87	0.57
6:N:1025:GLN:NE2	6:N:1025:GLN:HA	2.20	0.57
6:N:161:LEU:HD13	6:N:452:ILE:HD13	1.87	0.57
6:N:54:LYS:CD	6:N:55:ASP:H	2.17	0.57
7:O:17:TYR:O	7:O:21:VAL:HG23	2.05	0.57
2:Y:7:G:C8	2:Y:7:G:C5'	2.88	0.57
5:C:949:LYS:HA	11:C:1221:HOH:O	2.05	0.56
5:M:1050:GLN:OE1	6:N:1471:LEU:HA	2.04	0.56
5:M:286:SER:HB3	11:M:1441:HOH:O	2.05	0.56
5:M:578:VAL:CG2	5:M:579:VAL:HG12	2.34	0.56
5:M:716:LYS:HZ1	6:N:36:THR:HG23	1.69	0.56
5:M:871:LEU:HD11	5:M:992:MET:SD	2.44	0.56
6:N:1045:MET:HB3	6:N:1073:SER:HA	1.87	0.56
6:N:1057:VAL:HG13	6:N:1069:GLU:HB3	1.87	0.56
7:O:41:GLU:HB2	7:O:45:ARG:NE	2.19	0.56
4:A:225:PHE:HB2	11:A:325:HOH:O	2.05	0.56
4:A:52:ALA:HB2	4:A:170:VAL:O	2.04	0.56
5:C:338:GLU:O	5:C:341:THR:HG22	2.05	0.56
6:D:1436:SER:HB3	11:D:8024:HOH:O	2.05	0.56
7:E:19:LEU:O	7:E:23:VAL:HG23	2.05	0.56
1:G:22:DC:H4'	5:C:388:ARG:CD	2.33	0.56
4:L:43:ILE:O	4:L:47:SER:HB3	2.05	0.56
5:M:292:ARG:HH11	5:M:299:LYS:HD3	1.70	0.56
5:M:805:ARG:HB3	5:M:805:ARG:HH11	1.70	0.56
6:N:1091:SER:OG	6:N:1234:THR:HG23	2.04	0.56
6:N:714:GLN:NE2	6:N:765:SER:HA	2.20	0.56
6:N:824:ASN:HD22	6:N:824:ASN:C	2.09	0.56
2:Y:8:C:H5'	11:Y:1683:HOH:O	2.04	0.56
4:B:201:THR:HG21	4:B:205:VAL:HG23	1.87	0.56
5:C:186:VAL:HG11	11:C:1130:HOH:O	2.05	0.56
5:C:148:PHE:CZ	5:C:281:LEU:HB3	2.39	0.56
5:C:943:VAL:HG23	5:C:985:GLY:H	1.70	0.56
6:D:1226:ALA:HB2	11:D:8257:HOH:O	2.05	0.56
6:D:136:ASP:HB3	6:D:455:ARG:HE	1.70	0.56
6:D:703:ASN:ND2	6:D:704:ARG:H	2.03	0.56
7:E:41:GLU:HG2	7:E:42:PRO:HD3	1.87	0.56
7:E:59:ASN:N	7:E:59:ASN:HD22	2.02	0.56
4:L:92:PRO:HA	4:L:146:ARG:NH2	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:1054:THR:HG21	5:M:1079:PRO:HB3	1.87	0.56
5:M:121:MET:CE	5:M:125:GLY:HA2	2.34	0.56
5:M:257:VAL:HA	11:M:1334:HOH:O	2.04	0.56
6:N:1189:ARG:HD2	6:N:1204:CYS:SG	2.46	0.56
6:N:1238:MET:HA	6:N:1241:PHE:CE2	2.40	0.56
6:N:36:THR:C	6:N:38:LYS:H	2.07	0.56
6:N:794:GLN:HG3	6:N:795:VAL:N	2.20	0.56
6:N:80:VAL:HG12	6:N:81:THR:O	2.05	0.56
6:N:799:LYS:HE2	6:N:824:ASN:O	2.04	0.56
6:N:828:LYS:HG2	6:N:863:VAL:HG22	1.86	0.56
5:M:886:LEU:HD12	6:N:951:ILE:HG13	1.87	0.56
5:C:159:ILE:HD13	11:C:1523:HOH:O	2.06	0.56
5:C:412:ALA:HB1	5:C:419:THR:HG21	1.87	0.56
6:D:1042:ARG:O	6:D:1057:VAL:HB	2.04	0.56
6:D:1236:LEU:HD11	6:D:1361:VAL:HG23	1.88	0.56
6:D:758:GLU:HA	6:D:762:GLN:NE2	2.20	0.56
5:C:676:ILE:HD13	6:D:948:THR:HB	1.88	0.56
6:D:696:HIS:NE2	7:E:54:LEU:HD11	2.20	0.56
7:E:80:VAL:HG22	11:E:151:HOH:O	2.06	0.56
4:L:92:PRO:HA	4:L:146:ARG:CZ	2.35	0.56
5:M:39:ARG:HG3	5:M:39:ARG:HH11	1.68	0.56
5:M:546:LEU:HD12	5:M:565:GLN:NE2	2.18	0.56
6:N:1493:LYS:O	6:N:1496:GLU:HG2	2.04	0.56
6:N:806:PHE:HE1	6:N:813:LEU:HB3	1.69	0.56
7:O:13:VAL:HG21	7:O:19:LEU:HB2	1.88	0.56
7:O:84:ARG:HD3	11:O:1385:HOH:O	2.05	0.56
1:X:2:DC:H2"	1:X:3:DC:C6	2.40	0.56
4:B:160:ASP:HB3	11:B:345:HOH:O	2.05	0.56
4:A:42:ARG:NH2	4:B:34:VAL:HB	2.20	0.56
5:C:333:ILE:HD13	5:C:467:ILE:HG13	1.86	0.56
5:C:577:PRO:HA	5:C:671:ASN:ND2	2.20	0.56
5:C:838:LYS:O	5:C:839:LEU:HD23	2.06	0.56
6:D:116:LEU:HD11	6:D:464:LEU:HB3	1.86	0.56
6:D:117:ASP:N	6:D:150:ARG:NH1	2.53	0.56
6:D:36:THR:C	6:D:38:LYS:H	2.09	0.56
6:D:65:ARG:H	6:D:68:PHE:HE1	1.51	0.56
6:D:700:VAL:HG22	6:D:718:PRO:HG3	1.87	0.56
6:D:754:PHE:HE1	7:E:28:GLN:HE22	1.53	0.56
6:D:847:ASP:O	6:D:851:LEU:HG	2.06	0.56
4:L:187:GLY:HA3	11:L:397:HOH:O	2.05	0.56
5:M:48:PHE:O	5:M:52:PHE:HB2	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:532:MET:HB3	11:M:1310:HOH:O	2.04	0.56
5:M:611:ILE:HG13	5:M:625:LEU:HD21	1.87	0.56
5:M:668:LEU:HD13	5:M:995:MET:HE2	1.87	0.56
6:N:1271:LYS:NZ	6:N:1331:ASP:HB2	2.20	0.56
6:N:481:MET:HE3	6:N:1388:ARG:HG3	1.88	0.56
6:N:47:GLU:OE1	6:N:53:ILE:HB	2.06	0.56
6:N:704:ARG:HD3	6:N:738:ALA:HB2	1.87	0.56
6:N:988:ARG:O	6:N:992:ILE:HG13	2.05	0.56
4:A:54:THR:HB	4:A:143:ARG:CG	2.35	0.56
4:B:16:GLN:HG3	11:B:397:HOH:O	2.05	0.56
1:G:16:DG:H5''	5:C:1031:ARG:HB3	1.88	0.56
5:C:284:ARG:HG3	5:C:285:LEU:N	2.19	0.56
6:D:117:ASP:HB2	6:D:495:ARG:HH21	1.69	0.56
6:D:1267:ARG:HG2	6:D:1267:ARG:O	2.05	0.56
6:D:29:PRO:HG3	6:D:549:ASN:HD21	1.69	0.56
5:M:457:ALA:N	5:M:540:PHE:O	2.36	0.56
5:M:577:PRO:HG3	5:M:993:PHE:CE1	2.41	0.56
6:N:119:SER:HB2	6:N:123:LEU:CB	2.33	0.56
6:N:1336:LEU:HA	6:N:1344:VAL:HG21	1.86	0.56
6:N:792:ILE:O	6:N:878:GLY:HA3	2.04	0.56
4:B:117:VAL:HG22	11:B:392:HOH:O	2.06	0.56
5:C:12:VAL:HG13	5:C:13:ILE:CG1	2.36	0.56
5:C:232:GLU:O	5:C:235:LEU:HB3	2.05	0.56
5:C:451:LEU:C	5:C:452:ILE:HD12	2.26	0.56
5:C:437:ARG:HA	5:C:467:ILE:HG21	1.86	0.56
5:C:693:GLU:HA	5:C:696:LYS:HG3	1.88	0.56
5:C:697:ARG:O	5:C:699:PHE:N	2.39	0.56
5:C:804:VAL:HG11	5:C:824:ARG:NH2	2.19	0.56
6:D:136:ASP:OD1	6:D:463:GLN:HB3	2.05	0.56
6:D:964:LEU:HD22	6:D:1058:ARG:HH21	1.70	0.56
2:H:11:C:O2'	2:H:12:G:H5''	2.05	0.56
4:K:178:ALA:HB2	5:M:864:GLY:N	2.21	0.56
4:K:206:THR:HG23	4:K:207:PRO:HD2	1.88	0.56
4:K:92:PRO:HD3	11:K:1047:HOH:O	2.05	0.56
5:M:307:LEU:HD12	5:M:310:LEU:HD23	1.87	0.56
5:M:626:ARG:HH22	5:M:637:LEU:HD13	1.70	0.56
5:M:600:ASP:OD1	5:M:651:LYS:HB2	2.05	0.56
6:N:180:LYS:HD2	6:N:180:LYS:H	1.69	0.56
11:M:1366:HOH:O	6:N:6:ARG:HB2	2.04	0.56
6:N:853:VAL:HG11	6:N:860:LEU:HG	1.88	0.56
6:N:960:LYS:NZ	6:N:1041:LEU:HD13	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:46:PRO:C	7:O:47:LYS:HG2	2.25	0.56
1:X:14:DT:H5'	1:X:14:DT:H6	1.70	0.56
5:C:265:ARG:NH1	5:C:267:TYR:HB3	2.20	0.56
6:D:1124:GLN:HG2	6:D:1133:ARG:HG3	1.88	0.56
5:M:516:ARG:HE	6:N:1068:LEU:HD13	1.69	0.56
5:M:516:ARG:HH21	6:N:1068:LEU:HB3	1.71	0.56
6:N:24:GLY:HA3	6:N:49:ILE:HG12	1.87	0.56
5:M:1070:ILE:HG21	6:N:655:PRO:HB2	1.88	0.56
5:C:162:ILE:HD12	5:C:172:ILE:HB	1.86	0.56
5:C:265:ARG:HD2	5:C:267:TYR:HB3	1.88	0.56
5:C:654:LEU:HD13	5:C:664:GLY:N	2.21	0.56
6:D:1102:THR:HB	11:D:8257:HOH:O	2.04	0.56
6:D:116:LEU:HD13	6:D:118:LEU:HD11	1.87	0.56
6:D:1091:SER:HB3	6:D:1234:THR:OG1	2.05	0.56
6:D:703:ASN:HD22	6:D:704:ARG:H	1.53	0.56
6:D:906:GLN:HB3	6:D:911:LEU:HD11	1.88	0.56
7:E:30:LEU:O	7:E:35:PHE:HA	2.06	0.56
4:L:101:LEU:HA	11:L:368:HOH:O	2.06	0.56
5:M:172:ILE:HG23	5:M:184:MET:HE3	1.87	0.56
5:M:260:LEU:HB2	11:M:1400:HOH:O	2.05	0.56
5:M:695:LEU:HD11	11:M:1250:HOH:O	2.05	0.56
6:N:883:ALA:HB2	11:N:9040:HOH:O	2.04	0.56
4:B:124:ASN:ND2	4:B:127:LEU:HD22	2.21	0.56
5:C:410:ILE:HD12	5:C:438:ILE:HG13	1.88	0.56
5:C:439:CYS:HB2	5:C:541:SER:HB2	1.87	0.56
5:C:897:LEU:HD23	5:C:924:VAL:HG21	1.88	0.56
6:D:28:LYS:HB2	6:D:41:ARG:NH1	2.19	0.56
6:D:137:PRO:HD2	6:D:453:ASP:CG	2.27	0.56
6:D:714:GLN:NE2	6:D:765:SER:HA	2.20	0.56
7:E:27:ALA:CB	7:E:61:VAL:HG12	2.35	0.56
7:E:40:LEU:HB3	7:E:72:ARG:HH21	1.68	0.56
3:I:3:DA:H3'	11:I:500:HOH:O	2.05	0.56
4:L:197:LEU:HD23	4:L:199:ILE:HG13	1.87	0.56
5:M:290:LEU:HB3	5:M:302:VAL:HG12	1.88	0.56
6:N:1353:GLN:HB3	6:N:1357:ARG:HE	1.70	0.56
6:N:150:ARG:HD3	6:N:464:LEU:HD21	1.88	0.56
6:N:482:LYS:HE2	6:N:1384:PRO:HG2	1.88	0.56
5:M:1034:GLU:H	6:N:619:LEU:HD13	1.71	0.56
4:A:102:LYS:HZ2	4:A:139:ASN:HD21	1.54	0.56
5:C:233:GLU:HB3	11:C:1182:HOH:O	2.06	0.56
5:C:358:ARG:HA	5:C:361:MET:HG2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:474:VAL:HG12	5:C:531:PHE:HA	1.88	0.56
5:C:578:VAL:HG13	5:C:671:ASN:CB	2.29	0.56
5:C:680:ASP:HB2	5:C:682:TYR:CE2	2.40	0.56
6:D:1222:GLY:O	6:D:1225:ALA:HB3	2.06	0.56
5:M:1057:SER:HB2	6:N:622:ARG:O	2.05	0.56
5:M:569:VAL:HG12	5:M:996:LYS:O	2.07	0.56
6:N:783:ARG:CA	6:N:1028:ALA:HA	2.26	0.56
5:M:1050:GLN:HE22	6:N:1470:ARG:C	2.09	0.56
7:O:13:VAL:HG13	7:O:75:PHE:CZ	2.41	0.56
7:O:27:ALA:CB	7:O:61:VAL:HG12	2.35	0.56
7:O:54:LEU:HG	7:O:58:PRO:HG2	1.88	0.56
2:Y:8:C:O5'	2:Y:8:C:H6	1.89	0.56
5:C:150:PRO:HA	5:C:158:TYR:HB3	1.89	0.55
5:C:166:PRO:HD2	5:C:263:ASP:O	2.06	0.55
6:D:1336:LEU:HD22	6:D:1421:LEU:HB2	1.87	0.55
6:D:1197:ARG:HB3	6:D:1396:GLU:CG	2.36	0.55
6:D:710:ARG:CG	6:D:772:PRO:HG2	2.34	0.55
6:D:957:PRO:CG	6:D:1007:VAL:HA	2.36	0.55
6:D:1209:LEU:HD11	7:E:16:LYS:HD2	1.88	0.55
7:E:31:LEU:HD21	7:E:60:ALA:HB2	1.88	0.55
4:K:32:PHE:O	4:K:36:LEU:HG	2.05	0.55
4:K:94:LEU:HD11	4:K:119:ASP:CG	2.25	0.55
4:L:101:LEU:HD11	4:L:113:ASP:HB3	1.89	0.55
4:L:59:GLU:CG	4:L:137:ARG:HH22	2.18	0.55
5:M:697:ARG:O	5:M:699:PHE:N	2.38	0.55
6:N:1121:PRO:CD	6:N:1346:ARG:HH21	2.14	0.55
6:N:165:LYS:HG2	6:N:448:GLU:OE2	2.06	0.55
5:C:1016:ILE:CD1	5:C:1016:ILE:H	2.16	0.55
5:C:1020:PRO:O	5:C:1021:LEU:HD12	2.07	0.55
5:C:267:TYR:HB2	5:C:272:ALA:CB	2.37	0.55
5:C:850:ALA:HA	6:D:632:VAL:HG11	1.87	0.55
5:C:965:GLU:O	5:C:969:GLN:HG2	2.05	0.55
5:C:676:ILE:HG21	5:C:988:VAL:HG13	1.88	0.55
6:D:462:GLN:HG2	6:D:466:LYS:NZ	2.21	0.55
6:D:114:THR:HG22	6:D:495:ARG:HA	1.87	0.55
6:D:700:VAL:HG12	6:D:749:VAL:HG12	1.88	0.55
6:D:804:LEU:HD23	6:D:804:LEU:H	1.71	0.55
4:K:112:ARG:HG2	4:K:125:PRO:CB	2.37	0.55
5:M:946:ARG:HB3	5:M:946:ARG:NH1	2.07	0.55
6:N:1016:PRO:HB3	11:N:9351:HOH:O	2.04	0.55
6:N:120:ALA:HB2	11:N:9298:HOH:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:1258:ARG:NH1	6:N:1268:PRO:HB3	2.16	0.55
6:N:834:THR:HG22	6:N:838:ARG:NH1	2.21	0.55
2:Y:9:G:C8	2:Y:9:G:H5'	2.41	0.55
4:B:30:ARG:HH22	5:C:854:PRO:CG	2.20	0.55
4:B:48:ILE:HG13	11:B:331:HOH:O	2.07	0.55
5:C:472:ARG:HG2	5:C:483:VAL:HG22	1.88	0.55
5:C:759:THR:HB	5:C:785:VAL:CG1	2.33	0.55
5:C:92:ALA:HB2	5:C:120:LEU:HD11	1.87	0.55
6:D:473:LEU:O	6:D:477:LEU:HG	2.06	0.55
6:D:808:THR:OG1	6:D:809:PRO:HD3	2.07	0.55
4:L:58:ILE:HG22	4:L:61:VAL:H	1.71	0.55
5:M:134:ARG:HD3	5:M:392:SER:HB3	1.86	0.55
5:M:173:ASP:HB2	5:M:185:LYS:NZ	2.22	0.55
5:M:943:VAL:HG23	5:M:985:GLY:H	1.72	0.55
6:N:1165:TYR:CE2	6:N:1214:PRO:HB3	2.42	0.55
6:N:402:PRO:HA	6:N:443:VAL:HG23	1.88	0.55
4:A:183:ASP:HB3	11:A:321:HOH:O	2.07	0.55
5:C:136:ILE:CG2	5:C:336:VAL:HG22	2.36	0.55
5:C:401:LEU:HD21	5:C:565:GLN:HE21	1.71	0.55
5:C:527:GLU:OE1	5:C:528:GLU:HG3	2.06	0.55
5:C:780:GLU:HG2	11:C:1242:HOH:O	2.06	0.55
4:B:30:ARG:HH22	5:C:854:PRO:HG2	1.72	0.55
6:D:1007:VAL:HG12	6:D:1011:PHE:CE2	2.40	0.55
6:D:887:ALA:HB3	11:D:8116:HOH:O	2.06	0.55
4:K:57:TYR:CE2	4:K:59:GLU:HA	2.41	0.55
5:M:115:LEU:HD12	5:M:115:LEU:O	2.06	0.55
5:M:265:ARG:HB3	5:M:267:TYR:CD2	2.42	0.55
5:M:138:SER:HB3	5:M:333:ILE:HG23	1.88	0.55
4:K:72:LYS:HE3	5:M:641:PRO:O	2.06	0.55
5:M:975:TYR:HA	5:M:982:PRO:HA	1.89	0.55
5:C:139:GLN:O	5:C:333:ILE:HA	2.07	0.55
5:C:5:ARG:NE	5:C:8:ARG:HH12	2.00	0.55
6:D:117:ASP:H	6:D:150:ARG:HH12	1.55	0.55
5:M:285:LEU:O	5:M:285:LEU:HD23	2.06	0.55
5:M:987:ILE:HG12	6:N:948:THR:HG21	1.88	0.55
6:N:1209:LEU:HG	6:N:1219:GLU:OE1	2.07	0.55
6:N:1335:LEU:CD2	6:N:1344:VAL:HG22	2.27	0.55
4:A:153:ALA:HA	4:A:156:HIS:NE2	2.22	0.55
4:B:41:ARG:HD2	4:B:177:VAL:CG2	2.37	0.55
5:C:1045:ALA:HB1	5:C:1048:THR:HB	1.89	0.55
5:C:431:HIS:NE2	5:C:432:ARG:HB2	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:794:GLN:HB3	6:D:1017:PHE:HZ	1.72	0.55
6:D:112:ILE:HB	6:D:512:MET:SD	2.46	0.55
6:D:1481:VAL:HG12	6:D:1481:VAL:O	2.07	0.55
6:D:801:GLY:HA2	11:D:8362:HOH:O	2.06	0.55
5:M:433:THR:CG2	5:M:488:ALA:HB1	2.35	0.55
5:M:626:ARG:HH12	5:M:637:LEU:CB	2.17	0.55
6:N:957:PRO:HG2	6:N:1007:VAL:HG22	1.87	0.55
6:N:1027:GLY:HA2	11:N:9239:HOH:O	2.06	0.55
6:N:1105:ILE:HD13	11:N:9367:HOH:O	2.05	0.55
6:N:119:SER:N	6:N:123:LEU:HD22	2.17	0.55
6:N:161:LEU:HD22	6:N:452:ILE:HG21	1.87	0.55
6:N:116:LEU:HD21	6:N:464:LEU:HD22	1.88	0.55
6:N:52:PRO:HD2	6:N:85:VAL:CG2	2.32	0.55
6:N:827:ILE:H	6:N:827:ILE:HD12	1.72	0.55
1:X:17:DC:H2''	1:X:18:DG:C5'	2.37	0.55
5:C:140:ILE:CG2	5:C:333:ILE:HG13	2.34	0.55
5:C:141:HIS:HA	11:C:1222:HOH:O	2.06	0.55
5:C:411:SER:OG	5:C:413:LEU:HD12	2.07	0.55
5:C:949:LYS:HD3	6:D:796:ARG:NH2	2.19	0.55
6:D:554:LEU:HD21	6:D:571:LYS:CE	2.36	0.55
1:G:18:DG:H8	1:G:18:DG:H5'	1.72	0.55
4:K:177:VAL:O	5:M:864:GLY:CA	2.55	0.55
4:L:205:VAL:HG11	11:L:322:HOH:O	2.05	0.55
5:M:1067:TYR:CE1	5:M:1071:ILE:HD11	2.41	0.55
5:M:176:VAL:C	5:M:178:PRO:HD3	2.27	0.55
5:M:141:HIS:CB	5:M:418:LEU:HD23	2.33	0.55
4:K:72:LYS:HG3	5:M:641:PRO:HB2	1.87	0.55
5:M:660:ALA:HB1	5:M:667:ALA:O	2.06	0.55
5:M:719:PRO:HB2	11:M:1137:HOH:O	2.07	0.55
5:M:730:SER:O	5:M:734:LEU:HD13	2.07	0.55
5:M:752:GLY:O	6:N:679:ARG:HG2	2.06	0.55
4:K:181:VAL:HG21	5:M:939:ARG:NH1	2.20	0.55
6:N:137:PRO:HB2	6:N:138:LYS:HD3	1.89	0.55
6:N:43:GLY:N	11:N:9087:HOH:O	2.40	0.55
6:N:18:ILE:CG2	6:N:518:PRO:HG3	2.22	0.55
4:A:206:THR:HG23	4:A:208:LEU:H	1.72	0.55
4:B:55:SER:OG	4:B:143:ARG:HD3	2.06	0.55
5:C:290:LEU:HB3	5:C:302:VAL:HG12	1.88	0.55
5:C:437:ARG:NE	5:C:469:THR:HB	2.20	0.55
5:C:397:GLU:OE2	5:C:633:GLN:HG2	2.07	0.55
5:C:753:ASP:O	5:C:792:VAL:HG23	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1147:ARG:HB3	6:D:1188:VAL:CG2	2.37	0.55
6:D:119:SER:N	6:D:123:LEU:HD22	2.18	0.55
6:D:1495:ILE:HG22	6:D:1499:ARG:HE	1.72	0.55
4:K:150:TYR:CE2	4:K:152:PRO:HG3	2.42	0.55
4:K:161:ARG:HA	11:K:728:HOH:O	2.07	0.55
4:K:5:LYS:O	4:K:8:ALA:HB2	2.07	0.55
5:M:1022:GLY:HA3	5:M:1026:GLN:O	2.07	0.55
5:M:1098:ASP:HB2	6:N:21:TRP:CZ2	2.42	0.55
5:M:535:SER:HB3	5:M:537:LYS:HZ2	1.71	0.55
6:N:1097:LYS:O	6:N:1101:VAL:HG23	2.07	0.55
6:N:123:LEU:O	6:N:126:VAL:HB	2.07	0.55
6:N:1425:THR:HG22	6:N:1429:LEU:CD1	2.36	0.55
6:N:183:GLU:HG2	6:N:184:GLU:N	2.21	0.55
6:N:737:ASN:ND2	10:N:4999:APC:O3'	2.37	0.55
6:N:840:LYS:HE2	6:N:841:TYR:CE2	2.42	0.55
4:B:154:GLU:CD	4:B:155:LYS:HZ1	2.10	0.55
5:C:182:VAL:HG12	5:C:193:LEU:CD1	2.37	0.55
5:C:194:VAL:HG12	5:C:204:GLN:HE22	1.72	0.55
5:C:374:ASN:ND2	5:C:377:PRO:HD3	2.21	0.55
6:D:1105:ILE:HD12	6:D:1373:ARG:NH2	2.19	0.55
6:D:1266:ARG:HG2	6:D:1267:ARG:N	2.20	0.55
6:D:1389:LEU:HG	6:D:1390:LEU:HG	1.89	0.55
6:D:30:GLU:HB3	6:D:40:GLU:HB3	1.89	0.55
6:D:57:GLU:HG2	6:D:58:CYS:N	2.21	0.55
6:D:899:LEU:HD12	6:D:900:ILE:HG23	1.88	0.55
5:M:12:VAL:HB	5:M:472:ARG:NH2	2.22	0.55
5:M:139:GLN:HE21	5:M:418:LEU:HD22	1.72	0.55
5:M:239:PHE:CE1	5:M:254:VAL:HB	2.33	0.55
5:M:609:ASN:ND2	5:M:609:ASN:N	2.54	0.55
4:K:30:ARG:HH12	5:M:938:LYS:HD2	1.70	0.55
6:N:1393:GLN:HB2	6:N:1398:TRP:CZ2	2.42	0.55
6:N:1457:ASP:O	6:N:1459:LEU:HD12	2.07	0.55
6:N:696:HIS:CD2	7:O:59:ASN:HB2	2.41	0.55
4:B:181:VAL:HB	11:B:355:HOH:O	2.06	0.55
4:B:7:LYS:HG2	11:B:368:HOH:O	2.07	0.55
5:C:751:PRO:HA	5:C:792:VAL:HB	1.89	0.55
6:D:119:SER:HB2	6:D:123:LEU:CB	2.37	0.55
6:D:403:PHE:CD2	6:D:444:VAL:HG23	2.41	0.55
6:D:474:GLU:O	6:D:478:LEU:HG	2.06	0.55
6:D:618:LEU:HB3	6:D:619:LEU:HD23	1.89	0.55
6:D:630:VAL:HA	6:D:744:GLN:CG	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:12:DG:H2''	1:G:13:DT:O5'	2.06	0.55
2:H:3:G:H1'	11:C:1128:HOH:O	2.06	0.55
4:K:73:GLU:OE1	4:K:130:ALA:HA	2.06	0.55
5:M:173:ASP:O	5:M:184:MET:HA	2.06	0.55
5:M:700:TYR:CB	5:M:833:LEU:HD22	2.37	0.55
4:A:53:VAL:HG13	4:A:142:VAL:HG12	1.89	0.54
4:B:24:VAL:HG22	4:B:196:THR:HB	1.90	0.54
5:C:1:MET:CG	5:C:900:ARG:HH22	2.19	0.54
5:C:20:GLU:O	5:C:24:GLU:HG2	2.07	0.54
5:C:313:LEU:CB	5:C:321:GLU:HG3	2.37	0.54
5:C:714:ASP:HB2	5:C:818:GLY:O	2.07	0.54
6:D:1425:THR:HG21	11:D:8492:HOH:O	2.06	0.54
6:D:447:VAL:HG23	6:D:448:GLU:N	2.21	0.54
6:D:675:ARG:HA	6:D:678:GLU:CD	2.27	0.54
6:D:630:VAL:HA	6:D:744:GLN:HG2	1.89	0.54
6:D:827:ILE:HG22	6:D:837:GLY:HA2	1.88	0.54
6:D:890:VAL:HG11	6:D:922:LEU:CD1	2.37	0.54
2:H:7:G:C5'	2:H:7:G:C8	2.91	0.54
4:L:219:ARG:HB2	11:L:344:HOH:O	2.06	0.54
5:M:587:VAL:HG11	5:M:666:LEU:HD22	1.88	0.54
5:M:716:LYS:NZ	6:N:36:THR:HA	2.21	0.54
6:N:1125:PRO:C	6:N:1130:ARG:HH12	2.11	0.54
6:N:1192:LEU:HD22	6:N:1345:GLU:HG2	1.89	0.54
6:N:1263:PHE:O	6:N:1424:VAL:HG12	2.07	0.54
6:N:1500:LYS:HB3	11:N:9412:HOH:O	2.07	0.54
6:N:482:LYS:HB2	6:N:1388:ARG:NH2	2.21	0.54
6:N:520:LEU:CD1	6:N:521:PRO:HD2	2.35	0.54
6:N:584:ASN:CG	6:N:590:PRO:HD2	2.27	0.54
7:O:13:VAL:HG11	7:O:18:ARG:HB3	1.89	0.54
2:Y:7:G:H8	2:Y:7:G:O5'	1.90	0.54
5:C:1032:PHE:O	5:C:1033:GLY:O	2.26	0.54
5:C:814:GLU:HB3	11:C:1562:HOH:O	2.06	0.54
5:C:842:ARG:HH21	5:C:993:PHE:HB3	1.73	0.54
6:D:1087:ARG:HD2	6:D:1256:LEU:HD22	1.89	0.54
6:D:445:ARG:HG2	6:D:445:ARG:HH11	1.71	0.54
6:D:115:LEU:HD13	6:D:502:PHE:CD1	2.42	0.54
6:D:967:ALA:HA	11:D:8411:HOH:O	2.06	0.54
5:M:244:PRO:CD	5:M:245:GLY:H	2.20	0.54
5:M:15:LEU:HG	5:M:458:TYR:CE1	2.43	0.54
5:M:607:ASP:HB2	5:M:610:ARG:O	2.06	0.54
5:M:666:LEU:HD11	5:M:668:LEU:HD21	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:171:LEU:HD21	6:N:192:ALA:CB	2.37	0.54
6:N:141:ILE:HD13	6:N:450:TYR:O	2.07	0.54
4:A:83:LYS:HZ3	4:A:168:ASP:HB2	1.72	0.54
5:C:1046:ALA:HB2	6:D:1476:THR:H	1.72	0.54
5:C:200:LEU:HD13	5:C:300:ASP:CG	2.27	0.54
5:C:367:LEU:O	5:C:371:LYS:HB3	2.06	0.54
5:C:413:LEU:HD11	5:C:452:ILE:HD11	1.89	0.54
5:C:508:ILE:HG13	5:C:526:PRO:HB3	1.89	0.54
5:C:526:PRO:HG2	11:C:1239:HOH:O	2.06	0.54
5:C:715:THR:HG22	5:C:717:LEU:HG	1.90	0.54
6:D:119:SER:HB2	6:D:123:LEU:HD13	1.88	0.54
6:D:133:ILE:HG12	6:D:153:LEU:O	2.07	0.54
6:D:165:LYS:HD3	6:D:448:GLU:CD	2.27	0.54
6:D:685:ASP:HA	6:D:688:TRP:CD1	2.41	0.54
4:K:152:PRO:HB3	4:K:154:GLU:OE2	2.07	0.54
4:L:59:GLU:CG	4:L:139:ASN:HD22	2.20	0.54
5:M:1060:ILE:HG23	5:M:1061:GLU:H	1.73	0.54
5:M:250:ARG:HG2	5:M:253:ALA:HB3	1.90	0.54
5:M:674:VAL:HG12	5:M:990:GLY:O	2.07	0.54
5:M:851:LYS:HE2	5:M:852:ILE:O	2.08	0.54
6:N:111:LYS:HG2	6:N:1452:ILE:HD11	1.89	0.54
6:N:1120:VAL:O	6:N:1185:GLU:HA	2.08	0.54
6:N:98:PRO:C	6:N:458:ALA:HB3	2.27	0.54
4:A:149:GLY:O	4:A:171:PHE:HB2	2.08	0.54
5:C:1060:ILE:HG23	5:C:1061:GLU:N	2.23	0.54
5:C:12:VAL:HG12	5:C:534:VAL:HG13	1.89	0.54
5:C:198:ARG:HH11	5:C:204:GLN:HG2	1.71	0.54
5:C:289:THR:O	5:C:291:ALA:N	2.40	0.54
5:C:292:ARG:HD2	5:C:299:LYS:HE2	1.90	0.54
5:C:432:ARG:HH22	6:D:1053:PHE:HZ	1.55	0.54
6:D:137:PRO:HD2	6:D:453:ASP:OD2	2.07	0.54
6:D:204:LEU:HD12	6:D:396:VAL:HB	1.88	0.54
6:D:971:LEU:HG	6:D:972:LEU:HD22	1.89	0.54
4:L:54:THR:HG22	4:L:158:ILE:HG13	1.89	0.54
4:L:81:ASN:ND2	4:L:127:LEU:HD11	2.22	0.54
5:M:1008:ARG:NH2	5:M:1012:PRO:O	2.41	0.54
5:M:598:GLU:HG3	5:M:623:TYR:OH	2.08	0.54
5:M:983:ILE:HG21	5:M:987:ILE:CD1	2.37	0.54
6:N:28:LYS:HB3	6:N:41:ARG:HD2	1.89	0.54
7:O:28:GLN:CB	7:O:32:ARG:HH22	2.21	0.54
7:O:51:LEU:CD2	7:O:52:GLU:H	2.19	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:5:C:H5'	5:M:764:GLU:OE2	2.06	0.54
4:B:99:LEU:HD13	4:B:144:VAL:HG21	1.90	0.54
5:C:897:LEU:O	5:C:899:GLN:HG2	2.08	0.54
6:D:1485:GLN:NE2	7:E:79:LEU:N	2.55	0.54
6:D:38:LYS:HG2	6:D:39:PRO:CD	2.37	0.54
6:D:622:ARG:HD2	11:D:8134:HOH:O	2.07	0.54
6:D:731:LEU:CD1	6:D:931:LEU:HB3	2.37	0.54
5:M:1008:ARG:NH1	5:M:1011:GLY:N	2.56	0.54
5:M:1060:ILE:HD12	5:M:1064:ASN:HD21	1.72	0.54
5:M:1067:TYR:CZ	5:M:1071:ILE:HD11	2.43	0.54
5:M:554:ASP:HB3	5:M:880:MET:HB2	1.87	0.54
6:N:1054:GLU:HB3	11:N:9098:HOH:O	2.07	0.54
6:N:1192:LEU:HD21	6:N:1372:VAL:HG13	1.89	0.54
6:N:1255:GLY:O	6:N:1259:VAL:HG23	2.08	0.54
5:M:1085:PHE:HE2	6:N:1468:LEU:HG	1.72	0.54
6:N:132:TYR:O	6:N:456:MET:HB3	2.06	0.54
6:N:462:GLN:CB	6:N:513:ILE:HD13	2.37	0.54
11:N:9184:HOH:O	7:O:80:VAL:HG21	2.08	0.54
4:B:33:GLY:O	4:B:195:LEU:HD13	2.08	0.54
5:C:16:PRO:HD2	5:C:458:TYR:HA	1.89	0.54
5:C:182:VAL:HG21	5:C:220:GLY:C	2.28	0.54
5:C:310:LEU:O	5:C:314:THR:HG23	2.07	0.54
5:C:479:VAL:HG23	11:C:1232:HOH:O	2.08	0.54
5:C:607:ASP:HB3	5:C:610:ARG:H	1.71	0.54
5:C:806:LEU:CD1	5:C:813:VAL:HG21	2.37	0.54
5:C:869:VAL:HA	11:C:1453:HOH:O	2.08	0.54
6:D:1373:ARG:HE	6:D:1374:GLN:HE21	1.56	0.54
6:D:135:LEU:HD13	6:D:148:GLU:HB2	1.89	0.54
6:D:203:ALA:HB1	11:D:8118:HOH:O	2.06	0.54
6:D:394:LEU:H	6:D:394:LEU:HD23	1.73	0.54
6:D:989:TYR:O	6:D:993:LEU:HG	2.08	0.54
4:L:92:PRO:HA	4:L:146:ARG:NH1	2.23	0.54
5:M:132:ALA:HB1	5:M:632:ASN:ND2	2.20	0.54
5:M:164:PRO:HB2	11:M:1226:HOH:O	2.07	0.54
5:M:89:THR:HG21	5:M:383:ARG:NH2	2.23	0.54
5:M:332:ARG:HA	5:M:465:GLY:O	2.07	0.54
5:M:943:VAL:HG11	5:M:973:VAL:HG21	1.90	0.54
6:N:141:ILE:H	6:N:141:ILE:HD12	1.73	0.54
6:N:754:PHE:HE2	6:N:1476:THR:HG21	1.72	0.54
4:A:115:LEU:HD22	11:A:317:HOH:O	2.07	0.54
4:A:6:LEU:HD11	11:A:387:HOH:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:577:PRO:HA	5:C:671:ASN:HD21	1.71	0.54
5:C:861:LEU:HD12	5:C:865:THR:HG23	1.88	0.54
6:D:133:ILE:CG2	6:D:454:ALA:HB1	2.37	0.54
6:D:62:LYS:HD2	6:D:75:ARG:HD2	1.90	0.54
6:D:685:ASP:HA	6:D:688:TRP:NE1	2.22	0.54
5:M:248:PRO:HA	11:M:1493:HOH:O	2.07	0.54
5:M:304:LEU:CD2	5:M:305:PRO:HD3	2.29	0.54
5:M:461:VAL:HA	11:M:1287:HOH:O	2.07	0.54
5:M:837:ASP:O	5:M:848:VAL:HG13	2.06	0.54
6:N:1246:VAL:HB	11:N:9392:HOH:O	2.07	0.54
7:O:41:GLU:HG2	7:O:42:PRO:CD	2.37	0.54
4:A:101:LEU:HB3	4:A:114:PHE:CD2	2.43	0.54
4:A:24:VAL:HG13	4:A:196:THR:HG22	1.89	0.54
5:C:496:ILE:HD12	5:C:496:ILE:N	2.23	0.54
5:C:833:LEU:HD11	5:C:839:LEU:HD21	1.89	0.54
5:C:668:LEU:O	5:C:995:MET:HB3	2.08	0.54
6:D:111:LYS:HG2	6:D:1452:ILE:HD11	1.90	0.54
6:D:165:LYS:HA	6:D:199:LEU:CD1	2.38	0.54
6:D:470:LEU:H	6:D:470:LEU:HD23	1.73	0.54
5:C:1017:THR:HB	6:D:613:ARG:NH2	2.22	0.54
11:B:382:HOH:O	6:D:685:ASP:HB3	2.08	0.54
6:D:708:LEU:HB3	6:D:1231:GLU:CB	2.35	0.54
6:D:926:LYS:HA	6:D:929:ARG:HD2	1.88	0.54
7:E:47:LYS:HA	7:E:54:LEU:HB3	1.88	0.54
4:K:14:ARG:HH22	4:K:24:VAL:HG23	1.73	0.54
4:L:159:LYS:HB2	11:L:316:HOH:O	2.08	0.54
5:M:1097:LEU:HD22	5:M:1097:LEU:N	2.13	0.54
6:N:90:MET:HE1	6:N:518:PRO:HB2	1.89	0.54
6:N:583:ASP:OD1	6:N:586:ARG:HG3	2.07	0.54
5:C:1101:THR:OG1	5:C:1109:VAL:HB	2.08	0.54
5:C:100:LEU:HD22	5:C:372:LEU:CD2	2.38	0.54
5:C:397:GLU:OE1	5:C:631:SER:HB2	2.08	0.54
6:D:1209:LEU:HD21	7:E:16:LYS:HZ1	1.73	0.54
6:D:471:GLU:O	6:D:474:GLU:HB3	2.08	0.54
6:D:799:LYS:O	6:D:829:VAL:HG22	2.08	0.54
5:M:620:LEU:H	5:M:620:LEU:HD12	1.72	0.54
6:N:776:GLU:HB3	6:N:912:LYS:HE2	1.90	0.54
4:A:91:ASN:ND2	4:A:93:SER:H	2.06	0.54
4:A:42:ARG:HH12	4:B:34:VAL:HG11	1.72	0.54
5:C:684:PHE:N	5:C:687:ALA:HB3	2.19	0.54
6:D:1003:VAL:HG11	6:D:1041:LEU:HD23	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:565:ILE:HB	6:D:566:ILE:HD12	1.90	0.54
11:B:374:HOH:O	6:D:851:LEU:HD11	2.07	0.54
6:D:964:LEU:HD21	6:D:1058:ARG:NE	2.22	0.54
4:L:137:ARG:C	4:L:137:ARG:HD3	2.28	0.54
4:L:5:LYS:O	4:L:8:ALA:HB2	2.07	0.54
5:M:1095:LEU:HB2	5:M:1097:LEU:HD23	1.89	0.54
5:M:225:SER:HB2	11:M:1245:HOH:O	2.08	0.54
5:M:468:ARG:HE	5:M:487:THR:CA	2.21	0.54
6:N:177:ALA:HB3	6:N:205:TYR:OH	2.08	0.54
6:N:436:GLU:HB2	6:N:445:ARG:HG3	1.89	0.54
6:N:131:LYS:HZ3	6:N:568:ARG:HB2	1.72	0.54
6:N:868:TYR:HB2	6:N:873:LEU:HD12	1.89	0.54
6:N:996:TRP:HB2	11:N:9079:HOH:O	2.07	0.54
4:A:22:GLU:OE2	4:A:198:ARG:HB3	2.08	0.53
5:C:497:ALA:HA	5:C:515:ALA:HA	1.90	0.53
5:C:758:ARG:HH22	5:C:788:THR:HB	1.73	0.53
5:C:911:GLU:HB3	5:C:912:PRO:HD3	1.90	0.53
6:D:127:LEU:HD22	6:D:460:ALA:HB3	1.90	0.53
6:D:32:ILE:HB	6:D:527:MET:HE3	1.90	0.53
6:D:600:LEU:HD12	6:D:600:LEU:H	1.72	0.53
6:D:754:PHE:CG	7:E:24:ALA:HB1	2.43	0.53
6:D:53:ILE:HA	6:D:86:ARG:NE	2.23	0.53
5:M:510:ALA:HB3	5:M:513:VAL:CG2	2.37	0.53
5:M:57:GLU:O	5:M:62:GLY:HA3	2.07	0.53
6:N:1122:LEU:HB3	11:N:9164:HOH:O	2.09	0.53
6:N:1462:LEU:O	6:N:1466:VAL:HG23	2.08	0.53
6:N:478:LEU:O	6:N:1388:ARG:NH2	2.42	0.53
5:C:157:ARG:NH1	5:C:217:LEU:HD22	2.23	0.53
5:C:285:LEU:HD12	5:C:288:ARG:O	2.07	0.53
2:H:13:C:C4'	5:C:409:ARG:HH22	2.13	0.53
6:D:22:SER:CB	6:D:92:HIS:HB3	2.37	0.53
3:I:11:DC:H5	11:I:331:HOH:O	1.91	0.53
4:L:73:GLU:HB3	4:L:77:GLU:CG	2.38	0.53
5:M:259:GLY:HA3	11:M:1270:HOH:O	2.08	0.53
5:M:34:VAL:HB	5:M:38:LYS:CG	2.38	0.53
4:K:72:LYS:HD2	5:M:606:VAL:HG11	1.90	0.53
6:N:1168:MET:CE	6:N:1171:VAL:HB	2.37	0.53
6:N:1262:LEU:HD21	6:N:1351:GLU:HG3	1.91	0.53
6:N:1191:PRO:HG2	6:N:1370:ILE:CD1	2.38	0.53
6:N:168:THR:CG2	6:N:206:ARG:HH12	2.21	0.53
6:N:462:GLN:HA	6:N:513:ILE:HD13	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:875:THR:HB	6:N:880:ILE:HD11	1.90	0.53
3:Z:10:DA:H5"	6:N:121:THR:HG21	1.89	0.53
5:C:1049:LEU:CD1	5:C:1053:LEU:HD11	2.39	0.53
5:C:1054:THR:HG22	5:C:1082:PRO:HG3	1.89	0.53
5:C:1105:LYS:HZ2	5:C:1107:ASN:HD22	1.55	0.53
5:C:134:ARG:HE	5:C:392:SER:HB3	1.72	0.53
5:C:136:ILE:HG22	5:C:336:VAL:HG22	1.88	0.53
5:C:438:ILE:HG23	5:C:453:THR:OG1	2.08	0.53
5:C:462:ASP:OD1	5:C:462:ASP:N	2.41	0.53
5:C:577:PRO:HG3	5:C:993:PHE:CE1	2.42	0.53
6:D:1063:GLU:HG3	6:D:1064:GLY:N	2.24	0.53
6:D:1184:GLN:HB2	6:N:559:ALA:HA	1.90	0.53
6:D:126:VAL:HG21	11:D:8125:HOH:O	2.07	0.53
6:D:955:VAL:HG11	6:D:1015:TYR:CE2	2.42	0.53
1:G:17:DC:H2"	1:G:18:DG:C5'	2.36	0.53
4:K:171:PHE:O	4:K:173:PRO:HD3	2.08	0.53
4:L:201:THR:HG21	4:L:205:VAL:HG23	1.90	0.53
4:L:94:LEU:HD11	4:L:119:ASP:HB3	1.91	0.53
5:M:512:ARG:HD3	5:M:523:ILE:HD11	1.90	0.53
6:N:1114:THR:CG2	6:N:1195:GLN:HB3	2.38	0.53
6:N:394:LEU:HG	6:N:396:VAL:CG2	2.38	0.53
6:N:473:LEU:O	6:N:477:LEU:HG	2.08	0.53
6:N:619:LEU:HD23	6:N:619:LEU:N	2.23	0.53
6:N:817:GLU:O	6:N:821:VAL:HG23	2.08	0.53
7:O:91:ARG:HG2	11:O:2238:HOH:O	2.08	0.53
4:A:62:LEU:HD13	11:A:334:HOH:O	2.08	0.53
4:B:5:LYS:O	4:B:8:ALA:HB2	2.08	0.53
5:C:274:ARG:HB2	5:C:285:LEU:CD1	2.38	0.53
6:D:1010:ASN:ND2	11:D:8083:HOH:O	2.41	0.53
6:D:781:PRO:O	6:D:786:ILE:HD11	2.07	0.53
6:D:957:PRO:HG2	6:D:1007:VAL:HA	1.89	0.53
5:M:1045:ALA:HB1	5:M:1048:THR:HB	1.90	0.53
5:M:205:GLU:HB2	11:M:1398:HOH:O	2.07	0.53
5:M:334:ARG:O	5:M:339:LEU:HD11	2.09	0.53
5:M:344:PHE:HE2	5:M:378:LEU:HD21	1.74	0.53
5:M:642:ARG:HD2	11:M:1230:HOH:O	2.08	0.53
6:N:1078:ARG:HH11	6:N:1078:ARG:HG3	1.72	0.53
6:N:878:GLY:HA2	6:N:881:LEU:HD23	1.90	0.53
6:N:95:LEU:HD13	6:N:515:GLU:C	2.28	0.53
4:A:102:LYS:NZ	4:A:139:ASN:HD21	2.06	0.53
4:A:159:LYS:HZ1	4:A:166:PRO:HD3	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:175:ARG:CZ	4:A:176:ARG:HD3	2.37	0.53
4:B:159:LYS:N	4:B:159:LYS:HD3	2.24	0.53
5:C:167:LYS:HE3	11:C:1598:HOH:O	2.08	0.53
5:C:309:TYR:HA	5:C:312:ALA:HB3	1.90	0.53
5:C:872:ASN:ND2	5:C:874:LEU:H	2.06	0.53
5:C:905:ILE:HG22	5:C:906:PHE:N	2.23	0.53
6:D:1376:MET:HE1	6:D:1421:LEU:HD22	1.90	0.53
6:D:152:LEU:HD11	11:D:8125:HOH:O	2.09	0.53
6:D:191:LEU:HD11	6:D:395:VAL:CG2	2.38	0.53
6:D:643:GLY:O	6:D:726:ILE:HG23	2.08	0.53
6:D:758:GLU:O	6:D:762:GLN:HG2	2.08	0.53
4:K:176:ARG:HG3	4:K:200:TRP:CE3	2.44	0.53
4:K:20:TYR:HD2	4:K:21:GLY:N	2.07	0.53
4:K:57:TYR:CZ	4:K:59:GLU:HA	2.43	0.53
4:K:9:PRO:HB3	4:K:25:LEU:CG	2.38	0.53
4:L:121:GLU:OE2	4:L:123:MET:HG2	2.09	0.53
4:L:58:ILE:HB	4:L:61:VAL:CG1	2.39	0.53
5:M:1019:GLN:HG2	5:M:1058:ASP:OD1	2.08	0.53
5:M:140:ILE:HD11	5:M:412:ALA:HB2	1.91	0.53
5:M:224:GLU:HB2	5:M:227:PHE:CD1	2.44	0.53
6:N:1148:VAL:HG13	6:N:1163:GLY:HA2	1.90	0.53
6:N:1231:GLU:HB3	6:N:1232:PRO:CD	2.38	0.53
1:X:17:DC:H4'	6:N:628:ARG:CD	2.38	0.53
6:N:800:LYS:HZ1	6:N:804:LEU:HD22	1.73	0.53
6:N:814:ALA:HB1	6:N:818:ARG:NH2	2.24	0.53
6:N:769:LEU:HD11	6:N:919:PHE:CZ	2.43	0.53
6:N:886:VAL:HG13	6:N:930:LEU:HD11	1.89	0.53
5:C:1006:HIS:HA	5:C:1027:PHE:CD1	2.43	0.53
6:D:806:PHE:HE1	6:D:813:LEU:HD23	1.72	0.53
6:D:864:VAL:HG12	6:D:865:THR:H	1.74	0.53
4:K:20:TYR:HD2	4:K:21:GLY:H	1.55	0.53
5:M:532:MET:HG2	5:M:533:ASP:O	2.08	0.53
11:K:1782:HOH:O	5:M:640:ARG:HG2	2.08	0.53
6:N:1112:CYS:SG	6:N:1195:GLN:HG2	2.49	0.53
6:N:700:VAL:HG22	6:N:718:PRO:HG3	1.91	0.53
6:N:996:TRP:CA	6:N:999:THR:HG22	2.29	0.53
1:X:22:DC:H4'	5:M:388:ARG:HG3	1.90	0.53
4:B:99:LEU:HD13	4:B:144:VAL:CG2	2.39	0.53
5:C:218:VAL:HG23	5:C:311:PHE:HE1	1.72	0.53
5:C:257:VAL:HG21	11:C:1481:HOH:O	2.08	0.53
5:C:329:GLY:HA3	5:C:489:THR:HG23	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:326:ASP:CB	5:C:431:HIS:HB2	2.37	0.53
6:D:1041:LEU:HD12	6:D:1058:ARG:HA	1.90	0.53
6:D:1221:VAL:HG12	6:D:1222:GLY:N	2.24	0.53
6:D:132:TYR:C	6:D:133:ILE:HD13	2.29	0.53
6:D:960:LYS:HE2	6:D:1041:LEU:HD22	1.91	0.53
7:E:25:LYS:HA	7:E:28:GLN:HE21	1.74	0.53
4:L:33:GLY:O	4:L:195:LEU:HD22	2.09	0.53
5:M:463:GLU:HB3	11:M:1525:HOH:O	2.09	0.53
5:M:515:ALA:HB3	5:M:524:VAL:CG2	2.39	0.53
6:N:679:ARG:HB2	6:N:682:ASP:CG	2.29	0.53
4:B:50:GLY:HA3	4:B:171:PHE:O	2.08	0.53
5:C:217:LEU:HD23	5:C:217:LEU:N	2.24	0.53
6:D:43:GLY:N	11:D:8160:HOH:O	2.41	0.53
6:D:592:THR:H	6:D:600:LEU:HD11	1.74	0.53
6:D:995:LEU:HD11	11:D:8411:HOH:O	2.08	0.53
7:E:18:ARG:HD3	11:E:116:HOH:O	2.09	0.53
2:Y:7:G:O6	5:M:1015:LEU:HB2	2.09	0.53
5:M:769:PRO:HG2	6:N:65:ARG:HD3	1.90	0.53
6:N:1271:LYS:HZ1	6:N:1331:ASP:HB2	1.72	0.53
5:C:305:PRO:HA	5:C:308:ARG:HB3	1.90	0.53
5:C:545:ASN:OD1	5:C:583:LEU:HD13	2.08	0.53
5:C:679:PHE:C	6:D:943:THR:HG22	2.29	0.53
5:C:881:ASN:HD22	5:C:881:ASN:H	1.55	0.53
6:D:1258:ARG:HG2	11:D:8324:HOH:O	2.09	0.53
6:D:1435:LEU:HD23	6:D:1467:ILE:HD12	1.91	0.53
6:D:181:ASP:O	6:D:204:LEU:HA	2.08	0.53
6:D:161:LEU:HD22	6:D:452:ILE:HD13	1.91	0.53
4:K:47:SER:HB3	4:K:217:ILE:HD13	1.90	0.53
4:K:218:LEU:HG	11:K:1711:HOH:O	2.09	0.53
5:M:142:ARG:HA	5:M:330:ASN:O	2.09	0.53
5:M:549:PHE:CG	5:M:886:LEU:HD23	2.43	0.53
5:M:644:VAL:HG22	5:M:647:GLN:OE1	2.08	0.53
6:N:1128:VAL:O	6:N:1129:THR:C	2.47	0.53
6:N:1200:VAL:HG22	6:N:1373:ARG:HH12	1.73	0.53
6:N:808:THR:OG1	6:N:809:PRO:HD3	2.09	0.53
7:O:73:LEU:HD12	7:O:73:LEU:N	2.24	0.53
4:B:206:THR:CG2	4:B:209:GLU:H	2.20	0.53
5:C:195:LEU:HG	5:C:238:LEU:CD1	2.38	0.53
5:C:442:GLU:HA	11:C:1416:HOH:O	2.08	0.53
5:C:798:GLY:HA3	5:C:828:ALA:O	2.09	0.53
5:C:957:LYS:HD3	5:C:961:GLU:OE1	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1037:GLN:OE1	6:D:1042:ARG:HD3	2.09	0.53
6:D:1176:LYS:HA	6:D:1179:GLU:OE1	2.09	0.53
6:D:1441:GLN:NE2	6:D:1442:ASN:HB2	2.25	0.53
6:D:695:ILE:HG21	6:D:720:LEU:HD11	1.89	0.53
6:D:827:ILE:O	6:D:837:GLY:HA3	2.09	0.53
6:D:971:LEU:HG	6:D:972:LEU:N	2.22	0.53
4:K:100:LEU:HG	4:K:101:LEU:N	2.22	0.53
4:K:49:PRO:HG3	11:K:867:HOH:O	2.09	0.53
4:L:10:VAL:HG23	4:L:26:GLU:O	2.09	0.53
5:M:1101:THR:HG21	5:M:1111:ILE:CG2	2.38	0.53
5:M:1101:THR:OG1	5:M:1109:VAL:HB	2.08	0.53
5:M:172:ILE:H	5:M:172:ILE:HD12	1.73	0.53
5:M:264:PRO:HB3	5:M:289:THR:HB	1.90	0.53
5:M:264:PRO:HB3	5:M:289:THR:CB	2.38	0.53
5:M:394:PHE:HD1	5:M:633:GLN:HE22	1.56	0.53
5:M:759:THR:HB	5:M:785:VAL:HG13	1.90	0.53
6:N:1086:LEU:HB2	6:N:1087:ARG:NH1	2.23	0.53
6:N:482:LYS:HB2	6:N:1388:ARG:HH21	1.73	0.53
6:N:792:ILE:HG13	6:N:881:LEU:HD21	1.91	0.53
1:X:12:DG:H2''	1:X:13:DT:H5'	1.90	0.53
4:A:186:LEU:HB3	4:A:192:LEU:CD1	2.39	0.52
4:B:28:LEU:HG	4:B:193:ASP:O	2.08	0.52
1:G:20:DG:H4'	5:C:394:PHE:CZ	2.44	0.52
5:C:443:THR:HA	5:C:452:ILE:O	2.09	0.52
5:C:1:MET:HG2	5:C:900:ARG:NH2	2.23	0.52
6:D:1269:LYS:NZ	6:D:1269:LYS:HB3	2.24	0.52
6:D:1465:ASN:ND2	6:D:1470:ARG:HE	2.05	0.52
5:C:1031:ARG:HH21	6:D:621:LYS:HG3	1.73	0.52
4:L:37:GLY:HA3	4:L:179:PHE:CD1	2.45	0.52
5:M:1008:ARG:HB2	5:M:1027:PHE:HB2	1.91	0.52
5:M:367:LEU:HB3	5:M:371:LYS:HG2	1.90	0.52
5:M:69:LEU:HB2	5:M:97:ARG:HB2	1.91	0.52
5:M:821:GLU:HB3	11:M:1453:HOH:O	2.08	0.52
5:M:953:VAL:HG22	5:M:966:LEU:HD11	1.90	0.52
6:N:1058:ARG:HG2	11:N:9214:HOH:O	2.08	0.52
11:Z:1999:HOH:O	6:N:1426:LYS:HG3	2.08	0.52
6:N:1503:VAL:HG21	11:N:9060:HOH:O	2.07	0.52
6:N:166:GLN:HG2	6:N:396:VAL:HG13	1.91	0.52
6:N:496:LEU:CD1	6:N:500:ARG:HG2	2.39	0.52
6:N:705:ALA:CB	6:N:706:PRO:HD3	2.39	0.52
5:M:949:LYS:HD3	6:N:796:ARG:HH22	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:882:PHE:O	6:N:886:VAL:HG23	2.08	0.52
5:C:1105:LYS:O	5:C:1107:ASN:N	2.42	0.52
5:C:251:ASP:HB3	5:C:252:LYS:HD2	1.91	0.52
5:C:260:LEU:HG	5:C:261:ILE:HG13	1.91	0.52
5:C:143:SER:HB2	5:C:276:LYS:NZ	2.24	0.52
6:D:610:LYS:HA	6:D:615:ARG:CD	2.39	0.52
7:E:32:ARG:HB2	7:E:32:ARG:HH11	1.74	0.52
4:L:43:ILE:HG21	4:L:214:ALA:HA	1.91	0.52
5:M:89:THR:HA	5:M:129:ILE:O	2.08	0.52
5:M:134:ARG:HH11	5:M:392:SER:HB3	1.74	0.52
5:M:260:LEU:CB	5:M:291:ALA:HB1	2.36	0.52
5:M:305:PRO:HA	5:M:308:ARG:HB3	1.91	0.52
5:M:456:ALA:HB1	5:M:538:GLN:O	2.09	0.52
4:K:70:GLY:H	5:M:607:ASP:CG	2.12	0.52
5:M:74:GLY:O	5:M:76:PRO:HD3	2.09	0.52
6:N:1053:PHE:CE1	6:N:1072:ILE:HD12	2.44	0.52
6:N:1236:LEU:HD11	6:N:1361:VAL:HG23	1.90	0.52
6:N:204:LEU:HD13	6:N:445:ARG:HE	1.72	0.52
6:N:520:LEU:HG	6:N:521:PRO:N	2.24	0.52
6:D:1081:GLY:HA2	6:D:1241:PHE:CD1	2.45	0.52
6:D:426:LYS:CE	6:D:427:VAL:HG23	2.40	0.52
6:D:975:GLU:OE1	6:D:975:GLU:HA	2.08	0.52
2:H:8:C:H6	2:H:8:C:O5'	1.92	0.52
4:K:163:ASN:HA	11:K:2179:HOH:O	2.10	0.52
4:K:180:GLN:HA	5:M:937:ASP:OD1	2.08	0.52
4:L:7:LYS:HE3	4:L:186:LEU:HD13	1.90	0.52
5:M:1092:LEU:HA	5:M:1095:LEU:CD1	2.39	0.52
5:M:218:VAL:HG22	5:M:221:LEU:CD2	2.39	0.52
5:M:432:ARG:NH2	6:N:1047:LYS:HD3	2.22	0.52
6:N:496:LEU:O	6:N:496:LEU:HD12	2.09	0.52
6:N:104:PHE:HD1	6:N:512:MET:HG2	1.74	0.52
6:N:789:LEU:O	6:N:793:THR:HG23	2.08	0.52
6:N:899:LEU:HD12	6:N:900:ILE:HG23	1.91	0.52
7:O:80:VAL:HG13	11:O:1385:HOH:O	2.09	0.52
4:B:12:THR:OG1	4:B:24:VAL:HB	2.10	0.52
4:B:43:ILE:HG23	4:B:47:SER:CB	2.40	0.52
5:C:1105:LYS:HD2	5:C:1107:ASN:ND2	2.25	0.52
5:C:110:GLU:HG3	5:C:369:PRO:HB3	1.92	0.52
5:C:230:ARG:HG2	5:C:230:ARG:HH11	1.73	0.52
5:C:290:LEU:HB3	5:C:302:VAL:CG1	2.39	0.52
5:C:487:THR:HB	5:C:490:GLU:HG3	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1248:GLY:HA2	6:D:1251:ASP:OD2	2.09	0.52
6:D:202:VAL:HG11	6:D:400:VAL:HG12	1.91	0.52
6:D:434:ARG:HB2	6:D:447:VAL:CG2	2.40	0.52
6:D:557:LEU:HD11	11:D:8469:HOH:O	2.08	0.52
6:D:628:ARG:HB2	11:D:8067:HOH:O	2.08	0.52
6:D:64:LYS:HD2	11:D:8441:HOH:O	2.09	0.52
4:L:43:ILE:HG23	4:L:47:SER:CB	2.39	0.52
5:M:1001:VAL:HG22	11:M:1555:HOH:O	2.09	0.52
2:Y:7:G:H22	5:M:1014:SER:CA	2.23	0.52
5:M:1105:LYS:O	5:M:1107:ASN:N	2.42	0.52
5:M:674:VAL:HG23	5:M:869:VAL:HG13	1.92	0.52
5:M:690:ILE:HD11	5:M:833:LEU:HD23	1.91	0.52
5:M:807:ARG:N	5:M:807:ARG:HE	2.05	0.52
5:M:850:ALA:HA	6:N:632:VAL:HG11	1.92	0.52
5:M:860:HIS:CE1	5:M:975:TYR:HB2	2.45	0.52
6:N:1118:ILE:HD12	11:N:9016:HOH:O	2.09	0.52
6:N:119:SER:CB	6:N:123:LEU:HB2	2.38	0.52
6:N:1121:PRO:CD	6:N:1346:ARG:HE	2.22	0.52
6:N:192:ALA:HB1	6:N:193:PRO:HD2	1.92	0.52
6:N:584:ASN:HD22	6:N:585:GLY:N	2.08	0.52
6:N:644:LEU:HD12	6:N:645:PRO:HD2	1.91	0.52
4:A:190:THR:HA	11:A:369:HOH:O	2.08	0.52
5:C:1062:GLY:HA2	11:C:1284:HOH:O	2.10	0.52
5:C:173:ASP:O	5:C:184:MET:HA	2.09	0.52
5:C:327:HIS:HA	5:C:431:HIS:CD2	2.44	0.52
5:C:538:GLN:HG3	5:C:539:VAL:N	2.24	0.52
5:C:559:LEU:HD23	5:C:563:ASN:OD1	2.10	0.52
5:C:816:LYS:HZ3	5:C:816:LYS:H	1.57	0.52
6:D:1118:ILE:HD11	11:D:8142:HOH:O	2.09	0.52
6:D:1112:CYS:CB	6:D:1195:GLN:HG2	2.29	0.52
6:D:1232:PRO:HA	6:D:1235:GLN:OE1	2.10	0.52
6:D:52:PRO:CG	6:D:80:VAL:HG13	2.39	0.52
6:D:600:LEU:HD12	6:D:600:LEU:N	2.25	0.52
6:D:820:GLU:HB2	6:D:836:VAL:HG11	1.92	0.52
6:D:95:LEU:HB3	6:D:515:GLU:O	2.09	0.52
6:D:989:TYR:CE1	6:D:993:LEU:HD21	2.44	0.52
4:L:27:PRO:HB3	4:L:192:LEU:HD22	1.91	0.52
5:M:328:LEU:HD13	5:M:433:THR:HB	1.90	0.52
5:M:470:PRO:HB2	5:M:534:VAL:HG21	1.92	0.52
5:M:5:ARG:HE	5:M:8:ARG:NH2	2.02	0.52
5:M:684:PHE:N	5:M:687:ALA:HB3	2.21	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:754:ILE:HG12	5:M:791:ARG:NH1	2.25	0.52
5:M:839:LEU:HD23	5:M:996:LYS:HA	1.92	0.52
6:N:109:PRO:HB3	6:N:494:LYS:NZ	2.25	0.52
6:N:1165:TYR:OH	6:N:1202:GLN:HG2	2.09	0.52
6:N:44:LEU:H	6:N:44:LEU:HD12	1.75	0.52
6:D:1184:GLN:HB2	6:N:559:ALA:CB	2.39	0.52
6:N:568:ARG:O	6:N:572:ARG:HG3	2.08	0.52
6:N:654:LYS:HB3	6:N:655:PRO:HD3	1.91	0.52
5:M:1071:ILE:O	6:N:659:LYS:HD3	2.09	0.52
6:N:787:LEU:CD1	6:N:1023:MET:HA	2.39	0.52
6:N:832:ARG:HB3	6:N:833:GLU:OE1	2.09	0.52
1:X:13:DT:OP1	6:N:1093:TYR:HE2	1.93	0.52
5:C:258:TYR:HB3	11:C:1335:HOH:O	2.08	0.52
6:D:142:LEU:CD2	6:D:146:PRO:HA	2.40	0.52
6:D:660:LYS:HD2	6:D:694:VAL:CG2	2.40	0.52
6:D:834:THR:HA	6:D:838:ARG:NH1	2.24	0.52
7:E:45:ARG:HG2	11:E:129:HOH:O	2.09	0.52
4:K:64:GLU:HA	4:K:165:ILE:HD13	1.91	0.52
4:L:109:VAL:O	4:L:129:ILE:HG12	2.09	0.52
5:M:1009:SER:OG	6:N:654:LYS:HD2	2.09	0.52
5:M:218:VAL:O	5:M:221:LEU:HG	2.10	0.52
5:M:18:LEU:HD22	5:M:404:LEU:HD21	1.91	0.52
5:M:516:ARG:NH2	6:N:1068:LEU:HB3	2.25	0.52
5:M:5:ARG:CZ	5:M:8:ARG:HH12	2.22	0.52
5:M:971:LYS:HG2	5:M:988:VAL:CB	2.40	0.52
6:N:1034:GLN:NE2	6:N:1243:THR:HB	2.25	0.52
6:N:1045:MET:HE2	6:N:1073:SER:CB	2.35	0.52
6:N:1440:PHE:O	6:N:1441:GLN:O	2.28	0.52
7:O:36:LYS:HA	7:O:36:LYS:HE2	1.90	0.52
4:A:14:ARG:HH22	4:A:24:VAL:CG2	2.23	0.52
5:C:22:GLN:C	5:C:121:MET:HE1	2.30	0.52
5:C:39:ARG:H	5:C:39:ARG:CD	2.03	0.52
5:C:13:ILE:HD11	5:C:483:VAL:HG21	1.92	0.52
5:C:9:ILE:HD12	5:C:9:ILE:H	1.75	0.52
6:D:615:ARG:HH22	6:D:1096:ARG:CD	2.22	0.52
6:D:1498:ALA:HB1	7:E:84:ARG:NH2	2.25	0.52
6:D:82:LYS:HD2	11:D:8499:HOH:O	2.08	0.52
7:E:48:MET:CB	7:E:54:LEU:HB2	2.39	0.52
4:K:73:GLU:CD	4:K:130:ALA:HA	2.30	0.52
4:L:206:THR:HG23	4:L:208:LEU:H	1.73	0.52
4:K:8:ALA:HB1	4:L:224:TYR:CE1	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:1008:ARG:HH12	5:M:1011:GLY:H	1.58	0.52
5:M:1019:GLN:HE22	6:N:616:GLN:HE22	1.58	0.52
5:M:589:ARG:HH11	5:M:589:ARG:HB2	1.73	0.52
5:M:757:GLY:HA2	5:M:789:SER:OG	2.10	0.52
6:N:1492:LEU:HD12	6:N:1493:LYS:HZ1	1.73	0.52
1:X:12:DG:H2"	1:X:13:DT:C5'	2.40	0.52
4:A:178:ALA:HB3	4:A:198:ARG:CG	2.37	0.52
4:A:222:LEU:HD13	4:B:218:LEU:HD23	1.90	0.52
5:C:65:VAL:CG2	5:C:101:ILE:HB	2.40	0.52
5:C:564:MET:SD	5:C:995:MET:HG3	2.50	0.52
5:C:748:GLU:CB	5:C:799:ILE:HD12	2.39	0.52
5:C:859:PRO:O	5:C:867:VAL:HG22	2.09	0.52
5:C:983:ILE:HB	11:C:1149:HOH:O	2.10	0.52
6:D:684:LYS:HD3	6:D:686:GLU:OE1	2.10	0.52
5:M:1032:PHE:HZ	5:M:1040:LEU:HD13	1.74	0.52
5:M:157:ARG:HG2	11:M:1381:HOH:O	2.09	0.52
5:M:352:ALA:HA	5:M:355:VAL:CG1	2.39	0.52
5:M:91:GLN:NE2	5:M:383:ARG:NH2	2.57	0.52
6:N:141:ILE:HD12	6:N:141:ILE:N	2.25	0.52
6:N:452:ILE:HG22	11:N:9064:HOH:O	2.10	0.52
6:N:610:LYS:HG3	11:N:9272:HOH:O	2.09	0.52
6:N:619:LEU:HD12	6:N:621:LYS:NZ	2.25	0.52
6:N:756:GLN:NE2	6:N:760:ARG:HD2	2.24	0.52
5:C:102:HIS:HB2	5:C:106:GLY:O	2.10	0.52
5:C:774:LEU:HD23	5:C:775:ARG:N	2.25	0.52
5:C:996:LYS:HE3	11:C:1151:HOH:O	2.10	0.52
6:D:543:LEU:O	6:D:546:ARG:HB2	2.10	0.52
6:D:651:GLU:HA	6:D:654:LYS:HZ2	1.73	0.52
6:D:731:LEU:HD13	6:D:931:LEU:HB3	1.91	0.52
4:K:156:HIS:CD2	4:K:157:GLY:N	2.77	0.52
4:L:216:GLU:HG3	4:L:220:GLU:OE1	2.10	0.52
5:M:212:GLY:HA3	5:M:218:VAL:HG21	1.91	0.52
5:M:565:GLN:OE1	5:M:842:ARG:HG2	2.10	0.52
6:N:1270:ALA:O	6:N:1329:ALA:HB3	2.09	0.52
6:N:204:LEU:HD12	6:N:396:VAL:CG2	2.40	0.52
6:N:656:PHE:HB3	6:N:694:VAL:HG11	1.92	0.52
7:O:54:LEU:HA	7:O:58:PRO:CG	2.39	0.52
4:B:124:ASN:N	4:B:125:PRO:HD3	2.23	0.52
5:C:1018:GLN:C	5:C:1019:GLN:HE21	2.14	0.52
5:C:1037:VAL:HG12	5:C:1041:GLU:OE2	2.10	0.52
5:C:20:GLU:OE2	5:C:460:ARG:NH1	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1267:ARG:NH1	6:D:1267:ARG:HB2	2.24	0.52
6:D:399:ARG:HD3	6:D:430:ASP:OD2	2.09	0.52
6:D:525:ARG:HB2	6:D:538:SER:CB	2.40	0.52
6:D:820:GLU:HA	6:D:825:ALA:O	2.10	0.52
4:K:1:MET:O	4:K:6:LEU:HD22	2.10	0.52
5:M:353:ARG:HA	11:M:1274:HOH:O	2.09	0.52
6:N:1403:LEU:O	6:N:1407:LEU:HD13	2.10	0.52
6:N:1440:PHE:CG	6:N:1441:GLN:N	2.78	0.52
6:N:616:GLN:NE2	11:N:9292:HOH:O	2.43	0.52
6:N:642:CYS:SG	6:N:716:PHE:HB2	2.50	0.52
5:M:1094:ALA:HA	6:N:90:MET:CE	2.39	0.52
7:O:67:GLU:HB3	7:O:73:LEU:HD11	1.91	0.52
4:A:163:ASN:HD21	5:C:744:ARG:NH2	2.08	0.51
4:A:67:THR:CG2	5:C:609:ASN:HD21	2.23	0.51
4:A:9:PRO:HD2	4:B:224:TYR:CE1	2.45	0.51
5:C:286:SER:HB3	5:C:299:LYS:HE3	1.92	0.51
6:D:206:ARG:CG	6:D:394:LEU:HD22	2.33	0.51
6:D:396:VAL:CG1	6:D:447:VAL:HA	2.36	0.51
5:M:1109:VAL:HA	6:N:3:LYS:HE3	1.92	0.51
5:M:576:ALA:HB3	5:M:900:ARG:HH11	1.75	0.51
5:M:557:ARG:NH1	5:M:879:ARG:HD3	2.25	0.51
6:N:1020:LEU:HD21	6:N:1035:ILE:CG2	2.40	0.51
6:N:396:VAL:CG1	6:N:447:VAL:HA	2.41	0.51
6:N:461:ILE:O	6:N:465:LEU:HB2	2.09	0.51
6:N:632:VAL:HG23	6:N:725:SER:HB2	1.92	0.51
6:N:709:HIS:CD2	6:N:709:HIS:H	2.28	0.51
6:N:95:LEU:H	6:N:95:LEU:CD1	2.20	0.51
6:N:960:LYS:HZ1	6:N:1041:LEU:HD13	1.75	0.51
4:A:138:LEU:O	4:A:138:LEU:HD23	2.10	0.51
4:A:188:GLN:HG3	4:A:189:ARG:H	1.74	0.51
5:C:144:PRO:N	5:C:276:LYS:NZ	2.58	0.51
5:C:157:ARG:HG3	5:C:314:THR:HG21	1.92	0.51
5:C:176:VAL:C	5:C:178:PRO:HD3	2.31	0.51
5:C:198:ARG:CZ	5:C:203:ASP:HA	2.39	0.51
5:C:843:HIS:CB	5:C:884:GLN:HG2	2.40	0.51
6:D:1098:LEU:CD2	6:D:1226:ALA:HA	2.38	0.51
6:D:1118:ILE:HG13	6:D:1192:LEU:HD13	1.92	0.51
6:D:831:GLY:HA3	11:D:8198:HOH:O	2.09	0.51
4:K:102:LYS:NZ	4:K:115:LEU:HD22	2.24	0.51
4:K:41:ARG:O	4:K:45:LEU:HD12	2.10	0.51
4:L:182:GLU:OE1	4:L:194:LYS:O	2.29	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:110:GLU:HG3	5:M:369:PRO:CB	2.29	0.51
5:M:97:ARG:HA	5:M:111:ASP:O	2.10	0.51
5:M:139:GLN:NE2	5:M:418:LEU:HD22	2.25	0.51
5:M:557:ARG:HD3	5:M:560:MET:SD	2.50	0.51
5:M:787:ASP:HB3	11:M:1300:HOH:O	2.09	0.51
6:N:1121:PRO:HA	6:N:1185:GLU:HG2	1.90	0.51
6:N:1248:GLY:O	6:N:1252:ILE:HG12	2.10	0.51
6:N:1267:ARG:HA	6:N:1271:LYS:HZ1	1.75	0.51
6:N:1496:GLU:HA	6:N:1499:ARG:CZ	2.40	0.51
6:N:35:ARG:HG3	6:N:35:ARG:HH11	1.75	0.51
6:N:50:PHE:CB	6:N:522:PRO:HG3	2.40	0.51
6:N:52:PRO:CG	6:N:80:VAL:HG13	2.39	0.51
6:N:754:PHE:O	6:N:758:GLU:HG2	2.10	0.51
4:A:26:GLU:HG3	4:A:184:THR:HG21	1.91	0.51
4:B:206:THR:HG23	4:B:208:LEU:H	1.75	0.51
5:C:141:HIS:C	5:C:331:ARG:HG2	2.31	0.51
5:C:194:VAL:CG1	5:C:204:GLN:HE22	2.22	0.51
5:C:841:ASN:HD21	5:C:845:ASN:N	2.08	0.51
6:D:813:LEU:HD12	6:D:814:ALA:N	2.26	0.51
7:E:39:VAL:HG22	7:E:67:GLU:HG2	1.92	0.51
1:G:19:DC:OP1	5:C:1001:VAL:HG11	2.10	0.51
4:L:102:LYS:HZ2	4:L:137:ARG:HG2	1.72	0.51
5:M:211:LEU:CD1	5:M:308:ARG:HA	2.40	0.51
5:M:771:GLU:O	5:M:775:ARG:HG2	2.11	0.51
5:M:841:ASN:HD21	5:M:845:ASN:H	1.58	0.51
6:N:703:ASN:ND2	6:N:704:ARG:N	2.58	0.51
6:N:879:ARG:NH1	6:N:879:ARG:HG3	2.25	0.51
6:N:889:ALA:CB	6:N:930:LEU:HD12	2.39	0.51
1:X:18:DG:H2''	1:X:19:DC:C5'	2.31	0.51
4:B:216:GLU:HA	4:B:219:ARG:NH1	2.25	0.51
5:C:163:ILE:HG13	5:C:163:ILE:O	2.08	0.51
5:C:547:ILE:HD13	5:C:550:LEU:HD13	1.91	0.51
5:C:605:LYS:HD2	5:C:612:VAL:HB	1.92	0.51
5:C:598:GLU:HG3	5:C:623:TYR:OH	2.10	0.51
5:C:946:ARG:HB3	5:C:946:ARG:NH1	2.25	0.51
5:C:552:HIS:CD2	6:D:1064:GLY:HA2	2.46	0.51
6:D:1464:GLU:HA	6:D:1467:ILE:CD1	2.40	0.51
6:D:483:HIS:ND1	6:D:483:HIS:N	2.59	0.51
6:D:690:ALA:O	6:D:694:VAL:HG23	2.10	0.51
6:D:762:GLN:HE22	7:E:20:THR:HG21	1.75	0.51
4:K:9:PRO:HB3	4:K:25:LEU:HG	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:36:LEU:O	4:L:39:PRO:HD2	2.10	0.51
5:M:173:ASP:OD1	5:M:185:LYS:HG3	2.11	0.51
5:M:804:VAL:HB	5:M:824:ARG:HB2	1.93	0.51
5:M:79:PRO:HD2	5:M:82:GLU:OE1	2.10	0.51
5:M:976:ASP:HB2	11:M:1439:HOH:O	2.10	0.51
6:N:1377:LYS:HE3	6:N:1394:VAL:HG13	1.92	0.51
6:N:172:PRO:HG2	6:N:175:VAL:CG2	2.41	0.51
5:M:1087:VAL:HG23	6:N:524:LEU:HD21	1.92	0.51
6:N:871:LYS:HB3	6:N:873:LEU:CD2	2.40	0.51
6:N:793:THR:CB	6:N:879:ARG:HD3	2.31	0.51
6:N:977:ALA:HB1	6:N:983:LEU:HD21	1.91	0.51
4:A:98:THR:HG22	11:A:364:HOH:O	2.09	0.51
4:B:102:LYS:NZ	4:B:137:ARG:NE	2.59	0.51
5:C:195:LEU:HG	5:C:238:LEU:HD12	1.91	0.51
5:C:343:GLN:HB2	5:C:385:PHE:CD2	2.46	0.51
5:C:328:LEU:HB3	5:C:488:ALA:HB2	1.93	0.51
5:C:640:ARG:O	5:C:642:ARG:HG2	2.10	0.51
5:C:678:PRO:O	6:D:943:THR:HA	2.10	0.51
6:D:145:VAL:CG2	6:D:146:PRO:HD2	2.33	0.51
6:D:1491:THR:O	6:D:1495:ILE:HD13	2.11	0.51
6:D:394:LEU:O	6:D:396:VAL:N	2.43	0.51
6:D:582:LEU:HD23	6:D:603:LEU:CD1	2.41	0.51
2:H:8:C:H2'	2:H:9:G:C8	2.46	0.51
4:K:158:ILE:O	4:K:159:LYS:HE2	2.11	0.51
4:L:124:ASN:HD21	4:L:127:LEU:HD22	1.74	0.51
4:L:202:ASP:HA	11:L:321:HOH:O	2.10	0.51
5:M:23:VAL:N	5:M:121:MET:HE1	2.25	0.51
5:M:351:LEU:HD22	5:M:377:PRO:HB2	1.92	0.51
5:M:855:VAL:HG11	11:M:1481:HOH:O	2.11	0.51
6:N:1090:ASP:HA	6:N:1093:TYR:HB2	1.91	0.51
6:N:701:LEU:HD12	6:N:701:LEU:H	1.74	0.51
4:A:88:ARG:HD2	4:A:121:GLU:OE1	2.10	0.51
4:A:5:LYS:O	4:A:8:ALA:HB2	2.10	0.51
4:B:40:LEU:O	4:B:44:LEU:HG	2.11	0.51
5:C:334:ARG:HG2	5:C:338:GLU:CD	2.31	0.51
5:C:432:ARG:HH12	6:D:1072:ILE:HD11	1.75	0.51
5:C:564:MET:HE1	5:C:995:MET:HB2	1.92	0.51
5:C:603:VAL:H	5:C:647:GLN:H	1.57	0.51
5:C:612:VAL:HG12	11:C:1460:HOH:O	2.10	0.51
5:C:835:VAL:HG13	5:C:836:GLY:N	2.25	0.51
6:D:1101:VAL:HG21	6:D:1424:VAL:HA	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:31:THR:HB	6:D:527:MET:HE1	1.92	0.51
6:D:540:LEU:HA	6:D:543:LEU:CD1	2.40	0.51
6:D:705:ALA:CB	6:D:706:PRO:HD3	2.40	0.51
7:E:58:PRO:C	7:E:59:ASN:HD22	2.13	0.51
4:L:24:VAL:HG13	4:L:196:THR:CG2	2.39	0.51
4:L:29:GLU:OE2	4:L:29:GLU:HA	2.10	0.51
5:M:549:PHE:HA	11:M:1469:HOH:O	2.10	0.51
5:M:879:ARG:HH21	6:N:1029:ARG:NH2	2.08	0.51
5:M:913:GLU:O	5:M:917:LEU:HG	2.11	0.51
6:N:1094:LEU:HB2	6:N:1260:ILE:CD1	2.38	0.51
6:N:1100:ASP:HB3	6:N:1428:ALA:HB1	1.92	0.51
6:N:1107:VAL:HA	6:N:1200:VAL:O	2.11	0.51
6:N:1129:THR:O	6:N:1130:ARG:HD2	2.11	0.51
6:N:1366:LYS:HA	6:N:1369:GLU:OE1	2.11	0.51
6:N:153:LEU:HD22	6:N:158:TYR:HB2	1.93	0.51
6:N:864:VAL:HB	11:N:9142:HOH:O	2.10	0.51
6:N:879:ARG:HH21	6:N:903:ASP:C	2.13	0.51
4:A:221:HIS:HA	4:A:224:TYR:HD2	1.76	0.51
4:B:40:LEU:HD21	4:B:215:VAL:HG12	1.93	0.51
5:C:1088:LEU:HD23	5:C:1089:VAL:N	2.26	0.51
5:C:217:LEU:HD23	5:C:217:LEU:H	1.76	0.51
5:C:52:PHE:CG	5:C:68:PHE:HB2	2.46	0.51
6:D:129:PHE:C	6:D:568:ARG:HH21	2.14	0.51
6:D:631:ILE:HG21	6:D:745:MET:SD	2.50	0.51
6:D:903:ASP:O	6:D:904:VAL:HG13	2.11	0.51
6:D:933:ALA:O	6:D:937:TYR:HD1	1.93	0.51
4:L:102:LYS:HD3	4:L:139:ASN:CB	2.35	0.51
5:M:1090:LYS:HE3	5:M:1112:PHE:CE1	2.42	0.51
5:M:163:ILE:HG13	5:M:163:ILE:O	2.09	0.51
5:M:64:LEU:HD13	5:M:359:MET:HG3	1.93	0.51
5:M:710:ILE:HD12	5:M:790:LEU:HB2	1.91	0.51
5:M:892:LEU:HD11	5:M:967:PHE:CE1	2.45	0.51
6:N:1033:GLN:O	6:N:1037:GLN:HG3	2.10	0.51
6:N:1042:ARG:HH21	6:N:1045:MET:HE2	1.76	0.51
6:N:1117:TYR:CE2	6:N:1151:ARG:HD3	2.45	0.51
6:N:1191:PRO:HB2	11:N:9021:HOH:O	2.10	0.51
6:N:1452:ILE:HG22	6:N:1453:ALA:N	2.25	0.51
6:N:415:VAL:O	6:N:432:TYR:HA	2.11	0.51
6:N:634:GLY:O	6:N:637:LEU:HB3	2.11	0.51
6:N:828:LYS:HD3	6:N:862:ASP:OD2	2.11	0.51
6:N:1476:THR:HG23	7:O:21:VAL:HG22	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:1008:ARG:NH2	5:C:1011:GLY:H	2.09	0.51
5:C:80:GLN:HE22	5:C:122:THR:HG23	1.76	0.51
5:C:147:TYR:HB3	11:C:1186:HOH:O	2.10	0.51
5:C:158:TYR:CE1	5:C:314:THR:HA	2.46	0.51
5:C:352:ALA:HA	5:C:355:VAL:CG1	2.41	0.51
5:C:573:ARG:CB	5:C:670:GLN:HE22	2.23	0.51
5:C:957:LYS:HD3	5:C:961:GLU:CD	2.30	0.51
5:C:878:SER:HA	6:D:1034:GLN:OE1	2.11	0.51
6:D:1347:TYR:CD2	6:D:1348:LEU:HD12	2.46	0.51
6:D:1101:VAL:HG23	6:D:1424:VAL:HG23	1.93	0.51
6:D:566:ILE:HD12	6:D:566:ILE:H	1.76	0.51
6:D:582:LEU:HD23	6:D:603:LEU:HD12	1.92	0.51
4:K:26:GLU:HG2	4:K:27:PRO:CA	2.40	0.51
4:L:160:ASP:HB3	4:L:161:ARG:HD2	1.92	0.51
5:M:169:GLY:HA2	5:M:263:ASP:OD1	2.11	0.51
5:M:550:LEU:HD12	5:M:550:LEU:O	2.10	0.51
5:M:5:ARG:HB2	5:M:8:ARG:NH2	2.21	0.51
6:N:542:ASP:O	6:N:546:ARG:HG3	2.10	0.51
6:N:62:LYS:HB2	6:N:73:CYS:SG	2.51	0.51
4:B:7:LYS:O	4:B:7:LYS:HD2	2.11	0.51
5:C:604:ALA:HB3	5:C:612:VAL:O	2.10	0.51
6:D:1040:GLY:O	6:D:1060:SER:HB3	2.11	0.51
6:D:1379:VAL:HG12	6:D:1419:PRO:HA	1.93	0.51
6:D:1441:GLN:CD	6:D:1442:ASN:HB2	2.31	0.51
6:D:154:THR:HG22	6:D:157:GLU:OE2	2.10	0.51
6:D:393:ILE:HG21	11:D:8118:HOH:O	2.11	0.51
6:D:413:ASP:O	6:D:435:VAL:HG23	2.11	0.51
6:D:671:LYS:HG3	11:D:8106:HOH:O	2.11	0.51
7:E:41:GLU:CG	7:E:42:PRO:HD3	2.41	0.51
5:M:1047:HIS:H	5:M:1047:HIS:CD2	2.28	0.51
5:M:160:ALA:HB3	5:M:174:LEU:HB2	1.93	0.51
6:N:1023:MET:HG2	6:N:1029:ARG:HB2	1.93	0.51
6:N:481:MET:SD	6:N:493:ARG:HA	2.51	0.51
7:O:10:PHE:CZ	7:O:16:LYS:HE3	2.46	0.51
4:A:14:ARG:HG3	4:A:14:ARG:HH11	1.75	0.51
4:B:48:ILE:HD12	4:B:48:ILE:H	1.76	0.51
4:B:89:PHE:HB3	4:B:94:LEU:CD1	2.39	0.51
5:C:1019:GLN:HE22	5:C:1058:ASP:CB	2.24	0.51
5:C:288:ARG:HB2	5:C:288:ARG:NH1	2.26	0.51
5:C:552:HIS:ND1	5:C:886:LEU:HD22	2.26	0.51
5:C:730:SER:O	5:C:734:LEU:HD13	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:3:ILE:HA	5:C:900:ARG:O	2.11	0.51
6:D:1151:ARG:HG2	6:D:1187:PRO:HB2	1.92	0.51
6:D:181:ASP:HA	6:D:205:TYR:CD1	2.46	0.51
6:D:785:ILE:HG13	6:D:939:PHE:HE2	1.74	0.51
7:E:27:ALA:HA	7:E:30:LEU:HD13	1.93	0.51
7:E:48:MET:HG2	7:E:49:GLN:N	2.26	0.51
7:E:33:HIS:CD2	7:E:89:MET:HG2	2.45	0.51
5:M:1016:ILE:HG12	5:M:1017:THR:N	2.26	0.51
5:M:628:PHE:HA	11:M:1256:HOH:O	2.10	0.51
5:M:660:ALA:HA	11:M:1443:HOH:O	2.11	0.51
5:M:571:LEU:HD21	5:M:700:TYR:HA	1.93	0.51
6:N:1087:ARG:HB3	6:N:1256:LEU:CD2	2.41	0.51
6:N:1379:VAL:HA	6:N:1420:LEU:HB2	1.92	0.51
6:N:155:ASP:N	11:N:9432:HOH:O	2.43	0.51
6:N:133:ILE:HD13	6:N:158:TYR:CD2	2.45	0.51
6:N:409:VAL:CG1	6:N:435:VAL:HG11	2.41	0.51
5:M:1007:ALA:HB2	6:N:648:MET:HG2	1.91	0.51
4:B:160:ASP:HA	11:B:363:HOH:O	2.09	0.50
5:C:1034:GLU:HG2	6:D:619:LEU:HD13	1.93	0.50
5:C:978:ARG:NH1	11:C:1599:HOH:O	2.44	0.50
6:D:1023:MET:O	6:D:1028:ALA:HB3	2.11	0.50
6:D:133:ILE:HG21	6:D:454:ALA:HB1	1.93	0.50
6:D:550:ARG:HA	6:D:550:ARG:NE	2.20	0.50
6:D:719:VAL:O	6:D:721:VAL:HG23	2.10	0.50
6:D:978:TYR:HB2	6:D:983:LEU:HD12	1.93	0.50
7:E:16:LYS:HA	11:E:128:HOH:O	2.10	0.50
5:M:1046:ALA:HB3	5:M:1047:HIS:HD2	1.76	0.50
5:M:15:LEU:H	5:M:15:LEU:HD12	1.77	0.50
5:M:692:GLU:O	5:M:696:LYS:HG3	2.10	0.50
5:M:773:LEU:O	5:M:777:ILE:HG13	2.11	0.50
6:N:1222:GLY:O	6:N:1225:ALA:HB3	2.11	0.50
6:N:50:PHE:HB3	6:N:522:PRO:HG3	1.92	0.50
6:N:710:ARG:C	6:N:712:GLY:H	2.14	0.50
5:C:148:PHE:HB2	5:C:313:LEU:CD2	2.41	0.50
5:C:338:GLU:HA	5:C:341:THR:HG22	1.93	0.50
5:C:468:ARG:CZ	5:C:485:TYR:O	2.59	0.50
5:C:328:LEU:C	5:C:488:ALA:HB3	2.30	0.50
5:C:51:THR:HG23	5:C:348:LEU:HD23	1.93	0.50
5:C:920:GLN:O	5:C:924:VAL:HG23	2.11	0.50
6:D:133:ILE:HG13	6:D:153:LEU:HD12	1.93	0.50
6:D:151:GLN:HA	11:D:8479:HOH:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:611:GLN:HG3	6:D:611:GLN:O	2.11	0.50
4:K:92:PRO:HG3	4:K:146:ARG:HH12	1.76	0.50
5:M:144:PRO:HB2	11:M:1136:HOH:O	2.11	0.50
5:M:289:THR:O	5:M:291:ALA:N	2.44	0.50
5:M:439:CYS:HB2	5:M:541:SER:HB3	1.92	0.50
5:M:888:THR:HG21	11:M:1248:HOH:O	2.10	0.50
5:M:916:GLU:HG3	5:M:917:LEU:HD23	1.93	0.50
5:M:943:VAL:HG11	5:M:973:VAL:CG2	2.41	0.50
6:N:1101:VAL:HG22	6:N:1428:ALA:HB2	1.94	0.50
6:N:1146:GLY:HA3	6:N:1207:TYR:CB	2.39	0.50
10:N:4999:APC:H8	10:N:4999:APC:H5'1	1.93	0.50
6:N:643:GLY:O	6:N:726:ILE:HG23	2.09	0.50
6:N:633:VAL:HB	6:N:740:PHE:CE1	2.46	0.50
6:N:937:TYR:N	6:N:937:TYR:CD1	2.79	0.50
4:A:111:ALA:HB3	4:A:124:ASN:O	2.11	0.50
1:G:18:DG:O4'	5:C:1002:GLU:HB3	2.11	0.50
5:C:1021:LEU:HD23	11:C:1374:HOH:O	2.11	0.50
5:C:1105:LYS:NZ	5:C:1107:ASN:HB2	2.26	0.50
5:C:436:GLY:HA2	5:C:456:ALA:CB	2.41	0.50
6:D:134:VAL:O	6:D:134:VAL:HG23	2.11	0.50
6:D:1403:LEU:O	6:D:1407:LEU:HB2	2.11	0.50
6:D:657:LEU:HB2	6:D:691:LEU:HD22	1.93	0.50
6:D:926:LYS:HA	6:D:929:ARG:CD	2.41	0.50
5:M:364:GLU:HB2	11:M:1318:HOH:O	2.10	0.50
5:M:589:ARG:HG3	5:M:596:TYR:CZ	2.46	0.50
5:M:702:SER:OG	5:M:831:ARG:HB2	2.11	0.50
5:M:726:ILE:HB	11:M:1385:HOH:O	2.10	0.50
5:M:852:ILE:N	5:M:852:ILE:HD12	2.26	0.50
5:M:537:LYS:HG3	5:M:905:ILE:CD1	2.42	0.50
6:N:1424:VAL:CG1	6:N:1425:THR:H	2.22	0.50
5:M:1115:LEU:CG	6:N:85:VAL:HG12	2.40	0.50
4:B:20:TYR:CE2	4:B:198:ARG:HB3	2.45	0.50
5:C:1019:GLN:N	5:C:1019:GLN:HE21	2.08	0.50
5:C:433:THR:C	5:C:435:TYR:H	2.15	0.50
5:C:610:ARG:HG3	5:C:622:GLU:HG3	1.94	0.50
5:C:737:LEU:HD21	5:C:741:GLY:CA	2.42	0.50
6:D:131:LYS:HG3	6:D:568:ARG:CG	2.41	0.50
6:D:434:ARG:H	6:D:447:VAL:CG2	2.20	0.50
6:D:150:ARG:HG3	6:D:464:LEU:HD22	1.93	0.50
6:D:87:ARG:HB2	6:D:523:ASP:HB3	1.93	0.50
1:G:18:DG:H5''	6:D:628:ARG:NH2	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:1087:VAL:HG22	5:M:1091:GLU:OE1	2.10	0.50
5:M:22:GLN:C	5:M:121:MET:HE1	2.32	0.50
5:M:218:VAL:HA	5:M:221:LEU:HD23	1.93	0.50
5:M:141:HIS:C	5:M:331:ARG:HG3	2.32	0.50
5:M:5:ARG:NE	5:M:8:ARG:NH1	2.57	0.50
5:M:862:PRO:HA	5:M:975:TYR:CE2	2.47	0.50
3:Z:10:DA:H5''	6:N:121:THR:CG2	2.41	0.50
2:Y:7:G:OP1	6:N:530:VAL:HG13	2.11	0.50
11:N:9174:HOH:O	7:O:81:PRO:HG2	2.11	0.50
2:Y:2:A:C3'	2:Y:2:A:H8	2.12	0.50
4:B:43:ILE:HG21	4:B:214:ALA:HA	1.94	0.50
5:C:1006:HIS:HD1	5:C:1027:PHE:HD1	1.60	0.50
5:C:185:LYS:HE2	5:C:190:LYS:HZ3	1.75	0.50
5:C:460:ARG:HB3	11:C:1158:HOH:O	2.11	0.50
5:C:597:ALA:CA	5:C:655:LEU:HD11	2.41	0.50
5:C:721:ARG:HA	5:C:820:ARG:NH2	2.26	0.50
5:C:732:ALA:HA	5:C:735:ARG:NH1	2.26	0.50
6:D:171:LEU:HD21	6:D:192:ALA:HB1	1.91	0.50
6:D:29:PRO:CB	6:D:549:ASN:HD21	2.23	0.50
11:C:1228:HOH:O	6:D:2:LYS:HA	2.11	0.50
6:D:542:ASP:OD2	6:D:542:ASP:N	2.42	0.50
4:K:177:VAL:O	5:M:864:GLY:HA2	2.12	0.50
4:K:24:VAL:HG22	4:K:196:THR:CG2	2.41	0.50
4:L:62:LEU:HD12	4:L:62:LEU:N	2.22	0.50
5:M:1055:LEU:HD11	5:M:1076:VAL:HB	1.94	0.50
5:M:395:LYS:HE3	5:M:407:LYS:HE2	1.92	0.50
5:M:757:GLY:HA2	5:M:789:SER:CB	2.42	0.50
5:M:807:ARG:N	5:M:807:ARG:NE	2.59	0.50
6:N:1020:LEU:HD21	6:N:1035:ILE:HG23	1.93	0.50
6:N:1195:GLN:HG3	6:N:1196:THR:N	2.27	0.50
2:Y:6:U:OP1	6:N:528:VAL:HG13	2.12	0.50
6:N:637:LEU:CD2	6:N:642:CYS:HA	2.41	0.50
6:N:896:ALA:O	6:N:900:ILE:HG23	2.12	0.50
7:O:54:LEU:HG	7:O:58:PRO:CG	2.42	0.50
5:C:275:TYR:HA	11:C:1297:HOH:O	2.11	0.50
5:C:22:GLN:NE2	5:C:407:LYS:HG2	2.26	0.50
2:H:14:G:P	5:C:409:ARG:HH12	2.35	0.50
5:C:630:ARG:HA	5:C:705:ILE:CD1	2.41	0.50
5:C:713:ARG:NH2	6:D:532:GLY:H	2.09	0.50
5:C:690:ILE:HD12	5:C:833:LEU:HD23	1.94	0.50
6:D:108:VAL:HG23	6:D:109:PRO:HD3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:155:ASP:O	6:D:159:ARG:N	2.41	0.50
6:D:470:LEU:HD12	6:D:503:LEU:CD2	2.42	0.50
5:M:1005:MET:HB2	6:N:648:MET:HE3	1.92	0.50
5:M:158:TYR:HE1	5:M:314:THR:HA	1.76	0.50
5:M:410:ILE:CD1	5:M:455:LEU:HB3	2.42	0.50
5:M:754:ILE:HG12	5:M:791:ARG:HH12	1.77	0.50
5:M:810:ASP:HB3	5:M:813:VAL:CG1	2.36	0.50
5:M:836:GLY:HA3	6:N:724:GLN:HE21	1.76	0.50
6:N:1240:THR:HB	6:N:1252:ILE:HD13	1.92	0.50
6:N:1267:ARG:HA	6:N:1331:ASP:HB2	1.94	0.50
6:N:613:ARG:HH11	6:N:616:GLN:HG2	1.76	0.50
6:N:758:GLU:HA	7:O:20:THR:CG2	2.42	0.50
6:N:890:VAL:HG23	6:N:890:VAL:O	2.11	0.50
7:O:28:GLN:HB3	7:O:32:ARG:NH2	2.25	0.50
4:B:174:VAL:HG13	4:B:200:TRP:O	2.12	0.50
4:B:26:GLU:HB3	4:B:194:LYS:HG3	1.93	0.50
5:C:301:GLU:O	5:C:305:PRO:HG2	2.12	0.50
5:C:580:MET:HB3	5:C:584:GLU:OE1	2.11	0.50
5:C:627:ARG:CG	5:C:628:PHE:H	2.25	0.50
5:C:702:SER:HB3	5:C:996:LYS:NZ	2.27	0.50
5:C:820:ARG:HB2	11:C:1271:HOH:O	2.12	0.50
6:D:1103:HIS:NE2	6:D:1463:LYS:HB2	2.27	0.50
6:D:1440:PHE:O	6:D:1441:GLN:O	2.30	0.50
6:D:902:LEU:H	6:D:902:LEU:HD23	1.75	0.50
7:E:68:LEU:CD1	7:E:73:LEU:HD22	2.41	0.50
5:M:120:LEU:HD13	5:M:121:MET:O	2.12	0.50
5:M:192:PRO:HB2	5:M:195:LEU:HB2	1.93	0.50
5:M:622:GLU:O	5:M:624:PRO:HD3	2.11	0.50
5:M:837:ASP:HA	5:M:999:HIS:CE1	2.46	0.50
5:M:876:VAL:O	5:M:879:ARG:O	2.30	0.50
6:N:1037:GLN:HG2	6:N:1042:ARG:HB2	1.93	0.50
6:N:1192:LEU:HD21	6:N:1372:VAL:CG1	2.42	0.50
6:N:1394:VAL:HG11	6:N:1397:LYS:HE2	1.94	0.50
6:N:150:ARG:CD	6:N:464:LEU:HD21	2.41	0.50
6:N:619:LEU:HB2	6:N:621:LYS:HD3	1.92	0.50
6:N:690:ALA:O	6:N:694:VAL:HG23	2.12	0.50
6:N:845:ASN:N	6:N:848:GLU:HG3	2.26	0.50
5:C:999:HIS:HD2	5:C:1004:LYS:NZ	2.10	0.50
5:C:290:LEU:H	5:C:290:LEU:HD23	1.75	0.50
5:C:564:MET:HE2	5:C:565:GLN:HA	1.93	0.50
5:C:57:GLU:O	5:C:62:GLY:HA3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:397:LYS:O	6:D:448:GLU:HB2	2.12	0.50
6:D:54:LYS:CD	6:D:55:ASP:H	2.25	0.50
6:D:562:ALA:HB1	6:D:567:ILE:HD11	1.94	0.50
6:D:634:GLY:CA	6:D:727:GLN:HE21	2.23	0.50
5:M:1020:PRO:O	5:M:1021:LEU:HD12	2.11	0.50
5:M:1034:GLU:HB3	6:N:619:LEU:CD2	2.40	0.50
5:M:5:ARG:NE	5:M:8:ARG:HH22	2.00	0.50
6:N:1237:THR:N	11:N:9434:HOH:O	2.45	0.50
6:N:1139:ASP:HB3	6:N:1357:ARG:NH2	2.27	0.50
6:N:475:LYS:HA	6:N:478:LEU:HG	1.94	0.50
6:N:52:PRO:HG2	6:N:80:VAL:HG13	1.93	0.50
6:N:79:GLU:HG3	11:N:9414:HOH:O	2.12	0.50
6:N:982:PHE:HB3	6:N:983:LEU:HD23	1.92	0.50
1:X:8:DT:H2"	1:X:9:DG:C8	2.46	0.50
4:B:62:LEU:HD12	4:B:62:LEU:H	1.77	0.50
5:C:265:ARG:HD2	5:C:267:TYR:CB	2.41	0.50
5:C:842:ARG:HG3	5:C:995:MET:HE1	1.93	0.50
6:D:1021:TYR:HA	11:D:8152:HOH:O	2.11	0.50
5:C:906:PHE:CZ	6:D:1067:VAL:HA	2.46	0.50
6:D:127:LEU:HD23	6:D:134:VAL:HG22	1.93	0.50
6:D:133:ILE:HG13	6:D:153:LEU:CD1	2.41	0.50
6:D:477:LEU:HD13	6:D:496:LEU:HA	1.94	0.50
6:D:510:GLU:O	6:D:513:ILE:HD12	2.12	0.50
6:D:100:ALA:HA	6:D:514:LEU:H	1.76	0.50
6:D:683:ILE:HG23	6:D:687:VAL:HG21	1.94	0.50
6:D:721:VAL:HG12	6:D:722:GLU:N	2.26	0.50
6:D:739:ASP:O	6:D:741:ASP:N	2.45	0.50
7:E:18:ARG:O	7:E:22:VAL:HG23	2.12	0.50
5:M:17:PRO:HG3	11:M:1503:HOH:O	2.12	0.50
5:M:22:GLN:OE1	5:M:407:LYS:HB3	2.12	0.50
5:M:290:LEU:HB3	5:M:302:VAL:CG1	2.41	0.50
5:M:32:ALA:HB2	11:M:1235:HOH:O	2.12	0.50
5:M:432:ARG:HH21	6:N:1048:PRO:HD2	1.77	0.50
6:N:1087:ARG:HE	6:N:1253:THR:HG23	1.77	0.50
6:N:1236:LEU:HD11	6:N:1361:VAL:CG2	2.42	0.50
6:N:637:LEU:HD12	6:N:641:GLN:OE1	2.12	0.50
6:N:714:GLN:CD	6:N:765:SER:HA	2.33	0.50
4:A:163:ASN:HD21	5:C:744:ARG:HH22	1.59	0.49
5:C:97:ARG:HA	5:C:111:ASP:O	2.12	0.49
5:C:113:VAL:O	5:C:115:LEU:HG	2.11	0.49
5:C:119:PRO:HG2	5:C:386:PHE:CD2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:408:ARG:CG	5:C:455:LEU:H	2.24	0.49
5:C:73:LEU:N	5:C:73:LEU:HD23	2.27	0.49
6:D:1128:VAL:O	6:D:1129:THR:C	2.50	0.49
6:D:1144:LEU:HD11	6:D:1186:VAL:CG2	2.37	0.49
6:D:1402:ALA:HB3	11:D:8309:HOH:O	2.11	0.49
6:D:1443:THR:O	6:D:1447:LEU:HD13	2.11	0.49
6:D:82:LYS:CB	6:D:84:ILE:HG12	2.42	0.49
6:D:926:LYS:HG3	11:D:8014:HOH:O	2.11	0.49
6:D:977:ALA:CB	6:D:983:LEU:HD21	2.42	0.49
2:H:7:G:H8	2:H:7:G:O5'	1.95	0.49
5:M:134:ARG:CD	5:M:392:SER:HB3	2.42	0.49
5:M:139:GLN:HE21	5:M:418:LEU:CD2	2.25	0.49
5:M:616:GLU:OE1	5:M:616:GLU:HA	2.11	0.49
5:M:77:PRO:HG2	5:M:117:HIS:NE2	2.27	0.49
6:N:1020:LEU:HD23	6:N:1021:TYR:N	2.27	0.49
6:N:1042:ARG:NH2	11:N:9443:HOH:O	2.45	0.49
6:N:1364:HIS:CE1	6:N:1366:LYS:HG3	2.47	0.49
6:N:143:ASN:OD1	6:N:145:VAL:HG12	2.11	0.49
6:N:1459:LEU:HD21	6:N:1468:LEU:HD22	1.93	0.49
6:N:1489:GLN:O	6:N:1493:LYS:HG2	2.12	0.49
6:N:502:PHE:CZ	6:N:509:PRO:HB3	2.46	0.49
6:N:787:LEU:HD21	6:N:1023:MET:HE2	1.94	0.49
6:N:838:ARG:NH1	6:N:838:ARG:HG2	2.26	0.49
6:N:864:VAL:HB	11:N:9057:HOH:O	2.11	0.49
3:Z:9:DG:H2''	3:Z:10:DA:C8	2.47	0.49
4:B:86:VAL:HG12	4:B:124:ASN:HB2	1.94	0.49
5:C:264:PRO:HD2	11:C:1410:HOH:O	2.12	0.49
5:C:577:PRO:HB2	5:C:580:MET:HG2	1.93	0.49
6:D:185:VAL:HG21	6:D:203:ALA:HB2	1.93	0.49
6:D:29:PRO:HB3	6:D:549:ASN:HD21	1.77	0.49
6:D:547:LEU:HB3	11:D:8068:HOH:O	2.11	0.49
6:D:634:GLY:CA	6:D:727:GLN:HG2	2.43	0.49
6:D:709:HIS:CD2	6:D:709:HIS:N	2.80	0.49
7:E:83:ASP:O	7:E:86:GLN:HG3	2.13	0.49
1:G:12:DG:H2''	1:G:13:DT:C5'	2.43	0.49
5:M:198:ARG:HE	5:M:198:ARG:HA	1.77	0.49
5:M:21:ILE:HD12	5:M:21:ILE:H	1.77	0.49
5:M:415:PRO:HD2	5:M:418:LEU:HD13	1.94	0.49
5:M:583:LEU:N	5:M:584:GLU:OE2	2.45	0.49
5:M:676:ILE:O	5:M:676:ILE:HG23	2.11	0.49
5:M:959:PRO:O	5:M:963:LEU:HG	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:1010:ASN:HB3	11:N:9288:HOH:O	2.12	0.49
6:N:522:PRO:HG2	6:N:523:ASP:N	2.26	0.49
5:M:1019:GLN:CD	6:N:616:GLN:HE22	2.15	0.49
5:C:260:LEU:HA	5:C:291:ALA:CB	2.42	0.49
5:C:64:LEU:HD22	5:C:359:MET:HG3	1.93	0.49
5:C:54:ILE:HG22	5:C:66:LEU:HB3	1.95	0.49
5:C:881:ASN:N	5:C:881:ASN:ND2	2.60	0.49
6:D:1143:GLY:O	6:D:1147:ARG:NE	2.45	0.49
6:D:1495:ILE:HG12	7:E:80:VAL:CG1	2.39	0.49
6:D:836:VAL:O	6:D:840:LYS:HG3	2.12	0.49
6:D:762:GLN:NE2	7:E:20:THR:OG1	2.45	0.49
4:L:103:ALA:HB1	4:L:107:LYS:CE	2.42	0.49
4:L:47:SER:HB2	4:L:217:ILE:HD13	1.95	0.49
5:M:276:LYS:O	5:M:280:LYS:HB3	2.12	0.49
6:N:957:PRO:HG3	6:N:1007:VAL:HA	1.94	0.49
6:N:996:TRP:CE2	6:N:1056:PRO:HG2	2.47	0.49
6:N:1189:ARG:NH1	6:N:1203:LYS:HB2	2.28	0.49
6:N:437:VAL:HG13	6:N:444:VAL:HG22	1.94	0.49
6:N:133:ILE:CG2	6:N:454:ALA:HB1	2.41	0.49
7:O:18:ARG:O	7:O:22:VAL:HG23	2.12	0.49
7:O:68:LEU:HD12	7:O:73:LEU:HD22	1.93	0.49
4:A:190:THR:HG23	11:A:369:HOH:O	2.12	0.49
4:A:68:ILE:HD12	4:A:68:ILE:N	2.27	0.49
4:A:83:LYS:HE2	4:A:170:VAL:HG13	1.93	0.49
4:B:62:LEU:HD13	4:B:63:HIS:CE1	2.47	0.49
5:C:1022:GLY:HA3	5:C:1026:GLN:O	2.12	0.49
5:C:674:VAL:CG2	5:C:869:VAL:HG13	2.42	0.49
5:C:689:VAL:HG11	5:C:870:ILE:HD11	1.94	0.49
5:C:876:VAL:O	5:C:879:ARG:O	2.30	0.49
5:C:8:ARG:N	5:C:907:ASP:OD2	2.45	0.49
6:D:1124:GLN:HG2	6:D:1133:ARG:CG	2.42	0.49
6:D:1258:ARG:HA	6:D:1261:GLU:OE2	2.12	0.49
6:D:1384:PRO:HG3	6:D:1389:LEU:HA	1.92	0.49
6:D:172:PRO:HG2	6:D:175:VAL:CG2	2.42	0.49
6:D:17:LYS:O	6:D:20:SER:HB3	2.12	0.49
6:D:519:VAL:HG12	6:D:544:TYR:CE2	2.48	0.49
6:D:737:ASN:O	6:D:737:ASN:CG	2.50	0.49
5:M:689:VAL:HG11	5:M:870:ILE:HD11	1.93	0.49
5:M:897:LEU:HD12	11:M:1461:HOH:O	2.12	0.49
4:A:199:ILE:HD12	4:A:199:ILE:N	2.26	0.49
5:C:1001:VAL:O	5:C:1001:VAL:HG12	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:304:LEU:HA	11:C:1215:HOH:O	2.12	0.49
5:C:490:GLU:HB3	5:C:493:ARG:CZ	2.42	0.49
5:C:496:ILE:HA	5:C:531:PHE:O	2.11	0.49
5:C:432:ARG:HH12	6:D:1072:ILE:CD1	2.25	0.49
6:D:1125:PRO:HB3	6:D:1130:ARG:NH1	2.27	0.49
6:D:1168:MET:HE3	6:D:1171:VAL:HG21	1.94	0.49
6:D:1374:GLN:OE1	6:D:1377:LYS:HD3	2.12	0.49
6:D:118:LEU:HD21	6:D:464:LEU:HD13	1.94	0.49
6:D:465:LEU:HD13	6:D:513:ILE:HD11	1.95	0.49
6:D:638:LYS:HD2	6:D:932:ASP:CG	2.33	0.49
2:H:16:G:H21	6:D:705:ALA:HB1	1.78	0.49
4:K:218:LEU:O	4:K:222:LEU:HD13	2.12	0.49
5:M:1016:ILE:HD13	5:M:1017:THR:H	1.78	0.49
5:M:340:MET:HG2	5:M:386:PHE:HE1	1.78	0.49
5:M:574:ALA:HB2	11:M:1443:HOH:O	2.12	0.49
5:M:736:ASP:HA	5:M:744:ARG:HH11	1.77	0.49
4:K:30:ARG:NH2	5:M:938:LYS:HD2	2.25	0.49
6:N:10:ILE:HG13	6:N:1434:TRP:CZ2	2.47	0.49
6:N:516:ALA:O	6:N:518:PRO:HD3	2.13	0.49
5:M:1009:SER:HB3	6:N:651:GLU:O	2.13	0.49
7:O:33:HIS:HB2	7:O:37:ASN:HD21	1.77	0.49
5:C:127:PHE:O	5:C:133:ASP:HA	2.12	0.49
5:C:150:PRO:HG3	5:C:158:TYR:HD2	1.78	0.49
5:C:165:LEU:HD11	11:C:1123:HOH:O	2.13	0.49
5:C:409:ARG:HD2	5:C:452:ILE:CG2	2.42	0.49
5:C:437:ARG:O	5:C:467:ILE:HD13	2.12	0.49
5:C:449:ILE:C	5:C:451:LEU:H	2.15	0.49
5:C:537:LYS:HD2	5:C:537:LYS:H	1.78	0.49
6:D:1087:ARG:HG3	6:D:1237:THR:CG2	2.40	0.49
6:D:108:VAL:CB	6:D:109:PRO:HD3	2.42	0.49
6:D:1263:PHE:O	6:D:1424:VAL:HG12	2.12	0.49
6:D:1418:LYS:HD3	6:D:1419:PRO:CD	2.42	0.49
6:D:138:LYS:HD2	6:D:450:TYR:OH	2.13	0.49
6:D:610:LYS:CA	6:D:615:ARG:HD3	2.42	0.49
6:D:926:LYS:HA	6:D:929:ARG:HH11	1.78	0.49
5:M:23:VAL:CA	5:M:121:MET:HE1	2.43	0.49
5:M:127:PHE:O	5:M:133:ASP:HA	2.13	0.49
5:M:319:GLY:HA3	11:M:1388:HOH:O	2.11	0.49
5:M:265:ARG:HH22	5:M:332:ARG:HH22	1.60	0.49
5:M:471:TYR:HB2	11:M:1201:HOH:O	2.11	0.49
5:M:561:GLY:HA2	5:M:564:MET:HG3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:837:ASP:HA	5:M:999:HIS:HE1	1.78	0.49
6:N:1139:ASP:O	6:N:1142:ALA:HB3	2.13	0.49
6:N:137:PRO:HD2	6:N:453:ASP:OD1	2.12	0.49
6:N:641:GLN:HB3	6:N:717:GLN:O	2.12	0.49
6:N:800:LYS:HE3	6:N:804:LEU:HB3	1.93	0.49
6:N:897:TRP:HA	6:N:900:ILE:CG1	2.37	0.49
6:N:947:ILE:HG23	11:N:9083:HOH:O	2.11	0.49
4:A:73:GLU:OE1	4:A:130:ALA:HA	2.12	0.49
4:B:102:LYS:HZ1	4:B:137:ARG:NE	2.11	0.49
5:C:101:ILE:HG22	5:C:102:HIS:N	2.27	0.49
5:C:1111:ILE:HD12	5:C:1112:PHE:H	1.78	0.49
5:C:162:ILE:HD12	5:C:172:ILE:CB	2.43	0.49
5:C:192:PRO:HB2	5:C:195:LEU:H	1.78	0.49
5:C:264:PRO:HB3	5:C:289:THR:CB	2.43	0.49
5:C:270:GLY:O	5:C:274:ARG:HD2	2.12	0.49
5:C:596:TYR:HB2	11:C:1524:HOH:O	2.12	0.49
5:C:841:ASN:N	5:C:841:ASN:ND2	2.60	0.49
5:C:89:THR:HA	5:C:129:ILE:O	2.12	0.49
6:D:108:VAL:HB	6:D:109:PRO:HD3	1.94	0.49
6:D:1211:MET:SD	6:D:1213:ARG:HG2	2.52	0.49
6:D:191:LEU:HG	6:D:197:SER:OG	2.13	0.49
6:D:613:ARG:O	6:D:616:GLN:HB3	2.13	0.49
6:D:899:LEU:HD13	6:D:914:LEU:CD2	2.37	0.49
6:D:957:PRO:O	6:D:960:LYS:HB3	2.13	0.49
7:E:38:THR:HG23	7:E:41:GLU:OE2	2.13	0.49
4:K:63:HIS:CD2	4:K:66:SER:HB2	2.48	0.49
5:M:1065:ALA:HB1	5:M:1077:PRO:CG	2.36	0.49
5:M:146:VAL:HG12	5:M:162:ILE:HA	1.93	0.49
5:M:250:ARG:HG3	5:M:250:ARG:HH11	1.78	0.49
5:M:31:GLN:NE2	5:M:71:TYR:OH	2.45	0.49
5:M:25:SER:CB	5:M:335:THR:HB	2.42	0.49
5:M:403:SER:O	5:M:407:LYS:HG3	2.13	0.49
5:M:902:ILE:O	5:M:904:PRO:HD3	2.12	0.49
6:N:1101:VAL:HG21	6:N:1424:VAL:HG23	1.95	0.49
6:N:1338:ALA:HB2	11:N:9199:HOH:O	2.12	0.49
6:N:151:GLN:HG3	6:N:152:LEU:H	1.78	0.49
5:C:141:HIS:CE1	5:C:334:ARG:HG3	2.47	0.49
5:C:150:PRO:HG3	5:C:158:TYR:CD2	2.47	0.49
5:C:162:ILE:O	5:C:164:PRO:HD3	2.12	0.49
5:C:265:ARG:O	5:C:288:ARG:HD2	2.13	0.49
5:C:537:LYS:HG3	5:C:545:ASN:HD21	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:918:LEU:HD23	5:C:968:LEU:HA	1.93	0.49
5:C:98:LEU:N	5:C:98:LEU:HD12	2.28	0.49
6:D:1000:THR:HG23	6:D:1001:GLU:N	2.28	0.49
6:D:1087:ARG:CG	6:D:1237:THR:HG21	2.41	0.49
6:D:1192:LEU:HD22	6:D:1345:GLU:CG	2.43	0.49
6:D:204:LEU:O	6:D:394:LEU:HD23	2.13	0.49
6:D:754:PHE:CE2	6:D:1476:THR:HG21	2.48	0.49
4:L:111:ALA:HB3	4:L:124:ASN:O	2.13	0.49
5:M:136:ILE:HD11	11:M:1417:HOH:O	2.12	0.49
5:M:374:ASN:HD22	5:M:377:PRO:HD3	1.76	0.49
6:N:116:LEU:HD22	6:N:118:LEU:HG	1.95	0.49
6:N:1156:LEU:HG	6:N:1177:ALA:HB2	1.94	0.49
6:N:1213:ARG:NH2	7:O:15:SER:HA	2.27	0.49
6:N:1487:VAL:HA	11:N:9036:HOH:O	2.11	0.49
6:N:1488:ASP:OD1	6:N:1488:ASP:N	2.46	0.49
6:N:827:ILE:O	6:N:837:GLY:HA3	2.12	0.49
4:A:173:PRO:HB2	4:A:205:VAL:HG22	1.94	0.49
4:B:176:ARG:HG3	4:B:200:TRP:CE3	2.47	0.49
5:C:1040:LEU:HD21	5:C:1048:THR:HG22	1.95	0.49
5:C:190:LYS:HB2	11:C:1219:HOH:O	2.13	0.49
5:C:313:LEU:HA	5:C:321:GLU:HG3	1.94	0.49
5:C:368:THR:N	5:C:369:PRO:HD2	2.28	0.49
5:C:433:THR:CG2	5:C:488:ALA:HB1	2.28	0.49
5:C:575:GLN:HG2	5:C:671:ASN:OD1	2.11	0.49
5:C:689:VAL:O	5:C:869:VAL:HG23	2.13	0.49
5:C:677:MET:HE1	5:C:974:LEU:HD23	1.94	0.49
6:D:184:GLU:HG3	11:D:8384:HOH:O	2.13	0.49
6:D:38:LYS:HZ1	6:D:59:ALA:HB1	1.77	0.49
6:D:883:ALA:HB2	11:D:8066:HOH:O	2.12	0.49
6:D:915:VAL:HG11	6:D:931:LEU:HD21	1.94	0.49
5:M:301:GLU:O	5:M:305:PRO:HG2	2.13	0.49
5:M:328:LEU:N	5:M:328:LEU:HD12	2.28	0.49
5:M:328:LEU:HD11	5:M:434:HIS:CD2	2.47	0.49
5:M:524:VAL:HG12	5:M:528:GLU:HB2	1.95	0.49
5:M:68:PHE:CZ	5:M:71:TYR:HD2	2.24	0.49
5:M:971:LYS:HE2	11:M:1216:HOH:O	2.13	0.49
6:N:1498:ALA:HB2	7:O:88:GLU:OE1	2.13	0.49
6:N:92:HIS:HA	6:N:517:VAL:O	2.13	0.49
6:N:538:SER:O	6:N:541:ASN:ND2	2.45	0.49
6:N:565:ILE:HD12	6:N:565:ILE:N	2.26	0.49
6:N:703:ASN:ND2	6:N:704:ARG:H	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:173:PRO:HA	4:B:202:ASP:OD2	2.13	0.49
4:B:57:TYR:CE2	4:B:161:ARG:HG2	2.48	0.49
5:C:46:ALA:O	5:C:49:ARG:HG2	2.13	0.49
5:C:722:ILE:O	5:C:722:ILE:HG23	2.13	0.49
5:C:762:LYS:HD2	5:C:786:LYS:CB	2.42	0.49
5:C:860:HIS:CE1	5:C:975:TYR:HB2	2.48	0.49
5:C:906:PHE:CD1	6:D:1067:VAL:HG13	2.48	0.49
6:D:192:ALA:HB1	6:D:193:PRO:HD2	1.94	0.49
6:D:737:ASN:ND2	10:D:3999:APC:O3'	2.38	0.49
6:D:396:VAL:CG1	6:D:447:VAL:HG12	2.42	0.49
6:D:508:ARG:HD2	6:D:509:PRO:HD2	1.94	0.49
6:D:729:HIS:CE1	6:D:731:LEU:HB2	2.48	0.49
4:L:176:ARG:HE	6:N:847:ASP:CG	2.17	0.49
5:M:433:THR:O	5:M:437:ARG:HD2	2.12	0.49
5:M:498:GLN:NE2	6:N:1068:LEU:HG	2.28	0.49
5:M:759:THR:HB	5:M:785:VAL:HG22	1.95	0.49
5:M:893:ALA:HB2	5:M:918:LEU:HD12	1.95	0.49
5:M:981:GLU:HG3	5:M:982:PRO:HD2	1.94	0.49
6:N:545:ARG:HB2	6:N:545:ARG:CZ	2.42	0.49
5:M:687:ALA:HB2	6:N:740:PHE:HB2	1.95	0.49
6:N:829:VAL:O	6:N:835:SER:HB3	2.12	0.49
5:C:18:LEU:HD22	5:C:404:LEU:CD2	2.43	0.48
5:C:276:LYS:O	5:C:280:LYS:HB2	2.12	0.48
5:C:439:CYS:SG	5:C:442:GLU:N	2.75	0.48
5:C:439:CYS:SG	5:C:442:GLU:HB2	2.52	0.48
5:C:853:LEU:HB2	5:C:858:MET:CE	2.42	0.48
5:C:579:VAL:CG1	5:C:887:GLU:HG3	2.33	0.48
6:D:1026:SER:C	6:D:1028:ALA:H	2.17	0.48
6:D:1033:GLN:N	11:D:8254:HOH:O	2.46	0.48
6:D:1102:THR:CG2	6:D:1370:ILE:HG22	2.42	0.48
6:D:1136:LYS:HB2	6:D:1139:ASP:OD1	2.13	0.48
6:D:1231:GLU:CG	6:D:1232:PRO:HD3	2.43	0.48
11:C:1216:HOH:O	6:D:606:ILE:HD11	2.12	0.48
6:D:675:ARG:HA	6:D:678:GLU:HG2	1.94	0.48
6:D:699:VAL:H	6:D:756:GLN:HE22	1.55	0.48
4:K:1:MET:O	4:K:6:LEU:HD13	2.12	0.48
4:L:89:PHE:CD1	4:L:120:VAL:HG13	2.48	0.48
4:L:124:ASN:ND2	4:L:127:LEU:HB2	2.28	0.48
4:L:24:VAL:HG12	4:L:26:GLU:OE2	2.13	0.48
5:M:127:PHE:HZ	5:M:336:VAL:HG11	1.78	0.48
5:M:250:ARG:HG2	5:M:253:ALA:CB	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:262:ALA:HB3	11:M:1334:HOH:O	2.13	0.48
5:M:174:LEU:HD13	5:M:307:LEU:HD13	1.94	0.48
5:M:376:ARG:NH1	5:M:376:ARG:HG3	2.28	0.48
5:M:490:GLU:HG2	5:M:493:ARG:CZ	2.42	0.48
5:M:630:ARG:HA	11:M:1247:HOH:O	2.12	0.48
5:M:642:ARG:HG3	5:M:657:ASP:OD2	2.13	0.48
5:M:673:LEU:HB3	5:M:868:ASP:OD1	2.13	0.48
5:M:95:TYR:CD2	5:M:114:PHE:HB2	2.47	0.48
6:N:1114:THR:O	6:N:1114:THR:HG23	2.13	0.48
6:N:470:LEU:CD2	6:N:470:LEU:H	2.24	0.48
6:N:729:HIS:CE1	6:N:731:LEU:H	2.31	0.48
6:N:739:ASP:O	6:N:741:ASP:N	2.45	0.48
2:Y:2:A:C4'	2:Y:2:A:C8	2.95	0.48
4:A:108:GLU:OE2	4:A:131:THR:HG22	2.13	0.48
4:A:180:GLN:HB3	4:A:182:GLU:OE2	2.11	0.48
4:B:111:ALA:HB3	4:B:124:ASN:O	2.12	0.48
5:C:1102:LEU:N	6:D:7:LYS:O	2.46	0.48
5:C:723:THR:HG23	5:C:725:ASP:H	1.78	0.48
6:D:1366:LYS:HA	6:D:1369:GLU:OE2	2.13	0.48
5:C:1049:LEU:CD2	6:D:1472:ILE:HD12	2.37	0.48
6:D:1217:ILE:HD12	6:D:1480:PHE:CE2	2.48	0.48
6:D:1483:PHE:CD1	6:D:1483:PHE:N	2.81	0.48
6:D:522:PRO:HG2	6:D:523:ASP:H	1.78	0.48
6:D:689:ASP:O	6:D:693:GLU:HG3	2.12	0.48
4:L:30:ARG:HB2	4:L:30:ARG:HH11	1.78	0.48
5:M:19:THR:HG22	5:M:404:LEU:CD1	2.41	0.48
5:M:217:LEU:HD12	5:M:311:PHE:CD2	2.48	0.48
5:M:302:VAL:O	5:M:306:THR:HG23	2.14	0.48
5:M:39:ARG:CD	5:M:39:ARG:H	2.18	0.48
5:M:642:ARG:NH1	11:M:1230:HOH:O	2.45	0.48
5:M:1043:TYR:CE1	6:N:710:ARG:HG3	2.48	0.48
6:N:646:LYS:NZ	6:N:722:GLU:HG2	2.28	0.48
4:A:150:TYR:OH	5:C:696:LYS:HA	2.12	0.48
4:B:115:LEU:O	4:B:115:LEU:HD12	2.13	0.48
5:C:119:PRO:HB2	11:C:1174:HOH:O	2.12	0.48
5:C:398:THR:HB	5:C:399:ASN:HD22	1.79	0.48
5:C:674:VAL:HG23	5:C:869:VAL:O	2.13	0.48
5:C:548:PRO:HG3	5:C:842:ARG:NH1	2.28	0.48
5:C:981:GLU:HG3	5:C:982:PRO:CD	2.43	0.48
6:D:164:GLY:O	6:D:199:LEU:HD12	2.13	0.48
6:D:764:LEU:HD12	6:D:766:ALA:H	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:174:VAL:HG13	4:L:200:TRP:O	2.13	0.48
5:M:98:LEU:HD21	5:M:373:VAL:HG21	1.95	0.48
5:M:736:ASP:HA	5:M:744:ARG:HH12	1.75	0.48
5:M:842:ARG:NH2	5:M:887:GLU:CD	2.66	0.48
6:N:1026:SER:C	6:N:1028:ALA:H	2.16	0.48
6:N:1220:ALA:O	6:N:1224:VAL:HG23	2.14	0.48
6:N:202:VAL:HB	6:N:398:ALA:O	2.13	0.48
6:N:543:LEU:HA	6:N:546:ARG:HG3	1.96	0.48
6:N:678:GLU:HB3	11:N:9222:HOH:O	2.13	0.48
6:N:959:GLU:O	6:N:963:TYR:HD1	1.96	0.48
6:N:757:ALA:CB	7:O:24:ALA:HB2	2.42	0.48
1:X:16:DG:N2	11:X:2005:HOH:O	2.46	0.48
5:C:1083:GLU:HA	5:C:1086:ARG:HE	1.79	0.48
5:C:98:LEU:HD13	5:C:110:GLU:O	2.13	0.48
5:C:622:GLU:O	5:C:624:PRO:HD3	2.14	0.48
6:D:1147:ARG:O	6:D:1166:LEU:HD23	2.12	0.48
6:D:1213:ARG:HH12	7:E:11:GLY:HA2	1.78	0.48
6:D:139:GLY:HA2	6:D:451:ASP:O	2.13	0.48
6:D:50:PHE:CB	6:D:522:PRO:HG3	2.43	0.48
6:D:827:ILE:H	6:D:827:ILE:HD12	1.77	0.48
6:D:881:LEU:HA	11:D:8376:HOH:O	2.13	0.48
4:L:73:GLU:OE1	4:L:130:ALA:HA	2.13	0.48
5:M:368:THR:N	5:M:369:PRO:HD2	2.29	0.48
5:M:52:PHE:HB3	5:M:53:PRO:HD3	1.95	0.48
5:M:880:MET:HE1	6:N:1243:THR:O	2.13	0.48
5:M:959:PRO:HB2	11:M:1487:HOH:O	2.13	0.48
6:N:1238:MET:HA	6:N:1241:PHE:HE2	1.76	0.48
6:N:119:SER:N	6:N:123:LEU:HB2	2.28	0.48
6:N:155:ASP:O	6:N:159:ARG:HB3	2.13	0.48
6:N:181:ASP:O	6:N:204:LEU:HA	2.13	0.48
6:N:606:ILE:HG23	11:N:9149:HOH:O	2.12	0.48
6:N:619:LEU:HG	6:N:621:LYS:HE2	1.94	0.48
6:N:759:ALA:O	6:N:763:MET:HB3	2.14	0.48
7:O:73:LEU:HD12	7:O:73:LEU:H	1.79	0.48
1:X:8:DT:H2"	1:X:9:DG:H8	1.77	0.48
5:C:415:PRO:HD2	5:C:418:LEU:HD13	1.95	0.48
5:C:601:GLY:HA3	5:C:615:TYR:HA	1.95	0.48
5:C:688:ILE:CG2	5:C:871:LEU:HD23	2.43	0.48
5:C:675:ALA:CA	5:C:989:VAL:HG13	2.43	0.48
6:D:1495:ILE:HG22	6:D:1499:ARG:NH2	2.28	0.48
6:D:133:ILE:HG13	6:D:153:LEU:HG	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:785:ILE:O	6:D:789:LEU:HG	2.14	0.48
5:M:1103:ASP:OD1	6:N:3:LYS:HD2	2.13	0.48
5:M:342:ASP:HA	5:M:345:ARG:CD	2.43	0.48
6:N:1378:TYR:O	6:N:1379:VAL:HG13	2.13	0.48
6:N:15:PRO:HB3	11:N:9303:HOH:O	2.12	0.48
6:N:399:ARG:HH21	6:N:431:VAL:HG22	1.78	0.48
6:N:584:ASN:HD21	6:N:590:PRO:HD2	1.77	0.48
6:N:92:HIS:CA	6:N:519:VAL:HG23	2.43	0.48
6:N:939:PHE:O	6:N:943:THR:HG23	2.13	0.48
1:X:12:DG:H2''	1:X:13:DT:O5'	2.14	0.48
2:Y:7:G:H5''	2:Y:7:G:C8	2.49	0.48
4:B:18:ARG:NH1	4:B:123:MET:HE1	2.14	0.48
4:B:23:PHE:HZ	4:B:207:PRO:HB2	1.78	0.48
5:C:1034:GLU:HA	5:C:1037:VAL:CG2	2.43	0.48
5:C:159:ILE:HD11	11:C:1246:HOH:O	2.13	0.48
5:C:168:ARG:HB2	11:C:1136:HOH:O	2.13	0.48
5:C:326:ASP:HB2	5:C:431:HIS:CG	2.49	0.48
5:C:409:ARG:NH1	5:C:444:PRO:HG2	2.28	0.48
6:D:110:SER:HB3	6:D:113:GLY:H	1.77	0.48
2:H:11:C:C2'	2:H:12:G:H5''	2.44	0.48
5:M:1012:PRO:HB2	5:M:1021:LEU:O	2.13	0.48
5:M:95:TYR:HD2	5:M:114:PHE:HB2	1.79	0.48
5:M:21:ILE:HD11	11:M:1541:HOH:O	2.13	0.48
5:M:218:VAL:HG22	5:M:221:LEU:HD21	1.94	0.48
5:M:260:LEU:HG	5:M:261:ILE:HG12	1.95	0.48
5:M:44:ILE:HD12	5:M:344:PHE:CD1	2.48	0.48
5:M:16:PRO:HG2	5:M:485:TYR:OH	2.14	0.48
5:M:607:ASP:HB3	5:M:609:ASN:H	1.79	0.48
5:M:61:LYS:HD3	5:M:61:LYS:O	2.14	0.48
6:N:1066:THR:HG22	6:N:1069:GLU:OE1	2.12	0.48
6:N:1441:GLN:OE1	6:N:1442:ASN:HB2	2.13	0.48
6:N:42:ASP:O	6:N:43:GLY:O	2.32	0.48
6:N:500:ARG:HG3	11:N:9399:HOH:O	2.14	0.48
6:N:95:LEU:HA	6:N:551:ASN:ND2	2.28	0.48
6:N:583:ASP:HB2	6:N:604:THR:OG1	2.14	0.48
6:N:613:ARG:HD3	6:N:613:ARG:HA	1.62	0.48
6:N:902:LEU:HB3	11:N:9040:HOH:O	2.13	0.48
7:O:41:GLU:N	7:O:42:PRO:CD	2.76	0.48
5:C:1103:ASP:OD1	5:C:1109:VAL:HG22	2.14	0.48
5:C:176:VAL:HG13	11:C:1142:HOH:O	2.14	0.48
5:C:205:GLU:O	5:C:209:ARG:HD2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:691:SER:HB2	5:C:858:MET:SD	2.53	0.48
5:C:758:ARG:NH2	5:C:788:THR:HB	2.29	0.48
6:D:963:TYR:HE2	6:D:1002:LYS:HB3	1.78	0.48
6:D:1381:VAL:HG13	11:D:8400:HOH:O	2.14	0.48
6:D:42:ASP:O	6:D:43:GLY:O	2.31	0.48
6:D:462:GLN:HA	6:D:513:ILE:HD13	1.94	0.48
6:D:762:GLN:CB	7:E:16:LYS:HE2	2.44	0.48
7:E:23:VAL:HG22	7:E:68:LEU:HD23	1.96	0.48
4:K:224:TYR:HD1	11:K:1342:HOH:O	1.96	0.48
4:L:124:ASN:N	4:L:125:PRO:HD3	2.29	0.48
4:L:173:PRO:HG3	11:L:367:HOH:O	2.14	0.48
5:M:260:LEU:HA	5:M:291:ALA:CB	2.43	0.48
5:M:626:ARG:HB3	5:M:626:ARG:HH11	1.79	0.48
5:M:767:PRO:HD3	11:M:1522:HOH:O	2.14	0.48
5:M:845:ASN:ND2	11:M:1407:HOH:O	2.46	0.48
6:N:1152:GLU:OE2	6:N:1154:GLU:HG3	2.13	0.48
6:N:1102:THR:HG22	6:N:1222:GLY:HA3	1.95	0.48
6:N:1378:TYR:HA	6:N:1395:LEU:H	1.78	0.48
6:N:490:ALA:HA	6:N:1390:LEU:CD1	2.44	0.48
2:Y:7:G:H8	2:Y:7:G:C5'	2.27	0.48
4:A:215:VAL:HG21	4:B:225:PHE:CD1	2.49	0.48
4:B:102:LYS:HZ2	4:B:139:ASN:HB2	1.78	0.48
5:C:265:ARG:H	5:C:289:THR:HG21	1.78	0.48
5:C:317:VAL:HG23	11:C:1254:HOH:O	2.14	0.48
5:C:562:SER:HB3	11:C:1416:HOH:O	2.12	0.48
5:C:405:ARG:NE	5:C:566:THR:HG21	2.28	0.48
5:C:587:VAL:HG23	11:C:1190:HOH:O	2.12	0.48
6:D:1112:CYS:HB2	6:D:1195:GLN:CG	2.32	0.48
6:D:119:SER:N	6:D:123:LEU:HB2	2.29	0.48
6:D:1381:VAL:HB	6:D:1389:LEU:O	2.14	0.48
6:D:562:ALA:HB1	6:D:567:ILE:CD1	2.44	0.48
6:D:644:LEU:HD23	6:D:718:PRO:CB	2.43	0.48
6:D:671:LYS:O	6:D:675:ARG:HG3	2.14	0.48
6:D:792:ILE:O	6:D:792:ILE:HG12	2.13	0.48
6:D:81:THR:HB	6:D:85:VAL:HG22	1.95	0.48
4:K:38:ASN:CB	5:M:980:GLY:HA3	2.40	0.48
4:L:23:PHE:O	4:L:196:THR:HA	2.14	0.48
4:L:226:SER:O	4:L:228:PRO:HD3	2.14	0.48
5:M:172:ILE:HG23	5:M:184:MET:SD	2.54	0.48
6:N:1098:LEU:HD23	6:N:1371:VAL:HG21	1.96	0.48
6:N:1336:LEU:CD1	6:N:1341:PRO:HG3	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:1383:ASP:HB2	6:N:1416:ALA:HB3	1.96	0.48
6:N:1499:ARG:HB2	6:N:1499:ARG:HH11	1.78	0.48
5:M:716:LYS:HZ1	6:N:36:THR:HA	1.78	0.48
6:N:394:LEU:HD21	6:N:445:ARG:CZ	2.43	0.48
6:N:93:ILE:HB	6:N:517:VAL:HB	1.96	0.48
5:M:1095:LEU:HD21	6:N:603:LEU:HB3	1.95	0.48
6:N:804:LEU:HD23	6:N:804:LEU:H	1.79	0.48
6:N:1484:THR:H	7:O:25:LYS:NZ	2.11	0.48
7:O:57:ASP:H	7:O:58:PRO:HD3	1.79	0.48
4:A:156:HIS:CD2	4:A:157:GLY:N	2.82	0.48
5:C:260:LEU:CD1	5:C:261:ILE:HG13	2.43	0.48
5:C:774:LEU:HD11	11:D:8351:HOH:O	2.14	0.48
5:C:833:LEU:HD13	5:C:996:LYS:HD2	1.96	0.48
6:D:1094:LEU:O	6:D:1098:LEU:HD13	2.14	0.48
6:D:1120:VAL:HB	6:D:1144:LEU:HD21	1.96	0.48
6:D:1221:VAL:O	6:D:1224:VAL:HB	2.14	0.48
6:D:153:LEU:HB3	11:D:8252:HOH:O	2.14	0.48
6:D:581:LEU:H	6:D:581:LEU:HD23	1.77	0.48
6:D:727:GLN:NE2	11:D:8105:HOH:O	2.46	0.48
7:E:5:GLY:HA3	7:E:8:LYS:HD2	1.96	0.48
1:G:23:DG:N2	11:G:185:HOH:O	2.46	0.48
4:K:36:LEU:O	4:K:39:PRO:HD2	2.14	0.48
5:M:129:ILE:HG22	5:M:130:ASN:N	2.29	0.48
5:M:21:ILE:HD12	5:M:21:ILE:N	2.29	0.48
5:M:256:TYR:HB2	11:M:1408:HOH:O	2.13	0.48
6:N:1109:GLU:CG	6:N:1201:CYS:HA	2.34	0.48
6:N:1223:ILE:H	6:N:1223:ILE:CD1	2.19	0.48
6:N:546:ARG:HH11	6:N:546:ARG:HB3	1.78	0.48
6:N:786:ILE:HD13	6:N:1027:GLY:CA	2.44	0.48
6:N:974:ILE:HD11	6:N:995:LEU:HD22	1.95	0.48
7:O:22:VAL:CG1	7:O:68:LEU:HD21	2.44	0.48
2:Y:7:G:H2'	2:Y:8:C:OP1	2.14	0.48
2:Y:9:G:C8	2:Y:9:G:C5'	2.97	0.48
4:B:153:ALA:HA	4:B:156:HIS:CE1	2.49	0.48
4:A:36:LEU:HD11	4:B:221:HIS:CD2	2.49	0.48
5:C:322:VAL:HG23	5:C:322:VAL:O	2.14	0.48
6:D:1097:LYS:O	6:D:1101:VAL:HG23	2.13	0.48
6:D:1105:ILE:HG23	6:D:1373:ARG:NH2	2.28	0.48
6:D:1462:LEU:HD21	6:D:1474:ALA:CB	2.42	0.48
6:D:93:ILE:HG13	6:D:519:VAL:CG2	2.43	0.48
5:C:681:GLY:O	6:D:633:VAL:HG11	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:675:ARG:HB3	6:D:675:ARG:CZ	2.43	0.48
6:D:650:LEU:HD23	6:D:691:LEU:CD2	2.43	0.48
6:D:769:LEU:HB2	6:D:919:PHE:CE1	2.49	0.48
3:I:4:DC:H2"	3:I:5:DG:O5'	2.14	0.48
4:L:7:LYS:HD2	4:L:7:LYS:O	2.14	0.48
5:M:1013:TYR:HB3	5:M:1018:GLN:OE1	2.13	0.48
5:M:101:ILE:HG22	5:M:102:HIS:N	2.29	0.48
5:M:1040:LEU:N	5:M:1040:LEU:HD12	2.29	0.48
5:M:91:GLN:NE2	5:M:383:ARG:HH22	2.12	0.48
5:M:684:PHE:HD2	11:N:9180:HOH:O	1.97	0.48
6:N:9:ARG:HA	6:N:1455:LYS:O	2.13	0.48
5:M:1030:GLN:HE22	6:N:628:ARG:HD3	1.78	0.48
4:A:150:TYR:CE1	5:C:696:LYS:HA	2.49	0.47
5:C:144:PRO:HA	5:C:163:ILE:CD1	2.44	0.47
5:C:193:LEU:N	5:C:193:LEU:HD12	2.29	0.47
5:C:433:THR:O	5:C:437:ARG:HD2	2.14	0.47
5:C:715:THR:CG2	5:C:717:LEU:HG	2.43	0.47
6:D:117:ASP:N	6:D:150:ARG:HH11	2.12	0.47
6:D:796:ARG:O	6:D:797:LYS:HD2	2.14	0.47
6:D:932:ASP:O	6:D:935:LYS:HB3	2.14	0.47
1:G:18:DG:H5"	6:D:628:ARG:HH22	1.79	0.47
4:K:213:GLN:O	4:K:217:ILE:HG13	2.13	0.47
5:M:152:PRO:HB2	11:M:1160:HOH:O	2.14	0.47
5:M:257:VAL:HG22	11:M:1151:HOH:O	2.13	0.47
5:M:129:ILE:HG13	5:M:386:PHE:HB3	1.96	0.47
5:M:503:LEU:HD23	5:M:507:ARG:O	2.14	0.47
5:M:604:ALA:HB3	5:M:612:VAL:O	2.14	0.47
5:M:571:LEU:HD21	5:M:700:TYR:CD2	2.49	0.47
5:M:780:GLU:HG3	5:M:781:LYS:HD3	1.96	0.47
5:M:833:LEU:HD21	5:M:839:LEU:HD11	1.96	0.47
5:M:969:GLN:CD	5:M:971:LYS:HE3	2.34	0.47
6:N:783:ARG:HH12	6:N:1029:ARG:NH2	2.12	0.47
6:N:1378:TYR:OH	6:N:1431:THR:HA	2.14	0.47
6:N:525:ARG:HB2	6:N:538:SER:CB	2.43	0.47
6:N:84:ILE:O	6:N:87:ARG:HG3	2.13	0.47
6:N:94:GLU:O	6:N:551:ASN:ND2	2.45	0.47
1:X:14:DT:H3'	6:N:610:LYS:HZ1	1.79	0.47
5:C:185:LYS:HB3	5:C:188:LYS:O	2.13	0.47
5:C:158:TYR:CD1	5:C:314:THR:HG22	2.44	0.47
5:C:31:GLN:HB3	5:C:71:TYR:HH	1.78	0.47
6:D:1124:GLN:HA	6:D:1125:PRO:HD3	1.65	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1147:ARG:HB2	6:D:1166:LEU:HD21	1.96	0.47
6:D:1147:ARG:HD2	6:D:1188:VAL:HG21	1.96	0.47
6:D:1228:SER:HA	11:D:8193:HOH:O	2.14	0.47
6:D:1087:ARG:NH2	6:D:1253:THR:HG22	2.27	0.47
6:D:1429:LEU:HG	6:D:1441:GLN:HG3	1.96	0.47
6:D:42:ASP:CG	6:D:48:ARG:HH22	2.18	0.47
6:D:440:VAL:CB	6:D:441:ARG:HH21	2.26	0.47
6:D:756:GLN:CG	6:D:760:ARG:HH11	2.25	0.47
6:D:796:ARG:NE	6:D:828:LYS:HZ2	2.12	0.47
6:D:902:LEU:HD13	11:D:8066:HOH:O	2.12	0.47
3:I:9:DG:H2"	3:I:10:DA:C8	2.50	0.47
4:K:111:ALA:HB3	4:K:124:ASN:O	2.13	0.47
4:K:2:LEU:HA	4:K:6:LEU:HD22	1.96	0.47
5:M:252:LYS:HZ2	5:M:296:GLY:HA3	1.77	0.47
5:M:487:THR:OG1	5:M:490:GLU:HG3	2.13	0.47
6:N:47:GLU:O	6:N:51:GLY:N	2.47	0.47
6:N:573:MET:HE2	11:N:9331:HOH:O	2.14	0.47
6:N:58:CYS:HA	6:N:78:VAL:HG11	1.96	0.47
6:N:838:ARG:HG2	6:N:838:ARG:HH11	1.79	0.47
6:N:861:GLN:H	6:N:861:GLN:NE2	2.12	0.47
7:O:57:ASP:N	7:O:58:PRO:HD3	2.30	0.47
4:A:171:PHE:O	4:A:173:PRO:HD3	2.15	0.47
4:A:26:GLU:HG2	4:A:27:PRO:HG3	1.96	0.47
4:A:73:GLU:H	4:A:73:GLU:CD	2.17	0.47
5:C:1102:LEU:HB2	6:D:7:LYS:HB2	1.96	0.47
5:C:31:GLN:HG2	5:C:31:GLN:O	2.14	0.47
5:C:77:PRO:HB2	5:C:78:PHE:CD1	2.49	0.47
6:D:1101:VAL:HG21	6:D:1424:VAL:CA	2.44	0.47
6:D:1441:GLN:OE1	6:D:1442:ASN:HB2	2.13	0.47
6:D:520:LEU:HD12	6:D:521:PRO:HD2	1.97	0.47
6:D:583:ASP:OD2	6:D:604:THR:HG21	2.14	0.47
6:D:619:LEU:N	6:D:619:LEU:HD23	2.29	0.47
5:M:287:GLY:O	5:M:288:ARG:C	2.52	0.47
5:M:620:LEU:N	5:M:620:LEU:HD12	2.29	0.47
5:M:734:LEU:HD11	11:M:1385:HOH:O	2.14	0.47
6:N:1130:ARG:HD3	11:N:9173:HOH:O	2.13	0.47
6:N:628:ARG:HG3	6:N:628:ARG:NH1	2.30	0.47
2:Y:7:G:O6	5:M:1015:LEU:N	2.45	0.47
3:Z:4:DC:H4'	11:Z:1418:HOH:O	2.15	0.47
4:A:101:LEU:HD22	4:A:114:PHE:CZ	2.49	0.47
4:B:64:GLU:HG2	4:B:64:GLU:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:158:TYR:HE1	5:C:314:THR:HA	1.79	0.47
5:C:18:LEU:HD22	5:C:404:LEU:HD21	1.95	0.47
5:C:244:PRO:CD	5:C:245:GLY:H	2.26	0.47
5:C:148:PHE:HZ	5:C:281:LEU:HB3	1.78	0.47
5:C:361:MET:HG3	5:C:371:LYS:HD2	1.96	0.47
5:C:437:ARG:HH21	5:C:469:THR:HG22	1.80	0.47
5:C:398:THR:HG21	5:C:567:GLN:C	2.34	0.47
4:A:67:THR:HG23	5:C:609:ASN:HD21	1.79	0.47
5:C:625:LEU:O	5:C:627:ARG:N	2.47	0.47
6:D:1033:GLN:O	6:D:1037:GLN:HG3	2.14	0.47
6:D:1200:VAL:N	11:D:8286:HOH:O	2.47	0.47
6:D:1262:LEU:HD23	6:D:1352:ILE:CG1	2.44	0.47
6:D:147:VAL:HG12	11:D:8415:HOH:O	2.14	0.47
6:D:159:ARG:HB3	6:D:163:TYR:OH	2.14	0.47
7:E:16:LYS:HD3	7:E:17:TYR:CE1	2.49	0.47
4:K:64:GLU:HG3	4:K:64:GLU:O	2.13	0.47
4:K:9:PRO:HB3	4:K:25:LEU:HD21	1.95	0.47
5:M:1067:TYR:HB3	11:M:1303:HOH:O	2.13	0.47
5:M:474:VAL:HG12	5:M:531:PHE:HA	1.96	0.47
5:M:610:ARG:NH1	5:M:612:VAL:HG23	2.30	0.47
5:M:65:VAL:HG12	5:M:67:ASP:OD2	2.14	0.47
5:M:734:LEU:HD21	11:M:1385:HOH:O	2.14	0.47
5:M:798:GLY:H	5:M:827:VAL:CG1	2.28	0.47
5:M:675:ALA:CA	5:M:989:VAL:HG12	2.38	0.47
6:N:1231:GLU:HB3	6:N:1232:PRO:HD3	1.96	0.47
5:M:1049:LEU:HD23	6:N:1472:ILE:HD12	1.95	0.47
6:N:394:LEU:O	6:N:396:VAL:N	2.47	0.47
5:M:764:GLU:HG3	6:N:54:LYS:HD3	1.96	0.47
6:N:610:LYS:HB2	11:N:9190:HOH:O	2.15	0.47
6:N:756:GLN:HE22	6:N:760:ARG:HB3	1.80	0.47
6:N:820:GLU:HA	6:N:825:ALA:O	2.15	0.47
6:N:95:LEU:N	6:N:95:LEU:HD12	2.24	0.47
7:O:26:ARG:NH1	7:O:29:GLN:HE21	2.13	0.47
4:B:154:GLU:HB3	4:B:155:LYS:HZ2	1.78	0.47
4:B:40:LEU:HD22	4:B:211:LEU:CD1	2.43	0.47
5:C:144:PRO:N	5:C:276:LYS:HZ2	2.12	0.47
5:C:759:THR:HG21	5:C:783:ARG:NH2	2.30	0.47
6:D:1220:ALA:HB1	6:D:1223:ILE:CD1	2.40	0.47
6:D:683:ILE:N	6:D:683:ILE:HD12	2.29	0.47
6:D:783:ARG:HA	6:D:1028:ALA:CA	2.29	0.47
6:D:876:SER:O	6:D:880:ILE:HG12	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:884:ARG:HG2	11:D:8116:HOH:O	2.14	0.47
5:M:310:LEU:O	5:M:314:THR:HG23	2.14	0.47
5:M:537:LYS:H	5:M:537:LYS:CD	2.20	0.47
6:N:1023:MET:HG2	6:N:1029:ARG:H	1.80	0.47
6:N:1268:PRO:HD3	6:N:1331:ASP:HB2	1.96	0.47
6:N:493:ARG:CZ	6:N:1391:GLU:HA	2.45	0.47
7:O:8:LYS:O	7:O:12:MET:HG3	2.14	0.47
7:O:13:VAL:HG12	7:O:14:ASP:N	2.29	0.47
4:A:79:ILE:HG21	4:A:165:ILE:HD11	1.94	0.47
4:B:45:LEU:HD21	6:D:855:HIS:NE2	2.30	0.47
5:C:260:LEU:C	5:C:260:LEU:HD12	2.34	0.47
5:C:626:ARG:N	5:C:639:GLN:HE21	2.13	0.47
5:C:722:ILE:CD1	5:C:823:VAL:HG21	2.39	0.47
5:C:874:LEU:HD11	6:D:787:LEU:HD23	1.97	0.47
6:D:1107:VAL:HA	6:D:1200:VAL:O	2.14	0.47
6:D:1160:LEU:CD1	6:D:1174:LEU:HD21	2.42	0.47
6:D:1223:ILE:HG22	6:D:1227:GLN:NE2	2.16	0.47
6:D:138:LYS:HE2	11:D:8030:HOH:O	2.14	0.47
6:D:401:TYR:HB2	11:D:8164:HOH:O	2.14	0.47
6:D:634:GLY:HA3	6:D:727:GLN:HG2	1.97	0.47
6:D:23:TYR:O	6:D:91:GLY:HA2	2.14	0.47
5:M:68:PHE:HZ	5:M:71:TYR:CD2	2.23	0.47
5:M:86:LYS:HD2	11:M:1208:HOH:O	2.14	0.47
5:M:7:GLY:O	5:M:8:ARG:NE	2.48	0.47
6:N:1220:ALA:CB	6:N:1223:ILE:HD13	2.27	0.47
6:N:119:SER:H	6:N:123:LEU:HB2	1.79	0.47
6:N:493:ARG:NH2	6:N:1391:GLU:HA	2.29	0.47
6:N:1432:LYS:HA	11:N:9333:HOH:O	2.13	0.47
6:N:520:LEU:HD11	6:N:524:LEU:HD23	1.96	0.47
5:M:764:GLU:CB	6:N:54:LYS:HD3	2.44	0.47
5:M:1090:LYS:CD	6:N:90:MET:HG3	2.40	0.47
4:B:117:VAL:HG11	11:B:324:HOH:O	2.14	0.47
6:D:638:LYS:HD2	6:D:932:ASP:OD1	2.14	0.47
5:M:172:ILE:HG23	5:M:184:MET:CE	2.45	0.47
5:M:27:ARG:HD3	5:M:28:ARG:N	2.29	0.47
5:M:331:ARG:CB	5:M:331:ARG:HH11	2.27	0.47
5:M:430:VAL:HG13	6:N:1075:HIS:ND1	2.30	0.47
5:M:462:ASP:CG	5:M:463:GLU:N	2.67	0.47
5:M:589:ARG:HG3	5:M:596:TYR:CE1	2.50	0.47
6:N:1197:ARG:HB2	6:N:1197:ARG:HH11	1.80	0.47
6:N:127:LEU:HD13	6:N:128:TYR:CD2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:204:LEU:O	6:N:394:LEU:HD23	2.14	0.47
6:N:666:ILE:HG13	6:N:666:ILE:H	1.41	0.47
2:Y:8:C:H2'	2:Y:9:G:N7	2.30	0.47
4:A:101:LEU:HD23	4:A:140:MET:HG2	1.95	0.47
4:B:124:ASN:HD21	4:B:127:LEU:HD22	1.78	0.47
5:C:1008:ARG:NH2	5:C:1011:GLY:N	2.62	0.47
5:C:1030:GLN:NE2	5:C:1030:GLN:HA	2.29	0.47
5:C:1115:LEU:HG	6:D:85:VAL:HG12	1.97	0.47
5:C:287:GLY:O	5:C:288:ARG:C	2.53	0.47
5:C:322:VAL:HB	11:C:1379:HOH:O	2.15	0.47
5:C:564:MET:HG3	5:C:565:GLN:N	2.29	0.47
4:A:69:PRO:HA	5:C:607:ASP:OD1	2.14	0.47
5:C:874:LEU:HD11	6:D:787:LEU:CD2	2.44	0.47
6:D:137:PRO:HD3	6:D:455:ARG:HH21	1.80	0.47
6:D:1496:GLU:HA	6:D:1499:ARG:CZ	2.44	0.47
6:D:206:ARG:HB2	6:D:392:SER:O	2.14	0.47
6:D:398:ALA:HA	6:D:446:VAL:O	2.15	0.47
6:D:455:ARG:CB	6:D:460:ALA:CA	2.86	0.47
6:D:800:LYS:HE3	6:D:804:LEU:HD13	1.96	0.47
6:D:97:THR:HG21	6:D:571:LYS:HZ3	1.80	0.47
4:K:177:VAL:O	5:M:864:GLY:HA3	2.15	0.47
4:L:161:ARG:HD2	4:L:161:ARG:N	2.30	0.47
4:L:43:ILE:HG23	4:L:47:SER:HB3	1.97	0.47
4:L:81:ASN:O	4:L:127:LEU:HD21	2.15	0.47
5:M:1056:LYS:HD3	6:N:625:TYR:CD1	2.50	0.47
5:M:1090:LYS:HG2	5:M:1112:PHE:CZ	2.48	0.47
5:M:119:PRO:HG2	5:M:386:PHE:CD2	2.49	0.47
5:M:162:ILE:HB	5:M:172:ILE:HB	1.96	0.47
5:M:437:ARG:C	5:M:438:ILE:HD12	2.35	0.47
5:M:689:VAL:HG11	5:M:870:ILE:CD1	2.44	0.47
5:M:45:GLN:HE21	5:M:68:PHE:HE2	1.62	0.47
5:M:769:PRO:HG2	6:N:65:ARG:CD	2.45	0.47
5:M:926:PHE:HD2	5:M:930:LYS:HE3	1.80	0.47
6:N:1204:CYS:C	11:N:9238:HOH:O	2.51	0.47
6:N:1353:GLN:HG2	6:N:1368:ILE:CD1	2.45	0.47
6:N:634:GLY:HA2	6:N:727:GLN:HE21	1.79	0.47
4:B:58:ILE:HD13	4:B:140:MET:HB3	1.96	0.47
5:C:204:GLN:OE1	5:C:222:MET:HA	2.15	0.47
5:C:26:TYR:CD2	5:C:121:MET:HB2	2.49	0.47
5:C:573:ARG:HG2	5:C:670:GLN:OE1	2.15	0.47
5:C:688:ILE:N	11:C:1474:HOH:O	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:964:LYS:NZ	5:C:968:LEU:HD21	2.29	0.47
6:D:135:LEU:HB2	6:D:148:GLU:O	2.15	0.47
6:D:1384:PRO:HG3	6:D:1389:LEU:CA	2.45	0.47
6:D:1462:LEU:HD23	6:D:1473:PRO:HD2	1.96	0.47
6:D:173:PRO:HB2	11:D:8270:HOH:O	2.13	0.47
6:D:720:LEU:H	6:D:720:LEU:HD12	1.80	0.47
6:D:53:ILE:HA	6:D:86:ARG:CZ	2.44	0.47
7:E:64:ALA:O	7:E:68:LEU:HD13	2.14	0.47
2:H:10:G:C2'	2:H:11:C:H5'	2.45	0.47
5:M:1031:ARG:NH1	6:N:621:LYS:HZ2	2.13	0.47
5:M:376:ARG:HH11	5:M:376:ARG:HG3	1.80	0.47
5:M:603:VAL:H	5:M:647:GLN:H	1.63	0.47
5:M:78:PHE:HB3	5:M:82:GLU:OE1	2.14	0.47
5:M:996:LYS:HE3	11:M:1161:HOH:O	2.14	0.47
6:N:519:VAL:HA	6:N:544:TYR:OH	2.15	0.47
5:M:1070:ILE:HG23	6:N:656:PHE:CD1	2.50	0.47
4:L:152:PRO:HG2	6:N:857:ILE:HD12	1.96	0.47
4:A:89:PHE:HZ	4:A:146:ARG:HB2	1.80	0.47
4:A:73:GLU:CD	4:A:130:ALA:HA	2.35	0.47
4:B:162:ILE:HD12	4:B:163:ASN:N	2.29	0.47
1:G:19:DC:P	5:C:1001:VAL:HB	2.55	0.47
5:C:1016:ILE:HG12	5:C:1017:THR:N	2.29	0.47
5:C:1036:GLU:O	5:C:1039:ALA:HB3	2.14	0.47
5:C:470:PRO:HD3	5:C:485:TYR:HE2	1.79	0.47
5:C:769:PRO:HB3	11:D:8366:HOH:O	2.15	0.47
5:C:553:ASP:OD1	5:C:843:HIS:HB3	2.14	0.47
5:C:937:ASP:HB2	5:C:940:GLU:CG	2.43	0.47
6:D:116:LEU:HD22	6:D:118:LEU:CD2	2.45	0.47
6:D:1472:ILE:HD13	6:D:1472:ILE:N	2.29	0.47
6:D:704:ARG:HH12	6:D:743:ASP:CB	2.28	0.47
2:H:7:G:H5"	2:H:7:G:C8	2.50	0.47
4:K:112:ARG:HG2	4:K:125:PRO:CA	2.45	0.47
4:L:140:MET:HG2	4:L:141:GLU:N	2.28	0.47
4:L:222:LEU:HA	4:L:225:PHE:CE1	2.50	0.47
5:M:625:LEU:O	5:M:627:ARG:N	2.48	0.47
5:M:688:ILE:CD1	5:M:847:GLY:HA3	2.45	0.47
5:M:69:LEU:HD21	5:M:99:GLN:HG3	1.97	0.47
6:N:1156:LEU:HD21	6:N:1177:ALA:HA	1.97	0.47
6:N:1221:VAL:HG12	6:N:1222:GLY:N	2.30	0.47
6:N:1476:THR:C	6:N:1478:SER:N	2.67	0.47
6:N:26:VAL:HG21	6:N:519:VAL:HG11	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:439:LEU:HG	11:N:9125:HOH:O	2.15	0.47
6:N:756:GLN:O	6:N:756:GLN:NE2	2.48	0.47
6:N:711:LEU:HD21	6:N:768:ASN:HB2	1.95	0.47
6:N:845:ASN:ND2	6:N:846:PRO:HD2	2.30	0.47
6:N:884:ARG:HG2	11:N:9101:HOH:O	2.14	0.47
7:O:38:THR:HG21	7:O:63:TRP:CZ3	2.50	0.47
1:X:21:DC:H3'	11:X:589:HOH:O	2.14	0.47
4:A:48:ILE:CD1	4:A:210:ALA:HB1	2.44	0.47
4:B:110:LYS:HD3	4:B:112:ARG:HG2	1.97	0.47
4:B:51:THR:HG23	11:B:316:HOH:O	2.15	0.47
5:C:1095:LEU:HD22	6:D:101:HIS:CE1	2.49	0.47
5:C:146:VAL:CG2	5:C:162:ILE:HG23	2.43	0.47
5:C:437:ARG:HG2	5:C:467:ILE:O	2.15	0.47
5:C:674:VAL:HG11	5:C:992:MET:HB3	1.97	0.47
6:D:1191:PRO:HB3	6:D:1370:ILE:HD13	1.95	0.47
6:D:130:SER:HB3	6:D:132:TYR:CE1	2.50	0.47
6:D:710:ARG:C	6:D:712:GLY:H	2.18	0.47
6:D:796:ARG:HH21	6:D:828:LYS:CE	2.27	0.47
6:D:896:ALA:O	6:D:899:LEU:HD12	2.15	0.47
2:H:8:C:H2'	2:H:9:G:N7	2.30	0.47
4:L:34:VAL:HA	4:L:179:PHE:HE1	1.79	0.47
5:M:151:ASP:OD1	5:M:154:ARG:HB3	2.15	0.47
5:M:806:LEU:HD11	5:M:824:ARG:HH22	1.79	0.47
5:M:822:VAL:CB	5:M:824:ARG:HH21	2.28	0.47
5:M:876:VAL:HG13	5:M:881:ASN:HD21	1.79	0.47
6:N:1118:ILE:HG12	6:N:1193:THR:HG23	1.97	0.47
6:N:1442:ASN:CG	6:N:1444:THR:HB	2.36	0.47
6:N:1462:LEU:HD21	6:N:1474:ALA:HB3	1.97	0.47
4:A:175:ARG:NH2	4:A:176:ARG:HD3	2.30	0.46
4:A:88:ARG:NH1	4:A:89:PHE:O	2.47	0.46
4:B:27:PRO:C	4:B:28:LEU:HD23	2.35	0.46
5:C:1103:ASP:N	5:C:1107:ASN:O	2.44	0.46
5:C:265:ARG:HD2	5:C:267:TYR:CG	2.50	0.46
5:C:292:ARG:HB2	5:C:299:LYS:HG2	1.97	0.46
5:C:580:MET:HB3	5:C:584:GLU:CD	2.35	0.46
4:A:133:GLU:OE1	5:C:605:LYS:HB3	2.16	0.46
5:C:394:PHE:CE1	5:C:632:ASN:HB3	2.49	0.46
5:C:69:LEU:C	5:C:70:GLU:HG2	2.35	0.46
5:C:737:LEU:HD21	5:C:741:GLY:C	2.36	0.46
5:C:872:ASN:ND2	5:C:874:LEU:N	2.63	0.46
5:C:900:ARG:NH1	11:C:1210:HOH:O	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:999:HIS:HB2	11:C:1358:HOH:O	2.15	0.46
5:C:1098:ASP:O	6:D:10:ILE:HA	2.15	0.46
6:D:1198:TYR:HE2	6:D:1377:LYS:HD2	1.80	0.46
6:D:161:LEU:HD21	6:D:452:ILE:CG2	2.27	0.46
6:D:118:LEU:HD13	6:D:461:ILE:HD12	1.97	0.46
6:D:502:PHE:HA	11:D:8084:HOH:O	2.14	0.46
6:D:502:PHE:CZ	6:D:509:PRO:HB3	2.50	0.46
6:D:843:PHE:CE1	6:D:864:VAL:HG11	2.50	0.46
7:E:54:LEU:HA	7:E:58:PRO:CG	2.44	0.46
2:H:4:U:O2'	2:H:5:C:H5'	2.15	0.46
4:K:111:ALA:HB2	4:K:127:LEU:CD2	2.45	0.46
4:K:177:VAL:HG13	4:K:199:ILE:CD1	2.45	0.46
4:L:94:LEU:HD11	4:L:119:ASP:HB2	1.97	0.46
5:M:2:GLU:O	5:M:3:ILE:HD13	2.15	0.46
5:M:678:PRO:HD2	11:N:9146:HOH:O	2.14	0.46
5:M:498:GLN:HE22	6:N:1067:VAL:CG1	2.28	0.46
6:N:1121:PRO:HB2	6:N:1135:ARG:HH12	1.79	0.46
6:N:1122:LEU:HD11	6:N:1186:VAL:HG23	1.97	0.46
6:N:1149:LEU:HD23	6:N:1187:PRO:O	2.15	0.46
6:N:1389:LEU:HG	6:N:1390:LEU:H	1.79	0.46
6:N:10:ILE:HD11	6:N:1434:TRP:NE1	2.30	0.46
6:N:134:VAL:CG1	6:N:152:LEU:HD22	2.45	0.46
6:N:462:GLN:O	6:N:466:LYS:HG3	2.15	0.46
6:N:481:MET:CE	6:N:1388:ARG:HG3	2.44	0.46
6:N:493:ARG:HD2	6:N:494:LYS:N	2.30	0.46
7:O:91:ARG:HH11	7:O:92:LEU:HD21	1.80	0.46
2:Y:15:C:H2'	2:Y:16:G:C8	2.50	0.46
4:A:7:LYS:HE3	4:A:186:LEU:HD22	1.97	0.46
4:A:42:ARG:HH12	4:B:34:VAL:CG1	2.28	0.46
5:C:172:ILE:H	5:C:172:ILE:HD12	1.80	0.46
5:C:193:LEU:N	5:C:193:LEU:CD1	2.78	0.46
5:C:207:LEU:HD22	5:C:221:LEU:HD13	1.97	0.46
5:C:292:ARG:HD2	5:C:299:LYS:CE	2.46	0.46
5:C:713:ARG:HH22	6:D:532:GLY:H	1.62	0.46
5:C:718:GLY:HA3	5:C:761:PHE:CE1	2.50	0.46
5:C:859:PRO:HB3	5:C:974:LEU:CD2	2.44	0.46
6:D:1100:ASP:HB3	6:D:1428:ALA:HB1	1.97	0.46
6:D:136:ASP:OD2	6:D:464:LEU:HD23	2.15	0.46
6:D:1468:LEU:HD23	6:D:1468:LEU:O	2.15	0.46
6:D:540:LEU:HA	6:D:543:LEU:HD11	1.97	0.46
6:D:647:ARG:HA	6:D:650:LEU:HD12	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:66:GLN:O	6:D:69:GLU:HB3	2.16	0.46
6:D:69:GLU:HG2	6:D:70:GLY:N	2.30	0.46
6:D:871:LYS:NZ	6:N:442:ASN:HD22	2.13	0.46
5:C:1100:GLN:HB3	6:D:9:ARG:HH21	1.80	0.46
7:E:48:MET:HB2	7:E:54:LEU:HB2	1.96	0.46
2:H:9:G:C5'	2:H:9:G:C8	2.98	0.46
4:K:181:VAL:H	5:M:937:ASP:CG	2.19	0.46
4:L:124:ASN:HD21	4:L:127:LEU:HB2	1.80	0.46
5:M:512:ARG:HB3	5:M:523:ILE:HD11	1.97	0.46
5:M:689:VAL:CG1	5:M:690:ILE:H	2.25	0.46
5:M:751:PRO:HB2	6:N:680:GLN:NE2	2.30	0.46
5:M:79:PRO:HA	5:M:90:TYR:HE2	1.80	0.46
5:M:897:LEU:HD11	5:M:920:GLN:HB3	1.97	0.46
5:M:911:GLU:HB2	5:M:912:PRO:HD3	1.97	0.46
5:M:940:GLU:HG3	11:M:1220:HOH:O	2.15	0.46
5:M:862:PRO:HD3	5:M:973:VAL:O	2.14	0.46
5:M:668:LEU:HD13	5:M:995:MET:CE	2.44	0.46
6:N:1381:VAL:HB	6:N:1389:LEU:O	2.14	0.46
5:M:1050:GLN:NE2	6:N:1471:LEU:N	2.58	0.46
6:N:133:ILE:HB	6:N:153:LEU:CD1	2.45	0.46
6:N:33:ASN:O	6:N:36:THR:O	2.33	0.46
6:N:434:ARG:NH2	6:N:447:VAL:HG11	2.29	0.46
6:N:452:ILE:HB	11:N:9092:HOH:O	2.14	0.46
6:N:92:HIS:HA	6:N:519:VAL:HG23	1.96	0.46
4:B:170:VAL:HG23	4:B:170:VAL:O	2.16	0.46
4:B:206:THR:HG23	4:B:208:LEU:N	2.29	0.46
5:C:212:GLY:HA3	5:C:218:VAL:HG21	1.96	0.46
5:C:456:ALA:HA	5:C:541:SER:HA	1.97	0.46
5:C:494:TYR:HD2	5:C:530:GLU:HB3	1.81	0.46
5:C:600:ASP:OD1	5:C:651:LYS:HB2	2.15	0.46
6:D:119:SER:HB2	6:D:123:LEU:N	2.29	0.46
6:D:164:GLY:HA3	11:D:8094:HOH:O	2.15	0.46
4:K:26:GLU:HG3	4:K:184:THR:HG21	1.95	0.46
4:K:200:TRP:HZ2	11:M:1430:HOH:O	1.97	0.46
5:M:677:MET:HB3	5:M:987:ILE:HD13	1.96	0.46
5:M:798:GLY:HA3	5:M:828:ALA:O	2.15	0.46
5:M:831:ARG:NH1	5:M:999:HIS:HB3	2.31	0.46
6:N:1252:ILE:HA	11:N:9048:HOH:O	2.14	0.46
6:N:133:ILE:HG22	6:N:455:ARG:N	2.30	0.46
6:N:1369:GLU:HA	6:N:1372:VAL:HG12	1.97	0.46
6:N:396:VAL:C	6:N:398:ALA:N	2.69	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:564:GLU:O	6:N:567:ILE:HG13	2.16	0.46
6:N:799:LYS:HB3	6:N:826:PRO:HG2	1.97	0.46
6:N:890:VAL:HG12	6:N:926:LYS:CD	2.35	0.46
6:N:793:THR:OG1	6:N:905:PRO:HA	2.14	0.46
4:A:156:HIS:CD2	4:A:157:GLY:H	2.32	0.46
4:A:18:ARG:O	4:A:207:PRO:HD3	2.15	0.46
5:C:159:ILE:CG2	5:C:175:GLU:HB2	2.45	0.46
5:C:197:LEU:HB3	5:C:202:TYR:HB2	1.97	0.46
5:C:75:GLU:HA	5:C:76:PRO:HD3	1.79	0.46
6:D:116:LEU:HG	6:D:468:LEU:CD1	2.46	0.46
6:D:117:ASP:O	6:D:150:ARG:HD2	2.16	0.46
6:D:1394:VAL:HB	6:D:1397:LYS:HB2	1.97	0.46
6:D:407:VAL:HG13	6:D:422:ALA:HB2	1.97	0.46
6:D:844:ALA:O	6:D:867:ARG:HB3	2.15	0.46
5:C:889:HIS:CE1	6:D:951:ILE:HG22	2.50	0.46
2:H:5:C:H6	2:H:5:C:O5'	1.98	0.46
4:L:102:LYS:HD2	4:L:138:LEU:O	2.15	0.46
4:L:184:THR:CG2	4:L:194:LYS:HB2	2.45	0.46
4:L:43:ILE:HD12	4:L:217:ILE:CG2	2.45	0.46
4:L:39:PRO:HD3	11:L:348:HOH:O	2.16	0.46
5:M:286:SER:OG	5:M:299:LYS:HE3	2.15	0.46
5:M:381:ALA:HB2	11:M:1457:HOH:O	2.15	0.46
5:M:401:LEU:HG	5:M:402:SER:N	2.29	0.46
5:M:611:ILE:HD11	5:M:641:PRO:HG3	1.97	0.46
5:M:739:GLU:OE2	5:M:744:ARG:HA	2.14	0.46
5:M:948:GLU:OE1	5:M:955:PRO:HA	2.16	0.46
6:N:1335:LEU:HD13	6:N:1347:TYR:CE2	2.50	0.46
6:N:18:ILE:HG23	6:N:518:PRO:CG	2.23	0.46
6:N:204:LEU:HB3	6:N:445:ARG:HH21	1.81	0.46
6:N:792:ILE:HD13	6:N:793:THR:CG2	2.44	0.46
6:N:820:GLU:CB	6:N:836:VAL:HG21	2.45	0.46
6:N:911:LEU:O	6:N:915:VAL:HG23	2.14	0.46
5:M:984:GLU:HG3	6:N:944:THR:O	2.15	0.46
1:X:15:DC:H2"	1:X:16:DG:H8	1.80	0.46
4:A:101:LEU:HD22	4:A:114:PHE:CE2	2.49	0.46
4:A:173:PRO:O	4:A:201:THR:HG22	2.16	0.46
5:C:1046:ALA:HB3	6:D:1476:THR:HB	1.98	0.46
5:C:198:ARG:HD3	5:C:228:ALA:HA	1.98	0.46
5:C:605:LYS:CD	5:C:612:VAL:HB	2.45	0.46
6:D:123:LEU:HD11	6:D:152:LEU:CD2	2.39	0.46
6:D:399:ARG:HH11	6:D:430:ASP:CB	2.25	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:434:ARG:HB2	6:D:447:VAL:HG22	1.98	0.46
4:K:52:ALA:HB2	4:K:170:VAL:O	2.15	0.46
5:M:109:LYS:HE2	5:M:111:ASP:HA	1.97	0.46
5:M:217:LEU:HD12	5:M:311:PHE:HA	1.96	0.46
5:M:326:ASP:OD1	5:M:427:VAL:HG22	2.14	0.46
5:M:468:ARG:HB3	5:M:486:MET:O	2.14	0.46
5:M:61:LYS:NZ	11:M:1290:HOH:O	2.48	0.46
4:K:30:ARG:NH1	5:M:938:LYS:HD2	2.31	0.46
6:N:1146:GLY:O	6:N:1207:TYR:N	2.48	0.46
6:N:1221:VAL:O	6:N:1224:VAL:HB	2.15	0.46
6:D:1184:GLN:N	6:N:559:ALA:O	2.47	0.46
6:N:637:LEU:CD1	6:N:641:GLN:HB2	2.45	0.46
5:C:1083:GLU:CG	5:C:1086:ARG:HH21	2.25	0.46
5:C:181:VAL:HG12	5:C:182:VAL:N	2.30	0.46
5:C:226:VAL:HG13	5:C:227:PHE:CD1	2.51	0.46
5:C:732:ALA:HA	5:C:735:ARG:CZ	2.45	0.46
5:C:737:LEU:HD21	5:C:741:GLY:N	2.30	0.46
6:D:1002:LYS:HA	11:D:8149:HOH:O	2.16	0.46
6:D:1335:LEU:CD2	6:D:1344:VAL:HG22	2.46	0.46
6:D:785:ILE:HG22	6:D:789:LEU:CD1	2.36	0.46
4:K:23:PHE:O	4:K:196:THR:HA	2.16	0.46
4:K:224:TYR:HB3	4:L:9:PRO:CB	2.45	0.46
5:M:1047:HIS:N	5:M:1047:HIS:CD2	2.83	0.46
5:M:689:VAL:O	5:M:869:VAL:HG23	2.15	0.46
5:M:937:ASP:O	5:M:941:VAL:HG23	2.16	0.46
5:M:939:ARG:CB	5:M:982:PRO:HG3	2.33	0.46
6:N:400:VAL:O	6:N:400:VAL:HG13	2.16	0.46
6:N:654:LYS:NZ	6:N:654:LYS:HB2	2.31	0.46
6:N:880:ILE:O	6:N:883:ALA:HB3	2.15	0.46
5:M:1093:GLN:HB3	6:N:90:MET:SD	2.55	0.46
4:A:86:VAL:HG12	4:A:124:ASN:HB2	1.97	0.46
5:C:445:GLU:HA	5:C:449:ILE:HD12	1.97	0.46
5:C:902:ILE:O	5:C:904:PRO:HD3	2.15	0.46
5:C:971:LYS:HB2	5:C:986:PRO:HB2	1.97	0.46
6:D:1042:ARG:NH2	6:D:1061:PHE:HZ	2.12	0.46
6:D:1213:ARG:HH12	7:E:10:PHE:C	2.19	0.46
6:D:1393:GLN:HE22	6:D:1394:VAL:HB	1.80	0.46
6:D:618:LEU:HD12	6:D:1439:SER:HB3	1.96	0.46
5:C:1082:PRO:HD2	6:D:1468:LEU:O	2.15	0.46
6:D:436:GLU:HB2	6:D:445:ARG:CG	2.45	0.46
6:D:987:GLU:O	6:D:991:GLN:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:68:ILE:HG21	11:L:362:HOH:O	2.15	0.46
5:M:146:VAL:CG2	5:M:281:LEU:HD11	2.46	0.46
5:M:260:LEU:HA	5:M:291:ALA:HB2	1.98	0.46
5:M:467:ILE:HG23	11:M:1287:HOH:O	2.15	0.46
5:M:748:GLU:HA	5:M:799:ILE:HD13	1.97	0.46
6:N:30:GLU:HB3	6:N:40:GLU:HB3	1.96	0.46
6:N:611:GLN:O	6:N:611:GLN:HG3	2.14	0.46
5:C:1081:VAL:HG23	11:C:1198:HOH:O	2.16	0.46
5:C:1101:THR:HG23	5:C:1109:VAL:O	2.16	0.46
5:C:218:VAL:O	5:C:221:LEU:HG	2.16	0.46
5:C:232:GLU:O	5:C:236:ILE:HD12	2.16	0.46
5:C:522:VAL:HG21	11:C:1425:HOH:O	2.15	0.46
5:C:524:VAL:HG13	5:C:528:GLU:HB2	1.98	0.46
5:C:545:ASN:OD1	5:C:583:LEU:HD22	2.16	0.46
5:C:834:GLN:HE21	5:C:834:GLN:HB2	1.58	0.46
6:D:786:ILE:CG2	6:D:1026:SER:HB3	2.37	0.46
6:D:1031:ASN:HB3	6:D:1034:GLN:CD	2.36	0.46
6:D:1101:VAL:HG12	6:D:1374:GLN:HB3	1.97	0.46
6:D:31:THR:HB	6:D:527:MET:CE	2.46	0.46
6:D:438:ASP:HB2	6:D:445:ARG:NH1	2.31	0.46
6:D:785:ILE:H	6:D:785:ILE:CD1	2.13	0.46
6:D:939:PHE:O	6:D:943:THR:HG23	2.16	0.46
5:M:1036:GLU:O	5:M:1039:ALA:HB3	2.16	0.46
5:M:567:GLN:HG2	11:M:1537:HOH:O	2.15	0.46
5:M:694:LEU:HD21	5:M:868:ASP:OD2	2.15	0.46
5:M:906:PHE:CZ	6:N:1067:VAL:HA	2.51	0.46
6:N:1145:TYR:HD2	6:N:1168:MET:SD	2.39	0.46
6:N:1209:LEU:CD2	6:N:1210:SER:H	2.28	0.46
6:N:1402:ALA:HB2	6:N:1415:VAL:CG2	2.46	0.46
6:N:403:PHE:CE2	6:N:444:VAL:HG23	2.51	0.46
6:N:397:LYS:HB3	6:N:448:GLU:CB	2.46	0.46
6:N:62:LYS:HG3	6:N:75:ARG:HD2	1.98	0.46
6:N:960:LYS:HD3	11:N:9374:HOH:O	2.15	0.46
6:N:984:THR:CG2	6:N:987:GLU:H	2.29	0.46
1:X:15:DC:H2"	1:X:16:DG:C8	2.51	0.46
5:C:231:PRO:HD2	11:C:1261:HOH:O	2.16	0.46
5:C:401:LEU:CD2	5:C:565:GLN:HE21	2.29	0.46
5:C:418:LEU:HD12	5:C:418:LEU:N	2.31	0.46
5:C:437:ARG:HG2	5:C:467:ILE:HB	1.98	0.46
5:C:516:ARG:HH21	6:D:1068:LEU:HB3	1.81	0.46
5:C:404:LEU:HD22	5:C:591:SER:HB3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1228:SER:O	6:D:1232:PRO:CD	2.58	0.46
6:D:783:ARG:HH22	6:D:1239:ARG:HH22	1.64	0.46
6:D:33:ASN:HB2	6:D:40:GLU:OE1	2.16	0.46
6:D:749:VAL:HA	6:D:750:PRO:HD3	1.82	0.46
6:D:800:LYS:CE	6:D:804:LEU:HD22	2.43	0.46
6:D:951:ILE:HD13	6:D:951:ILE:O	2.16	0.46
4:K:185:ARG:O	4:K:185:ARG:HD2	2.15	0.46
5:M:1008:ARG:HH12	5:M:1011:GLY:N	2.14	0.46
5:M:745:ILE:CD1	5:M:745:ILE:H	2.22	0.46
5:M:864:GLY:O	5:M:866:PRO:HD3	2.15	0.46
5:M:674:VAL:HG21	5:M:871:LEU:HG	1.98	0.46
5:M:91:GLN:NE2	5:M:117:HIS:O	2.49	0.46
6:N:1112:CYS:CB	6:N:1195:GLN:HG2	2.44	0.46
6:N:1349:VAL:HA	6:N:1368:ILE:HG21	1.98	0.46
6:N:543:LEU:CD1	6:N:581:LEU:HA	2.38	0.46
6:N:707:THR:HG22	6:N:712:GLY:HA3	1.96	0.46
6:N:968:ASP:O	6:N:971:LEU:HB3	2.16	0.46
6:N:974:ILE:CD1	6:N:995:LEU:HD22	2.45	0.46
6:N:760:ARG:NH1	7:O:61:VAL:HG23	2.27	0.46
5:C:124:ASP:OD1	5:C:124:ASP:N	2.48	0.46
5:C:169:GLY:CA	5:C:263:ASP:HB3	2.44	0.46
5:C:217:LEU:HD11	5:C:314:THR:OG1	2.16	0.46
5:C:322:VAL:HG13	11:C:1193:HOH:O	2.14	0.46
5:C:333:ILE:HD12	5:C:333:ILE:N	2.31	0.46
5:C:737:LEU:HD21	5:C:741:GLY:H	1.81	0.46
5:C:758:ARG:HG2	5:C:758:ARG:HH11	1.81	0.46
6:D:1166:LEU:HD12	6:D:1171:VAL:HG22	1.98	0.46
6:D:19:ARG:H	6:D:19:ARG:HG2	1.51	0.46
6:D:407:VAL:HA	6:D:422:ALA:CB	2.46	0.46
6:D:443:VAL:CG1	6:D:445:ARG:HH22	2.29	0.46
6:D:617:ASN:HA	11:D:8092:HOH:O	2.15	0.46
6:D:638:LYS:NZ	11:D:8121:HOH:O	2.48	0.46
6:D:71:LYS:HB2	6:D:71:LYS:HZ3	1.79	0.46
6:D:899:LEU:HB3	6:D:921:ARG:NH1	2.31	0.46
6:D:926:LYS:HG2	6:D:929:ARG:NH1	2.30	0.46
7:E:37:ASN:HD22	7:E:89:MET:CE	2.29	0.46
1:G:6:DT:H71	11:G:2394:HOH:O	2.16	0.46
4:L:175:ARG:HD3	4:L:202:ASP:HB3	1.98	0.46
5:M:1019:GLN:NE2	11:N:9292:HOH:O	2.48	0.46
5:M:1060:ILE:CD1	5:M:1064:ASN:HD21	2.29	0.46
5:M:342:ASP:O	5:M:346:VAL:HG23	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:433:THR:C	5:M:435:TYR:H	2.18	0.46
5:M:568:ALA:HB3	11:M:1233:HOH:O	2.15	0.46
6:N:1002:LYS:HA	11:N:9185:HOH:O	2.15	0.46
6:N:115:LEU:HB2	6:N:498:VAL:HG11	1.98	0.46
6:N:1353:GLN:HG2	6:N:1368:ILE:HD11	1.98	0.46
6:N:1366:LYS:O	6:N:1370:ILE:HG12	2.15	0.46
6:N:1394:VAL:HB	6:N:1397:LYS:CB	2.43	0.46
6:N:30:GLU:HB3	6:N:40:GLU:CB	2.45	0.46
6:N:481:MET:HE3	6:N:496:LEU:HD23	1.98	0.46
6:N:491:LYS:O	6:N:491:LYS:HD2	2.16	0.46
5:M:1031:ARG:HE	6:N:621:LYS:HB3	1.80	0.46
6:N:644:LEU:HD12	6:N:645:PRO:CD	2.46	0.46
6:N:65:ARG:HA	6:N:65:ARG:HD2	1.70	0.46
6:N:902:LEU:HD13	11:N:9040:HOH:O	2.14	0.46
6:N:959:GLU:O	6:N:963:TYR:CD1	2.70	0.46
5:C:219:GLN:HA	5:C:222:MET:HE2	1.98	0.45
5:C:5:ARG:HB2	5:C:5:ARG:HE	1.65	0.45
5:C:950:LEU:HB3	5:C:952:LEU:CD2	2.44	0.45
5:C:430:VAL:HG12	6:D:1078:ARG:HG3	1.98	0.45
6:D:1123:PHE:CZ	6:D:1178:ALA:HB1	2.51	0.45
6:D:1218:GLY:HA2	11:D:8043:HOH:O	2.15	0.45
6:D:496:LEU:HD21	6:D:1388:ARG:CG	2.44	0.45
6:D:14:SER:O	6:D:17:LYS:N	2.49	0.45
6:D:639:LEU:HD12	6:D:640:HIS:H	1.81	0.45
5:M:100:LEU:HD12	5:M:101:ILE:O	2.16	0.45
5:M:1043:TYR:HA	6:N:710:ARG:NH1	2.30	0.45
5:M:195:LEU:O	5:M:199:VAL:HG23	2.16	0.45
5:M:352:ALA:CA	5:M:355:VAL:HG12	2.44	0.45
4:K:198:ARG:NH2	5:M:932:GLU:HB3	2.30	0.45
6:N:1051:GLU:HB3	11:N:9122:HOH:O	2.15	0.45
6:N:1262:LEU:HD21	6:N:1351:GLU:CG	2.46	0.45
6:N:1192:LEU:HD22	6:N:1345:GLU:CG	2.46	0.45
6:N:631:ILE:HG21	6:N:745:MET:HG3	1.97	0.45
6:N:783:ARG:NH1	6:N:1029:ARG:CZ	2.79	0.45
6:N:770:LEU:HD11	6:N:919:PHE:HE2	1.80	0.45
5:C:146:VAL:HG13	5:C:162:ILE:HA	1.97	0.45
5:C:189:ARG:HD3	5:C:190:LYS:H	1.81	0.45
5:C:203:ASP:O	5:C:207:LEU:HB2	2.16	0.45
5:C:573:ARG:CB	5:C:573:ARG:HH11	2.19	0.45
5:C:669:GLY:HA3	5:C:995:MET:HA	1.98	0.45
6:D:1098:LEU:CD2	6:D:1229:ILE:HD12	2.44	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:114:THR:HB	6:D:498:VAL:HG21	1.98	0.45
3:I:8:DA:H1'	3:I:9:DG:C5'	2.46	0.45
4:K:39:PRO:O	4:K:43:ILE:HG12	2.17	0.45
4:L:121:GLU:OE1	4:L:123:MET:HG2	2.16	0.45
5:M:192:PRO:HD2	5:M:195:LEU:HD22	1.98	0.45
5:M:211:LEU:HD22	11:M:1152:HOH:O	2.17	0.45
5:M:146:VAL:HG21	5:M:281:LEU:HD11	1.98	0.45
5:M:30:LEU:HD12	5:M:30:LEU:O	2.17	0.45
5:M:44:ILE:HG23	5:M:344:PHE:CE1	2.47	0.45
5:M:688:ILE:HD12	5:M:847:GLY:HA3	1.99	0.45
4:K:198:ARG:HH22	5:M:932:GLU:CB	2.26	0.45
6:N:1136:LYS:O	6:N:1140:ILE:HG13	2.15	0.45
6:N:119:SER:OG	6:N:123:LEU:HD13	2.16	0.45
6:N:1380:GLU:OE2	6:N:1390:LEU:HA	2.15	0.45
6:N:206:ARG:HG3	6:N:206:ARG:HH11	1.81	0.45
6:N:409:VAL:HG11	6:N:435:VAL:HG21	1.98	0.45
6:N:470:LEU:HD23	6:N:470:LEU:H	1.81	0.45
6:N:772:PRO:HB2	11:N:9024:HOH:O	2.15	0.45
7:O:41:GLU:HG2	7:O:42:PRO:N	2.31	0.45
5:C:10:ARG:HH11	5:C:11:GLU:H	1.63	0.45
5:C:398:THR:HG21	5:C:567:GLN:CA	2.46	0.45
5:C:640:ARG:HA	11:C:1183:HOH:O	2.16	0.45
5:C:832:LYS:HE3	11:C:1519:HOH:O	2.15	0.45
6:D:1135:ARG:HD2	6:D:1139:ASP:OD2	2.17	0.45
6:D:1207:TYR:HA	6:D:1214:PRO:HA	1.97	0.45
6:D:1402:ALA:HB2	6:D:1415:VAL:CG2	2.46	0.45
6:D:508:ARG:NH1	11:D:8038:HOH:O	2.50	0.45
6:D:530:VAL:HB	6:D:534:ARG:HB2	1.99	0.45
6:D:884:ARG:HA	11:D:8116:HOH:O	2.16	0.45
6:D:896:ALA:O	6:D:900:ILE:HG23	2.17	0.45
4:K:16:GLN:NE2	11:K:788:HOH:O	2.47	0.45
4:L:112:ARG:H	4:L:112:ARG:HG2	1.48	0.45
4:L:50:GLY:HA3	4:L:171:PHE:O	2.16	0.45
4:L:59:GLU:HG2	4:L:139:ASN:HD22	1.80	0.45
5:M:350:ARG:HB3	5:M:377:PRO:HB3	1.97	0.45
5:M:479:VAL:HG22	5:M:506:ASN:HA	1.98	0.45
5:M:577:PRO:HB3	5:M:842:ARG:NH1	2.31	0.45
5:M:801:VAL:HG23	5:M:802:ARG:N	2.31	0.45
6:N:169:TYR:HB3	6:N:195:VAL:HG11	1.99	0.45
6:N:31:THR:OG1	6:N:32:ILE:N	2.49	0.45
6:N:465:LEU:HD22	6:N:510:GLU:HA	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:756:GLN:HE21	6:N:760:ARG:HD2	1.82	0.45
6:N:796:ARG:NE	6:N:828:LYS:NZ	2.61	0.45
5:M:1115:LEU:O	6:N:89:ARG:CZ	2.64	0.45
6:N:907:GLU:O	6:N:911:LEU:HG	2.15	0.45
6:N:95:LEU:HA	6:N:551:ASN:HD21	1.81	0.45
6:N:963:TYR:H	6:N:963:TYR:HD1	1.63	0.45
4:A:186:LEU:HB2	11:A:361:HOH:O	2.17	0.45
4:A:206:THR:HG23	4:A:208:LEU:N	2.31	0.45
5:C:1008:ARG:HB2	5:C:1027:PHE:HB2	1.99	0.45
5:C:1055:LEU:HD22	5:C:1066:ALA:CB	2.37	0.45
5:C:1063:ARG:O	5:C:1066:ALA:HB3	2.16	0.45
5:C:265:ARG:HB3	5:C:267:TYR:CE2	2.51	0.45
5:C:385:PHE:O	5:C:389:SER:HB2	2.16	0.45
5:C:403:SER:O	5:C:407:LYS:HD3	2.16	0.45
5:C:431:HIS:CD2	5:C:432:ARG:N	2.85	0.45
5:C:523:ILE:HG23	5:C:523:ILE:O	2.17	0.45
5:C:401:LEU:HD22	5:C:546:LEU:HD13	1.99	0.45
5:C:569:VAL:HA	5:C:570:PRO:HD3	1.85	0.45
5:C:625:LEU:HA	5:C:639:GLN:NE2	2.24	0.45
5:C:810:ASP:HA	5:C:811:PRO:HD3	1.68	0.45
6:D:136:ASP:HB3	6:D:137:PRO:CD	2.33	0.45
6:D:1376:MET:CE	6:D:1421:LEU:HD22	2.46	0.45
6:D:165:LYS:HA	6:D:199:LEU:HD13	1.97	0.45
6:D:396:VAL:CG1	6:D:398:ALA:HB2	2.46	0.45
6:D:44:LEU:O	6:D:525:ARG:NH2	2.49	0.45
6:D:606:ILE:O	6:D:613:ARG:HB2	2.16	0.45
6:D:819:GLY:HA2	11:D:8465:HOH:O	2.17	0.45
4:K:158:ILE:HA	11:K:1352:HOH:O	2.15	0.45
4:K:41:ARG:HA	4:K:44:LEU:HD12	1.97	0.45
5:M:1007:ALA:HB1	6:N:652:LEU:CD1	2.46	0.45
5:M:310:LEU:HD11	11:M:1381:HOH:O	2.15	0.45
5:M:468:ARG:NE	5:M:487:THR:HG23	2.32	0.45
5:M:479:VAL:HG21	5:M:503:LEU:CD1	2.46	0.45
5:M:601:GLY:HA3	5:M:615:TYR:HA	1.97	0.45
5:M:77:PRO:HG2	5:M:117:HIS:CE1	2.51	0.45
5:M:9:ILE:HD11	5:M:537:LYS:HZ3	1.81	0.45
6:N:106:LYS:CE	6:N:125:GLN:HE22	2.30	0.45
5:M:817:PRO:O	6:N:532:GLY:HA2	2.15	0.45
6:N:781:PRO:O	6:N:786:ILE:HD11	2.17	0.45
6:N:800:LYS:HE3	6:N:804:LEU:HD22	1.98	0.45
4:A:9:PRO:HB3	4:A:25:LEU:CG	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:48:ILE:HG22	4:B:173:PRO:HD2	1.99	0.45
5:C:146:VAL:HG11	5:C:306:THR:CB	2.41	0.45
5:C:168:ARG:HH11	5:C:168:ARG:HG3	1.82	0.45
5:C:260:LEU:HA	5:C:291:ALA:HB2	1.97	0.45
6:D:1344:VAL:HG12	6:D:1348:LEU:CD1	2.46	0.45
6:D:1476:THR:O	6:D:1482:ARG:HA	2.17	0.45
6:D:618:LEU:CD1	6:D:1439:SER:HB3	2.47	0.45
6:D:68:PHE:HZ	11:D:8399:HOH:O	1.98	0.45
6:D:794:GLN:OE1	6:D:905:PRO:HG3	2.15	0.45
7:E:45:ARG:HB2	7:E:45:ARG:HE	1.62	0.45
1:G:15:DC:H2''	1:G:16:DG:H8	1.82	0.45
4:K:13:VAL:HG22	4:K:23:PHE:HD1	1.82	0.45
4:K:94:LEU:HD11	4:K:119:ASP:HB3	1.98	0.45
4:L:2:LEU:O	4:L:6:LEU:HD23	2.16	0.45
5:M:1105:LYS:C	5:M:1107:ASN:HD22	2.19	0.45
5:M:122:THR:HB	5:M:124:ASP:OD1	2.17	0.45
5:M:165:LEU:HA	5:M:166:PRO:O	2.16	0.45
5:M:250:ARG:NH1	5:M:250:ARG:HG3	2.31	0.45
5:M:43:GLY:HA2	5:M:341:THR:HG21	1.96	0.45
5:M:375:SER:HA	11:M:1564:HOH:O	2.14	0.45
5:M:769:PRO:HD2	6:N:65:ARG:NE	2.32	0.45
6:N:1476:THR:C	6:N:1478:SER:H	2.19	0.45
6:N:152:LEU:HD23	6:N:152:LEU:N	2.31	0.45
6:N:204:LEU:HD12	6:N:396:VAL:HG21	1.97	0.45
6:N:41:ARG:CD	6:N:42:ASP:H	2.28	0.45
6:N:497:GLU:O	6:N:500:ARG:HB2	2.16	0.45
3:Z:4:DC:H2''	3:Z:5:DG:O5'	2.16	0.45
5:C:1016:ILE:HD13	5:C:1016:ILE:N	2.24	0.45
5:C:329:GLY:CA	5:C:489:THR:HG23	2.46	0.45
5:C:51:THR:CG2	5:C:348:LEU:HD23	2.46	0.45
5:C:833:LEU:CD1	5:C:996:LYS:HD2	2.47	0.45
5:C:567:GLN:HB2	5:C:997:LEU:HD12	1.98	0.45
6:D:1057:VAL:HG13	6:D:1069:GLU:HB3	1.98	0.45
6:D:1135:ARG:HB3	6:D:1140:ILE:CG1	2.47	0.45
6:D:1198:TYR:N	11:D:8501:HOH:O	2.48	0.45
6:D:1389:LEU:HD13	11:D:8087:HOH:O	2.17	0.45
6:D:36:THR:O	6:D:38:LYS:N	2.49	0.45
6:D:32:ILE:HD12	6:D:527:MET:HG2	1.97	0.45
6:D:1213:ARG:NH2	7:E:10:PHE:O	2.44	0.45
3:I:3:DA:H4'	5:C:423:ALA:HB1	1.97	0.45
4:L:73:GLU:HB3	4:L:77:GLU:HG3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:139:GLN:HA	5:M:411:SER:O	2.17	0.45
5:M:31:GLN:CD	5:M:34:VAL:HG23	2.36	0.45
5:M:662:GLU:HG2	5:M:663:ASN:CG	2.37	0.45
5:M:695:LEU:O	5:M:695:LEU:HD23	2.16	0.45
5:M:690:ILE:CG2	5:M:852:ILE:HG13	2.47	0.45
5:M:876:VAL:HG12	5:M:876:VAL:O	2.17	0.45
6:N:1031:ASN:HB3	6:N:1034:GLN:OE1	2.15	0.45
5:M:516:ARG:CZ	6:N:1068:LEU:HD13	2.44	0.45
1:X:13:DT:OP1	6:N:1093:TYR:CE2	2.70	0.45
6:N:1412:LYS:NZ	6:N:1414:PRO:HG3	2.32	0.45
6:N:1475:GLY:O	6:N:1478:SER:HB3	2.16	0.45
6:N:168:THR:OG1	6:N:206:ARG:NH2	2.49	0.45
6:N:179:VAL:HG21	6:N:191:LEU:HD23	1.99	0.45
6:D:1153:VAL:CG1	6:N:561:GLY:HA3	2.41	0.45
6:N:618:LEU:HD22	6:N:619:LEU:HD22	1.98	0.45
6:N:682:ASP:N	6:N:682:ASP:OD1	2.49	0.45
6:N:701:LEU:N	6:N:701:LEU:HD12	2.32	0.45
6:N:845:ASN:H	6:N:848:GLU:HG3	1.81	0.45
6:N:945:SER:OG	6:N:947:ILE:HG13	2.16	0.45
7:O:28:GLN:HB3	7:O:32:ARG:HH12	1.82	0.45
4:A:41:ARG:HH11	4:A:177:VAL:HB	1.82	0.45
5:C:160:ALA:HB3	5:C:174:LEU:HB2	1.97	0.45
5:C:570:PRO:O	5:C:702:SER:HB2	2.16	0.45
5:C:603:VAL:O	5:C:646:GLY:HA2	2.16	0.45
5:C:56:GLU:CB	5:C:64:LEU:HD23	2.46	0.45
5:C:837:ASP:OD1	5:C:999:HIS:NE2	2.50	0.45
5:C:551:GLU:HB3	5:C:906:PHE:CD2	2.52	0.45
5:C:910:LYS:HG3	5:C:912:PRO:HD2	1.99	0.45
6:D:1102:THR:HG23	6:D:1370:ILE:HG22	1.99	0.45
6:D:1406:ARG:HB2	6:D:1412:LYS:HZ3	1.82	0.45
6:D:10:ILE:HD11	6:D:1434:TRP:CE2	2.51	0.45
6:D:576:GLU:HA	6:D:579:ASP:OD2	2.17	0.45
6:D:992:ILE:HG21	11:D:8500:HOH:O	2.16	0.45
6:D:1484:THR:O	7:E:25:LYS:HD3	2.17	0.45
2:H:9:G:C5'	2:H:9:G:H8	2.30	0.45
4:K:58:ILE:HG21	4:K:68:ILE:CD1	2.46	0.45
5:M:615:TYR:HB3	5:M:617:ASP:OD1	2.16	0.45
5:M:829:GLN:NE2	5:M:831:ARG:HH21	2.15	0.45
5:M:899:GLN:HG3	5:M:901:TYR:CZ	2.51	0.45
5:M:987:ILE:HG12	6:N:948:THR:CG2	2.46	0.45
6:N:1232:PRO:O	6:N:1236:LEU:HG	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:515:GLU:HG3	11:N:9303:HOH:O	2.16	0.45
6:N:587:ARG:HG2	6:N:587:ARG:HH11	1.81	0.45
5:M:1034:GLU:CB	6:N:619:LEU:HD13	2.45	0.45
6:N:784:ASP:HB3	6:N:939:PHE:CE2	2.51	0.45
4:A:13:VAL:HG22	4:A:23:PHE:CD1	2.51	0.45
4:B:97:VAL:HG13	11:B:325:HOH:O	2.17	0.45
5:C:1060:ILE:O	5:C:1063:ARG:HG2	2.15	0.45
6:D:998:GLU:O	6:D:1002:LYS:HG3	2.17	0.45
5:C:906:PHE:CE1	6:D:1067:VAL:HG13	2.52	0.45
6:D:1225:ALA:HB2	6:D:1367:HIS:ND1	2.32	0.45
6:D:1261:GLU:O	6:D:1264:GLU:O	2.35	0.45
6:D:1492:LEU:HD22	6:D:1492:LEU:O	2.16	0.45
6:D:407:VAL:HA	6:D:422:ALA:HB2	1.99	0.45
6:D:633:VAL:HG22	6:D:635:PRO:HD3	1.98	0.45
6:D:974:ILE:O	6:D:983:LEU:HD11	2.16	0.45
7:E:80:VAL:HG11	7:E:85:LEU:HD23	1.98	0.45
5:M:806:LEU:O	5:M:821:GLU:HB2	2.17	0.45
5:M:844:GLY:O	5:M:846:LYS:HG3	2.16	0.45
5:M:860:HIS:CE1	5:M:977:GLY:HA2	2.52	0.45
6:N:1262:LEU:HD23	6:N:1352:ILE:HA	1.99	0.45
6:N:36:THR:O	6:N:38:LYS:N	2.49	0.45
6:N:777:PRO:HG2	6:N:916:TYR:HB2	1.98	0.45
6:N:954:ALA:HB1	6:N:1039:CYS:SG	2.57	0.45
6:N:969:ARG:O	6:N:973:GLN:HG3	2.17	0.45
6:N:987:GLU:O	6:N:991:GLN:HG3	2.16	0.45
6:N:993:LEU:HA	11:N:9079:HOH:O	2.17	0.45
11:A:316:HOH:O	4:B:148:VAL:HG23	2.17	0.45
4:B:213:GLN:HG2	11:B:331:HOH:O	2.17	0.45
5:C:14:PRO:HB2	11:C:1307:HOH:O	2.17	0.45
5:C:22:GLN:OE1	5:C:407:LYS:HB3	2.16	0.45
5:C:76:PRO:HA	5:C:77:PRO:HD3	1.89	0.45
5:C:855:VAL:HG13	5:C:856:GLU:OE2	2.17	0.45
6:D:1345:GLU:O	6:D:1349:VAL:HG23	2.16	0.45
5:C:1046:ALA:O	6:D:1472:ILE:HD11	2.16	0.45
6:D:33:ASN:O	6:D:36:THR:O	2.34	0.45
6:D:525:ARG:HB2	6:D:538:SER:OG	2.17	0.45
11:C:1135:HOH:O	6:D:750:PRO:HB3	2.16	0.45
1:G:15:DC:H2"	1:G:16:DG:C8	2.52	0.45
4:K:189:ARG:HG3	4:K:191:ASP:OD1	2.17	0.45
4:L:19:GLU:N	4:L:19:GLU:OE2	2.49	0.45
4:L:1:MET:HB2	11:L:357:HOH:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:243:ARG:HB3	11:M:1168:HOH:O	2.16	0.45
5:M:265:ARG:H	5:M:289:THR:HG21	1.80	0.45
5:M:358:ARG:HB3	5:M:371:LYS:O	2.17	0.45
5:M:564:MET:SD	5:M:565:GLN:N	2.90	0.45
5:M:689:VAL:CG1	5:M:690:ILE:N	2.79	0.45
5:M:882:LEU:HD23	5:M:882:LEU:N	2.32	0.45
6:N:1147:ARG:CB	6:N:1188:VAL:HG21	2.44	0.45
6:N:1209:LEU:O	6:N:1210:SER:C	2.54	0.45
6:N:1336:LEU:HD11	6:N:1341:PRO:HG3	1.99	0.45
6:N:28:LYS:CG	6:N:29:PRO:HD2	2.47	0.45
6:N:542:ASP:HA	6:N:545:ARG:NE	2.30	0.45
6:N:634:GLY:N	6:N:635:PRO:HD3	2.32	0.45
6:N:837:GLY:O	6:N:841:TYR:CD1	2.70	0.45
4:L:45:LEU:HD22	6:N:851:LEU:CD2	2.47	0.45
7:O:84:ARG:HB3	11:O:1385:HOH:O	2.15	0.45
5:C:248:PRO:HG3	11:C:1252:HOH:O	2.17	0.45
5:C:54:ILE:CG2	5:C:66:LEU:HB3	2.47	0.45
5:C:703:ILE:CD1	5:C:703:ILE:H	2.17	0.45
5:C:813:VAL:HG22	5:C:814:GLU:N	2.32	0.45
5:C:899:GLN:NE2	5:C:901:TYR:OH	2.50	0.45
6:D:1010:ASN:HB3	11:D:8019:HOH:O	2.17	0.45
6:D:1102:THR:HG22	6:D:1222:GLY:HA3	1.99	0.45
6:D:1369:GLU:HA	6:D:1372:VAL:HG12	1.98	0.45
6:D:1426:LYS:HA	6:D:1429:LEU:HD13	1.99	0.45
6:D:1465:ASN:ND2	6:D:1471:LEU:O	2.50	0.45
6:D:484:PRO:HB3	6:D:488:ARG:NE	2.17	0.45
5:C:1095:LEU:CD2	6:D:582:LEU:HD22	2.43	0.45
6:D:761:ILE:HG12	7:E:65:MET:HE1	1.99	0.45
5:M:36:PRO:HB2	5:M:70:GLU:HG2	1.98	0.45
5:M:817:PRO:C	5:M:819:VAL:H	2.20	0.45
5:M:798:GLY:H	5:M:827:VAL:HG11	1.82	0.45
6:N:127:LEU:HD12	6:N:127:LEU:H	1.82	0.45
6:N:675:ARG:O	6:N:678:GLU:HG2	2.17	0.45
6:N:777:PRO:CG	6:N:916:TYR:HB2	2.47	0.45
6:N:876:SER:HB3	11:N:9301:HOH:O	2.17	0.45
5:M:678:PRO:HG2	6:N:943:THR:HA	1.99	0.45
1:X:14:DT:H3'	6:N:610:LYS:HZ3	1.81	0.45
1:X:6:DT:H2''	1:X:7:DC:C5	2.52	0.45
2:Y:8:C:H2'	2:Y:9:G:C8	2.52	0.45
4:A:179:PHE:HB2	4:A:195:LEU:CD1	2.45	0.44
4:A:20:TYR:HE2	4:A:198:ARG:HB2	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:83:LYS:HG3	4:A:170:VAL:HG21	1.98	0.44
5:C:1008:ARG:HH12	5:C:1010:THR:HA	1.81	0.44
5:C:1084:SER:HA	5:C:1087:VAL:HG12	1.99	0.44
5:C:689:VAL:HG21	5:C:870:ILE:HD12	1.99	0.44
6:D:1119:SER:O	6:D:1121:PRO:HD3	2.16	0.44
6:D:1147:ARG:O	6:D:1165:TYR:HA	2.18	0.44
6:D:1487:VAL:HG12	6:D:1488:ASP:N	2.31	0.44
6:D:112:ILE:HD11	6:D:461:ILE:CG2	2.47	0.44
6:D:6:ARG:HH11	6:D:6:ARG:HG2	1.82	0.44
6:D:950:GLY:O	6:D:953:ASP:HB2	2.16	0.44
4:L:102:LYS:HE3	4:L:104:GLU:CG	2.43	0.44
5:M:1003:ASP:OD1	5:M:1004:LYS:HG2	2.16	0.44
5:M:199:VAL:HG13	5:M:235:LEU:HG	1.99	0.44
5:M:265:ARG:HB3	5:M:267:TYR:CZ	2.52	0.44
5:M:334:ARG:HG3	11:M:1156:HOH:O	2.17	0.44
5:M:461:VAL:HG13	5:M:465:GLY:HA2	1.98	0.44
5:M:490:GLU:HG2	5:M:493:ARG:NH2	2.32	0.44
5:M:400:PRO:HG2	5:M:593:ALA:CB	2.47	0.44
5:M:80:GLN:HE21	5:M:84:ARG:NH2	2.15	0.44
6:N:1151:ARG:HG2	6:N:1187:PRO:CB	2.45	0.44
6:N:1231:GLU:HA	6:N:1234:THR:OG1	2.17	0.44
6:N:1425:THR:O	6:N:1429:LEU:HD12	2.16	0.44
6:N:754:PHE:CZ	6:N:1476:THR:HG21	2.52	0.44
6:N:700:VAL:HG13	6:N:718:PRO:HG2	2.00	0.44
6:N:793:THR:O	6:N:879:ARG:HD3	2.17	0.44
6:N:999:THR:HA	6:N:1002:LYS:HD2	1.98	0.44
4:B:84:GLU:OE1	4:B:127:LEU:HD11	2.17	0.44
5:C:1038:TRP:HA	5:C:1041:GLU:OE1	2.17	0.44
5:C:422:ARG:HB2	11:C:1579:HOH:O	2.17	0.44
5:C:532:MET:HG2	5:C:533:ASP:N	2.32	0.44
5:C:674:VAL:HG12	5:C:990:GLY:O	2.18	0.44
5:C:783:ARG:HG2	5:C:785:VAL:HB	1.98	0.44
5:C:817:PRO:C	5:C:819:VAL:H	2.20	0.44
6:D:1014:ASN:O	6:D:1016:PRO:HD3	2.17	0.44
6:D:116:LEU:HD11	6:D:464:LEU:CB	2.46	0.44
6:D:1183:ILE:O	6:D:1183:ILE:HG13	2.16	0.44
6:D:1184:GLN:HB2	6:N:559:ALA:CA	2.47	0.44
6:D:1271:LYS:HD3	6:D:1331:ASP:N	2.32	0.44
6:D:1232:PRO:HB3	6:D:1361:VAL:HG21	1.99	0.44
6:D:1377:LYS:O	6:D:1395:LEU:HB3	2.18	0.44
6:D:1486:VAL:CG1	7:E:22:VAL:HG13	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:15:PRO:O	6:D:19:ARG:HG2	2.18	0.44
6:D:584:ASN:CG	6:D:590:PRO:HD2	2.37	0.44
6:D:783:ARG:HH12	6:D:1239:ARG:NH2	2.15	0.44
5:C:676:ILE:O	6:D:948:THR:HB	2.17	0.44
4:K:26:GLU:HG2	4:K:27:PRO:N	2.32	0.44
4:L:94:LEU:HD21	4:L:119:ASP:HB2	1.99	0.44
5:M:13:ILE:HD12	5:M:13:ILE:O	2.17	0.44
5:M:670:GLN:NE2	5:M:699:PHE:O	2.51	0.44
5:M:853:LEU:HB3	5:M:858:MET:HE2	2.00	0.44
5:M:676:ILE:HG21	5:M:988:VAL:HG13	1.99	0.44
5:M:9:ILE:O	5:M:9:ILE:HD12	2.18	0.44
6:N:1472:ILE:O	6:N:1477:GLY:HA3	2.17	0.44
6:N:400:VAL:HG22	6:N:443:VAL:CG2	2.41	0.44
6:N:434:ARG:H	6:N:447:VAL:HG22	1.82	0.44
6:N:470:LEU:HD12	6:N:503:LEU:HD21	1.99	0.44
6:N:54:LYS:HE3	6:N:55:ASP:HB2	1.99	0.44
6:N:705:ALA:HB3	6:N:706:PRO:HD3	1.99	0.44
2:Y:4:U:O2'	2:Y:5:C:H5'	2.16	0.44
4:B:30:ARG:HB3	4:B:30:ARG:CZ	2.47	0.44
5:C:97:ARG:HB3	5:C:109:LYS:HE3	1.99	0.44
5:C:352:ALA:CA	5:C:355:VAL:HG12	2.47	0.44
5:C:44:ILE:HG22	5:C:45:GLN:N	2.31	0.44
5:C:595:LEU:HD22	5:C:625:LEU:HD23	2.00	0.44
5:C:748:GLU:HA	5:C:799:ILE:HD12	1.99	0.44
6:D:10:ILE:O	6:D:1451:ALA:HA	2.18	0.44
6:D:1432:LYS:HB3	6:D:1432:LYS:NZ	2.32	0.44
6:D:156:GLU:O	6:D:159:ARG:HB2	2.18	0.44
6:D:396:VAL:HB	6:D:398:ALA:HB3	1.98	0.44
6:D:420:VAL:O	6:D:421:LEU:HD23	2.17	0.44
6:D:471:GLU:H	6:D:471:GLU:HG2	1.52	0.44
6:D:525:ARG:HG2	6:D:525:ARG:O	2.17	0.44
6:D:593:ASN:HB2	11:D:8122:HOH:O	2.18	0.44
4:L:19:GLU:O	4:L:200:TRP:HA	2.18	0.44
4:L:201:THR:HG21	4:L:205:VAL:O	2.17	0.44
4:L:73:GLU:CD	4:L:130:ALA:HA	2.38	0.44
5:M:1013:TYR:CZ	5:M:1063:ARG:HD2	2.52	0.44
5:M:208:ALA:O	5:M:218:VAL:HG21	2.17	0.44
5:M:405:ARG:NH2	5:M:566:THR:CG2	2.79	0.44
5:M:780:GLU:HG3	5:M:781:LYS:H	1.83	0.44
5:M:859:PRO:HB3	5:M:974:LEU:HD23	1.99	0.44
6:N:35:ARG:HG3	6:N:35:ARG:NH1	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:1043:TYR:CE2	6:N:763:MET:HA	2.53	0.44
6:N:784:ASP:HB3	6:N:939:PHE:HE2	1.82	0.44
6:N:85:VAL:HG23	6:N:86:ARG:N	2.33	0.44
1:X:18:DG:P	6:N:628:ARG:HH21	2.40	0.44
2:Y:11:C:C2'	2:Y:12:G:H5''	2.47	0.44
3:Z:6:DC:P	6:N:1266:ARG:HH12	2.41	0.44
4:A:150:TYR:CZ	5:C:696:LYS:HA	2.53	0.44
4:A:47:SER:HB3	4:A:217:ILE:HD13	2.00	0.44
4:B:95:GLN:HA	4:B:146:ARG:HD2	1.99	0.44
4:A:219:ARG:HD3	4:B:219:ARG:HG3	1.99	0.44
5:C:172:ILE:HG12	11:C:1177:HOH:O	2.17	0.44
5:C:189:ARG:NH1	5:C:190:LYS:HD2	2.33	0.44
5:C:503:LEU:HD23	5:C:507:ARG:O	2.17	0.44
5:C:479:VAL:HG22	5:C:506:ASN:HA	1.99	0.44
5:C:52:PHE:O	5:C:54:ILE:N	2.50	0.44
5:C:553:ASP:OD1	5:C:881:ASN:HB2	2.17	0.44
5:C:721:ARG:CG	5:C:820:ARG:HH12	2.29	0.44
5:C:957:LYS:NZ	5:C:957:LYS:HB2	2.33	0.44
5:C:952:LEU:HB3	5:C:966:LEU:HD11	2.00	0.44
6:D:1000:THR:HG23	6:D:1001:GLU:H	1.82	0.44
6:D:651:GLU:HG2	11:D:8181:HOH:O	2.17	0.44
6:D:654:LYS:O	6:D:658:LEU:HG	2.17	0.44
2:H:7:G:C5'	2:H:7:G:H8	2.29	0.44
4:L:124:ASN:ND2	4:L:127:LEU:HD22	2.32	0.44
5:M:1084:SER:HA	5:M:1087:VAL:HG12	1.98	0.44
5:M:252:LYS:HD2	5:M:252:LYS:N	2.32	0.44
5:M:94:LEU:HD12	5:M:95:TYR:N	2.32	0.44
6:N:1262:LEU:HA	6:N:1262:LEU:HD12	1.77	0.44
6:N:436:GLU:OE2	6:N:445:ARG:HD3	2.18	0.44
6:N:530:VAL:HB	6:N:534:ARG:HB2	1.99	0.44
5:M:949:LYS:CD	6:N:796:ARG:HH22	2.29	0.44
6:N:1213:ARG:HH22	7:O:15:SER:HA	1.83	0.44
7:O:24:ALA:O	7:O:28:GLN:HG3	2.17	0.44
2:Y:16:G:H3'	11:Y:968:HOH:O	2.17	0.44
4:A:165:ILE:O	4:A:165:ILE:HG13	2.18	0.44
4:B:47:SER:OG	4:B:48:ILE:N	2.49	0.44
5:C:106:GLY:C	5:C:107:LEU:HD23	2.38	0.44
5:C:170:PRO:HB2	11:C:1335:HOH:O	2.17	0.44
5:C:189:ARG:HD3	5:C:190:LYS:N	2.33	0.44
5:C:393:GLN:HE21	5:C:393:GLN:HB2	1.62	0.44
5:C:492:ASP:OD2	5:C:518:LYS:HB3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:566:THR:O	5:C:566:THR:HG22	2.18	0.44
5:C:689:VAL:CG1	5:C:853:LEU:HD13	2.47	0.44
5:C:673:LEU:HD21	5:C:867:VAL:HG12	2.00	0.44
6:D:1344:VAL:HG11	6:D:1421:LEU:CD2	2.48	0.44
6:D:1380:GLU:HA	6:D:1391:GLU:O	2.18	0.44
6:D:15:PRO:HD3	6:D:511:TRP:CE3	2.52	0.44
6:D:554:LEU:HD12	6:D:570:GLU:HB3	2.00	0.44
6:D:550:ARG:NH1	6:D:573:MET:SD	2.88	0.44
6:D:800:LYS:HD3	6:D:800:LYS:O	2.18	0.44
6:D:875:THR:HG22	6:D:879:ARG:HB2	2.00	0.44
6:D:95:LEU:HD23	6:D:96:ALA:H	1.82	0.44
7:E:13:VAL:HG11	7:E:18:ARG:HB3	2.00	0.44
1:G:12:DG:H1'	1:G:13:DT:H5'	1.99	0.44
4:L:121:GLU:CD	4:L:123:MET:HG2	2.37	0.44
4:L:38:ASN:HB3	4:L:39:PRO:HD3	2.00	0.44
5:M:140:ILE:HG22	5:M:333:ILE:CD1	2.48	0.44
5:M:15:LEU:HD12	5:M:15:LEU:N	2.31	0.44
5:M:18:LEU:HD23	5:M:542:VAL:HG21	2.00	0.44
5:M:548:PRO:HB2	5:M:843:HIS:HE1	1.83	0.44
5:M:69:LEU:HD12	5:M:97:ARG:HB3	1.98	0.44
6:N:1149:LEU:HD22	6:N:1187:PRO:HG2	2.00	0.44
6:N:1139:ASP:HB3	6:N:1357:ARG:CZ	2.48	0.44
6:N:1336:LEU:CD2	6:N:1421:LEU:HB2	2.48	0.44
6:N:50:PHE:HB3	6:N:522:PRO:CD	2.47	0.44
5:M:1034:GLU:CB	6:N:619:LEU:HD22	2.44	0.44
6:N:899:LEU:CB	6:N:917:GLN:HG2	2.48	0.44
7:O:62:THR:HB	11:O:844:HOH:O	2.18	0.44
4:A:132:LEU:N	4:A:132:LEU:HD12	2.32	0.44
4:A:151:VAL:HB	4:A:169:ALA:HB3	2.00	0.44
4:B:48:ILE:N	4:B:48:ILE:HD12	2.32	0.44
5:C:69:LEU:CD1	5:C:109:LYS:HE3	2.45	0.44
5:C:148:PHE:HB2	5:C:313:LEU:HD22	1.99	0.44
5:C:235:LEU:C	5:C:235:LEU:HD23	2.37	0.44
5:C:41:ASN:O	5:C:46:ALA:HB2	2.17	0.44
5:C:473:ARG:HA	5:C:531:PHE:CD1	2.53	0.44
5:C:524:VAL:CG1	5:C:528:GLU:HB2	2.48	0.44
5:C:579:VAL:HB	5:C:890:LEU:HD21	1.98	0.44
5:C:650:ARG:CG	5:C:653:ASP:HB2	2.44	0.44
5:C:690:ILE:HG23	5:C:852:ILE:HA	1.99	0.44
5:C:549:PHE:CD2	5:C:886:LEU:HB3	2.52	0.44
6:D:1080:GLY:O	6:D:1083:ASP:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:119:SER:H	6:D:123:LEU:HB2	1.83	0.44
6:D:1201:CYS:SG	6:D:1204:CYS:HB2	2.57	0.44
6:D:1367:HIS:O	6:D:1371:VAL:HG23	2.17	0.44
6:D:33:ASN:HB2	6:D:40:GLU:OE2	2.18	0.44
4:L:7:LYS:HD2	4:L:7:LYS:C	2.37	0.44
5:M:1034:GLU:HB3	6:N:619:LEU:CD1	2.46	0.44
5:M:198:ARG:HG2	5:M:204:GLN:HE22	1.82	0.44
5:M:23:VAL:HA	5:M:121:MET:CE	2.48	0.44
5:M:496:ILE:HA	5:M:531:PHE:O	2.18	0.44
6:N:1147:ARG:O	6:N:1166:LEU:HD23	2.17	0.44
6:N:644:LEU:HD12	6:N:645:PRO:N	2.33	0.44
7:O:5:GLY:HA3	7:O:8:LYS:HD2	1.99	0.44
4:B:19:GLU:O	4:B:200:TRP:HA	2.18	0.44
4:B:58:ILE:HG21	4:B:61:VAL:HG23	2.00	0.44
5:C:329:GLY:CA	5:C:488:ALA:HB3	2.48	0.44
5:C:546:LEU:HD13	5:C:565:GLN:HE22	1.82	0.44
5:C:862:PRO:HD3	5:C:973:VAL:O	2.18	0.44
6:D:115:LEU:HD12	6:D:499:VAL:HG22	2.00	0.44
6:D:1432:LYS:HG2	6:D:1433:SER:N	2.33	0.44
6:D:1463:LYS:O	6:D:1467:ILE:HG13	2.18	0.44
6:D:123:LEU:CD1	6:D:152:LEU:HD22	2.41	0.44
4:L:143:ARG:NE	4:L:145:ASP:OD1	2.51	0.44
4:L:73:GLU:OE1	4:L:131:THR:N	2.51	0.44
5:M:284:ARG:O	5:M:301:GLU:HB2	2.18	0.44
5:M:728:HIS:C	5:M:729:LEU:HG	2.38	0.44
5:M:728:HIS:O	5:M:729:LEU:HG	2.17	0.44
6:N:1192:LEU:HD23	11:N:9021:HOH:O	2.17	0.44
6:N:121:THR:HB	11:N:9300:HOH:O	2.17	0.44
6:N:1259:VAL:HG11	6:N:1356:TYR:HH	1.81	0.44
6:N:124:GLU:O	6:N:127:LEU:HD12	2.18	0.44
6:N:131:LYS:NZ	6:N:568:ARG:HB2	2.32	0.44
6:N:637:LEU:HD11	6:N:642:CYS:N	2.33	0.44
6:N:711:LEU:HD22	6:N:714:GLN:NE2	2.33	0.44
6:N:884:ARG:CZ	6:N:884:ARG:HB3	2.45	0.44
6:N:955:VAL:HG11	6:N:1015:TYR:CE2	2.52	0.44
6:N:95:LEU:HA	6:N:551:ASN:OD1	2.17	0.44
1:X:13:DT:OP2	6:N:1096:ARG:NH2	2.45	0.44
5:C:288:ARG:HH11	5:C:288:ARG:CB	2.31	0.44
5:C:137:VAL:HG22	5:C:391:LEU:HG	2.00	0.44
5:C:964:LYS:O	5:C:968:LEU:HG	2.17	0.44
6:D:1098:LEU:HD21	6:D:1229:ILE:CD1	2.44	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:128:TYR:O	6:D:457:GLY:HA2	2.17	0.44
6:D:418:GLY:O	6:D:428:LYS:HB3	2.18	0.44
6:D:489:ARG:NH1	11:D:8508:HOH:O	2.49	0.44
6:D:554:LEU:CD1	6:D:571:LYS:HD3	2.45	0.44
6:D:615:ARG:NH2	6:D:1096:ARG:CZ	2.81	0.44
6:D:8:VAL:HG23	6:D:1457:ASP:CB	2.37	0.44
6:D:95:LEU:HD23	6:D:96:ALA:N	2.32	0.44
6:D:1481:VAL:HG22	7:E:18:ARG:HH21	1.83	0.44
7:E:41:GLU:HB2	7:E:45:ARG:CZ	2.48	0.44
4:K:185:ARG:HB2	11:K:1437:HOH:O	2.17	0.44
4:K:26:GLU:HG2	4:K:27:PRO:HA	1.99	0.44
4:K:34:VAL:HG23	4:K:179:PHE:HZ	1.82	0.44
4:K:44:LEU:HD13	4:K:177:VAL:HG11	2.00	0.44
5:M:1060:ILE:HG21	5:M:1083:GLU:OE1	2.17	0.44
5:M:12:VAL:HG13	5:M:13:ILE:HG13	2.00	0.44
5:M:165:LEU:HD12	5:M:166:PRO:C	2.38	0.44
5:M:41:ASN:O	5:M:46:ALA:HB2	2.18	0.44
5:M:479:VAL:HG21	5:M:503:LEU:HD11	1.98	0.44
5:M:721:ARG:HH21	5:M:783:ARG:NH1	2.15	0.44
5:M:808:ARG:NH2	5:M:820:ARG:NH2	2.65	0.44
5:M:84:ARG:HG2	5:M:131:GLY:O	2.18	0.44
5:M:854:PRO:HB2	5:M:856:GLU:CD	2.38	0.44
5:M:971:LYS:HG2	5:M:988:VAL:HB	2.00	0.44
6:N:493:ARG:HG2	6:N:1390:LEU:CB	2.43	0.44
6:N:578:VAL:O	6:N:581:LEU:HD23	2.17	0.44
6:N:984:THR:HG22	6:N:987:GLU:HG3	1.99	0.44
2:Y:10:G:C2'	2:Y:11:C:H5'	2.47	0.44
4:A:26:GLU:HG2	4:A:27:PRO:N	2.33	0.44
4:A:5:LYS:HE2	4:B:224:TYR:OH	2.18	0.44
5:C:1055:LEU:CD2	5:C:1066:ALA:HB2	2.37	0.44
5:C:127:PHE:CE1	5:C:136:ILE:HG12	2.53	0.44
5:C:355:VAL:CG2	5:C:372:LEU:HG	2.48	0.44
5:C:573:ARG:HD2	5:C:699:PHE:HA	2.00	0.44
5:C:874:LEU:C	5:C:877:PRO:HD2	2.38	0.44
6:D:1045:MET:O	6:D:1053:PHE:HD1	2.01	0.44
6:D:18:ILE:HD12	6:D:518:PRO:HG3	1.99	0.44
6:D:569:ASN:HA	6:D:572:ARG:NE	2.33	0.44
6:D:675:ARG:HA	6:D:678:GLU:CG	2.48	0.44
6:D:81:THR:HB	6:D:85:VAL:CG2	2.48	0.44
6:D:19:ARG:NE	6:D:94:GLU:OE1	2.51	0.44
3:I:4:DC:H3'	11:I:2461:HOH:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:102:LYS:HZ1	4:K:115:LEU:HD22	1.82	0.44
4:L:101:LEU:HD23	4:L:101:LEU:C	2.38	0.44
4:L:43:ILE:HD12	4:L:217:ILE:HG21	2.00	0.44
5:M:140:ILE:HD12	5:M:140:ILE:O	2.18	0.44
5:M:198:ARG:HG2	5:M:204:GLN:NE2	2.33	0.44
5:M:486:MET:HG3	5:M:490:GLU:HB2	2.00	0.44
6:N:1037:GLN:OE1	6:N:1042:ARG:HD2	2.17	0.44
6:N:1100:ASP:HB3	6:N:1428:ALA:CB	2.47	0.44
6:N:1102:THR:O	6:N:1102:THR:HG22	2.18	0.44
6:N:1221:VAL:O	6:N:1224:VAL:N	2.50	0.44
6:N:1478:SER:O	6:N:1482:ARG:N	2.51	0.44
6:N:1481:VAL:O	6:N:1481:VAL:HG12	2.18	0.44
6:N:163:TYR:HE1	6:N:198:ARG:HH12	1.66	0.44
6:N:486:ARG:CA	6:N:489:ARG:HG2	2.45	0.44
6:N:639:LEU:HD23	6:N:639:LEU:H	1.83	0.44
6:N:646:LYS:HG2	6:N:720:LEU:HB3	1.99	0.44
6:N:962:GLN:O	6:N:966:GLU:HG3	2.18	0.44
4:A:222:LEU:HD22	4:B:218:LEU:HD23	2.00	0.43
4:B:40:LEU:HD22	4:B:211:LEU:HD12	1.99	0.43
5:C:22:GLN:O	5:C:121:MET:HE1	2.17	0.43
5:C:279:GLU:HG3	5:C:280:LYS:N	2.33	0.43
5:C:285:LEU:HD23	5:C:285:LEU:O	2.18	0.43
5:C:409:ARG:HB3	5:C:454:SER:OG	2.17	0.43
5:C:563:ASN:O	5:C:567:GLN:HG2	2.18	0.43
5:C:703:ILE:HD11	11:C:1597:HOH:O	2.17	0.43
5:C:745:ILE:HD11	5:C:803:THR:OG1	2.18	0.43
1:G:11:DC:H5"	6:D:1442:ASN:ND2	2.33	0.43
6:D:26:VAL:HG11	6:D:44:LEU:HD23	2.00	0.43
6:D:393:ILE:HD12	11:D:8204:HOH:O	2.18	0.43
6:D:60:CYS:SG	6:D:62:LYS:HG3	2.58	0.43
6:D:632:VAL:O	6:D:727:GLN:HA	2.18	0.43
6:D:675:ARG:O	6:D:678:GLU:HG2	2.17	0.43
6:D:834:THR:CG2	6:D:838:ARG:HH11	2.27	0.43
7:E:28:GLN:HB2	7:E:28:GLN:HE21	1.56	0.43
5:M:177:GLU:N	5:M:178:PRO:HD3	2.32	0.43
5:M:52:PHE:O	5:M:54:ILE:N	2.51	0.43
5:M:578:VAL:HG21	5:M:991:GLN:O	2.18	0.43
5:M:669:GLY:HA3	5:M:995:MET:HA	1.99	0.43
5:M:940:GLU:N	11:M:1220:HOH:O	2.51	0.43
5:M:971:LYS:HG2	5:M:988:VAL:N	2.33	0.43
6:N:1045:MET:CB	6:N:1073:SER:HA	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:1164:ARG:NH1	6:N:1170:ASP:OD2	2.51	0.43
6:N:165:LYS:HG2	6:N:397:LYS:HD3	2.00	0.43
1:X:15:DC:P	6:N:610:LYS:HE2	2.58	0.43
2:Y:5:C:H6	2:Y:5:C:O5'	2.00	0.43
5:C:101:ILE:HD12	5:C:107:LEU:HD13	2.00	0.43
5:C:1058:ASP:O	5:C:1060:ILE:N	2.51	0.43
5:C:568:ALA:HB1	5:C:668:LEU:HB2	2.00	0.43
5:C:841:ASN:HD21	5:C:845:ASN:H	1.65	0.43
6:D:1066:THR:OG1	6:D:1067:VAL:N	2.51	0.43
6:D:1262:LEU:HD21	6:D:1351:GLU:CG	2.43	0.43
6:D:1438:ALA:CA	6:D:1446:VAL:HG11	2.48	0.43
6:D:56:TYR:C	6:D:80:VAL:HG11	2.38	0.43
6:D:827:ILE:HG23	6:D:840:LYS:NZ	2.33	0.43
4:K:114:PHE:O	4:K:116:PRO:HD3	2.18	0.43
4:L:86:VAL:HG12	4:L:124:ASN:HB2	1.99	0.43
4:L:83:LYS:HE2	4:L:168:ASP:HB2	2.00	0.43
5:M:1008:ARG:NH2	5:M:1020:PRO:HB3	2.33	0.43
5:M:147:TYR:CE2	5:M:280:LYS:HE2	2.52	0.43
5:M:307:LEU:CD1	5:M:310:LEU:HD23	2.48	0.43
5:M:573:ARG:HB3	5:M:670:GLN:OE1	2.18	0.43
5:M:672:VAL:HG12	5:M:699:PHE:HE1	1.82	0.43
5:M:842:ARG:NH2	5:M:887:GLU:OE1	2.51	0.43
6:N:1087:ARG:HB3	6:N:1237:THR:HG21	2.00	0.43
6:N:1165:TYR:HB2	11:N:9241:HOH:O	2.18	0.43
6:N:1261:GLU:O	6:N:1264:GLU:O	2.35	0.43
6:N:1383:ASP:HA	6:N:1384:PRO:HD3	1.71	0.43
11:M:1450:HOH:O	6:N:1456:LYS:HB3	2.17	0.43
6:N:155:ASP:O	6:N:159:ARG:N	2.49	0.43
6:N:204:LEU:HB3	6:N:445:ARG:NH2	2.32	0.43
6:N:732:VAL:HG12	6:N:732:VAL:O	2.18	0.43
11:M:1170:HOH:O	6:N:754:PHE:HB2	2.18	0.43
4:B:65:PHE:CE1	6:D:813:LEU:HD13	2.54	0.43
5:C:1031:ARG:CZ	6:D:621:LYS:NZ	2.81	0.43
5:C:360:LEU:HD22	11:C:1160:HOH:O	2.17	0.43
5:C:431:HIS:CG	5:C:432:ARG:H	2.35	0.43
5:C:124:ASP:OD2	5:C:592:LEU:HD12	2.19	0.43
5:C:71:TYR:HA	5:C:96:ALA:HB2	2.00	0.43
6:D:409:VAL:CG1	6:D:435:VAL:HG11	2.48	0.43
6:D:411:THR:HG23	6:D:436:GLU:HA	2.01	0.43
6:D:477:LEU:HD21	6:D:495:ARG:NH1	2.33	0.43
6:D:827:ILE:HG22	6:D:837:GLY:CA	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:957:PRO:HG3	6:D:1007:VAL:HA	2.00	0.43
7:E:41:GLU:H	7:E:41:GLU:CD	2.21	0.43
2:H:5:C:H2'	2:H:6:U:C5	2.52	0.43
4:K:133:GLU:OE2	4:K:134:GLU:HB2	2.17	0.43
4:K:30:ARG:HH22	5:M:938:LYS:CD	2.28	0.43
4:L:91:ASN:N	4:L:91:ASN:OD1	2.51	0.43
5:M:198:ARG:HE	5:M:198:ARG:CA	2.32	0.43
5:M:144:PRO:N	5:M:276:LYS:HZ3	2.15	0.43
5:M:342:ASP:HA	5:M:345:ARG:HD3	1.99	0.43
5:M:351:LEU:HD11	11:M:1564:HOH:O	2.17	0.43
5:M:569:VAL:HA	5:M:570:PRO:HD3	1.88	0.43
5:M:601:GLY:O	5:M:648:ARG:HA	2.18	0.43
5:M:677:MET:HE1	5:M:679:PHE:CD1	2.38	0.43
5:M:816:LYS:HB2	5:M:819:VAL:CG2	2.47	0.43
5:M:876:VAL:H	5:M:877:PRO:CD	2.31	0.43
5:M:873:PRO:O	5:M:877:PRO:HD3	2.18	0.43
6:N:154:THR:HG23	6:N:157:GLU:H	1.82	0.43
6:N:436:GLU:OE1	6:N:445:ARG:O	2.36	0.43
6:N:481:MET:HE1	6:N:493:ARG:HA	2.01	0.43
6:N:481:MET:CE	6:N:496:LEU:HD23	2.48	0.43
6:N:57:GLU:OE2	6:N:61:GLY:HA2	2.18	0.43
6:N:645:PRO:HG3	6:N:725:SER:O	2.18	0.43
6:N:813:LEU:HB2	6:N:839:LEU:HD21	1.99	0.43
6:N:53:ILE:HA	6:N:86:ARG:HD2	1.99	0.43
2:Y:9:G:C5'	2:Y:9:G:H8	2.30	0.43
4:A:48:ILE:HD11	4:A:210:ALA:HB1	2.00	0.43
5:C:142:ARG:NH2	5:C:325:ILE:HG12	2.34	0.43
5:C:256:TYR:CE1	5:C:293:PHE:HB2	2.53	0.43
5:C:466:PHE:O	5:C:468:ARG:N	2.52	0.43
5:C:36:PRO:CG	5:C:70:GLU:HB3	2.36	0.43
6:D:1046:GLN:HG2	6:D:1052:THR:CG2	2.44	0.43
6:D:1105:ILE:HG22	11:D:8286:HOH:O	2.17	0.43
6:D:1117:TYR:CE1	6:D:1187:PRO:HA	2.53	0.43
6:D:1471:LEU:HD21	6:D:1477:GLY:HA2	1.99	0.43
6:D:957:PRO:HG3	11:D:8019:HOH:O	2.17	0.43
6:D:1486:VAL:HG12	7:E:22:VAL:HG13	2.00	0.43
5:M:1003:ASP:OD2	6:N:724:GLN:NE2	2.52	0.43
5:M:166:PRO:HA	11:M:1128:HOH:O	2.17	0.43
5:M:328:LEU:HD11	5:M:434:HIS:HD2	1.82	0.43
5:M:462:ASP:HB3	5:M:468:ARG:CD	2.43	0.43
5:M:490:GLU:HG2	5:M:493:ARG:NH1	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:587:VAL:CG1	5:M:588:VAL:N	2.79	0.43
5:M:567:GLN:C	5:M:997:LEU:HD12	2.38	0.43
6:N:794:GLN:HG2	6:N:1017:PHE:CE1	2.53	0.43
5:M:879:ARG:HH21	6:N:1029:ARG:HH22	1.65	0.43
6:N:1209:LEU:HD21	7:O:17:TYR:OH	2.19	0.43
6:N:1453:ALA:O	6:N:1455:LYS:HG2	2.18	0.43
6:N:471:GLU:OE1	6:N:503:LEU:HD21	2.18	0.43
6:N:606:ILE:CG2	6:N:607:LEU:HG	2.48	0.43
6:N:615:ARG:NH2	6:N:1096:ARG:HD2	2.34	0.43
6:N:832:ARG:NE	6:N:832:ARG:HA	2.33	0.43
6:N:970:LYS:HE2	11:N:9402:HOH:O	2.18	0.43
7:O:21:VAL:HG12	7:O:25:LYS:HD2	1.99	0.43
7:O:65:MET:O	7:O:69:LEU:HD12	2.17	0.43
1:X:17:DC:O3'	6:N:628:ARG:NE	2.51	0.43
4:B:216:GLU:HA	4:B:219:ARG:HH12	1.83	0.43
5:C:250:ARG:HG2	5:C:253:ALA:HB3	2.00	0.43
5:C:610:ARG:HD3	5:C:622:GLU:CD	2.38	0.43
5:C:814:GLU:O	5:C:816:LYS:NZ	2.52	0.43
5:C:853:LEU:HB2	5:C:858:MET:HE2	2.01	0.43
5:C:976:ASP:HB3	5:C:979:THR:HG22	2.00	0.43
6:D:108:VAL:CG2	6:D:109:PRO:HD3	2.47	0.43
6:D:1122:LEU:O	6:D:1135:ARG:HB2	2.18	0.43
6:D:1209:LEU:O	6:D:1210:SER:C	2.53	0.43
6:D:1099:VAL:HG23	6:D:1226:ALA:HB1	2.00	0.43
6:D:1271:LYS:CE	6:D:1331:ASP:H	2.32	0.43
6:D:1406:ARG:CB	6:D:1412:LYS:HZ3	2.31	0.43
6:D:1436:SER:N	11:D:8024:HOH:O	2.49	0.43
6:D:415:VAL:O	6:D:432:TYR:HA	2.18	0.43
6:D:95:LEU:CD2	6:D:574:LEU:HD21	2.45	0.43
6:D:711:LEU:HD21	6:D:768:ASN:CB	2.49	0.43
6:D:899:LEU:HB3	6:D:921:ARG:HH12	1.83	0.43
4:K:116:PRO:HG3	11:K:2001:HOH:O	2.17	0.43
4:K:127:LEU:HA	11:K:827:HOH:O	2.17	0.43
4:K:55:SER:HB2	4:K:158:ILE:HB	2.00	0.43
4:L:52:ALA:HB2	4:L:170:VAL:C	2.38	0.43
5:M:1095:LEU:HB2	5:M:1097:LEU:CD2	2.47	0.43
5:M:1101:THR:C	5:M:1102:LEU:HD12	2.38	0.43
5:M:162:ILE:HB	5:M:172:ILE:HD13	2.00	0.43
5:M:37:GLU:HA	11:M:1579:HOH:O	2.18	0.43
5:M:39:ARG:HG3	5:M:39:ARG:NH1	2.29	0.43
5:M:399:ASN:O	5:M:400:PRO:C	2.57	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:853:LEU:O	5:M:858:MET:HE1	2.19	0.43
6:N:615:ARG:HH22	6:N:1096:ARG:CD	2.31	0.43
6:N:111:LYS:HG2	6:N:1452:ILE:CD1	2.48	0.43
6:N:1467:ILE:H	6:N:1467:ILE:HG13	1.55	0.43
6:N:40:GLU:HB3	6:N:41:ARG:H	1.68	0.43
4:A:19:GLU:O	4:A:200:TRP:HA	2.18	0.43
5:C:18:LEU:HD13	5:C:590:ASP:CB	2.48	0.43
5:C:230:ARG:HA	5:C:231:PRO:HD3	1.84	0.43
5:C:496:ILE:HG13	5:C:531:PHE:HB2	2.01	0.43
5:C:398:THR:OG1	5:C:566:THR:O	2.21	0.43
5:C:602:GLU:OE1	5:C:648:ARG:HG2	2.18	0.43
5:C:975:TYR:N	5:C:975:TYR:CD1	2.86	0.43
6:D:127:LEU:CD2	6:D:134:VAL:HG22	2.49	0.43
6:D:475:LYS:NZ	11:D:8306:HOH:O	2.51	0.43
6:D:522:PRO:HG2	6:D:523:ASP:N	2.33	0.43
6:D:52:PRO:HG2	6:D:80:VAL:HA	2.00	0.43
6:D:554:LEU:HD11	6:D:571:LYS:CD	2.48	0.43
6:D:683:ILE:HG23	6:D:687:VAL:CG2	2.48	0.43
6:D:695:ILE:HD13	6:D:720:LEU:HD11	2.00	0.43
6:D:716:PHE:CZ	6:D:765:SER:HB3	2.54	0.43
4:L:86:VAL:O	4:L:86:VAL:HG13	2.18	0.43
4:L:99:LEU:HD13	4:L:144:VAL:CG2	2.49	0.43
5:M:179:ASN:ND2	11:M:1597:HOH:O	2.50	0.43
5:M:666:LEU:HD11	5:M:668:LEU:CD2	2.48	0.43
5:M:771:GLU:HB2	11:M:1204:HOH:O	2.18	0.43
6:N:1148:VAL:HG11	6:N:1203:LYS:HB3	2.00	0.43
6:N:1101:VAL:HG13	6:N:1427:SER:OG	2.18	0.43
6:N:1431:THR:OG1	6:N:1432:LYS:N	2.51	0.43
6:N:41:ARG:HB2	11:N:9006:HOH:O	2.18	0.43
6:N:525:ARG:HB2	6:N:538:SER:HB3	2.00	0.43
6:N:62:LYS:HG3	6:N:75:ARG:HH11	1.84	0.43
6:N:781:PRO:HB3	6:N:785:ILE:CG2	2.49	0.43
6:N:893:GLU:O	6:N:896:ALA:HB3	2.18	0.43
6:N:961:LYS:HG2	11:N:9172:HOH:O	2.17	0.43
7:O:26:ARG:HE	7:O:30:LEU:HD12	1.84	0.43
7:O:67:GLU:HB3	7:O:73:LEU:CD1	2.48	0.43
4:B:100:LEU:O	4:B:115:LEU:HG	2.19	0.43
4:B:103:ALA:N	11:B:348:HOH:O	2.51	0.43
4:B:23:PHE:O	4:B:196:THR:HA	2.19	0.43
5:C:1118:LYS:O	5:C:1119:ARG:HB2	2.18	0.43
5:C:140:ILE:HG13	5:C:411:SER:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:631:SER:CB	5:C:637:LEU:HD11	2.45	0.43
5:C:815:LEU:HD23	11:C:1323:HOH:O	2.19	0.43
6:D:1098:LEU:HD11	6:D:1263:PHE:CE2	2.53	0.43
6:D:1422:MET:CE	6:D:1427:SER:HA	2.48	0.43
6:D:171:LEU:HD11	11:D:8204:HOH:O	2.19	0.43
6:D:33:ASN:HB2	6:D:40:GLU:CD	2.38	0.43
6:D:556:LYS:O	6:D:560:GLN:HG3	2.19	0.43
6:D:586:ARG:HH22	6:D:1444:THR:HG21	1.83	0.43
6:D:80:VAL:HG12	6:D:81:THR:O	2.18	0.43
6:D:849:ALA:O	6:D:853:VAL:HG23	2.18	0.43
4:L:223:THR:HG23	11:L:379:HOH:O	2.18	0.43
4:L:227:ASN:H	4:L:227:ASN:ND2	2.16	0.43
4:L:54:THR:CG2	4:L:158:ILE:HG13	2.48	0.43
5:M:285:LEU:HD12	5:M:288:ARG:O	2.19	0.43
5:M:31:GLN:NE2	5:M:31:GLN:O	2.52	0.43
5:M:771:GLU:O	5:M:771:GLU:HG2	2.19	0.43
5:M:834:GLN:HB3	11:M:1436:HOH:O	2.19	0.43
5:M:882:LEU:HD11	6:N:1038:LEU:HB3	2.00	0.43
6:N:12:LEU:HD21	6:N:104:PHE:CE1	2.52	0.43
6:N:396:VAL:CG1	6:N:447:VAL:HG12	2.47	0.43
6:N:826:PRO:O	6:N:836:VAL:HG13	2.18	0.43
6:N:994:GLN:O	6:N:998:GLU:HG3	2.17	0.43
7:O:70:THR:HG22	7:O:71:GLY:N	2.33	0.43
2:Y:5:C:H2'	2:Y:6:U:C5	2.50	0.43
5:C:1003:ASP:OD1	5:C:1004:LYS:HD3	2.19	0.43
5:C:17:PRO:O	5:C:20:GLU:HB3	2.19	0.43
5:C:250:ARG:HD2	11:C:1278:HOH:O	2.18	0.43
5:C:140:ILE:HA	5:C:332:ARG:O	2.18	0.43
5:C:493:ARG:HE	5:C:493:ARG:HB2	1.53	0.43
6:D:1336:LEU:CD1	6:D:1341:PRO:HG3	2.49	0.43
6:D:1438:ALA:O	6:D:1443:THR:HG22	2.18	0.43
6:D:400:VAL:CG2	6:D:443:VAL:HG21	2.48	0.43
6:D:470:LEU:H	6:D:470:LEU:CD2	2.31	0.43
6:D:496:LEU:HD11	6:D:1388:ARG:HG3	2.01	0.43
6:D:662:GLU:OE2	6:D:669:ASN:HA	2.18	0.43
6:D:699:VAL:H	6:D:756:GLN:HE21	1.62	0.43
6:D:782:SER:O	6:D:786:ILE:HG13	2.18	0.43
5:C:949:LYS:CD	6:D:796:ARG:HH22	2.24	0.43
6:D:867:ARG:HD2	6:D:867:ARG:O	2.19	0.43
6:D:935:LYS:HE3	11:D:8312:HOH:O	2.18	0.43
4:K:7:LYS:HD2	4:K:186:LEU:HD21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:151:ASP:OD2	5:M:152:PRO:HD2	2.19	0.43
5:M:194:VAL:CG1	5:M:221:LEU:HB2	2.48	0.43
5:M:352:ALA:C	5:M:355:VAL:HG12	2.39	0.43
5:M:672:VAL:HG12	5:M:699:PHE:CE1	2.54	0.43
5:M:805:ARG:NH1	5:M:807:ARG:HD3	2.34	0.43
5:M:99:GLN:NE2	5:M:109:LYS:HB2	2.33	0.43
6:N:1148:VAL:CG1	6:N:1163:GLY:HA2	2.48	0.43
6:N:1207:TYR:HA	6:N:1214:PRO:HA	2.00	0.43
6:N:106:LYS:HE2	6:N:125:GLN:HE22	1.84	0.43
6:N:179:VAL:CG1	6:N:183:GLU:HB3	2.45	0.43
6:N:207:PHE:HB3	11:N:9229:HOH:O	2.18	0.43
5:M:716:LYS:NZ	6:N:36:THR:HG23	2.31	0.43
6:N:399:ARG:NE	6:N:430:ASP:HB2	2.33	0.43
6:N:816:HIS:N	6:N:816:HIS:ND1	2.65	0.43
6:N:949:ILE:N	11:N:9020:HOH:O	2.51	0.43
4:A:108:GLU:HB3	4:A:110:LYS:CE	2.49	0.43
4:A:43:ILE:HD11	4:B:35:THR:HG21	2.00	0.43
5:C:1103:ASP:OD2	5:C:1108:PRO:O	2.37	0.43
5:C:145:GLY:H	5:C:163:ILE:HG13	1.83	0.43
5:C:258:TYR:N	5:C:258:TYR:CD2	2.84	0.43
5:C:441:VAL:O	5:C:559:LEU:HG	2.18	0.43
5:C:626:ARG:HG3	5:C:626:ARG:HH11	1.84	0.43
5:C:759:THR:HG23	11:C:1516:HOH:O	2.19	0.43
5:C:751:PRO:HA	5:C:792:VAL:CG1	2.49	0.43
5:C:7:GLY:H	5:C:904:PRO:HD2	1.84	0.43
5:C:714:ASP:N	5:C:818:GLY:O	2.52	0.43
5:C:875:GLY:O	5:C:879:ARG:HD2	2.19	0.43
5:C:909:ALA:HB1	5:C:914:ILE:CD1	2.47	0.43
5:C:981:GLU:HG3	5:C:982:PRO:HD3	2.01	0.43
6:D:787:LEU:HD13	6:D:1023:MET:HA	2.00	0.43
6:D:1262:LEU:HD23	6:D:1352:ILE:HG12	2.00	0.43
6:D:1268:PRO:HD2	6:D:1271:LYS:HD3	2.01	0.43
6:D:189:GLN:HG3	11:D:8023:HOH:O	2.19	0.43
6:D:440:VAL:CG2	6:D:441:ARG:HH21	2.32	0.43
5:M:1019:GLN:HA	5:M:1020:PRO:HD3	1.86	0.43
5:M:111:ASP:CG	5:M:112:GLU:HG2	2.39	0.43
5:M:193:LEU:HD22	5:M:307:LEU:HD21	2.00	0.43
5:M:553:ASP:OD2	5:M:883:GLY:HA3	2.18	0.43
6:N:1144:LEU:HA	6:N:1147:ARG:HG3	2.00	0.43
6:N:1424:VAL:CG1	6:N:1425:THR:N	2.82	0.43
6:N:191:LEU:HD22	6:N:393:ILE:HD13	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:456:MET:HG2	11:N:9491:HOH:O	2.18	0.43
6:N:525:ARG:CD	6:N:525:ARG:H	2.31	0.43
6:N:607:LEU:HD23	11:N:9149:HOH:O	2.19	0.43
7:O:28:GLN:CA	7:O:32:ARG:HH22	2.32	0.43
6:N:1498:ALA:CB	7:O:84:ARG:HE	2.31	0.43
4:A:215:VAL:HG11	4:B:225:PHE:HD1	1.84	0.43
5:C:1031:ARG:CZ	6:D:621:LYS:HZ2	2.32	0.43
5:C:262:ALA:O	5:C:264:PRO:O	2.37	0.43
5:C:894:GLY:HA2	5:C:901:TYR:OH	2.19	0.43
5:C:983:ILE:HG21	5:C:987:ILE:CD1	2.49	0.43
5:C:946:ARG:HD3	5:C:984:GLU:HB3	2.01	0.43
3:I:8:DA:OP1	6:D:1426:LYS:HE3	2.19	0.43
6:D:1441:GLN:NE2	6:D:1442:ASN:H	2.17	0.43
6:D:30:GLU:N	11:D:8061:HOH:O	2.52	0.43
6:D:497:GLU:O	6:D:500:ARG:HB2	2.19	0.43
6:D:764:LEU:HD12	6:D:765:SER:N	2.34	0.43
6:D:767:HIS:CE1	7:E:6:ILE:HG21	2.54	0.43
6:D:799:LYS:N	11:D:8279:HOH:O	2.52	0.43
6:D:820:GLU:HG3	6:D:836:VAL:HG11	1.99	0.43
1:G:23:DG:OP1	5:C:388:ARG:NH1	2.52	0.43
4:L:26:GLU:HB2	4:L:27:PRO:HA	2.01	0.43
4:L:70:GLY:N	11:L:402:HOH:O	2.50	0.43
4:L:76:VAL:HA	4:L:79:ILE:HG12	2.00	0.43
4:L:9:PRO:HB3	4:L:25:LEU:CD2	2.49	0.43
2:Y:7:G:N2	5:M:1014:SER:HA	2.32	0.43
5:M:175:GLU:HB3	5:M:183:SER:OG	2.18	0.43
5:M:290:LEU:HD23	5:M:290:LEU:N	2.32	0.43
5:M:299:LYS:HG3	11:M:1441:HOH:O	2.19	0.43
5:M:564:MET:CB	11:M:1517:HOH:O	2.67	0.43
5:M:822:VAL:HB	5:M:824:ARG:HH21	1.84	0.43
5:M:701:THR:CG2	5:M:830:LYS:HE2	2.46	0.43
5:M:851:LYS:HD2	5:M:852:ILE:H	1.84	0.43
6:N:1112:CYS:O	6:N:1189:ARG:NH2	2.52	0.43
6:N:1150:ALA:CB	6:N:1151:ARG:HD2	2.48	0.43
6:N:1264:GLU:HG3	6:N:1425:THR:OG1	2.19	0.43
5:M:1103:ASP:OD2	6:N:3:LYS:HD2	2.18	0.43
6:N:407:VAL:HA	6:N:422:ALA:CB	2.49	0.43
6:N:508:ARG:HD3	11:N:9337:HOH:O	2.18	0.43
6:N:695:ILE:CD1	6:N:718:PRO:HB2	2.48	0.43
6:N:826:PRO:HD2	6:N:829:VAL:HG22	2.00	0.43
6:N:953:ASP:OD2	6:N:953:ASP:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:5:DG:H3'	11:Z:945:HOH:O	2.18	0.43
5:C:139:GLN:HE21	5:C:334:ARG:CD	2.25	0.42
5:C:183:SER:OG	5:C:190:LYS:HG2	2.18	0.42
5:C:251:ASP:HB3	5:C:252:LYS:CD	2.48	0.42
5:C:265:ARG:NH1	11:C:1308:HOH:O	2.51	0.42
5:C:313:LEU:HD13	5:C:321:GLU:CG	2.49	0.42
5:C:399:ASN:ND2	5:C:402:SER:OG	2.52	0.42
5:C:500:ASN:HA	11:C:1162:HOH:O	2.19	0.42
5:C:583:LEU:O	5:C:587:VAL:HG23	2.20	0.42
5:C:614:ARG:HG3	5:C:620:LEU:CD2	2.43	0.42
5:C:599:GLU:HA	5:C:651:LYS:HG3	2.00	0.42
6:D:101:HIS:HD2	6:D:514:LEU:HD11	1.83	0.42
6:D:1123:PHE:CE2	6:D:1184:GLN:HA	2.54	0.42
6:D:133:ILE:HG13	6:D:153:LEU:CG	2.48	0.42
6:D:1344:VAL:HG12	6:D:1348:LEU:HD13	2.00	0.42
6:D:1490:LYS:HB2	7:E:93:TYR:OH	2.19	0.42
6:D:175:VAL:HG21	11:D:8081:HOH:O	2.19	0.42
6:D:397:LYS:HB3	6:D:448:GLU:CB	2.49	0.42
6:D:397:LYS:HD3	6:D:448:GLU:OE1	2.19	0.42
6:D:701:LEU:O	6:D:747:VAL:HA	2.20	0.42
6:D:739:ASP:OD1	6:D:741:ASP:OD1	2.37	0.42
6:D:786:ILE:CD1	6:D:908:LYS:HD3	2.49	0.42
7:E:41:GLU:N	7:E:42:PRO:CD	2.81	0.42
4:K:133:GLU:HG3	5:M:605:LYS:HA	2.01	0.42
4:L:59:GLU:HB2	4:L:137:ARG:CZ	2.49	0.42
5:M:141:HIS:NE2	5:M:332:ARG:HD2	2.34	0.42
5:M:208:ALA:HB3	5:M:209:ARG:NH2	2.33	0.42
5:M:436:GLY:HA2	5:M:538:GLN:C	2.35	0.42
5:M:458:TYR:CD1	5:M:458:TYR:N	2.86	0.42
5:M:519:GLY:HA3	11:M:1314:HOH:O	2.19	0.42
5:M:515:ALA:HB3	5:M:524:VAL:HG21	2.01	0.42
5:M:687:ALA:C	5:M:688:ILE:HG13	2.39	0.42
6:N:1153:VAL:O	6:N:1160:LEU:HG	2.19	0.42
6:N:586:ARG:HH22	6:N:1444:THR:HG21	1.84	0.42
5:M:874:LEU:HD23	6:N:783:ARG:HB3	2.01	0.42
6:N:860:LEU:HD22	6:N:881:LEU:HD23	2.01	0.42
6:N:963:TYR:HA	6:N:966:GLU:OE2	2.19	0.42
6:N:984:THR:HG23	6:N:987:GLU:H	1.84	0.42
7:O:51:LEU:HD12	11:O:1058:HOH:O	2.19	0.42
7:O:26:ARG:HD3	7:O:73:LEU:CD2	2.49	0.42
4:A:152:PRO:HB3	4:A:154:GLU:OE1	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:313:LEU:CA	5:C:321:GLU:HG3	2.48	0.42
5:C:352:ALA:O	5:C:355:VAL:HG12	2.19	0.42
1:G:23:DG:H5''	5:C:388:ARG:NH2	2.35	0.42
5:C:580:MET:CE	5:C:584:GLU:HG3	2.49	0.42
5:C:747:ALA:C	5:C:799:ILE:HG23	2.39	0.42
5:C:816:LYS:HB2	5:C:819:VAL:HG21	2.00	0.42
5:C:571:LEU:HD12	5:C:996:LYS:HZ2	1.84	0.42
6:D:1046:GLN:HG2	6:D:1052:THR:CA	2.49	0.42
6:D:1231:GLU:OE2	6:D:1232:PRO:HD3	2.18	0.42
6:D:171:LEU:HD21	6:D:192:ALA:HB3	2.00	0.42
6:D:26:VAL:HG11	6:D:44:LEU:CD2	2.48	0.42
6:D:564:GLU:HA	6:D:567:ILE:HD12	2.01	0.42
6:D:699:VAL:HG21	6:D:760:ARG:HB3	2.01	0.42
6:D:794:GLN:HB3	6:D:1017:PHE:CZ	2.51	0.42
6:D:893:GLU:O	6:D:896:ALA:HB3	2.20	0.42
6:D:969:ARG:HA	11:D:8045:HOH:O	2.19	0.42
4:L:106:PRO:HG3	4:L:133:GLU:O	2.19	0.42
5:M:1058:ASP:O	5:M:1060:ILE:N	2.51	0.42
5:M:1103:ASP:N	5:M:1107:ASN:O	2.49	0.42
5:M:12:VAL:HB	5:M:472:ARG:NH1	2.34	0.42
5:M:136:ILE:HA	5:M:136:ILE:HD13	1.93	0.42
5:M:191:PHE:HB2	5:M:192:PRO:HD3	2.01	0.42
5:M:235:LEU:HD21	11:M:1276:HOH:O	2.18	0.42
5:M:684:PHE:O	5:M:685:GLU:C	2.58	0.42
5:M:960:GLU:HG3	5:M:961:GLU:N	2.32	0.42
6:N:501:ALA:CB	6:N:1453:ALA:HB2	2.38	0.42
6:N:161:LEU:HB2	11:N:9073:HOH:O	2.19	0.42
6:N:407:VAL:HA	6:N:422:ALA:HB2	2.01	0.42
6:N:522:PRO:HA	6:N:525:ARG:NE	2.34	0.42
6:N:714:GLN:HE22	6:N:768:ASN:HD22	1.67	0.42
6:N:756:GLN:NE2	6:N:760:ARG:HB3	2.34	0.42
6:N:783:ARG:HG3	6:N:783:ARG:H	1.53	0.42
4:A:55:SER:HB2	4:A:158:ILE:HB	2.01	0.42
4:B:102:LYS:HZ3	4:B:139:ASN:HB2	1.84	0.42
4:B:169:ALA:HB1	4:B:171:PHE:CE2	2.54	0.42
5:C:259:GLY:O	5:C:290:LEU:O	2.37	0.42
5:C:267:TYR:N	5:C:267:TYR:CD2	2.87	0.42
5:C:297:GLU:HG3	11:C:1205:HOH:O	2.18	0.42
5:C:437:ARG:CB	5:C:467:ILE:HB	2.49	0.42
5:C:573:ARG:CD	5:C:670:GLN:HE22	2.32	0.42
6:D:1047:LYS:HG2	6:D:1053:PHE:CE2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:137:PRO:HG3	6:D:467:GLU:OE1	2.20	0.42
6:D:185:VAL:HG21	6:D:191:LEU:CD2	2.49	0.42
6:D:191:LEU:HB2	6:D:195:VAL:HG12	2.00	0.42
6:D:32:ILE:HD13	6:D:37:LEU:O	2.19	0.42
6:D:423:ASP:N	6:D:423:ASP:OD1	2.52	0.42
6:D:440:VAL:HB	6:D:441:ARG:NH2	2.30	0.42
6:D:625:TYR:CD1	6:D:625:TYR:N	2.88	0.42
6:D:711:LEU:HD22	6:D:714:GLN:NE2	2.34	0.42
6:D:701:LEU:CD1	6:D:715:ALA:HB2	2.49	0.42
6:D:829:VAL:O	6:D:835:SER:HB2	2.19	0.42
6:D:98:PRO:HG3	6:D:462:GLN:HE22	1.85	0.42
4:K:206:THR:HG23	4:K:207:PRO:CD	2.49	0.42
4:L:56:VAL:HG12	4:L:57:TYR:N	2.34	0.42
5:M:203:ASP:O	5:M:207:LEU:HB2	2.18	0.42
5:M:617:ASP:HB2	5:M:619:ARG:NE	2.33	0.42
5:M:869:VAL:HG22	5:M:871:LEU:HD23	2.01	0.42
6:N:206:ARG:NH1	6:N:206:ARG:HG3	2.34	0.42
6:N:45:PHE:HB3	6:N:86:ARG:HH22	1.83	0.42
6:N:631:ILE:HG21	6:N:745:MET:CG	2.49	0.42
6:N:63:TYR:HB3	6:N:68:PHE:CE1	2.54	0.42
6:N:840:LYS:HE2	6:N:841:TYR:HE2	1.84	0.42
4:A:221:HIS:HA	4:A:224:TYR:CD2	2.54	0.42
5:C:1085:PHE:O	5:C:1088:LEU:HB3	2.18	0.42
5:C:214:TYR:OH	5:C:312:ALA:HB2	2.19	0.42
5:C:362:GLY:HA2	5:C:371:LYS:NZ	2.34	0.42
5:C:399:ASN:O	5:C:400:PRO:C	2.57	0.42
5:C:588:VAL:HA	5:C:591:SER:OG	2.19	0.42
5:C:626:ARG:O	5:C:638:ASP:HA	2.19	0.42
5:C:695:LEU:HD11	5:C:832:LYS:HB3	2.02	0.42
5:C:690:ILE:HD11	5:C:833:LEU:HD23	2.00	0.42
5:C:86:LYS:HB2	5:C:88:LEU:HD23	2.01	0.42
6:D:1109:GLU:CG	6:D:1201:CYS:HA	2.31	0.42
6:D:193:PRO:HG2	11:D:8081:HOH:O	2.18	0.42
6:D:455:ARG:NH1	6:D:463:GLN:HG3	2.35	0.42
2:H:2:A:H2'	2:H:3:G:O5'	2.20	0.42
4:K:9:PRO:HB3	4:K:25:LEU:CD2	2.50	0.42
5:M:146:VAL:CG1	5:M:162:ILE:HG12	2.48	0.42
5:M:244:PRO:HD2	5:M:245:GLY:N	2.28	0.42
5:M:334:ARG:HA	5:M:338:GLU:OE2	2.19	0.42
5:M:364:GLU:O	5:M:367:LEU:HG	2.18	0.42
5:M:526:PRO:HA	5:M:529:VAL:CG2	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:526:PRO:HA	5:M:529:VAL:HG23	2.01	0.42
5:M:654:LEU:HD13	5:M:664:GLY:N	2.34	0.42
5:M:695:LEU:CD2	5:M:832:LYS:HD3	2.29	0.42
5:M:894:GLY:HA2	5:M:901:TYR:OH	2.19	0.42
6:N:409:VAL:HG12	6:N:435:VAL:HG11	2.01	0.42
6:N:441:ARG:HH22	6:N:445:ARG:NH2	2.16	0.42
6:N:462:GLN:CA	6:N:513:ILE:HD13	2.49	0.42
6:N:653:PHE:CD1	6:N:653:PHE:N	2.87	0.42
6:N:688:TRP:HA	6:N:688:TRP:CE3	2.54	0.42
6:N:903:ASP:O	6:N:904:VAL:HG13	2.19	0.42
6:N:921:ARG:HH11	6:N:921:ARG:CB	2.15	0.42
6:N:785:ILE:CG1	6:N:935:LYS:HA	2.43	0.42
2:Y:16:G:H5'	6:N:742:GLY:C	2.39	0.42
3:Z:8:DA:H1'	3:Z:9:DG:C5'	2.46	0.42
5:C:191:PHE:CE2	5:C:196:LEU:HD12	2.55	0.42
5:C:227:PHE:HB3	11:C:1552:HOH:O	2.20	0.42
5:C:352:ALA:C	5:C:355:VAL:HG12	2.39	0.42
5:C:609:ASN:N	5:C:609:ASN:ND2	2.63	0.42
5:C:663:ASN:C	5:C:665:PHE:H	2.23	0.42
5:C:689:VAL:CG1	5:C:690:ILE:N	2.82	0.42
5:C:807:ARG:C	11:C:1277:HOH:O	2.58	0.42
5:C:924:VAL:HG12	11:C:1285:HOH:O	2.18	0.42
5:C:839:LEU:CD2	5:C:996:LYS:HA	2.47	0.42
6:D:118:LEU:O	6:D:120:ALA:N	2.53	0.42
6:D:1389:LEU:HG	6:D:1390:LEU:N	2.24	0.42
6:D:29:PRO:HD3	11:D:8201:HOH:O	2.18	0.42
6:D:440:VAL:HB	6:D:441:ARG:NE	2.32	0.42
6:D:118:LEU:CD1	6:D:461:ILE:HD12	2.50	0.42
6:D:486:ARG:CA	6:D:489:ARG:HG2	2.47	0.42
6:D:114:THR:CG2	6:D:495:ARG:HA	2.49	0.42
6:D:79:GLU:HG2	6:D:80:VAL:N	2.33	0.42
6:D:817:GLU:HA	6:D:836:VAL:HG21	2.02	0.42
6:D:838:ARG:NH1	6:D:838:ARG:HG2	2.34	0.42
6:D:1487:VAL:HB	7:E:74:VAL:HG23	2.00	0.42
1:G:12:DG:H2''	1:G:13:DT:H5'	2.01	0.42
4:L:106:PRO:HA	4:L:133:GLU:O	2.20	0.42
4:L:56:VAL:HG22	4:L:142:VAL:HG12	2.01	0.42
4:L:142:VAL:HG23	4:L:142:VAL:O	2.18	0.42
4:L:182:GLU:OE1	4:L:194:LYS:HD2	2.20	0.42
5:M:1032:PHE:HB3	6:N:620:GLY:O	2.20	0.42
5:M:208:ALA:CB	5:M:209:ARG:HH21	2.32	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:566:THR:HG22	5:M:566:THR:O	2.18	0.42
5:M:602:GLU:OE1	5:M:648:ARG:HB3	2.18	0.42
5:M:937:ASP:OD2	5:M:939:ARG:HG2	2.20	0.42
6:N:955:VAL:HG11	6:N:1015:TYR:CZ	2.54	0.42
6:N:1365:ASP:O	6:N:1369:GLU:HG3	2.19	0.42
6:N:1401:GLU:OE2	6:N:1415:VAL:HG21	2.20	0.42
6:N:739:ASP:OD1	6:N:741:ASP:OD1	2.36	0.42
6:N:989:TYR:CE1	6:N:993:LEU:HD21	2.54	0.42
4:B:101:LEU:HD23	4:B:101:LEU:C	2.40	0.42
5:C:1111:ILE:H	5:C:1111:ILE:HG13	1.48	0.42
5:C:333:ILE:HG12	5:C:467:ILE:HD11	2.01	0.42
5:C:408:ARG:O	5:C:454:SER:HA	2.19	0.42
5:C:431:HIS:HD2	5:C:433:THR:OG1	2.03	0.42
5:C:606:VAL:HG23	5:C:645:VAL:HG12	2.02	0.42
5:C:620:LEU:HD11	11:C:1436:HOH:O	2.19	0.42
5:C:644:VAL:HB	11:C:1372:HOH:O	2.20	0.42
5:C:693:GLU:HA	5:C:696:LYS:HE3	2.00	0.42
5:C:77:PRO:HD3	5:C:91:GLN:O	2.20	0.42
5:C:710:ILE:CD1	5:C:790:LEU:HD13	2.49	0.42
5:C:895:TYR:HA	11:C:1275:HOH:O	2.20	0.42
5:C:1096:ALA:HB2	6:D:101:HIS:NE2	2.34	0.42
5:C:874:LEU:HA	6:D:1023:MET:SD	2.60	0.42
6:D:116:LEU:HD23	6:D:150:ARG:HH11	1.85	0.42
6:D:1121:PRO:HG3	6:D:1185:GLU:OE2	2.19	0.42
6:D:1211:MET:HE1	6:D:1213:ARG:HD3	2.00	0.42
6:D:54:LYS:CG	6:D:55:ASP:H	2.32	0.42
6:D:610:LYS:C	6:D:615:ARG:HD3	2.39	0.42
6:D:709:HIS:CD2	6:D:709:HIS:H	2.37	0.42
6:D:841:TYR:HB3	6:D:843:PHE:CZ	2.54	0.42
6:D:959:GLU:CD	6:D:959:GLU:N	2.73	0.42
2:H:9:G:N2	11:H:26:HOH:O	2.53	0.42
4:K:13:VAL:HG22	4:K:23:PHE:CD1	2.55	0.42
5:M:1060:ILE:O	5:M:1064:ASN:ND2	2.53	0.42
5:M:1111:ILE:HG13	5:M:1112:PHE:N	2.31	0.42
5:M:473:ARG:HG3	5:M:474:VAL:N	2.35	0.42
5:M:536:PRO:HB3	5:M:906:PHE:HD1	1.84	0.42
5:M:575:GLN:NE2	5:M:670:GLN:OE1	2.52	0.42
5:M:810:ASP:HA	5:M:811:PRO:HD3	1.67	0.42
5:M:833:LEU:HD11	5:M:839:LEU:HD21	2.01	0.42
5:M:889:HIS:HE1	6:N:951:ILE:H	1.67	0.42
6:N:1036:ARG:HH11	6:N:1036:ARG:HB3	1.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:1158:VAL:HG12	6:N:1159:ARG:N	2.35	0.42
6:N:166:GLN:OE1	6:N:396:VAL:HG22	2.20	0.42
6:N:131:LYS:HZ3	6:N:568:ARG:CB	2.32	0.42
6:N:656:PHE:HB3	6:N:694:VAL:CG1	2.50	0.42
1:X:19:DC:H3'	11:X:2000:HOH:O	2.19	0.42
4:A:161:ARG:HA	4:A:161:ARG:NE	2.34	0.42
4:B:142:VAL:HG23	4:B:142:VAL:O	2.18	0.42
5:C:137:VAL:N	5:C:391:LEU:HD21	2.33	0.42
5:C:140:ILE:HD11	5:C:412:ALA:HB2	2.01	0.42
5:C:966:LEU:HA	5:C:966:LEU:HD12	1.94	0.42
6:D:1103:HIS:HD2	6:D:1463:LYS:H	1.59	0.42
6:D:711:LEU:HD21	6:D:768:ASN:HB2	2.01	0.42
6:D:806:PHE:HE1	6:D:813:LEU:HB3	1.79	0.42
6:D:820:GLU:OE1	6:D:840:LYS:HE3	2.20	0.42
4:K:213:GLN:NE2	11:K:1765:HOH:O	2.51	0.42
4:L:189:ARG:HG3	4:L:189:ARG:O	2.19	0.42
4:L:75:VAL:O	4:L:79:ILE:HG23	2.19	0.42
5:M:1009:SER:OG	5:M:1010:THR:N	2.53	0.42
5:M:458:TYR:HD1	5:M:458:TYR:N	2.18	0.42
5:M:580:MET:O	5:M:902:ILE:HA	2.19	0.42
5:M:783:ARG:HE	5:M:785:VAL:CG1	2.32	0.42
5:M:69:LEU:HD12	5:M:97:ARG:CB	2.49	0.42
5:M:98:LEU:N	5:M:98:LEU:HD12	2.35	0.42
6:N:1047:LYS:HG2	6:N:1053:PHE:CE1	2.54	0.42
6:N:1055:VAL:HA	6:N:1056:PRO:HD3	1.90	0.42
6:N:1365:ASP:N	6:N:1365:ASP:OD2	2.53	0.42
6:N:137:PRO:HD2	6:N:453:ASP:CG	2.39	0.42
6:N:457:GLY:C	6:N:459:GLU:N	2.72	0.42
6:N:506:GLY:O	6:N:507:ASN:C	2.58	0.42
6:N:19:ARG:HE	6:N:516:ALA:CB	2.32	0.42
6:N:998:GLU:O	6:N:1002:LYS:HG3	2.20	0.42
4:A:184:THR:N	11:A:321:HOH:O	2.53	0.42
5:C:1105:LYS:HD2	5:C:1107:ASN:HD22	1.83	0.42
5:C:401:LEU:HD21	5:C:565:GLN:NE2	2.34	0.42
5:C:541:SER:OG	5:C:542:VAL:N	2.52	0.42
5:C:780:GLU:H	5:C:780:GLU:HG3	1.53	0.42
6:D:1072:ILE:HG12	11:D:8010:HOH:O	2.20	0.42
6:D:1341:PRO:O	6:D:1343:ALA:N	2.52	0.42
6:D:462:GLN:HG2	6:D:466:LYS:HZ2	1.85	0.42
6:D:470:LEU:HD21	11:D:8038:HOH:O	2.19	0.42
6:D:54:LYS:HB3	6:D:57:GLU:OE2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:698:LYS:HE3	6:D:698:LYS:HB3	1.92	0.42
6:D:695:ILE:HD13	6:D:720:LEU:CD1	2.50	0.42
6:D:87:ARG:NH2	11:D:8227:HOH:O	2.53	0.42
6:D:780:LYS:HD2	6:D:912:LYS:HB2	2.02	0.42
7:E:66:LYS:HD2	7:E:69:LEU:HD23	2.02	0.42
3:I:3:DA:O4'	5:C:423:ALA:HB2	2.20	0.42
5:M:1111:ILE:HG12	5:M:1111:ILE:H	1.43	0.42
5:M:628:PHE:CZ	5:M:703:ILE:HD13	2.55	0.42
5:M:677:MET:HE3	5:M:678:PRO:O	2.19	0.42
6:N:879:ARG:HH11	6:N:879:ARG:CG	2.32	0.42
4:A:182:GLU:HG2	4:A:194:LYS:HG2	2.02	0.42
4:A:8:ALA:HB1	4:B:224:TYR:CE1	2.51	0.42
4:B:81:ASN:O	4:B:127:LEU:HD21	2.20	0.42
5:C:139:GLN:HA	5:C:411:SER:O	2.19	0.42
5:C:431:HIS:CD2	5:C:432:ARG:HB2	2.55	0.42
5:C:442:GLU:HG2	5:C:454:SER:H	1.84	0.42
5:C:719:PRO:HD2	11:C:1241:HOH:O	2.20	0.42
6:D:116:LEU:HD23	6:D:150:ARG:NH1	2.35	0.42
6:D:127:LEU:CD1	6:D:128:TYR:N	2.80	0.42
6:D:1444:THR:OG1	6:D:1445:HIS:N	2.53	0.42
6:D:1451:ALA:O	6:D:1452:ILE:C	2.57	0.42
6:D:48:ARG:HB3	6:D:48:ARG:HE	1.53	0.42
7:E:33:HIS:CE1	7:E:89:MET:HB3	2.55	0.42
3:I:13:DG:H2"	3:I:14:DG:C8	2.55	0.42
4:K:107:LYS:HD3	4:K:108:GLU:O	2.20	0.42
4:L:58:ILE:HG21	4:L:61:VAL:HB	2.00	0.42
4:L:73:GLU:CB	4:L:77:GLU:HG3	2.50	0.42
5:M:1035:MET:H	5:M:1035:MET:HG3	1.65	0.42
5:M:20:GLU:OE2	5:M:460:ARG:HD3	2.20	0.42
5:M:909:ALA:CB	5:M:914:ILE:HD11	2.47	0.42
6:N:1078:ARG:NH1	6:N:1078:ARG:HG3	2.34	0.42
6:N:1221:VAL:O	6:N:1222:GLY:C	2.58	0.42
6:N:1415:VAL:HG22	11:N:9043:HOH:O	2.19	0.42
6:N:19:ARG:HH11	6:N:19:ARG:HG3	1.85	0.42
6:N:403:PHE:CD2	6:N:444:VAL:HG23	2.55	0.42
6:N:574:LEU:O	6:N:578:VAL:HG23	2.19	0.42
6:N:596:SER:HB3	6:N:598:ARG:NE	2.35	0.42
6:N:600:LEU:HD12	6:N:600:LEU:H	1.83	0.42
6:N:673:ALA:O	6:N:677:LEU:HD12	2.19	0.42
6:N:683:ILE:HG23	6:N:687:VAL:HG21	2.01	0.42
4:A:70:GLY:O	4:A:132:LEU:HA	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:152:PRO:HG2	6:D:857:ILE:HD12	2.01	0.42
4:B:22:GLU:HG2	4:B:198:ARG:HG2	2.00	0.42
5:C:182:VAL:HG12	5:C:193:LEU:HD13	2.01	0.42
5:C:208:ALA:HB1	5:C:218:VAL:CG1	2.50	0.42
5:C:208:ALA:O	5:C:218:VAL:HG21	2.19	0.42
5:C:537:LYS:CG	5:C:545:ASN:HD21	2.33	0.42
5:C:598:GLU:O	5:C:651:LYS:HG3	2.20	0.42
5:C:71:TYR:HA	5:C:96:ALA:CB	2.50	0.42
5:C:577:PRO:HA	5:C:993:PHE:CD2	2.54	0.42
6:D:1001:GLU:O	6:D:1004:THR:HB	2.20	0.42
6:D:1341:PRO:O	6:D:1344:VAL:N	2.53	0.42
6:D:461:ILE:O	6:D:465:LEU:HB2	2.18	0.42
6:D:50:PHE:HB3	6:D:522:PRO:CG	2.46	0.42
6:D:82:LYS:HB2	11:D:8499:HOH:O	2.20	0.42
7:E:59:ASN:ND2	7:E:59:ASN:N	2.68	0.42
4:K:91:ASN:HB3	11:K:1721:HOH:O	2.20	0.42
4:L:25:LEU:CD2	4:L:28:LEU:HD21	2.40	0.42
5:M:63:GLY:HA3	5:M:103:LYS:HG3	2.02	0.42
5:M:1049:LEU:HD23	6:N:1472:ILE:CD1	2.49	0.42
5:M:536:PRO:CD	5:M:537:LYS:HZ2	2.17	0.42
5:M:456:ALA:HA	5:M:541:SER:HA	2.01	0.42
5:M:549:PHE:HE2	5:M:887:GLU:HA	1.85	0.42
5:M:605:LYS:O	5:M:611:ILE:HA	2.20	0.42
5:M:728:HIS:NE2	5:M:775:ARG:NH1	2.67	0.42
5:M:757:GLY:HA2	5:M:789:SER:HB3	2.02	0.42
5:M:872:ASN:HD21	5:M:874:LEU:HD13	1.85	0.42
5:M:917:LEU:HB3	11:M:1461:HOH:O	2.20	0.42
6:N:1137:ARG:HG3	11:N:9103:HOH:O	2.19	0.42
6:N:1463:LYS:O	6:N:1467:ILE:HG13	2.19	0.42
6:N:397:LYS:HB3	6:N:448:GLU:HB3	2.01	0.42
6:N:446:VAL:O	6:N:447:VAL:O	2.38	0.42
6:N:628:ARG:HG3	6:N:628:ARG:HH11	1.84	0.42
6:N:632:VAL:O	6:N:727:GLN:HA	2.20	0.42
6:N:804:LEU:HD12	6:N:830:ALA:O	2.20	0.42
6:N:859:ASP:HB3	6:N:861:GLN:NE2	2.35	0.42
7:O:47:LYS:CA	7:O:54:LEU:HB3	2.49	0.42
2:Y:7:G:H22	5:M:1014:SER:HA	1.84	0.42
4:A:89:PHE:CE2	4:A:146:ARG:HB2	2.55	0.41
5:C:1084:SER:O	5:C:1087:VAL:HG12	2.20	0.41
5:C:129:ILE:CG1	5:C:134:ARG:HD3	2.50	0.41
5:C:186:VAL:HG23	5:C:187:ASN:N	2.26	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:243:ARG:N	5:C:244:PRO:HD3	2.32	0.41
2:H:13:C:C3'	5:C:409:ARG:HH22	2.32	0.41
5:C:564:MET:HE3	5:C:564:MET:O	2.20	0.41
5:C:848:VAL:HG12	5:C:849:VAL:N	2.35	0.41
6:D:1042:ARG:HD2	6:D:1045:MET:CE	2.50	0.41
6:D:105:VAL:HG12	11:D:8237:HOH:O	2.20	0.41
6:D:1495:ILE:HG22	6:D:1499:ARG:NE	2.35	0.41
6:D:566:ILE:N	6:D:566:ILE:HD12	2.35	0.41
6:D:581:LEU:HG	6:D:582:LEU:N	2.35	0.41
5:C:1031:ARG:NH1	6:D:621:LYS:NZ	2.68	0.41
6:D:789:LEU:HD13	6:D:911:LEU:HD21	2.02	0.41
6:D:82:LYS:C	6:D:84:ILE:N	2.74	0.41
6:D:890:VAL:HG23	6:D:890:VAL:O	2.19	0.41
6:D:926:LYS:HB3	6:D:926:LYS:HE2	1.93	0.41
4:K:14:ARG:HH11	4:K:14:ARG:HG3	1.85	0.41
4:K:30:ARG:HD2	4:K:30:ARG:HA	1.87	0.41
4:L:143:ARG:NH1	4:L:158:ILE:HG21	2.35	0.41
4:L:43:ILE:HG23	4:L:217:ILE:HG21	2.02	0.41
5:M:1013:TYR:CE1	5:M:1020:PRO:HG3	2.55	0.41
5:M:263:ASP:HB2	5:M:264:PRO:HD3	2.02	0.41
5:M:292:ARG:HD2	5:M:299:LYS:CE	2.49	0.41
5:M:745:ILE:HG21	11:M:1187:HOH:O	2.19	0.41
5:M:756:VAL:O	5:M:789:SER:CB	2.66	0.41
5:M:842:ARG:HH22	5:M:887:GLU:CD	2.23	0.41
5:M:940:GLU:O	5:M:943:VAL:HG12	2.19	0.41
5:M:842:ARG:HG3	5:M:995:MET:HE3	2.02	0.41
6:N:1000:THR:HG23	6:N:1001:GLU:N	2.34	0.41
6:N:107:ASP:O	6:N:108:VAL:C	2.57	0.41
6:N:1206:GLY:O	6:N:1215:VAL:HG23	2.20	0.41
6:N:1267:ARG:HD2	6:N:1271:LYS:HE2	2.01	0.41
6:N:12:LEU:HD23	6:N:12:LEU:HA	1.84	0.41
6:N:1381:VAL:HG22	6:N:1398:TRP:CZ2	2.54	0.41
6:N:1399:ASP:O	6:N:1403:LEU:HB2	2.19	0.41
6:N:206:ARG:CG	6:N:394:LEU:HD22	2.36	0.41
6:N:485:SER:HA	11:N:9344:HOH:O	2.19	0.41
5:C:636:ALA:HB3	5:C:703:ILE:CD1	2.33	0.41
5:C:68:PHE:HZ	5:C:71:TYR:HD2	1.68	0.41
5:C:704:HIS:O	5:C:829:GLN:OE1	2.38	0.41
5:C:873:PRO:O	5:C:877:PRO:HD3	2.20	0.41
5:C:89:THR:O	5:C:91:GLN:HG3	2.20	0.41
6:D:960:LYS:NZ	6:D:1040:GLY:O	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:12:LEU:HD21	6:D:104:PHE:CZ	2.55	0.41
6:D:1248:GLY:O	6:D:1252:ILE:HG12	2.20	0.41
6:D:1472:ILE:O	6:D:1477:GLY:HA3	2.19	0.41
6:D:134:VAL:HA	6:D:151:GLN:O	2.19	0.41
6:D:522:PRO:HA	6:D:525:ARG:NE	2.34	0.41
6:D:984:THR:HG23	6:D:986:ARG:H	1.84	0.41
7:E:44:GLU:HA	11:E:110:HOH:O	2.20	0.41
4:L:106:PRO:HG3	4:L:134:GLU:CD	2.41	0.41
4:L:175:ARG:HG2	4:L:175:ARG:H	1.61	0.41
4:L:9:PRO:HB3	4:L:25:LEU:HG	2.03	0.41
5:M:1016:ILE:CG1	5:M:1017:THR:N	2.82	0.41
5:M:217:LEU:HD13	11:M:1269:HOH:O	2.20	0.41
5:M:274:ARG:HG3	5:M:285:LEU:HD22	2.02	0.41
5:M:354:GLY:O	5:M:358:ARG:HD3	2.19	0.41
5:M:39:ARG:NH2	11:M:1341:HOH:O	2.52	0.41
5:M:957:LYS:NZ	5:M:957:LYS:HB2	2.35	0.41
6:N:1209:LEU:HD13	11:N:9248:HOH:O	2.20	0.41
6:N:1363:LEU:O	6:N:1363:LEU:HD12	2.20	0.41
6:N:1498:ALA:HB1	7:O:84:ARG:HE	1.86	0.41
6:N:394:LEU:HD11	6:N:445:ARG:HH12	1.81	0.41
6:N:52:PRO:CB	6:N:80:VAL:HG13	2.50	0.41
6:N:66:GLN:O	6:N:69:GLU:HB3	2.20	0.41
6:N:709:HIS:CD2	6:N:709:HIS:N	2.89	0.41
2:Y:7:G:H22	5:M:1014:SER:N	2.17	0.41
4:A:111:ALA:CB	4:A:127:LEU:HD23	2.42	0.41
4:A:128:HIS:HE1	4:A:131:THR:HG23	1.86	0.41
4:B:132:LEU:HD23	4:B:136:GLY:O	2.20	0.41
4:A:42:ARG:HH22	4:B:34:VAL:HB	1.85	0.41
5:C:1006:HIS:HA	5:C:1027:PHE:HD1	1.83	0.41
5:C:115:LEU:H	5:C:115:LEU:HG	1.70	0.41
5:C:182:VAL:CG2	5:C:220:GLY:O	2.67	0.41
5:C:468:ARG:NH2	11:C:1462:HOH:O	2.53	0.41
5:C:6:PHE:N	5:C:6:PHE:CD1	2.88	0.41
5:C:552:HIS:HD2	6:D:1064:GLY:HA2	1.86	0.41
6:D:1464:GLU:HA	6:D:1467:ILE:HD11	2.02	0.41
6:D:412:GLY:HA2	6:D:434:ARG:NH1	2.34	0.41
6:D:420:VAL:C	6:D:421:LEU:HD23	2.40	0.41
6:D:481:MET:CE	6:D:493:ARG:HB2	2.47	0.41
7:E:28:GLN:HG2	7:E:32:ARG:HH22	1.86	0.41
7:E:8:LYS:O	7:E:12:MET:HG3	2.20	0.41
4:K:41:ARG:HG3	4:K:177:VAL:CG1	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:91:ASN:O	4:K:94:LEU:HD12	2.20	0.41
4:L:48:ILE:HG22	4:L:173:PRO:HD2	2.03	0.41
4:L:88:ARG:HD2	4:L:123:MET:SD	2.61	0.41
5:M:211:LEU:HD11	5:M:308:ARG:HA	2.02	0.41
5:M:29:ALA:HB2	5:M:337:GLY:HA3	2.01	0.41
5:M:666:LEU:HD12	5:M:667:ALA:N	2.35	0.41
5:M:670:GLN:NE2	5:M:699:PHE:CG	2.88	0.41
5:M:913:GLU:O	5:M:916:GLU:HB3	2.20	0.41
5:M:1070:ILE:HG23	6:N:656:PHE:HD1	1.84	0.41
6:N:704:ARG:CZ	6:N:737:ASN:O	2.69	0.41
5:C:1016:ILE:HG12	5:C:1017:THR:H	1.84	0.41
5:C:98:LEU:C	5:C:109:LYS:HD2	2.40	0.41
6:D:1100:ASP:HB3	6:D:1428:ALA:CB	2.49	0.41
6:D:1110:ALA:O	6:D:1111:ASP:C	2.58	0.41
6:D:124:GLU:O	6:D:128:TYR:HB2	2.19	0.41
6:D:1236:LEU:HD12	6:D:1359:GLN:HB3	2.03	0.41
6:D:496:LEU:HD12	6:D:500:ARG:HG2	2.03	0.41
6:D:754:PHE:O	6:D:758:GLU:HG2	2.20	0.41
6:D:783:ARG:HD2	6:D:1029:ARG:HG2	2.02	0.41
6:D:972:LEU:HD23	11:D:8045:HOH:O	2.19	0.41
6:D:98:PRO:HA	6:D:515:GLU:HA	2.01	0.41
4:K:181:VAL:O	5:M:938:LYS:N	2.54	0.41
4:K:36:LEU:HD11	11:L:365:HOH:O	2.20	0.41
4:K:42:ARG:HH11	5:M:978:ARG:CA	2.28	0.41
5:M:1067:TYR:O	5:M:1071:ILE:HG12	2.20	0.41
5:M:23:VAL:HG13	11:M:1414:HOH:O	2.20	0.41
5:M:13:ILE:HG23	5:M:483:VAL:HG21	2.02	0.41
5:M:632:ASN:HB3	5:M:633:GLN:NE2	2.35	0.41
6:N:1124:GLN:HA	6:N:1125:PRO:HD3	1.60	0.41
6:N:1155:VAL:HG12	11:N:9051:HOH:O	2.20	0.41
6:N:493:ARG:CG	6:N:1390:LEU:HB2	2.45	0.41
6:N:1440:PHE:C	6:N:1440:PHE:CD2	2.93	0.41
5:M:1085:PHE:CE2	6:N:1468:LEU:HG	2.52	0.41
6:N:159:ARG:NH2	11:N:9468:HOH:O	2.53	0.41
6:N:470:LEU:HD12	6:N:503:LEU:CD2	2.50	0.41
6:N:633:VAL:C	6:N:635:PRO:HD3	2.40	0.41
6:N:782:SER:O	6:N:786:ILE:HG13	2.20	0.41
6:N:899:LEU:HB3	6:N:917:GLN:HG2	2.01	0.41
3:Z:13:DG:H2"	3:Z:14:DG:C8	2.55	0.41
5:C:118:ILE:HG22	5:C:382:ILE:HD13	2.01	0.41
5:C:137:VAL:CG2	5:C:391:LEU:HG	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:603:VAL:HG11	5:C:606:VAL:HG22	2.03	0.41
5:C:669:GLY:C	5:C:670:GLN:HG2	2.41	0.41
5:C:692:GLU:O	5:C:696:LYS:HG3	2.20	0.41
5:C:715:THR:HA	11:C:1542:HOH:O	2.20	0.41
5:C:791:ARG:O	5:C:793:PRO:HD3	2.20	0.41
5:C:842:ARG:HG3	5:C:995:MET:CE	2.51	0.41
5:C:569:VAL:HG13	5:C:996:LYS:HZ3	1.84	0.41
6:D:1046:GLN:HG2	6:D:1052:THR:CB	2.51	0.41
6:D:112:ILE:HA	6:D:512:MET:HE3	2.02	0.41
6:D:1154:GLU:HB3	6:N:563:PRO:HB3	2.01	0.41
6:D:1481:VAL:HG11	7:E:18:ARG:CA	2.42	0.41
6:D:1481:VAL:HG22	7:E:18:ARG:NE	2.28	0.41
6:D:28:LYS:HD2	11:D:8201:HOH:O	2.20	0.41
6:D:510:GLU:HG2	11:D:8320:HOH:O	2.20	0.41
6:D:702:LEU:N	6:D:702:LEU:HD12	2.35	0.41
6:D:906:GLN:HB3	6:D:911:LEU:CD1	2.49	0.41
7:E:43:GLU:HG3	7:E:43:GLU:H	1.69	0.41
2:H:2:A:C2'	2:H:3:G:O5'	2.68	0.41
4:K:174:VAL:HG13	4:K:200:TRP:O	2.20	0.41
4:K:94:LEU:HD11	4:K:119:ASP:CB	2.51	0.41
5:M:259:GLY:O	5:M:290:LEU:O	2.38	0.41
5:M:25:SER:OG	5:M:335:THR:HB	2.20	0.41
5:M:292:ARG:HB2	5:M:299:LYS:HG2	2.02	0.41
5:M:309:TYR:HA	5:M:312:ALA:HB3	2.02	0.41
5:M:217:LEU:CD1	5:M:311:PHE:HA	2.50	0.41
5:M:580:MET:HE1	5:M:665:PHE:CZ	2.55	0.41
5:M:780:GLU:HG3	5:M:781:LYS:N	2.35	0.41
5:M:928:LYS:O	5:M:932:GLU:HG3	2.21	0.41
6:N:1114:THR:O	6:N:1114:THR:CG2	2.68	0.41
6:N:1330:ILE:HB	6:N:1347:TYR:OH	2.20	0.41
6:N:710:ARG:C	6:N:712:GLY:N	2.74	0.41
6:N:800:LYS:CE	6:N:804:LEU:HD13	2.50	0.41
6:N:8:VAL:HG12	6:N:9:ARG:N	2.34	0.41
1:X:11:DC:H2''	1:X:12:DG:H8	1.85	0.41
1:X:12:DG:H2'	1:X:13:DT:H72	2.02	0.41
5:C:1012:PRO:HB2	5:C:1021:LEU:O	2.20	0.41
5:C:141:HIS:CD2	5:C:141:HIS:C	2.93	0.41
5:C:265:ARG:HB2	11:C:1165:HOH:O	2.21	0.41
5:C:318:PRO:HB2	11:C:1545:HOH:O	2.20	0.41
5:C:348:LEU:HD12	5:C:348:LEU:HA	1.90	0.41
5:C:668:LEU:HD12	5:C:668:LEU:H	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:673:LEU:CD2	5:C:867:VAL:HG12	2.50	0.41
5:C:754:ILE:HD12	5:C:789:SER:HB3	2.02	0.41
5:C:764:GLU:HG3	6:D:54:LYS:HZ3	1.85	0.41
6:D:1153:VAL:HG12	6:D:1155:VAL:HG22	2.02	0.41
6:D:1457:ASP:O	6:D:1459:LEU:HD12	2.21	0.41
6:D:1485:GLN:HG2	6:D:1485:GLN:H	1.75	0.41
6:D:641:GLN:HB3	6:D:717:GLN:O	2.20	0.41
6:D:838:ARG:HH11	6:D:838:ARG:HG2	1.86	0.41
6:D:1494:ALA:HB1	7:E:88:GLU:OE2	2.21	0.41
2:H:7:G:H2'	2:H:8:C:OP1	2.20	0.41
5:M:1008:ARG:HA	5:M:1027:PHE:CD2	2.54	0.41
5:M:23:VAL:HA	11:M:1414:HOH:O	2.21	0.41
5:M:395:LYS:HE2	5:M:403:SER:CB	2.36	0.41
5:M:713:ARG:HB3	5:M:720:GLU:OE2	2.20	0.41
5:M:80:GLN:HE21	5:M:84:ARG:HH21	1.68	0.41
5:M:983:ILE:HG22	5:M:983:ILE:O	2.20	0.41
5:M:993:PHE:HE1	5:M:995:MET:HE2	1.85	0.41
6:N:1406:ARG:HE	6:N:1407:LEU:HD12	1.84	0.41
6:N:63:TYR:HB3	6:N:68:PHE:CD1	2.55	0.41
6:N:716:PHE:O	6:N:718:PRO:HD3	2.21	0.41
6:N:729:HIS:HE1	6:N:731:LEU:HG	1.85	0.41
2:Y:16:G:O3'	6:N:741:ASP:OD1	2.39	0.41
6:N:937:TYR:H	6:N:937:TYR:HD1	1.66	0.41
6:N:956:ILE:HA	6:N:957:PRO:HD3	1.93	0.41
7:O:9:LEU:HB3	7:O:19:LEU:CD2	2.50	0.41
4:B:229:GLN:HB2	4:B:229:GLN:HE21	1.62	0.41
5:C:263:ASP:C	5:C:264:PRO:O	2.59	0.41
5:C:358:ARG:CA	5:C:361:MET:HG2	2.51	0.41
5:C:443:THR:HG21	6:D:1078:ARG:NH2	2.36	0.41
5:C:491:GLU:CB	11:C:1287:HOH:O	2.68	0.41
5:C:595:LEU:HD12	11:C:1444:HOH:O	2.21	0.41
5:C:694:LEU:HD21	5:C:868:ASP:CB	2.47	0.41
6:D:1107:VAL:HG12	6:D:1217:ILE:HA	2.02	0.41
6:D:1223:ILE:HD11	6:D:1462:LEU:HD12	2.03	0.41
6:D:1393:GLN:NE2	6:D:1394:VAL:HB	2.36	0.41
6:D:717:GLN:HG2	11:D:8027:HOH:O	2.21	0.41
6:D:764:LEU:HD23	6:D:767:HIS:CD2	2.54	0.41
1:G:14:DT:H5''	11:D:8242:HOH:O	2.21	0.41
4:L:11:PHE:CE1	4:L:23:PHE:HB3	2.55	0.41
5:M:1092:LEU:HD23	5:M:1095:LEU:HD13	2.03	0.41
5:M:158:TYR:CZ	5:M:313:LEU:HG	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:469:THR:OG1	5:M:470:PRO:HD2	2.21	0.41
5:M:668:LEU:H	5:M:668:LEU:HD12	1.86	0.41
5:M:738:ASP:HB2	5:M:744:ARG:HB3	2.02	0.41
5:M:73:LEU:HD12	5:M:73:LEU:O	2.21	0.41
6:N:1134:LEU:HB3	11:N:9479:HOH:O	2.20	0.41
6:N:701:LEU:O	6:N:747:VAL:HA	2.21	0.41
6:N:709:HIS:HA	6:N:1227:GLN:HB3	2.01	0.41
6:N:916:TYR:O	6:N:919:PHE:HB3	2.19	0.41
7:O:93:TYR:HA	7:O:94:PRO:HD2	1.87	0.41
4:A:178:ALA:HA	11:C:1156:HOH:O	2.20	0.41
5:C:1079:PRO:HB2	11:D:8463:HOH:O	2.19	0.41
5:C:185:LYS:HE2	5:C:190:LYS:NZ	2.35	0.41
5:C:242:LEU:HD11	11:C:1327:HOH:O	2.21	0.41
5:C:599:GLU:OE2	5:C:619:ARG:NH2	2.54	0.41
5:C:639:GLN:HG2	11:C:1396:HOH:O	2.19	0.41
6:D:1086:LEU:HA	11:D:8250:HOH:O	2.21	0.41
6:D:1197:ARG:CB	6:D:1396:GLU:HG3	2.45	0.41
6:D:185:VAL:HG11	6:D:197:SER:OG	2.20	0.41
6:D:446:VAL:O	6:D:447:VAL:O	2.39	0.41
6:D:525:ARG:HA	6:D:526:PRO:HD3	1.73	0.41
7:E:76:GLY:N	7:E:79:LEU:HD22	2.36	0.41
1:G:6:DT:H2'	1:G:7:DC:C5	2.55	0.41
2:H:14:G:C2'	2:H:15:C:H5'	2.48	0.41
4:L:124:ASN:CG	4:L:127:LEU:HB2	2.41	0.41
4:L:81:ASN:HD21	4:L:127:LEU:HD11	1.85	0.41
4:K:224:TYR:HB3	4:L:9:PRO:CG	2.51	0.41
5:M:1021:LEU:HA	11:M:1512:HOH:O	2.21	0.41
5:M:1096:ALA:O	6:N:13:ALA:CB	2.68	0.41
5:M:393:GLN:NE2	5:M:406:HIS:HE1	2.18	0.41
5:M:674:VAL:HG11	5:M:992:MET:HB3	2.02	0.41
6:N:1007:VAL:HA	11:N:9288:HOH:O	2.21	0.41
6:N:1117:TYR:CD2	6:N:1117:TYR:N	2.88	0.41
6:N:1406:ARG:HE	6:N:1407:LEU:CD1	2.33	0.41
6:N:1425:THR:HG22	6:N:1429:LEU:HD12	2.01	0.41
6:N:407:VAL:HG12	6:N:409:VAL:H	1.85	0.41
6:N:28:LYS:CB	6:N:41:ARG:HD2	2.50	0.41
6:N:769:LEU:HD11	6:N:919:PHE:CE2	2.56	0.41
6:N:832:ARG:HA	6:N:832:ARG:CZ	2.51	0.41
6:N:879:ARG:HH11	6:N:879:ARG:HG3	1.84	0.41
6:N:965:GLU:HA	6:N:965:GLU:OE1	2.20	0.41
7:O:19:LEU:O	7:O:23:VAL:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:15:DC:OP2	6:N:610:LYS:HE2	2.21	0.41
4:B:65:PHE:CD1	4:B:65:PHE:N	2.88	0.41
5:C:1067:TYR:HB3	11:C:1435:HOH:O	2.21	0.41
5:C:140:ILE:HD13	5:C:331:ARG:CZ	2.51	0.41
5:C:385:PHE:HA	5:C:389:SER:OG	2.21	0.41
5:C:676:ILE:HD13	5:C:676:ILE:O	2.21	0.41
5:C:690:ILE:HG13	5:C:694:LEU:HD12	2.01	0.41
6:D:1063:GLU:HG3	6:D:1064:GLY:H	1.84	0.41
6:D:434:ARG:HB2	6:D:447:VAL:HG21	2.03	0.41
6:D:703:ASN:ND2	6:D:704:ARG:N	2.67	0.41
4:L:209:GLU:HG2	11:L:361:HOH:O	2.21	0.41
5:M:471:TYR:CD2	5:M:533:ASP:HA	2.56	0.41
5:M:878:SER:OG	6:N:1029:ARG:HD2	2.20	0.41
6:N:1336:LEU:HD22	6:N:1421:LEU:HB2	2.03	0.41
6:N:1437:ALA:C	6:N:1446:VAL:HG21	2.40	0.41
6:N:1472:ILE:HB	6:N:1474:ALA:O	2.21	0.41
6:N:165:LYS:O	6:N:167:GLU:HG3	2.20	0.41
6:N:89:ARG:O	6:N:521:PRO:HB3	2.20	0.41
6:N:648:MET:HE2	11:N:9201:HOH:O	2.20	0.41
6:N:728:LEU:HD12	6:N:729:HIS:N	2.36	0.41
6:N:749:VAL:HA	6:N:750:PRO:HD3	1.87	0.41
6:N:875:THR:HG22	6:N:879:ARG:HB2	2.03	0.41
6:N:791:TYR:CD2	6:N:945:SER:HB2	2.56	0.41
3:Z:5:DG:H1'	3:Z:6:DC:H5'	2.01	0.41
4:A:154:GLU:H	4:A:154:GLU:CD	2.24	0.41
4:B:64:GLU:CA	4:B:165:ILE:HD13	2.48	0.41
5:C:1046:ALA:HA	6:D:1472:ILE:CG1	2.44	0.41
5:C:150:PRO:HA	5:C:158:TYR:HD2	1.86	0.41
5:C:172:ILE:HG23	5:C:184:MET:CE	2.51	0.41
5:C:957:LYS:HG2	5:C:961:GLU:CB	2.51	0.41
6:D:1492:LEU:HD11	11:D:8102:HOH:O	2.21	0.41
6:D:470:LEU:N	6:D:470:LEU:HD23	2.36	0.41
6:D:938:GLY:O	6:D:942:SER:HB3	2.21	0.41
6:D:996:TRP:CE3	6:D:996:TRP:HA	2.56	0.41
7:E:4:PRO:HG3	11:E:115:HOH:O	2.21	0.41
4:K:10:VAL:HG12	4:K:12:THR:HG22	2.02	0.41
4:K:14:ARG:HB2	4:K:14:ARG:CZ	2.50	0.41
4:K:159:LYS:NZ	4:K:164:ALA:O	2.50	0.41
4:K:173:PRO:HB2	4:K:205:VAL:HG22	2.03	0.41
5:M:140:ILE:HG13	5:M:411:SER:O	2.20	0.41
5:M:193:LEU:HD21	11:M:1471:HOH:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:280:LYS:HB2	5:M:280:LYS:NZ	2.35	0.41
5:M:495:THR:HG21	5:M:524:VAL:HG11	2.03	0.41
5:M:704:HIS:HA	11:M:1346:HOH:O	2.21	0.41
5:M:848:VAL:HG12	5:M:849:VAL:N	2.36	0.41
5:M:86:LYS:HZ3	5:M:812:GLY:H	1.69	0.41
6:N:119:SER:HB2	6:N:123:LEU:N	2.31	0.41
6:N:1336:LEU:CA	6:N:1344:VAL:HG21	2.50	0.41
6:N:708:LEU:HD22	6:N:1234:THR:OG1	2.21	0.41
6:N:796:ARG:O	6:N:828:LYS:HD2	2.21	0.41
4:B:137:ARG:CZ	4:B:139:ASN:HB3	2.51	0.41
4:B:80:LEU:HA	4:B:83:LYS:HD2	2.03	0.41
5:C:1030:GLN:O	6:D:622:ARG:HA	2.21	0.41
5:C:160:ALA:HB2	5:C:310:LEU:HB2	2.02	0.41
5:C:438:ILE:HA	5:C:455:LEU:HA	2.03	0.41
5:C:468:ARG:NE	5:C:485:TYR:O	2.54	0.41
5:C:606:VAL:HG11	5:C:643:VAL:O	2.21	0.41
5:C:808:ARG:NH2	5:C:820:ARG:CZ	2.84	0.41
5:C:876:VAL:H	5:C:877:PRO:CD	2.33	0.41
5:C:945:ARG:NE	11:C:1564:HOH:O	2.54	0.41
6:D:1003:VAL:O	6:D:1006:ALA:HB3	2.21	0.41
6:D:1117:TYR:HB2	6:D:1188:VAL:O	2.21	0.41
3:I:7:DC:OP2	6:D:1266:ARG:NE	2.54	0.41
6:D:1191:PRO:CB	6:D:1370:ILE:HD13	2.51	0.41
6:D:1425:THR:HG22	6:D:1429:LEU:CD1	2.50	0.41
6:D:1429:LEU:HD12	6:D:1440:PHE:HE1	1.85	0.41
6:D:1435:LEU:HB2	6:D:1457:ASP:OD2	2.21	0.41
6:D:36:THR:C	6:D:38:LYS:N	2.75	0.41
6:D:456:MET:N	6:D:459:GLU:OE1	2.49	0.41
5:C:911:GLU:OE1	6:D:951:ILE:HD12	2.21	0.41
1:G:12:DG:H2'	1:G:13:DT:H72	2.02	0.41
1:G:8:DT:H2''	1:G:9:DG:C8	2.55	0.41
4:L:26:GLU:HB3	4:L:194:LYS:HG3	2.03	0.41
4:L:49:PRO:HG3	11:L:364:HOH:O	2.20	0.41
5:M:102:HIS:CE1	5:M:365:ASP:HA	2.55	0.41
5:M:674:VAL:CG2	5:M:871:LEU:HG	2.51	0.41
5:M:874:LEU:CD1	5:M:874:LEU:H	2.34	0.41
6:N:954:ALA:C	6:N:1039:CYS:SG	2.99	0.41
6:N:1041:LEU:O	6:N:1041:LEU:HD23	2.21	0.41
6:N:1147:ARG:HB3	6:N:1188:VAL:CG2	2.50	0.41
6:N:1406:ARG:NE	6:N:1407:LEU:HD12	2.36	0.41
6:N:1438:ALA:CA	6:N:1446:VAL:HG11	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:180:LYS:CG	6:N:183:GLU:HB2	2.31	0.41
6:N:47:GLU:HG3	6:N:51:GLY:O	2.21	0.41
6:N:668:PRO:HB3	11:N:9371:HOH:O	2.20	0.41
6:N:773:ALA:HB2	11:N:9308:HOH:O	2.21	0.41
4:B:48:ILE:HA	4:B:49:PRO:HD3	1.88	0.40
4:B:66:SER:O	4:B:75:VAL:HG23	2.21	0.40
4:B:80:LEU:HG	6:D:844:ALA:HA	2.02	0.40
5:C:1065:ALA:HB3	11:C:1284:HOH:O	2.20	0.40
5:C:174:LEU:O	5:C:310:LEU:HD22	2.22	0.40
5:C:250:ARG:HG2	5:C:253:ALA:CB	2.51	0.40
5:C:436:GLY:O	5:C:459:ALA:CB	2.65	0.40
5:C:52:PHE:CE1	5:C:66:LEU:HG	2.56	0.40
6:D:1403:LEU:HD22	11:D:8028:HOH:O	2.21	0.40
6:D:495:ARG:O	6:D:499:VAL:HG23	2.21	0.40
6:D:645:PRO:CD	6:D:726:ILE:HG12	2.51	0.40
6:D:972:LEU:HD13	6:D:972:LEU:HA	1.94	0.40
1:G:11:DC:H2"	1:G:12:DG:H8	1.85	0.40
4:K:101:LEU:HD23	4:K:101:LEU:C	2.41	0.40
4:K:44:LEU:HD13	4:K:177:VAL:CG1	2.51	0.40
4:L:172:SER:HA	4:L:173:PRO:HD3	1.88	0.40
5:M:1:MET:HE3	11:M:1165:HOH:O	2.21	0.40
5:M:256:TYR:HE1	11:M:1452:HOH:O	2.04	0.40
5:M:494:TYR:HB3	5:M:530:GLU:OE2	2.21	0.40
5:M:572:ILE:HD11	5:M:701:THR:CB	2.51	0.40
5:M:685:GLU:HG3	5:M:686:ASP:N	2.36	0.40
5:M:776:SER:HA	5:M:780:GLU:HB3	2.02	0.40
4:K:38:ASN:CG	5:M:980:GLY:CA	2.89	0.40
6:N:1213:ARG:HD2	6:N:1214:PRO:N	2.35	0.40
6:N:127:LEU:HA	6:N:132:TYR:HD1	1.86	0.40
6:N:434:ARG:HH22	6:N:447:VAL:HG11	1.86	0.40
6:N:137:PRO:HD2	6:N:453:ASP:CB	2.50	0.40
6:N:50:PHE:HB3	6:N:522:PRO:CG	2.51	0.40
6:N:792:ILE:H	6:N:792:ILE:HG22	1.63	0.40
6:N:800:LYS:HZ1	6:N:804:LEU:HD13	1.86	0.40
6:N:957:PRO:HG3	11:N:9288:HOH:O	2.20	0.40
4:A:107:LYS:HE2	4:A:113:ASP:OD2	2.21	0.40
4:A:182:GLU:N	4:A:182:GLU:OE2	2.54	0.40
5:C:1008:ARG:NH1	5:C:1010:THR:HA	2.37	0.40
5:C:1078:GLU:HA	5:C:1079:PRO:HD3	1.93	0.40
5:C:1095:LEU:HD23	5:C:1095:LEU:HA	1.93	0.40
5:C:1090:LYS:HE2	5:C:1112:PHE:CE1	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:150:PRO:HA	5:C:158:TYR:CD2	2.56	0.40
5:C:164:PRO:HD2	5:C:170:PRO:O	2.20	0.40
5:C:267:TYR:O	5:C:268:ASP:C	2.59	0.40
5:C:260:LEU:CB	5:C:291:ALA:HB1	2.37	0.40
5:C:327:HIS:CD2	5:C:431:HIS:NE2	2.88	0.40
5:C:410:ILE:HD12	5:C:438:ILE:HG12	2.00	0.40
5:C:474:VAL:HG23	5:C:478:VAL:O	2.21	0.40
5:C:605:LYS:O	5:C:611:ILE:HA	2.21	0.40
5:C:80:GLN:HB3	5:C:80:GLN:HE21	1.63	0.40
5:C:80:GLN:HG2	5:C:90:TYR:CE2	2.56	0.40
5:C:874:LEU:HD12	5:C:874:LEU:N	2.30	0.40
5:C:5:ARG:HB3	5:C:902:ILE:HD12	2.02	0.40
5:C:958:THR:CG2	5:C:961:GLU:HB2	2.46	0.40
6:D:1093:TYR:CE1	6:D:1097:LYS:HE2	2.57	0.40
6:D:1184:GLN:HB2	6:N:559:ALA:HB1	2.02	0.40
5:C:1053:LEU:CD1	6:D:1466:VAL:HG22	2.51	0.40
6:D:34:TYR:O	6:D:35:ARG:C	2.60	0.40
6:D:141:ILE:CD1	6:D:450:TYR:HB3	2.48	0.40
6:D:965:GLU:HA	6:D:968:ASP:HB3	2.02	0.40
6:D:999:THR:O	6:D:1002:LYS:HB2	2.21	0.40
1:G:20:DG:H3'	11:G:38:HOH:O	2.20	0.40
4:K:101:LEU:HD12	4:K:114:PHE:N	2.36	0.40
4:K:159:LYS:HA	4:K:159:LYS:HD3	1.90	0.40
4:K:219:ARG:HG2	4:L:222:LEU:HD12	2.03	0.40
4:L:70:GLY:O	4:L:132:LEU:HA	2.21	0.40
4:L:137:ARG:CZ	4:L:139:ASN:HB3	2.52	0.40
4:L:185:ARG:NH1	11:L:381:HOH:O	2.55	0.40
11:K:1711:HOH:O	4:L:222:LEU:HD11	2.21	0.40
4:L:90:LEU:O	4:L:90:LEU:HD12	2.21	0.40
5:M:474:VAL:HG13	5:M:530:GLU:C	2.42	0.40
5:M:395:LYS:O	5:M:633:GLN:NE2	2.54	0.40
5:M:80:GLN:HG2	5:M:90:TYR:CZ	2.56	0.40
6:N:996:TRP:CZ2	6:N:1056:PRO:HG2	2.57	0.40
6:N:1105:ILE:HA	11:N:9367:HOH:O	2.21	0.40
6:N:1271:LYS:HZ3	6:N:1271:LYS:HB2	1.86	0.40
6:N:493:ARG:NE	6:N:1390:LEU:O	2.54	0.40
6:N:646:LYS:HG3	6:N:721:VAL:O	2.20	0.40
6:N:701:LEU:HD13	6:N:748:HIS:HB2	2.03	0.40
6:N:955:VAL:HG11	6:N:1015:TYR:OH	2.21	0.40
3:Z:3:DA:H1'	11:Z:824:HOH:O	2.20	0.40
4:A:156:HIS:HD2	4:A:157:GLY:N	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:175:ARG:HH21	4:A:176:ARG:HE	1.68	0.40
5:C:97:ARG:HB3	5:C:109:LYS:CE	2.51	0.40
5:C:408:ARG:NE	5:C:542:VAL:HG23	2.37	0.40
5:C:697:ARG:HG3	5:C:697:ARG:O	2.21	0.40
5:C:710:ILE:HB	5:C:790:LEU:CD2	2.43	0.40
5:C:909:ALA:CB	5:C:914:ILE:HD11	2.45	0.40
5:C:676:ILE:HG22	5:C:988:VAL:O	2.21	0.40
6:D:1046:GLN:HG2	6:D:1052:THR:HA	2.03	0.40
6:D:1071:PHE:HB3	11:D:8010:HOH:O	2.22	0.40
6:D:107:ASP:O	6:D:108:VAL:C	2.60	0.40
6:D:1117:TYR:CD1	6:D:1187:PRO:HA	2.57	0.40
6:D:1221:VAL:O	6:D:1222:GLY:C	2.59	0.40
6:D:1477:GLY:O	6:D:1478:SER:C	2.59	0.40
6:D:400:VAL:O	6:D:402:PRO:HD3	2.20	0.40
6:D:421:LEU:HD21	6:D:429:SER:OG	2.21	0.40
6:D:456:MET:HG3	11:D:8208:HOH:O	2.21	0.40
6:D:681:ARG:HB2	6:D:681:ARG:HE	1.66	0.40
6:D:796:ARG:C	6:D:797:LYS:HD2	2.42	0.40
6:D:810:GLU:C	6:D:813:LEU:HG	2.39	0.40
4:K:42:ARG:NH2	4:L:31:GLY:O	2.40	0.40
5:M:217:LEU:HD11	5:M:314:THR:OG1	2.21	0.40
5:M:141:HIS:CA	5:M:331:ARG:HG3	2.52	0.40
5:M:437:ARG:HB3	5:M:467:ILE:HB	2.03	0.40
5:M:610:ARG:HD2	5:M:622:GLU:HG3	2.04	0.40
5:M:626:ARG:NH1	5:M:629:TYR:HB2	2.37	0.40
5:M:720:GLU:OE1	5:M:758:ARG:HD2	2.21	0.40
5:M:909:ALA:HB1	5:M:914:ILE:CD1	2.48	0.40
5:M:80:GLN:HG2	5:M:90:TYR:CE1	2.57	0.40
6:N:1087:ARG:CB	6:N:1256:LEU:HD22	2.49	0.40
6:N:12:LEU:HD21	6:N:104:PHE:CZ	2.57	0.40
6:N:168:THR:HG21	6:N:206:ARG:HH12	1.86	0.40
6:N:415:VAL:HG12	6:N:416:ALA:N	2.37	0.40
6:N:525:ARG:HB2	6:N:538:SER:HB2	2.03	0.40
1:X:12:DG:C8	1:X:13:DT:H72	2.56	0.40
2:Y:12:G:C8	2:Y:12:G:C5'	2.96	0.40
4:B:43:ILE:HG23	4:B:47:SER:HB3	2.02	0.40
4:B:43:ILE:HG23	4:B:47:SER:OG	2.20	0.40
4:B:67:THR:HB	4:B:74:ASP:OD1	2.21	0.40
5:C:431:HIS:CD2	5:C:433:THR:OG1	2.74	0.40
5:C:739:GLU:HG2	5:C:739:GLU:H	1.62	0.40
5:C:773:LEU:O	5:C:777:ILE:HG13	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:782:ALA:O	5:C:784:ASP:N	2.54	0.40
6:D:1221:VAL:O	6:D:1224:VAL:N	2.54	0.40
6:D:700:VAL:HG13	6:D:718:PRO:HG2	2.03	0.40
6:D:789:LEU:O	6:D:793:THR:HG23	2.21	0.40
6:D:817:GLU:O	6:D:821:VAL:HG23	2.21	0.40
6:D:1481:VAL:CG2	7:E:18:ARG:HE	2.30	0.40
1:G:14:DT:C2'	1:G:15:DC:H5'	2.49	0.40
2:H:16:G:H5'	6:D:742:GLY:HA3	2.04	0.40
4:K:67:THR:HG22	5:M:627:ARG:HH21	1.87	0.40
4:K:88:ARG:NH1	4:K:88:ARG:HG2	2.37	0.40
4:K:35:THR:HG23	4:L:39:PRO:HA	2.03	0.40
4:L:58:ILE:HG22	4:L:61:VAL:HB	2.03	0.40
5:M:1091:GLU:HA	6:N:520:LEU:HD13	2.03	0.40
5:M:139:GLN:OE1	5:M:415:PRO:HD3	2.22	0.40
5:M:684:PHE:CG	5:M:685:GLU:N	2.90	0.40
5:M:926:PHE:CD2	5:M:930:LYS:HE3	2.55	0.40
6:N:1108:ARG:NH1	11:N:9097:HOH:O	2.54	0.40
6:N:135:LEU:HD22	6:N:147:VAL:HG23	2.02	0.40
6:N:44:LEU:CD1	6:N:44:LEU:H	2.34	0.40
6:N:501:ALA:HB1	6:N:1453:ALA:CB	2.40	0.40
5:M:1034:GLU:H	6:N:619:LEU:HB3	1.79	0.40
6:N:691:LEU:HG	6:N:720:LEU:HD21	2.02	0.40
4:A:82:LEU:CD2	4:A:142:VAL:HG11	2.43	0.40
4:A:206:THR:CG2	4:A:209:GLU:H	2.32	0.40
4:B:165:ILE:HA	4:B:166:PRO:HD3	1.95	0.40
5:C:1019:GLN:HE22	5:C:1058:ASP:HB2	1.86	0.40
5:C:182:VAL:HG12	5:C:193:LEU:HD11	2.02	0.40
5:C:144:PRO:CG	5:C:265:ARG:NH2	2.80	0.40
5:C:300:ASP:OD2	5:C:303:PHE:HB3	2.22	0.40
5:C:160:ALA:HB1	5:C:306:THR:OG1	2.21	0.40
5:C:520:GLU:HA	5:C:521:PRO:HD3	1.96	0.40
5:C:626:ARG:HG2	11:C:1192:HOH:O	2.21	0.40
5:C:636:ALA:CB	5:C:703:ILE:HD13	2.34	0.40
5:C:743:VAL:HG13	5:C:800:VAL:HG11	2.02	0.40
5:C:7:GLY:O	5:C:8:ARG:HD2	2.21	0.40
6:D:1037:GLN:CG	6:D:1042:ARG:HB3	2.47	0.40
6:D:1083:ASP:OD2	6:D:1241:PHE:HB3	2.21	0.40
6:D:1269:LYS:HZ2	6:D:1269:LYS:HB3	1.85	0.40
6:D:506:GLY:O	6:D:507:ASN:C	2.59	0.40
5:C:1006:HIS:O	6:D:627:GLY:HA2	2.21	0.40
6:D:630:VAL:HA	6:D:744:GLN:HG3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:51:GLY:HA3	6:D:86:ARG:HA	2.04	0.40
3:I:8:DA:H2"	3:I:9:DG:OP2	2.22	0.40
4:K:170:VAL:HG13	11:M:1536:HOH:O	2.20	0.40
4:K:18:ARG:O	4:K:207:PRO:HD3	2.22	0.40
4:L:133:GLU:HB3	4:L:134:GLU:H	1.62	0.40
5:M:324:ASP:HA	11:M:1465:HOH:O	2.22	0.40
6:N:1047:LYS:HB3	6:N:1048:PRO:CD	2.51	0.40
6:N:1044:LEU:HD13	6:N:1052:THR:HG21	2.04	0.40
6:N:112:ILE:O	6:N:112:ILE:HD12	2.22	0.40
6:N:1147:ARG:O	6:N:1165:TYR:HA	2.21	0.40
6:N:637:LEU:HD21	6:N:641:GLN:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	227/315 (72%)	206 (91%)	14 (6%)	7 (3%)	4	23
4	B	227/315 (72%)	206 (91%)	15 (7%)	6 (3%)	5	27
4	K	227/315 (72%)	208 (92%)	13 (6%)	6 (3%)	5	27
4	L	227/315 (72%)	206 (91%)	15 (7%)	6 (3%)	5	27
5	C	1117/1119 (100%)	919 (82%)	136 (12%)	62 (6%)	2	10
5	M	1117/1119 (100%)	923 (83%)	133 (12%)	61 (6%)	2	10
6	D	1258/1524 (82%)	1051 (84%)	149 (12%)	58 (5%)	2	14
6	N	1258/1524 (82%)	1058 (84%)	140 (11%)	60 (5%)	2	13
7	E	93/99 (94%)	76 (82%)	11 (12%)	6 (6%)	1	7
7	O	93/99 (94%)	74 (80%)	12 (13%)	7 (8%)	1	5
All	All	5844/6744 (87%)	4927 (84%)	638 (11%)	279 (5%)	2	13

All (279) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	29	GLU
4	A	187	GLY
4	B	29	GLU
4	B	187	GLY
5	C	178	PRO
5	C	231	PRO
5	C	244	PRO
5	C	288	ARG
5	C	290	LEU
5	C	369	PRO
5	C	462	ASP
5	C	465	GLY
5	C	548	PRO
5	C	627	ARG
5	C	680	ASP
5	C	727	PRO
5	C	908	GLY
5	C	1033	GLY
5	C	1106	ASP
6	D	40	GLU
6	D	43	GLY
6	D	55	ASP
6	D	137	PRO
6	D	447	VAL
6	D	705	ALA
6	D	742	GLY
6	D	832	ARG
6	D	844	ALA
6	D	1028	ALA
6	D	1129	THR
6	D	1389	LEU
6	D	1441	GLN
7	E	42	PRO
4	K	29	GLU
4	K	187	GLY
4	L	29	GLU
4	L	187	GLY
5	M	170	PRO
5	M	178	PRO
5	M	191	PHE
5	M	231	PRO
5	M	244	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	M	288	ARG
5	M	290	LEU
5	M	369	PRO
5	M	462	ASP
5	M	465	GLY
5	M	548	PRO
5	M	680	ASP
5	M	727	PRO
5	M	908	GLY
5	M	1033	GLY
5	M	1106	ASP
6	N	40	GLU
6	N	43	GLY
6	N	55	ASP
6	N	137	PRO
6	N	447	VAL
6	N	705	ALA
6	N	742	GLY
6	N	832	ARG
6	N	844	ALA
6	N	1028	ALA
6	N	1129	THR
6	N	1389	LEU
6	N	1441	GLN
7	O	42	PRO
5	C	40	GLU
5	C	44	ILE
5	C	59	LYS
5	C	152	PRO
5	C	156	GLY
5	C	170	PRO
5	C	191	PHE
5	C	251	ASP
5	C	363	SER
5	C	418	LEU
5	C	457	ALA
5	C	529	VAL
5	C	626	ARG
5	C	698	ASP
5	C	783	ARG
5	C	784	ASP
5	C	864	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	C	1059	ASP
6	D	34	TYR
6	D	120	ALA
6	D	164	GLY
6	D	620	GLY
6	D	740	PHE
6	D	803	GLY
6	D	1208	ASP
6	D	1342	GLU
6	D	1385	GLY
6	D	1452	ILE
6	D	1454	GLY
7	E	53	GLY
7	E	58	PRO
5	M	40	GLU
5	M	44	ILE
5	M	59	LYS
5	M	152	PRO
5	M	156	GLY
5	M	223	ASP
5	M	251	ASP
5	M	363	SER
5	M	418	LEU
5	M	529	VAL
5	M	626	ARG
5	M	627	ARG
5	M	698	ASP
5	M	905	ILE
5	M	1005	MET
5	M	1059	ASP
6	N	120	ALA
6	N	164	GLY
6	N	594	PRO
6	N	620	GLY
6	N	740	PHE
6	N	803	GLY
6	N	1125	PRO
6	N	1208	ASP
6	N	1221	VAL
6	N	1385	GLY
6	N	1424	VAL
6	N	1452	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	N	1454	GLY
7	O	53	GLY
7	O	58	PRO
4	A	3	ASP
5	C	74	GLY
5	C	164	PRO
5	C	188	LYS
5	C	223	ASP
5	C	262	ALA
5	C	268	ASP
5	C	325	ILE
5	C	424	GLY
5	C	517	ARG
5	C	740	GLU
5	C	808	ARG
6	D	37	LEU
6	D	96	ALA
6	D	110	SER
6	D	395	VAL
6	D	507	ASN
6	D	594	PRO
6	D	696	HIS
6	D	822	ALA
6	D	924	MET
6	D	1125	PRO
6	D	1196	THR
6	D	1341	PRO
7	E	43	GLU
4	L	191	ASP
5	M	74	GLY
5	M	164	PRO
5	M	188	LYS
5	M	268	ASP
5	M	424	GLY
5	M	457	ALA
5	M	517	ARG
5	M	808	ARG
5	M	864	GLY
5	M	984	GLU
6	N	37	LEU
6	N	96	ALA
6	N	395	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	N	397	LYS
6	N	507	ASN
6	N	539	ASP
6	N	807	ALA
6	N	830	ALA
6	N	924	MET
6	N	1196	THR
6	N	1269	LYS
7	O	43	GLU
5	C	80	GLN
5	C	180	GLY
5	C	282	GLY
5	C	984	GLU
5	C	1004	LYS
5	C	1024	LYS
5	C	1045	ALA
6	D	808	THR
6	D	830	ALA
6	D	1221	VAL
6	D	1244	GLY
6	D	1269	LYS
6	D	1390	LEU
4	K	3	ASP
5	M	180	GLY
5	M	262	ALA
5	M	767	PRO
5	M	1024	LYS
6	N	34	TYR
6	N	110	SER
6	N	735	ALA
6	N	808	THR
6	N	822	ALA
6	N	1244	GLY
7	O	32	ARG
7	O	82	GLU
5	C	767	PRO
5	C	877	PRO
6	D	31	THR
6	D	807	ALA
7	E	82	GLU
5	M	80	GLN
5	M	264	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	M	877	PRO
5	M	1004	LYS
5	M	1045	ALA
6	N	181	ASP
6	N	601	ARG
6	N	1390	LEU
4	A	118	ALA
4	B	48	ILE
4	B	191	ASP
5	C	11	GLU
5	C	264	PRO
5	C	905	ILE
5	C	1114	GLY
6	D	406	ASP
6	D	483	HIS
6	D	525	ARG
6	D	530	VAL
6	D	601	ARG
4	L	48	ILE
5	M	740	GLU
5	M	781	LYS
6	N	24	GLY
6	N	483	HIS
6	N	696	HIS
6	N	1222	GLY
6	N	1341	PRO
5	C	646	GLY
5	C	779	GLY
7	E	5	GLY
4	L	157	GLY
5	M	144	PRO
5	M	646	GLY
5	M	779	GLY
5	M	1114	GLY
6	N	136	ASP
6	N	526	PRO
6	N	1214	PRO
4	A	157	GLY
4	B	157	GLY
5	C	1079	PRO
6	D	565	ILE
6	D	1214	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	K	9	PRO
5	M	53	PRO
4	A	9	PRO
5	C	53	PRO
6	D	134	VAL
6	D	136	ASP
6	D	1050	GLY
4	K	125	PRO
4	K	157	GLY
4	L	125	PRO
5	M	282	GLY
5	M	876	VAL
6	N	146	PRO
6	N	530	VAL
4	A	125	PRO
4	B	125	PRO
6	D	484	PRO
6	D	595	GLY
5	M	336	VAL
6	N	484	PRO
6	N	595	GLY
6	N	1050	GLY
5	C	876	VAL
6	D	98	PRO
6	D	1222	GLY
6	N	565	ILE
7	O	5	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	202/273 (74%)	162 (80%)	40 (20%)	1	7
4	B	202/273 (74%)	159 (79%)	43 (21%)	1	5
4	K	202/273 (74%)	162 (80%)	40 (20%)	1	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	202/273 (74%)	150 (74%)	52 (26%)	0	3
5	C	941/941 (100%)	704 (75%)	237 (25%)	0	3
5	M	941/941 (100%)	713 (76%)	228 (24%)	0	3
6	D	1063/1279 (83%)	825 (78%)	238 (22%)	1	4
6	N	1063/1279 (83%)	833 (78%)	230 (22%)	1	5
7	E	84/88 (96%)	59 (70%)	25 (30%)	0	1
7	O	84/88 (96%)	68 (81%)	16 (19%)	1	8
All	All	4984/5708 (87%)	3835 (77%)	1149 (23%)	1	4

All (1149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	5	LYS
4	A	9	PRO
4	A	15	THR
4	A	26	GLU
4	A	29	GLU
4	A	47	SER
4	A	60	ASP
4	A	74	ASP
4	A	84	GLU
4	A	88	ARG
4	A	89	PHE
4	A	92	PRO
4	A	99	LEU
4	A	100	LEU
4	A	101	LEU
4	A	102	LYS
4	A	104	GLU
4	A	115	LEU
4	A	127	LEU
4	A	138	LEU
4	A	140	MET
4	A	141	GLU
4	A	142	VAL
4	A	143	ARG
4	A	148	VAL
4	A	168	ASP
4	A	174	VAL
4	A	176	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	180	GLN
4	A	182	GLU
4	A	183	ASP
4	A	185	ARG
4	A	189	ARG
4	A	191	ASP
4	A	193	ASP
4	A	200	TRP
4	A	201	THR
4	A	206	THR
4	A	218	LEU
4	A	219	ARG
4	B	1	MET
4	B	2	LEU
4	B	3	ASP
4	B	4	SER
4	B	7	LYS
4	B	25	LEU
4	B	26	GLU
4	B	28	LEU
4	B	32	PHE
4	B	41	ARG
4	B	42	ARG
4	B	47	SER
4	B	60	ASP
4	B	62	LEU
4	B	63	HIS
4	B	65	PHE
4	B	66	SER
4	B	67	THR
4	B	73	GLU
4	B	77	GLU
4	B	81	ASN
4	B	85	LEU
4	B	89	PHE
4	B	90	LEU
4	B	93	SER
4	B	95	GLN
4	B	112	ARG
4	B	122	ILE
4	B	140	MET
4	B	155	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	156	HIS
4	B	159	LYS
4	B	163	ASN
4	B	189	ARG
4	B	195	LEU
4	B	196	THR
4	B	197	LEU
4	B	201	THR
4	B	206	THR
4	B	213	GLN
4	B	216	GLU
4	B	221	HIS
4	B	229	GLN
5	C	1	MET
5	C	2	GLU
5	C	8	ARG
5	C	9	ILE
5	C	10	ARG
5	C	13	ILE
5	C	26	TYR
5	C	30	LEU
5	C	34	VAL
5	C	38	LYS
5	C	39	ARG
5	C	40	GLU
5	C	41	ASN
5	C	48	PHE
5	C	49	ARG
5	C	51	THR
5	C	65	VAL
5	C	70	GLU
5	C	73	LEU
5	C	80	GLN
5	C	82	GLU
5	C	91	GLN
5	C	95	TYR
5	C	98	LEU
5	C	105	THR
5	C	114	PHE
5	C	115	LEU
5	C	117	HIS
5	C	121	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	C	123	GLU
5	C	124	ASP
5	C	127	PHE
5	C	133	ASP
5	C	139	GLN
5	C	142	ARG
5	C	147	TYR
5	C	148	PHE
5	C	151	ASP
5	C	152	PRO
5	C	158	TYR
5	C	161	SER
5	C	163	ILE
5	C	170	PRO
5	C	171	TRP
5	C	177	GLU
5	C	178	PRO
5	C	183	SER
5	C	184	MET
5	C	187	ASN
5	C	188	LYS
5	C	193	LEU
5	C	194	VAL
5	C	196	LEU
5	C	198	ARG
5	C	205	GLU
5	C	217	LEU
5	C	221	LEU
5	C	225	SER
5	C	233	GLU
5	C	235	LEU
5	C	237	ARG
5	C	238	LEU
5	C	241	LEU
5	C	243	ARG
5	C	252	LYS
5	C	254	VAL
5	C	260	LEU
5	C	266	ARG
5	C	267	TYR
5	C	268	ASP
5	C	274	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	C	275	TYR
5	C	278	GLU
5	C	279	GLU
5	C	284	ARG
5	C	285	LEU
5	C	286	SER
5	C	290	LEU
5	C	293	PHE
5	C	294	GLU
5	C	295	ASP
5	C	301	GLU
5	C	309	TYR
5	C	321	GLU
5	C	327	HIS
5	C	330	ASN
5	C	334	ARG
5	C	345	ARG
5	C	351	LEU
5	C	359	MET
5	C	360	LEU
5	C	363	SER
5	C	365	ASP
5	C	366	SER
5	C	367	LEU
5	C	368	THR
5	C	385	PHE
5	C	387	SER
5	C	390	GLN
5	C	393	GLN
5	C	394	PHE
5	C	397	GLU
5	C	398	THR
5	C	399	ASN
5	C	405	ARG
5	C	408	ARG
5	C	413	LEU
5	C	419	THR
5	C	421	GLU
5	C	422	ARG
5	C	426	ASP
5	C	433	THR
5	C	435	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	C	441	VAL
5	C	445	GLU
5	C	453	THR
5	C	455	LEU
5	C	460	ARG
5	C	469	THR
5	C	484	VAL
5	C	491	GLU
5	C	492	ASP
5	C	498	GLN
5	C	503	LEU
5	C	507	ARG
5	C	508	ILE
5	C	518	LYS
5	C	525	SER
5	C	527	GLU
5	C	538	GLN
5	C	560	MET
5	C	562	SER
5	C	564	MET
5	C	567	GLN
5	C	569	VAL
5	C	573	ARG
5	C	578	VAL
5	C	586	ARG
5	C	590	ASP
5	C	602	GLU
5	C	605	LYS
5	C	609	ASN
5	C	610	ARG
5	C	611	ILE
5	C	617	ASP
5	C	620	LEU
5	C	638	ASP
5	C	639	GLN
5	C	644	VAL
5	C	647	GLN
5	C	649	VAL
5	C	657	ASP
5	C	668	LEU
5	C	676	ILE
5	C	677	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	C	679	PHE
5	C	684	PHE
5	C	699	PHE
5	C	701	THR
5	C	703	ILE
5	C	705	ILE
5	C	707	ARG
5	C	714	ASP
5	C	715	THR
5	C	721	ARG
5	C	727	PRO
5	C	729	LEU
5	C	739	GLU
5	C	740	GLU
5	C	748	GLU
5	C	753	ASP
5	C	766	GLU
5	C	770	GLU
5	C	774	LEU
5	C	780	GLU
5	C	784	ASP
5	C	805	ARG
5	C	807	ARG
5	C	814	GLU
5	C	816	LYS
5	C	821	GLU
5	C	825	VAL
5	C	834	GLN
5	C	841	ASN
5	C	846	LYS
5	C	856	GLU
5	C	858	MET
5	C	865	THR
5	C	868	ASP
5	C	870	ILE
5	C	872	ASN
5	C	881	ASN
5	C	890	LEU
5	C	900	ARG
5	C	904	PRO
5	C	923	GLU
5	C	937	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	C	938	LYS
5	C	939	ARG
5	C	946	ARG
5	C	950	LEU
5	C	953	VAL
5	C	958	THR
5	C	960	GLU
5	C	961	GLU
5	C	963	LEU
5	C	966	LEU
5	C	971	LYS
5	C	981	GLU
5	C	988	VAL
5	C	989	VAL
5	C	995	MET
5	C	999	HIS
5	C	1002	GLU
5	C	1005	MET
5	C	1016	ILE
5	C	1019	GLN
5	C	1021	LEU
5	C	1031	ARG
5	C	1035	MET
5	C	1040	LEU
5	C	1051	GLU
5	C	1052	MET
5	C	1061	GLU
5	C	1064	ASN
5	C	1072	LYS
5	C	1080	SER
5	C	1085	PHE
5	C	1097	LEU
5	C	1098	ASP
5	C	1101	THR
5	C	1104	GLU
5	C	1105	LYS
5	C	1108	PRO
5	C	1110	ASP
5	C	1111	ILE
5	C	1118	LYS
6	D	6	ARG
6	D	8	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	D	16	GLU
6	D	29	PRO
6	D	34	TYR
6	D	41	ARG
6	D	42	ASP
6	D	45	PHE
6	D	56	TYR
6	D	57	GLU
6	D	58	CYS
6	D	68	PHE
6	D	69	GLU
6	D	75	ARG
6	D	76	CYS
6	D	82	LYS
6	D	85	VAL
6	D	87	ARG
6	D	95	LEU
6	D	97	THR
6	D	101	HIS
6	D	103	TRP
6	D	108	VAL
6	D	111	LYS
6	D	116	LEU
6	D	124	GLU
6	D	127	LEU
6	D	128	TYR
6	D	133	ILE
6	D	145	VAL
6	D	149	LYS
6	D	151	GLN
6	D	152	LEU
6	D	155	ASP
6	D	161	LEU
6	D	163	TYR
6	D	169	TYR
6	D	180	LYS
6	D	189	GLN
6	D	196	VAL
6	D	198	ARG
6	D	199	LEU
6	D	206	ARG
6	D	207	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	D	407	VAL
6	D	410	SER
6	D	423	ASP
6	D	430	ASP
6	D	443	VAL
6	D	445	ARG
6	D	447	VAL
6	D	452	ILE
6	D	456	MET
6	D	465	LEU
6	D	470	LEU
6	D	474	GLU
6	D	481	MET
6	D	483	HIS
6	D	485	SER
6	D	493	ARG
6	D	496	LEU
6	D	505	SER
6	D	508	ARG
6	D	513	ILE
6	D	519	VAL
6	D	522	PRO
6	D	523	ASP
6	D	525	ARG
6	D	538	SER
6	D	542	ASP
6	D	543	LEU
6	D	546	ARG
6	D	550	ARG
6	D	554	LEU
6	D	570	GLU
6	D	586	ARG
6	D	590	PRO
6	D	594	PRO
6	D	607	LEU
6	D	611	GLN
6	D	615	ARG
6	D	619	LEU
6	D	621	LYS
6	D	626	SER
6	D	639	LEU
6	D	642	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	D	644	LEU
6	D	651	GLU
6	D	659	LYS
6	D	662	GLU
6	D	669	ASN
6	D	670	VAL
6	D	676	MET
6	D	678	GLU
6	D	679	ARG
6	D	682	ASP
6	D	691	LEU
6	D	692	GLU
6	D	698	LYS
6	D	703	ASN
6	D	709	HIS
6	D	710	ARG
6	D	724	GLN
6	D	733	CYS
6	D	734	GLU
6	D	736	PHE
6	D	737	ASN
6	D	739	ASP
6	D	740	PHE
6	D	741	ASP
6	D	743	ASP
6	D	744	GLN
6	D	754	PHE
6	D	758	GLU
6	D	762	GLN
6	D	763	MET
6	D	764	LEU
6	D	782	SER
6	D	783	ARG
6	D	785	ILE
6	D	791	TYR
6	D	796	ARG
6	D	808	THR
6	D	810	GLU
6	D	811	GLU
6	D	824	ASN
6	D	826	PRO
6	D	827	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	D	832	ARG
6	D	833	GLU
6	D	834	THR
6	D	838	ARG
6	D	842	VAL
6	D	859	ASP
6	D	863	VAL
6	D	868	TYR
6	D	869	MET
6	D	876	SER
6	D	879	ARG
6	D	897	TRP
6	D	899	LEU
6	D	904	VAL
6	D	907	GLU
6	D	913	ASP
6	D	914	LEU
6	D	922	LEU
6	D	932	ASP
6	D	947	ILE
6	D	951	ILE
6	D	959	GLU
6	D	971	LEU
6	D	975	GLU
6	D	980	MET
6	D	982	PHE
6	D	983	LEU
6	D	988	ARG
6	D	991	GLN
6	D	1005	GLN
6	D	1014	ASN
6	D	1038	LEU
6	D	1044	LEU
6	D	1052	THR
6	D	1060	SER
6	D	1062	ARG
6	D	1063	GLU
6	D	1066	THR
6	D	1067	VAL
6	D	1070	TYR
6	D	1074	SER
6	D	1083	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	D	1084	THR
6	D	1090	ASP
6	D	1093	TYR
6	D	1096	ARG
6	D	1100	ASP
6	D	1112	CYS
6	D	1114	THR
6	D	1118	ILE
6	D	1119	SER
6	D	1127	GLU
6	D	1134	LEU
6	D	1135	ARG
6	D	1139	ASP
6	D	1151	ARG
6	D	1152	GLU
6	D	1155	VAL
6	D	1164	ARG
6	D	1166	LEU
6	D	1167	SER
6	D	1196	THR
6	D	1197	ARG
6	D	1207	TYR
6	D	1211	MET
6	D	1214	PRO
6	D	1231	GLU
6	D	1232	PRO
6	D	1234	THR
6	D	1237	THR
6	D	1242	HIS
6	D	1256	LEU
6	D	1257	PRO
6	D	1259	VAL
6	D	1260	ILE
6	D	1264	GLU
6	D	1267	ARG
6	D	1271	LYS
6	D	1330	ILE
6	D	1331	ASP
6	D	1332	PRO
6	D	1337	GLU
6	D	1344	VAL
6	D	1346	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	D	1347	TYR
6	D	1354	LYS
6	D	1363	LEU
6	D	1365	ASP
6	D	1376	MET
6	D	1383	ASP
6	D	1389	LEU
6	D	1393	GLN
6	D	1395	LEU
6	D	1397	LYS
6	D	1403	LEU
6	D	1415	VAL
6	D	1422	MET
6	D	1424	VAL
6	D	1426	LYS
6	D	1429	LEU
6	D	1434	TRP
6	D	1436	SER
6	D	1440	PHE
6	D	1441	GLN
6	D	1464	GLU
6	D	1465	ASN
6	D	1470	ARG
6	D	1472	ILE
6	D	1483	PHE
6	D	1488	ASP
7	E	28	GLN
7	E	30	LEU
7	E	31	LEU
7	E	32	ARG
7	E	40	LEU
7	E	41	GLU
7	E	42	PRO
7	E	47	LYS
7	E	49	GLN
7	E	51	LEU
7	E	57	ASP
7	E	67	GLU
7	E	68	LEU
7	E	69	LEU
7	E	70	THR
7	E	72	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	E	74	VAL
7	E	77	GLU
7	E	79	LEU
7	E	81	PRO
7	E	82	GLU
7	E	83	ASP
7	E	85	LEU
7	E	86	GLN
7	E	94	PRO
4	K	1	MET
4	K	5	LYS
4	K	9	PRO
4	K	20	TYR
4	K	26	GLU
4	K	45	LEU
4	K	49	PRO
4	K	54	THR
4	K	58	ILE
4	K	64	GLU
4	K	80	LEU
4	K	86	VAL
4	K	89	PHE
4	K	92	PRO
4	K	93	SER
4	K	96	THR
4	K	99	LEU
4	K	102	LYS
4	K	109	VAL
4	K	116	PRO
4	K	126	ASP
4	K	127	LEU
4	K	131	THR
4	K	134	GLU
4	K	143	ARG
4	K	145	ASP
4	K	167	VAL
4	K	179	PHE
4	K	180	GLN
4	K	182	GLU
4	K	183	ASP
4	K	189	ARG
4	K	197	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	K	201	THR
4	K	204	SER
4	K	206	THR
4	K	208	LEU
4	K	216	GLU
4	K	219	ARG
4	K	229	GLN
4	L	1	MET
4	L	3	ASP
4	L	4	SER
4	L	7	LYS
4	L	10	VAL
4	L	11	PHE
4	L	15	THR
4	L	20	TYR
4	L	26	GLU
4	L	30	ARG
4	L	41	ARG
4	L	47	SER
4	L	51	THR
4	L	58	ILE
4	L	60	ASP
4	L	61	VAL
4	L	62	LEU
4	L	63	HIS
4	L	64	GLU
4	L	66	SER
4	L	67	THR
4	L	73	GLU
4	L	77	GLU
4	L	80	LEU
4	L	81	ASN
4	L	89	PHE
4	L	95	GLN
4	L	100	LEU
4	L	115	LEU
4	L	117	VAL
4	L	122	ILE
4	L	132	LEU
4	L	140	MET
4	L	151	VAL
4	L	160	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L	161	ARG
4	L	163	ASN
4	L	172	SER
4	L	176	ARG
4	L	177	VAL
4	L	179	PHE
4	L	182	GLU
4	L	184	THR
4	L	190	THR
4	L	191	ASP
4	L	196	THR
4	L	200	TRP
4	L	206	THR
4	L	223	THR
4	L	224	TYR
4	L	226	SER
4	L	227	ASN
5	M	1	MET
5	M	10	ARG
5	M	26	TYR
5	M	27	ARG
5	M	30	LEU
5	M	31	GLN
5	M	33	ASP
5	M	39	ARG
5	M	42	VAL
5	M	51	THR
5	M	95	TYR
5	M	98	LEU
5	M	99	GLN
5	M	100	LEU
5	M	107	LEU
5	M	115	LEU
5	M	117	HIS
5	M	118	ILE
5	M	120	LEU
5	M	126	SER
5	M	128	ILE
5	M	133	ASP
5	M	141	HIS
5	M	142	ARG
5	M	148	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	M	158	TYR
5	M	170	PRO
5	M	173	ASP
5	M	177	GLU
5	M	178	PRO
5	M	179	ASN
5	M	182	VAL
5	M	186	VAL
5	M	188	LYS
5	M	190	LYS
5	M	193	LEU
5	M	194	VAL
5	M	198	ARG
5	M	205	GLU
5	M	209	ARG
5	M	210	GLU
5	M	216	GLU
5	M	218	VAL
5	M	221	LEU
5	M	222	MET
5	M	224	GLU
5	M	225	SER
5	M	227	PHE
5	M	230	ARG
5	M	233	GLU
5	M	241	LEU
5	M	243	ARG
5	M	252	LYS
5	M	260	LEU
5	M	261	ILE
5	M	264	PRO
5	M	266	ARG
5	M	267	TYR
5	M	271	GLU
5	M	281	LEU
5	M	285	LEU
5	M	289	THR
5	M	290	LEU
5	M	293	PHE
5	M	294	GLU
5	M	301	GLU
5	M	303	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	M	304	LEU
5	M	309	TYR
5	M	320	HIS
5	M	323	ASP
5	M	331	ARG
5	M	332	ARG
5	M	342	ASP
5	M	344	PHE
5	M	350	ARG
5	M	351	LEU
5	M	359	MET
5	M	361	MET
5	M	365	ASP
5	M	367	LEU
5	M	376	ARG
5	M	383	ARG
5	M	387	SER
5	M	388	ARG
5	M	393	GLN
5	M	394	PHE
5	M	401	LEU
5	M	413	LEU
5	M	419	THR
5	M	422	ARG
5	M	425	PHE
5	M	426	ASP
5	M	433	THR
5	M	440	PRO
5	M	443	THR
5	M	458	TYR
5	M	471	TYR
5	M	472	ARG
5	M	474	VAL
5	M	480	THR
5	M	485	TYR
5	M	487	THR
5	M	489	THR
5	M	503	LEU
5	M	511	GLU
5	M	516	ARG
5	M	517	ARG
5	M	520	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	M	530	GLU
5	M	537	LYS
5	M	543	ASN
5	M	553	ASP
5	M	554	ASP
5	M	572	ILE
5	M	579	VAL
5	M	581	THR
5	M	585	GLU
5	M	586	ARG
5	M	589	ARG
5	M	599	GLU
5	M	602	GLU
5	M	607	ASP
5	M	609	ASN
5	M	613	VAL
5	M	616	GLU
5	M	617	ASP
5	M	620	LEU
5	M	625	LEU
5	M	627	ARG
5	M	628	PHE
5	M	645	VAL
5	M	647	GLN
5	M	654	LEU
5	M	662	GLU
5	M	668	LEU
5	M	671	ASN
5	M	677	MET
5	M	678	PRO
5	M	679	PHE
5	M	686	ASP
5	M	699	PHE
5	M	701	THR
5	M	706	GLU
5	M	711	GLU
5	M	715	THR
5	M	717	LEU
5	M	727	PRO
5	M	728	HIS
5	M	731	GLU
5	M	736	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	M	737	LEU
5	M	738	ASP
5	M	739	GLU
5	M	745	ILE
5	M	748	GLU
5	M	750	LYS
5	M	751	PRO
5	M	765	SER
5	M	766	GLU
5	M	769	PRO
5	M	780	GLU
5	M	781	LYS
5	M	783	ARG
5	M	784	ASP
5	M	785	VAL
5	M	787	ASP
5	M	794	PRO
5	M	803	THR
5	M	805	ARG
5	M	806	LEU
5	M	807	ARG
5	M	814	GLU
5	M	824	ARG
5	M	834	GLN
5	M	841	ASN
5	M	856	GLU
5	M	857	ASP
5	M	862	PRO
5	M	868	ASP
5	M	870	ILE
5	M	878	SER
5	M	881	ASN
5	M	884	GLN
5	M	904	PRO
5	M	907	ASP
5	M	913	GLU
5	M	916	GLU
5	M	918	LEU
5	M	920	GLN
5	M	937	ASP
5	M	938	LYS
5	M	946	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	M	953	VAL
5	M	958	THR
5	M	960	GLU
5	M	966	LEU
5	M	981	GLU
5	M	984	GLU
5	M	988	VAL
5	M	997	LEU
5	M	999	HIS
5	M	1003	ASP
5	M	1005	MET
5	M	1006	HIS
5	M	1008	ARG
5	M	1016	ILE
5	M	1017	THR
5	M	1018	GLN
5	M	1021	LEU
5	M	1027	PHE
5	M	1035	MET
5	M	1054	THR
5	M	1055	LEU
5	M	1058	ASP
5	M	1060	ILE
5	M	1074	GLU
5	M	1075	ASP
5	M	1078	GLU
5	M	1081	VAL
5	M	1085	PHE
5	M	1092	LEU
5	M	1095	LEU
5	M	1097	LEU
5	M	1098	ASP
5	M	1103	ASP
5	M	1110	ASP
5	M	1115	LEU
6	N	4	GLU
6	N	9	ARG
6	N	20	SER
6	N	21	TRP
6	N	36	THR
6	N	40	GLU
6	N	41	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	N	42	ASP
6	N	44	LEU
6	N	56	TYR
6	N	57	GLU
6	N	64	LYS
6	N	65	ARG
6	N	67	ARG
6	N	68	PHE
6	N	69	GLU
6	N	75	ARG
6	N	76	CYS
6	N	79	GLU
6	N	87	ARG
6	N	95	LEU
6	N	97	THR
6	N	98	PRO
6	N	101	HIS
6	N	108	VAL
6	N	112	ILE
6	N	116	LEU
6	N	122	GLU
6	N	123	LEU
6	N	124	GLU
6	N	127	LEU
6	N	131	LYS
6	N	133	ILE
6	N	138	LYS
6	N	145	VAL
6	N	147	VAL
6	N	148	GLU
6	N	149	LYS
6	N	150	ARG
6	N	152	LEU
6	N	153	LEU
6	N	155	ASP
6	N	157	GLU
6	N	159	ARG
6	N	163	TYR
6	N	166	GLN
6	N	167	GLU
6	N	176	ASP
6	N	178	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	N	180	LYS
6	N	199	LEU
6	N	405	ASP
6	N	406	ASP
6	N	414	ARG
6	N	430	ASP
6	N	434	ARG
6	N	450	TYR
6	N	451	ASP
6	N	455	ARG
6	N	456	MET
6	N	462	GLN
6	N	464	LEU
6	N	465	LEU
6	N	469	ASP
6	N	470	LEU
6	N	471	GLU
6	N	477	LEU
6	N	493	ARG
6	N	496	LEU
6	N	507	ASN
6	N	511	TRP
6	N	512	MET
6	N	513	ILE
6	N	522	PRO
6	N	523	ASP
6	N	525	ARG
6	N	537	THR
6	N	538	SER
6	N	539	ASP
6	N	542	ASP
6	N	544	TYR
6	N	550	ARG
6	N	564	GLU
6	N	565	ILE
6	N	567	ILE
6	N	576	GLU
6	N	581	LEU
6	N	584	ASN
6	N	594	PRO
6	N	617	ASN
6	N	619	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	N	629	SER
6	N	635	PRO
6	N	639	LEU
6	N	641	GLN
6	N	647	ARG
6	N	660	LYS
6	N	666	ILE
6	N	669	ASN
6	N	680	GLN
6	N	682	ASP
6	N	688	TRP
6	N	692	GLU
6	N	699	VAL
6	N	701	LEU
6	N	707	THR
6	N	709	HIS
6	N	728	LEU
6	N	733	CYS
6	N	734	GLU
6	N	737	ASN
6	N	739	ASP
6	N	740	PHE
6	N	741	ASP
6	N	743	ASP
6	N	754	PHE
6	N	769	LEU
6	N	792	ILE
6	N	794	GLN
6	N	797	LYS
6	N	817	GLU
6	N	818	ARG
6	N	823	LEU
6	N	824	ASN
6	N	836	VAL
6	N	838	ARG
6	N	840	LYS
6	N	841	TYR
6	N	847	ASP
6	N	861	GLN
6	N	864	VAL
6	N	868	TYR
6	N	881	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	N	888	GLU
6	N	897	TRP
6	N	902	LEU
6	N	907	GLU
6	N	913	ASP
6	N	914	LEU
6	N	921	ARG
6	N	930	LEU
6	N	939	PHE
6	N	947	ILE
6	N	951	ILE
6	N	952	ASP
6	N	953	ASP
6	N	968	ASP
6	N	976	GLN
6	N	982	PHE
6	N	983	LEU
6	N	985	ASP
6	N	988	ARG
6	N	1001	GLU
6	N	1017	PHE
6	N	1032	PRO
6	N	1034	GLN
6	N	1039	CYS
6	N	1041	LEU
6	N	1042	ARG
6	N	1046	GLN
6	N	1053	PHE
6	N	1060	SER
6	N	1062	ARG
6	N	1063	GLU
6	N	1070	TYR
6	N	1083	ASP
6	N	1088	THR
6	N	1093	TYR
6	N	1097	LYS
6	N	1098	LEU
6	N	1100	ASP
6	N	1109	GLU
6	N	1112	CYS
6	N	1115	THR
6	N	1116	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	N	1129	THR
6	N	1130	ARG
6	N	1144	LEU
6	N	1151	ARG
6	N	1155	VAL
6	N	1160	LEU
6	N	1164	ARG
6	N	1166	LEU
6	N	1170	ASP
6	N	1179	GLU
6	N	1197	ARG
6	N	1198	TYR
6	N	1204	CYS
6	N	1207	TYR
6	N	1208	ASP
6	N	1211	MET
6	N	1213	ARG
6	N	1219	GLU
6	N	1228	SER
6	N	1232	PRO
6	N	1237	THR
6	N	1238	MET
6	N	1242	HIS
6	N	1251	ASP
6	N	1257	PRO
6	N	1262	LEU
6	N	1264	GLU
6	N	1271	LYS
6	N	1334	GLN
6	N	1337	GLU
6	N	1345	GLU
6	N	1348	LEU
6	N	1350	GLU
6	N	1380	GLU
6	N	1381	VAL
6	N	1383	ASP
6	N	1389	LEU
6	N	1391	GLU
6	N	1397	LYS
6	N	1412	LYS
6	N	1415	VAL
6	N	1418	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	N	1422	MET
6	N	1429	LEU
6	N	1431	THR
6	N	1432	LYS
6	N	1433	SER
6	N	1440	PHE
6	N	1441	GLN
6	N	1452	ILE
6	N	1471	LEU
6	N	1472	ILE
6	N	1478	SER
6	N	1489	GLN
6	N	1492	LEU
7	O	26	ARG
7	O	30	LEU
7	O	43	GLU
7	O	46	PRO
7	O	48	MET
7	O	56	ASP
7	O	59	ASN
7	O	69	LEU
7	O	72	ARG
7	O	78	ASN
7	O	81	PRO
7	O	82	GLU
7	O	86	GLN
7	O	89	MET
7	O	94	PRO
7	O	96	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (154) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	91	ASN
4	A	124	ASN
4	A	163	ASN
4	A	180	GLN
4	A	221	HIS
4	B	81	ASN
4	B	95	GLN
4	B	124	ASN
4	B	128	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	B	139	ASN
4	B	180	GLN
4	B	221	HIS
4	B	229	GLN
5	C	22	GLN
5	C	80	GLN
5	C	130	ASN
5	C	139	GLN
5	C	187	ASN
5	C	320	HIS
5	C	327	HIS
5	C	330	ASN
5	C	343	GLN
5	C	390	GLN
5	C	393	GLN
5	C	399	ASN
5	C	406	HIS
5	C	431	HIS
5	C	434	HIS
5	C	500	ASN
5	C	543	ASN
5	C	552	HIS
5	C	565	GLN
5	C	567	GLN
5	C	609	ASN
5	C	639	GLN
5	C	663	ASN
5	C	671	ASN
5	C	834	GLN
5	C	841	ASN
5	C	872	ASN
5	C	881	ASN
5	C	889	HIS
5	C	899	GLN
5	C	1019	GLN
5	C	1030	GLN
5	C	1050	GLN
5	C	1100	GLN
5	C	1107	ASN
6	D	143	ASN
6	D	166	GLN
6	D	463	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	D	549	ASN
6	D	552	ASN
6	D	616	GLN
6	D	636	GLN
6	D	703	ASN
6	D	709	HIS
6	D	714	GLN
6	D	727	GLN
6	D	737	ASN
6	D	756	GLN
6	D	762	GLN
6	D	824	ASN
6	D	917	GLN
6	D	962	GLN
6	D	1005	GLN
6	D	1010	ASN
6	D	1014	ASN
6	D	1033	GLN
6	D	1103	HIS
6	D	1172	HIS
6	D	1227	GLN
6	D	1334	GLN
6	D	1359	GLN
6	D	1441	GLN
6	D	1465	ASN
6	D	1485	GLN
7	E	28	GLN
7	E	29	GLN
7	E	33	HIS
7	E	37	ASN
7	E	86	GLN
4	K	16	GLN
4	K	63	HIS
4	K	95	GLN
4	K	124	ASN
4	K	156	HIS
4	K	180	GLN
4	K	212	ASN
4	K	213	GLN
4	K	229	GLN
4	L	81	ASN
4	L	95	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L	124	ASN
4	L	227	ASN
5	M	31	GLN
5	M	91	GLN
5	M	139	GLN
5	M	204	GLN
5	M	374	ASN
5	M	393	GLN
5	M	406	HIS
5	M	543	ASN
5	M	552	HIS
5	M	556	ASN
5	M	565	GLN
5	M	567	GLN
5	M	575	GLN
5	M	609	ASN
5	M	633	GLN
5	M	639	GLN
5	M	671	ASN
5	M	704	HIS
5	M	829	GLN
5	M	841	ASN
5	M	872	ASN
5	M	881	ASN
5	M	889	HIS
5	M	899	GLN
5	M	1050	GLN
5	M	1064	ASN
5	M	1107	ASN
6	N	125	GLN
6	N	442	ASN
6	N	507	ASN
6	N	529	GLN
6	N	549	ASN
6	N	575	GLN
6	N	584	ASN
6	N	616	GLN
6	N	617	ASN
6	N	680	GLN
6	N	696	HIS
6	N	703	ASN
6	N	714	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	N	727	GLN
6	N	737	ASN
6	N	744	GLN
6	N	756	GLN
6	N	824	ASN
6	N	845	ASN
6	N	861	GLN
6	N	906	GLN
6	N	976	GLN
6	N	1010	ASN
6	N	1014	ASN
6	N	1025	GLN
6	N	1033	GLN
6	N	1124	GLN
6	N	1202	GLN
6	N	1465	ASN
7	O	29	GLN
7	O	78	ASN
7	O	86	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	H	16/16 (100%)	10 (62%)	8 (50%)
2	Y	16/16 (100%)	10 (62%)	8 (50%)
All	All	32/32 (100%)	20 (62%)	16 (50%)

All (20) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	H	2	A
2	H	3	G
2	H	6	U
2	H	7	G
2	H	8	C
2	H	9	G
2	H	10	G
2	H	12	G
2	H	13	C
2	H	15	C
2	Y	2	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Y	3	G
2	Y	6	U
2	Y	7	G
2	Y	8	C
2	Y	9	G
2	Y	10	G
2	Y	12	G
2	Y	13	C
2	Y	15	C

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	H	1	G
2	H	6	U
2	H	7	G
2	H	8	C
2	H	9	G
2	H	12	G
2	H	13	C
2	H	15	C
2	Y	1	G
2	Y	6	U
2	Y	7	G
2	Y	8	C
2	Y	9	G
2	Y	12	G
2	Y	13	C
2	Y	15	C

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 8 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
10	APC	D	3999	9	27,33,33	1.39	3 (11%)	31,52,52	1.97	8 (25%)
10	APC	N	4999	9	27,33,33	1.25	4 (14%)	31,52,52	1.93	7 (22%)

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
10	APC	D	3999	9	-	8/15/38/38	0/3/3/3
10	APC	N	4999	9	-	8/15/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	3999	APC	PB-O2B	-3.54	1.48	1.56
10	D	3999	APC	PB-O3B	3.53	1.62	1.58
10	D	3999	APC	PA-O2A	-3.13	1.49	1.56
10	N	4999	APC	PB-O3B	3.13	1.61	1.58
10	N	4999	APC	PB-O2B	-3.02	1.49	1.56
10	N	4999	APC	PA-O2A	-2.80	1.49	1.56
10	N	4999	APC	PA-O5'	2.06	1.60	1.57

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	N	4999	APC	C1'-N9-C4	-6.01	116.08	126.64
10	D	3999	APC	C1'-N9-C4	-5.65	116.72	126.64
10	D	3999	APC	C5-C6-N6	4.52	127.21	120.35
10	N	4999	APC	C5-C6-N6	4.29	126.87	120.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	N	4999	APC	PG-O3B-PB	-3.73	119.47	132.62
10	D	3999	APC	PG-O3B-PB	-3.68	119.65	132.62
10	D	3999	APC	O2A-PA-O1A	3.01	120.11	110.07
10	N	4999	APC	O2A-PA-O1A	2.97	119.98	110.07
10	N	4999	APC	O2B-PB-O1B	2.95	119.93	110.07
10	D	3999	APC	O2B-PB-O1B	2.90	119.75	110.07
10	D	3999	APC	O2'-C2'-C3'	-2.88	102.51	111.82
10	N	4999	APC	C2'-C3'-C4'	2.40	107.31	102.64
10	D	3999	APC	C2'-C3'-C4'	2.34	107.20	102.64
10	D	3999	APC	C3'-C2'-C1'	2.19	104.28	100.98
10	N	4999	APC	C3'-C2'-C1'	2.08	104.11	100.98

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	3999	APC	PA-C3A-PB-O1B
10	D	3999	APC	PA-C3A-PB-O3B
10	D	3999	APC	PB-C3A-PA-O1A
10	D	3999	APC	PB-C3A-PA-O5'
10	D	3999	APC	O4'-C4'-C5'-O5'
10	N	4999	APC	PA-C3A-PB-O1B
10	N	4999	APC	PA-C3A-PB-O3B
10	N	4999	APC	PB-C3A-PA-O1A
10	N	4999	APC	PB-C3A-PA-O5'
10	N	4999	APC	C5'-O5'-PA-O2A
10	N	4999	APC	O4'-C4'-C5'-O5'
10	N	4999	APC	C4'-C5'-O5'-PA
10	D	3999	APC	C3'-C4'-C5'-O5'
10	D	3999	APC	C4'-C5'-O5'-PA
10	N	4999	APC	PA-C3A-PB-O2B
10	D	3999	APC	C5'-O5'-PA-O2A

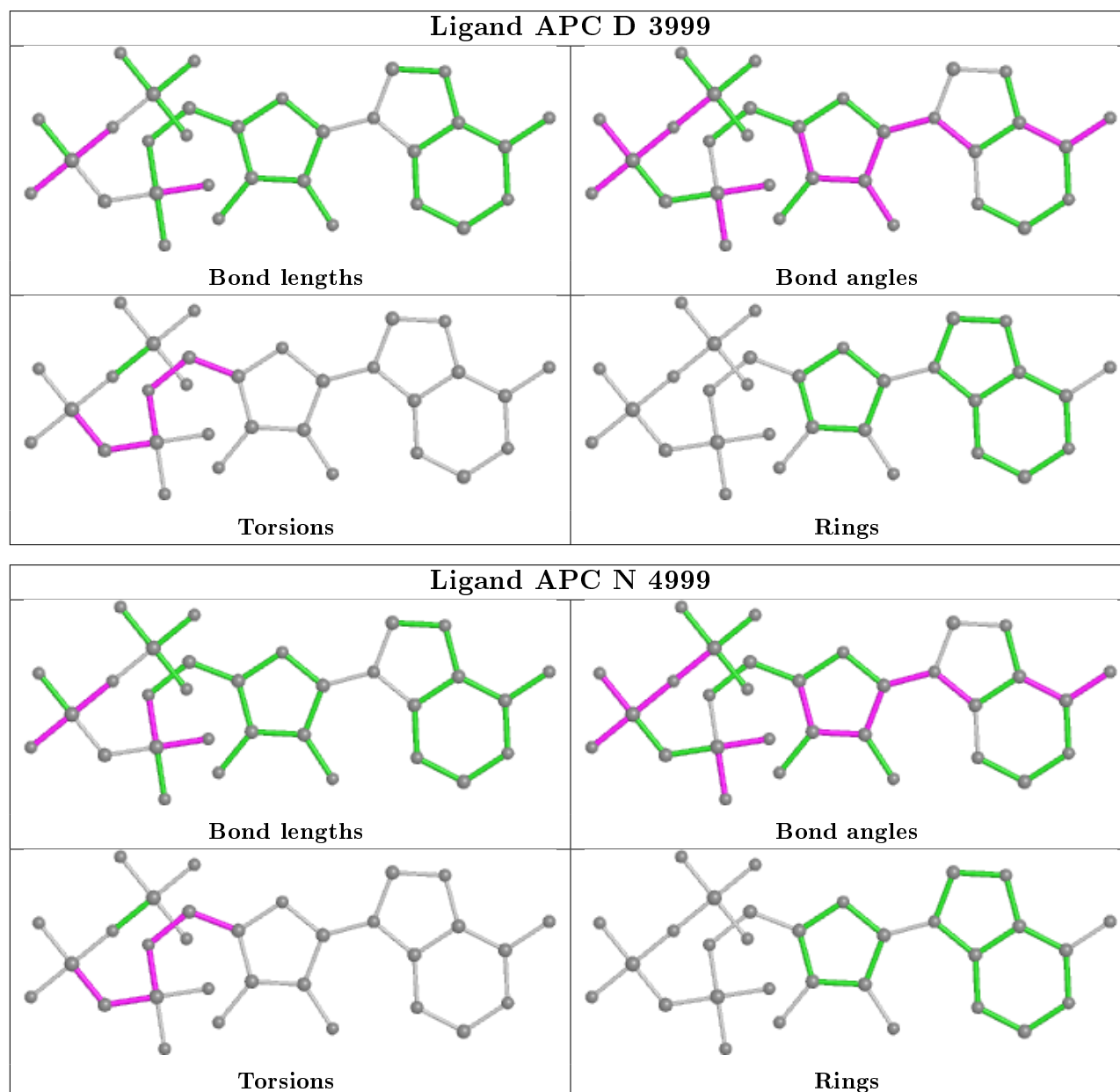
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	3999	APC	2	0
10	N	4999	APC	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	G	23/23 (100%)	-0.73	0 100 100	22, 46, 76, 79	0
1	X	23/23 (100%)	-0.67	0 100 100	21, 38, 71, 90	0
2	H	16/16 (100%)	-0.58	0 100 100	36, 56, 100, 102	0
2	Y	16/16 (100%)	-0.62	0 100 100	21, 73, 101, 103	0
3	I	13/14 (92%)	-0.89	0 100 100	49, 65, 74, 85	0
3	Z	13/14 (92%)	-0.86	0 100 100	54, 67, 80, 81	0
4	A	229/315 (72%)	-0.62	0 100 100	41, 66, 86, 94	0
4	B	229/315 (72%)	-0.55	2 (0%) 84 63	43, 70, 85, 101	0
4	K	229/315 (72%)	-0.61	1 (0%) 92 79	41, 65, 81, 93	0
4	L	229/315 (72%)	-0.60	0 100 100	38, 68, 80, 90	0
5	C	1119/1119 (100%)	-0.60	3 (0%) 94 84	26, 64, 86, 101	0
5	M	1119/1119 (100%)	-0.58	6 (0%) 91 75	25, 65, 89, 109	0
6	D	1264/1524 (82%)	-0.65	5 (0%) 92 79	23, 61, 83, 100	0
6	N	1264/1524 (82%)	-0.66	5 (0%) 92 79	26, 60, 84, 100	0
7	E	95/99 (95%)	-0.66	0 100 100	35, 59, 74, 82	0
7	O	95/99 (95%)	-0.67	0 100 100	45, 66, 80, 84	0
All	All	5976/6850 (87%)	-0.62	22 (0%) 92 79	21, 64, 86, 109	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	D	416	ALA	4.9
4	B	147	GLY	4.3
6	D	391	ALA	3.5
6	N	427	VAL	3.2
6	D	192	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	D	392	SER	3.0
6	N	416	ALA	2.8
6	N	391	ALA	2.8
5	M	936	VAL	2.7
6	N	421	LEU	2.7
5	C	1001	VAL	2.6
5	C	185	LYS	2.6
4	B	148	VAL	2.4
6	N	177	ALA	2.3
5	M	306	THR	2.3
6	D	619	LEU	2.3
5	M	174	LEU	2.2
5	M	418	LEU	2.2
5	C	309	TYR	2.1
5	M	172	ILE	2.1
5	M	183	SER	2.1
4	K	44	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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(\AA^2)	Q<0.9
8	ZN	N	5058	1/1	0.97	0.09	66,66,66,66	0
10	APC	D	3999	31/31	0.97	0.16	41,49,52,54	0
9	MG	N	9002	1/1	0.98	0.09	23,23,23,23	0
10	APC	N	4999	31/31	0.98	0.16	45,49,51,54	0
8	ZN	D	4058	1/1	0.99	0.09	66,66,66,66	0
8	ZN	D	6112	1/1	0.99	0.14	59,59,59,59	0

Continued on next page...

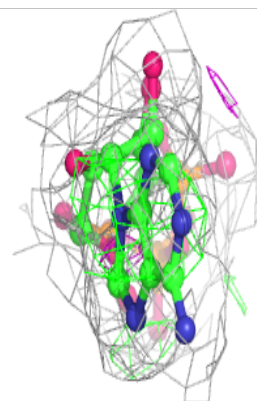
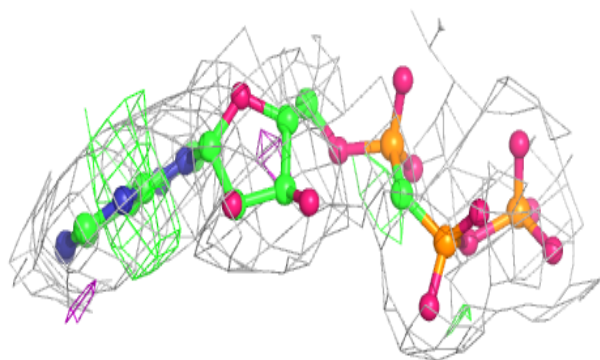
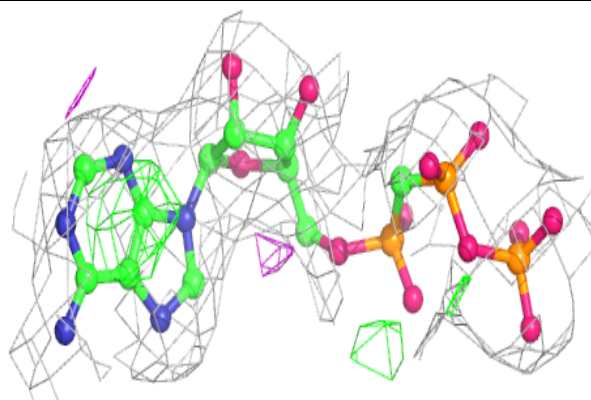
Continued from previous page...

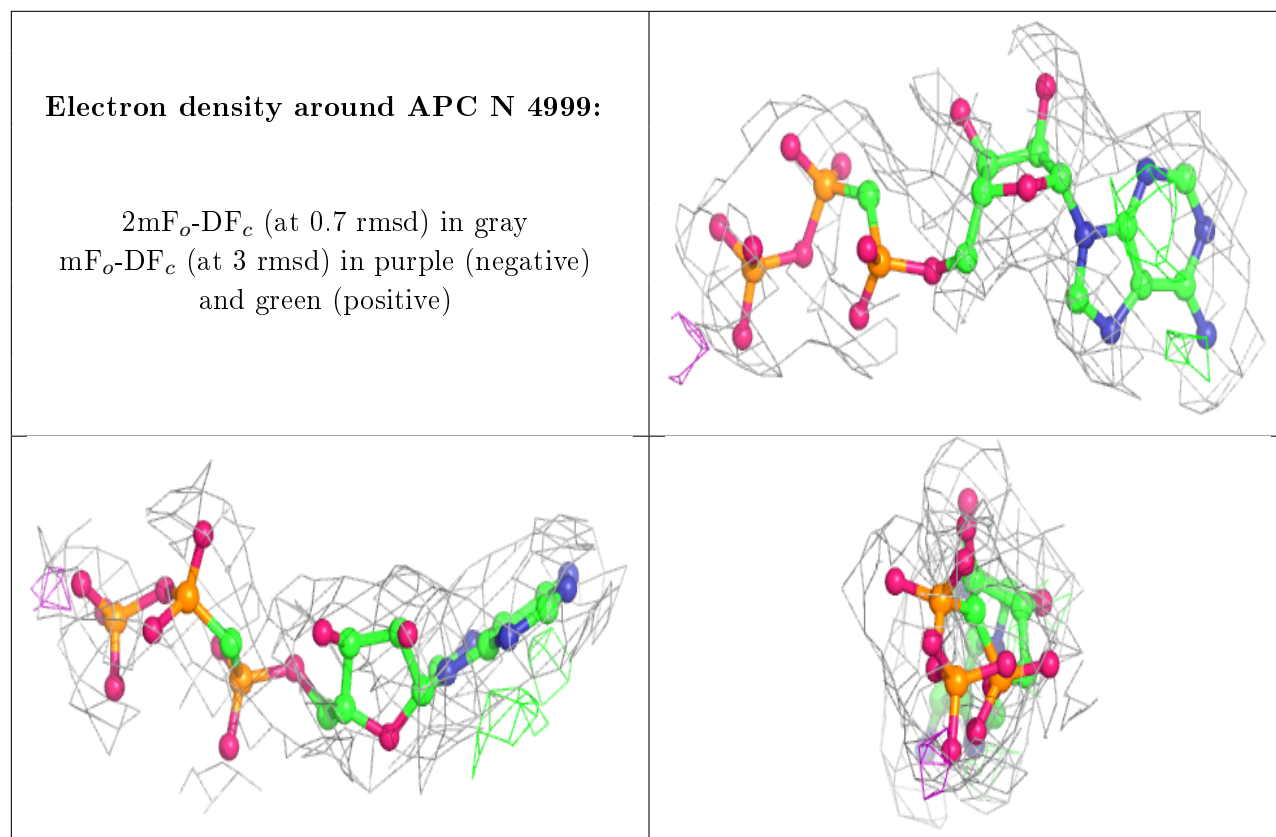
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	MG	N	9001	1/1	0.99	0.11	21,21,21,21	0
9	MG	D	8002	1/1	0.99	0.09	25,25,25,25	0
9	MG	D	8001	1/1	0.99	0.10	23,23,23,23	0
8	ZN	N	7112	1/1	1.00	0.13	65,65,65,65	0

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 APC D 3999:

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.