



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2020 – 03:19 PM BST

PDB ID : 4F5X
Title : Location of the dsRNA-dependent polymerase, VP1, in rotavirus particles
Authors : Estrozi, L.F.; Settembre, E.C.; Goret, G.; McClain, B.; Zhang, X.; Chen, J.Z.; Grigorieff, N.; Harrison, S.C.
Deposited on : 2012-05-13
Resolution : 5.00 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
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

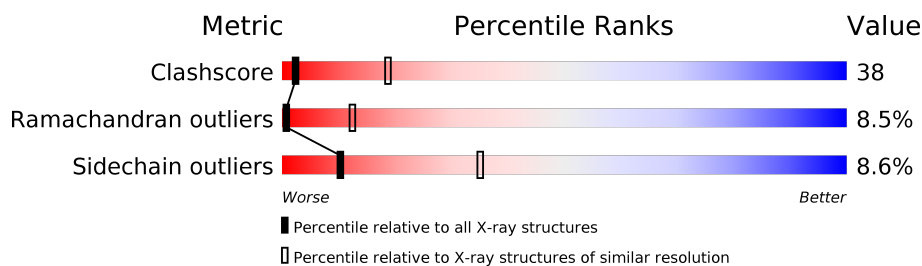
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1000 (6.16-3.82)
Ramachandran outliers	138981	1146 (6.20-3.80)
Sidechain outliers	138945	1122 (6.20-3.80)


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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	880	
1	B	880	
2	C	397	
2	D	397	
2	E	397	
2	F	397	
2	G	397	
2	H	397	

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Mol	Chain	Length	Quality of chain
2	I	397	 58% 33% 9%
2	J	397	 58% 34% 8% .
2	K	397	 59% 33% 8% .
2	L	397	 57% 35% 7% .
2	M	397	 58% 35% 6% .
2	N	397	 56% 34% 9% .
2	O	397	 57% 33% 9% .
3	W	1089	 40% 44% 5% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 62014 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called VP2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	781	Total	C	N	O	S	0	0	0
			6374	4049	1099	1190	36			
1	B	810	Total	C	N	O	S	0	0	0
			6624	4211	1138	1239	36			

- Molecule 2 is a protein called Intermediate capsid protein VP6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	D	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	E	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	F	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	G	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	H	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	I	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	J	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	K	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	L	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	M	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	N	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			

- Molecule 3 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	W	975	Total	C	N	O	S	0	0	0
			7905	5081	1308	1482	34			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

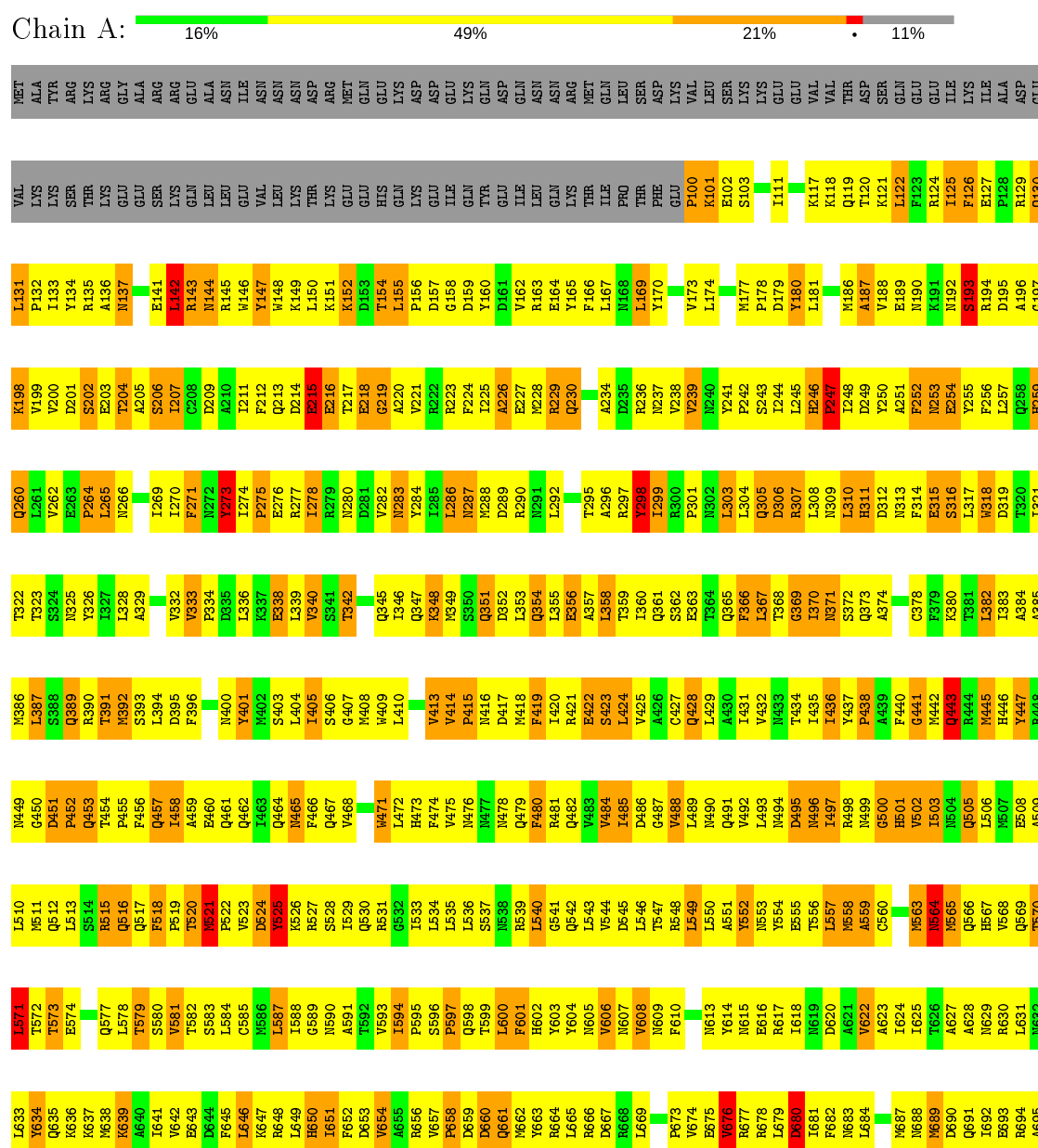
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	1	Total	Zn	0	0
			1	1		
4	I	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

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

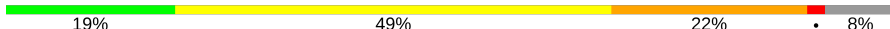
Note EDS failed to run properly.

• Molecule 1: VP2 protein

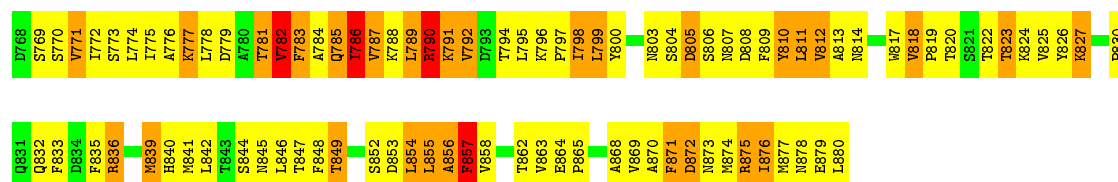


S896	V757	S821	K159	VAL	K135	K198	H259	T323	S388	G450	L513	B574	K636	V703
D697	A768	T822	K158	LYS	A136	V199	Q260	S394	Q889	D461	S514	Q577	K637	I704
K698	L759	T823	K157	TYR	M137	D201	L261	N325	R390	P452	R515	Q577	K638	I705
I699	V760	K824	SER	ARG	G138	D201	V262	Y326	T391	Q463	Q516	L577	K639	A706
A700	G761	E139	THR	LYS	E263	S202	E263	I327	M392	T454	Q517	T579	A640	A707
G701	A762	Y825	LYS	ARG	E203	E203	P264	L328	S393	P455	F518	S580	A641	A708
G702	L763	K827	GLU	GLY	E141	T204	L265	A329	L394	F456	P519	V581	V642	A709
V703	L764	Q828	GLU	ALA	E142	A205	N266	V333	D395	Q457	T520	T582	V645	K710
I704	F765	P830	SER	ARG	L143	S206	N267	V333	F396	I458	M521	S583	F645	G711
I705	F765	P830	ARG	ARG	N144	I207	I270	L336	T397	E489	R524	C585	L646	L712
A706	S769	F833	GLU	GLU	R145	I207	I270	L336	T399	I463	Y525	E586	L649	M717
Y707	S770	D834	ALA	ALA	W146	A210	F271	K337	T399	I463	Y525	E586	L650	Y718
D708	V771	D834	ASN	ASN	Y147	I211	N272	K337	N400	I463	Y525	E586	L650	Y718
D709	I772	F835	ILE	ILE	W148	F212	Y273	L339	Y401	Q464	K526	I588	I651	
M710	S773	R836	ASN	ASN	K149	Q213	I274	V340	M465	M465	R527	S589	F652	V721
Q711	L774	N837	ASN	ASN	L150	D214	P275	S403	F466	F466	S528	K590	D653	N722
L712	I775	S838	ASP	ASP	K151	E215	E276	T342	Q467	Q467	L404	A591	V654	I723
E713	A776	M839	ASP	ASP	K152	E216	R277	Q345	S406	W471	Q530	T592	A655	A724
D714	K777	H840	ARG	ARG	D153	T217	I278	Q346	Q407	L472	R531	Y593	B656	B725
E715	L778	M841	MET	MET	T154	E218	R279	Q347	Q408	L472	G532	I594	V657	B726
E716	D779	L842	GLN	GLN	L155	G219	M288	Q347	M408	L472	I533	P595	V658	L727
M717	A780	T843	GLU	GLU	P156	A220	N283	K348	H473	H473	L534	S596	D659	D728
Y718	Y781	Y88	LYS	LYS	D157	V221	Y284	N349	F474	F474	L535	P597	D660	G729
G719	F782	N845	ASP	ASP	G158	R222	Y285	A357	V475	V475	L536	Q598	D661	F730
Y720	V783	L846	ASP	ASP	D159	R223	I286	D852	T412	T412	S537	S599	Q662	Q731
V721	A784	T847	GLU	GLU	Y160	P224	L286	L353	V413	M477	M538	L600	V663	
M722	Q785	F848	LYS	LYS	D161	I225	N287	Q354	V414	M478	R539	F601	R664	N734
I723	L786	T849	GLN	GLN	L162	A226	M288	Q354	V414	M478	R539	F601	R664	N734
A724	Y787	P850	ASP	ASP	P163	E227	Y288	Q354	V414	M478	R539	F601	R664	N734
R725	K788	Y851	GLN	GLN	E164	M228	Y288	Q354	V414	M478	R539	F601	R664	N734
N726	L789	S852	ASN	ASN	Y165	R229	Y288	Q354	V414	M478	R539	F601	R664	N734
L727	L793	D853	ASN	ASN	F166	Q230	S294	L292	L292	L292	Q361	R421	D670	K739
D728	T794	L854	ARG	ARG	L167	Q231	T295	Q361	R421	D670	Q361	R421	D670	K739
G729	L795	L855	MET	MET	M168	Q232	A296	Q361	R421	D670	Q361	R421	D670	K739
F730	K796	A856	GLN	GLN	L169	Q233	R297	Q361	R421	D670	Q361	R421	D670	K739
Q731	P797	F857	LEU	LEU	Y170	A234	Y298	Q361	R421	D670	Q361	R421	D670	K739
K732	I798	S859	SER	SER	V173	D235	R300	Q361	R421	D670	Q361	R421	D670	K739
I733	L799	D860	ASP	ASP	L174	R236	R300	Q361	R421	D670	Q361	R421	D670	K739
M734	Y800	D861	LYS	LYS	T175	N237	P301	Q361	R421	D670	Q361	R421	D670	K739
L735	L800	T862	VAL	VAL	E109	V238	N302	Q361	R421	D670	Q361	R421	D670	K739
E736	K801	T862	LEU	LEU	E109	V238	N302	Q361	R421	D670	Q361	R421	D670	K739
E737	I802	V863	SER	SER	M177	N240	L303	Q361	R421	D670	Q361	R421	D670	K739
L738	N803	E864	LYS	LYS	I111	Y241	Q305	Q361	R421	D670	Q361	R421	D670	K739
M739	S804	P865	LYS	LYS	K112	P242	R306	Q361	R421	D670	Q361	R421	D670	K739
K740	D805	I866	GLU	GLU	P113	S243	R307	Q361	R421	D670	Q361	R421	D670	K739
T741	S806	N867	GLU	GLU	K117	I244	L308	Q361	R421	D670	Q361	R421	D670	K739
G742	N807	A868	VAL	VAL	Q119	H246	L310	Q361	R421	D670	Q361	R421	D670	K739
Y744	D808	V869	VAL	VAL	Q119	P247	H311	Q361	R421	D670	Q361	R421	D670	K739
A745	F809	K184	THR	THR	Q119	P247	H311	Q361	R421	D670	Q361	R421	D670	K739
Q746	F871	F871	ASP	ASP	L185	I248	D312	Q361	R421	D670	Q361	R421	D670	K739
I747	L811	D872	SER	SER	M186	D249	N313	Q361	R421	D670	Q361	R421	D670	K739
L751	V812	N873	GLN	GLN	N190	Y250	F314	Q361	R421	D670	Q361	R421	D670	K739
M750	A813	M874	GLU	GLU	K191	A251	E315	Q361	R421	D670	Q361	R421	D670	K739
L752	N814	R875	GLU	GLU	K191	F252	S316	Q361	R421	D670	Q361	R421	D670	K739
L753	Y815	I876	ILE	ILE	N192	N253	L317	Q361	R421	D670	Q361	R421	D670	K739
M753	D816	M877	LYS	LYS	S193	E254	H318	Q361	R421	D670	Q361	R421	D670	K739
Q754	W817	E877	ILE	ILE	R194	Y255	D319	Q361	R421	D670	Q361	R421	D670	K739
M755	V818	E878	ALA	ALA	D195	F256	T320	Q361	R421	D670	Q361	R421	D670	K739
Q756	P819	L880	ASP	ASP	A196	L257	I321	Q361	R421	D670	Q361	R421	D670	K739
T756	T820		GLU	GLU	G197	Q258	T322	Q361	R421	D670	Q361	R421	D670	K739

• Molecule 1: VP2 protein

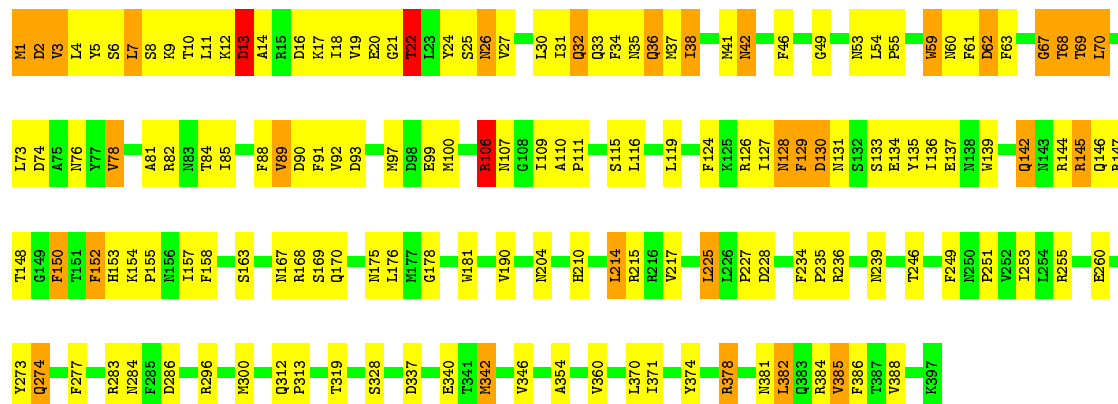
Chain B:  19% 49% 22% 8%

MET	VAL	R135	K198	H259	T323	S388	G450	L513	B574	K636	V703
ALA	LYS	A136	V199	Q260	S394	Q889	D461	S514	Q577	K637	I704
TYR	LYS	M137	D201	L261	N325	R390	P452	R515	Q577	K638	I705
ARG	SER	G138	D201	V262	Y326	T391	Q463	Q516	L577	A640	A706
LYS	THR	E139	E263	E263	I327	M392	T454	Q517	T579	A641	A707
ARG	LYS	K140	S202	P264	L328	S393	P455	F518	S580	V642	A708
GLY	GLU	E141	T204	L265	A329	L394	F456	P519	V581	V642	A709
ALA	GLU	L142	A205	N266	V333	D395	Q457	T520	T582	F645	K710
ARG	SER	R143	S206	N267	V333	F396	I458	M521	S583	L646	G711
ARG	ARG	N144	I207	I270	L336	T397	E489	R524	C585	L646	L712
GLU	GLU	R145	I207	I270	L336	T399	I463	Y525	E586	L649	M717
ALA	ALA	W146	A210	F271	K337	T399	I463	Y525	E586	L650	Y718
ASN	ASN	Y147	I211	N272	K337	N400	I463	Y525	E586	L650	Y718
ILE	ILE	W148	F212	Y273	L339	Y401	Q464	K526	I588	I651	
ASN	ASN	K149	Q213	I274	V340	M465	M465	R527	S589	F652	V721
ASN	ASN	L150	D214	P275	S403	F466	F466	S528	K590	D653	N722
L712	L776	K151	E215	E276	T342	Q467	Q467	L404	A591	V654	I723
ASP	ASP	K152	E216	R277	Q345	S406	W471	Q530	T592	A655	A724
ASP	ASP	D153	T217	I278	Q346	Q407	L472	R531	Y593	B656	B725
ARG	ARG	T154	E218	R279	Q347	Q408	L472	G532	I594	V657	B726
MET	MET	L155	G219	M288	Q347	M408	L472	I533	P595	V658	L727
GLN	GLU	P156	A220	N283	K348	H473	H473	L534	S596	D659	D728
LYS	LYS	D157	V221	Y284	N349	F474	F474	L535	P597	D660	G729
ASP	ASP	G158	R222	Y285	A357	V475	V475	L536	Q598	D661	F730
ASP	ASP	D159	R223	I286	D852	T412	T412	S537	S599	Q662	Q731
GLU	GLU	Y160	P224	L286	L353	V413	M477	M538	L600	V663	
LYS	LYS	D161	I225	N287	Q354	V414	M478	R539	F601	R664	N734
GLN	GLN	L162	A226	M288	Q354	V414	M478	R539	F601	R664	N734
ASP	ASP	P163	E227	Y288	Q354	V414	M478	R539	F601	R664	N734
GLN	GLN	E164	M228	Y288	Q354	V414	M478	R539	F601	R664	N734
P86	P86	Y165	R229	Y288	Q354	V414	M478	R539	F601	R664	N734
S853	S853	F166	Q230	S294	L292	L292	L292	Q361	R421	D670	K739
L854	L854	L167	Q231	T295	Q361	R421	D670	Q361	R421	D670	K739
L855	L855	M168	Q232	A296	Q361	R421	D670	Q361	R421	D670	K739
K101	K101	L169	Q233	R297	Q361	R421	D670	Q361	R421	D670	K739
F857	F857	Y170	A234	Y298	Q361	R421	D670	Q361	R421	D670	K739
S858	S858	V173	D235	R300	Q361	R421	D670	Q361	R421	D670	K739
I798	I798	L174	R236	R300	Q361	R421	D670	Q361	R421	D670	K739
L799	L799	T175	N237	P301	Q361	R421	D670	Q361	R421	D670	K739
Y800	Y800	E109	V238	N302	Q361	R421	D670	Q361	R421	D670	K739
K801	K801	E109	V238	N302	Q361	R421	D670	Q361	R421	D670	K739
I802	I802	M177	N240	L303	Q361	R421	D670	Q361	R421	D670	K739
N803	N803	I111	Y241	Q305	Q361	R421	D670	Q361	R421	D670	K739
L738	L738	K112	P242	R306	Q361	R421	D670	Q361	R421	D670	K739
M739	M739	P113	S243	R307	Q361	R421	D670	Q361	R421	D670	K739
D805	D805	K117	I244	L308	Q361	R421	D670	Q361	R421	D670	K739



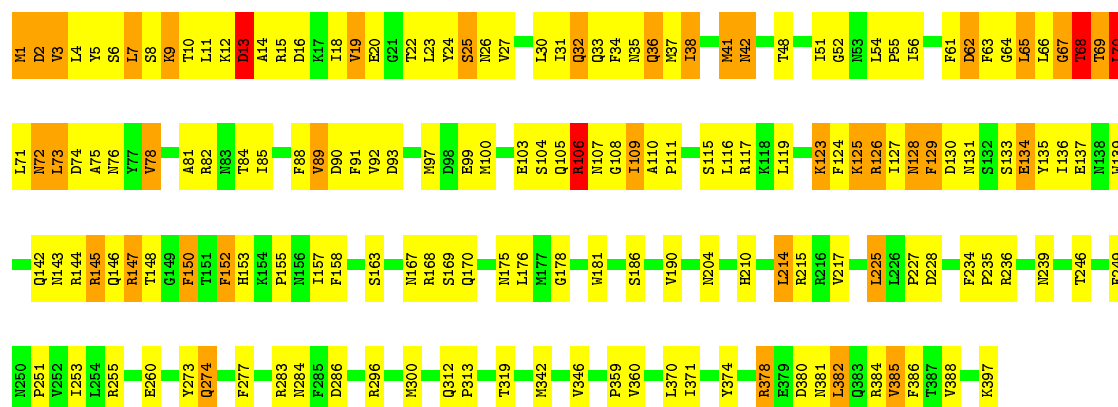
• Molecule 2: Intermediate capsid protein VP6

Chain C: 60% 31% 8%



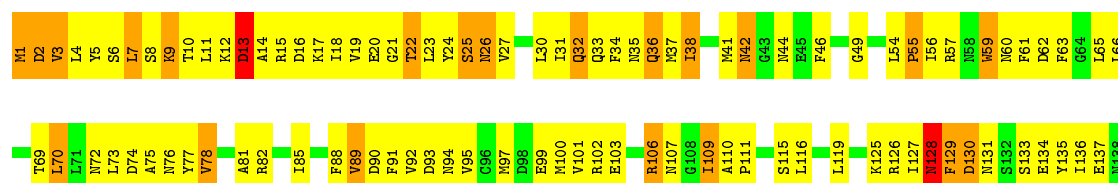
• Molecule 2: Intermediate capsid protein VP6

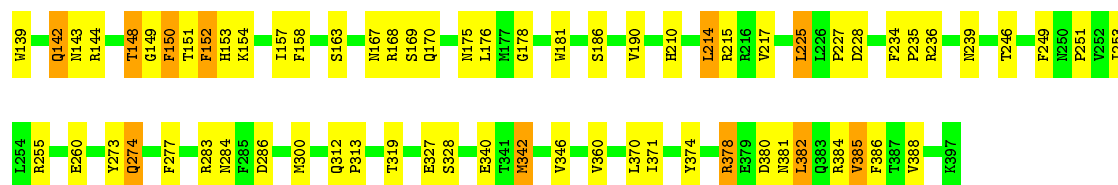
Chain D: 57% 32% 9%



• Molecule 2: Intermediate capsid protein VP6

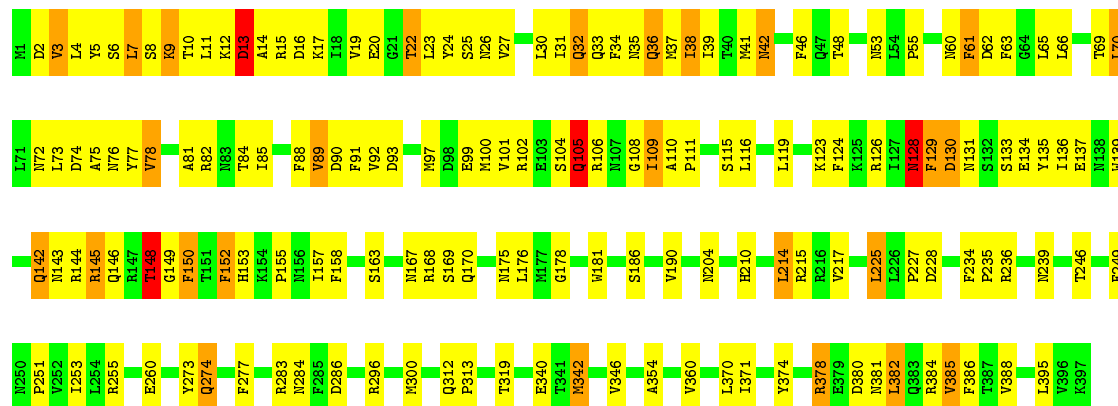
Chain E: 58% 33% 8%





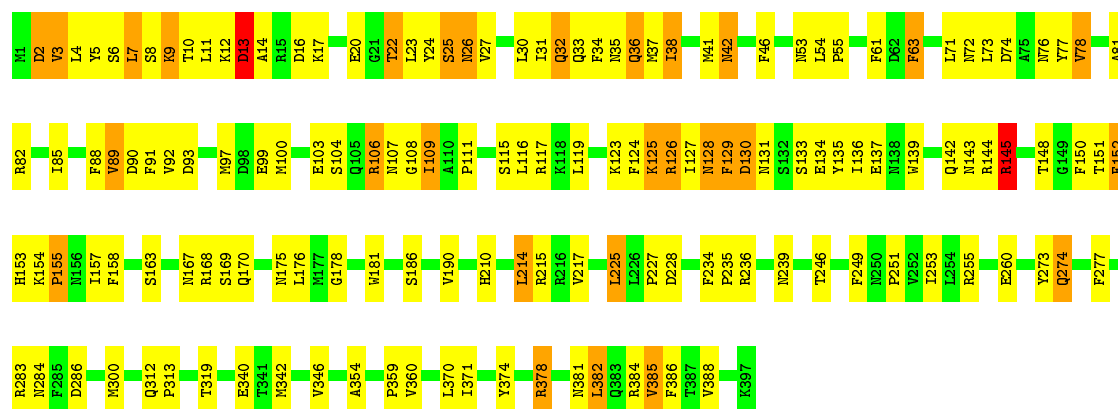
• Molecule 2: Intermediate capsid protein VP6

Chain F: 59% 34% 7%



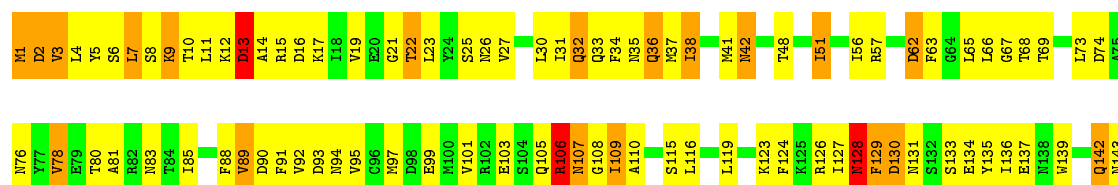
• Molecule 2: Intermediate capsid protein VP6

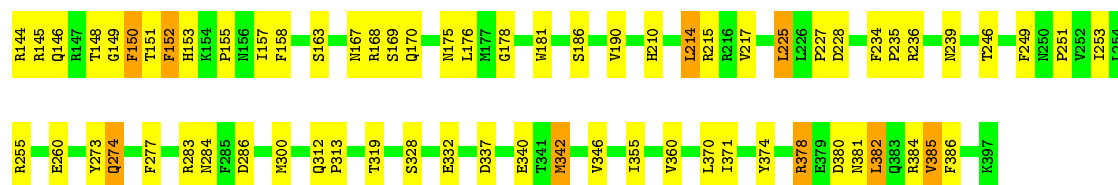
Chain G: 62% 30% 7%



• Molecule 2: Intermediate capsid protein VP6

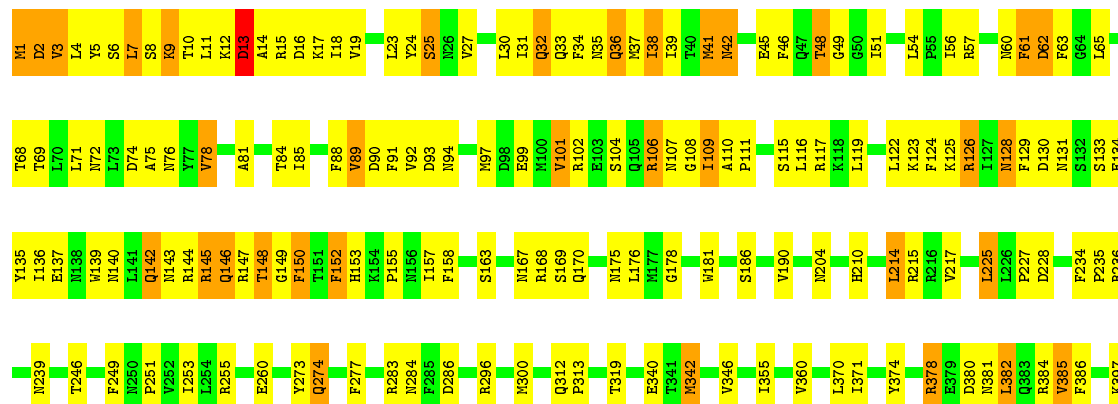
Chain H: 60% 32% 7%





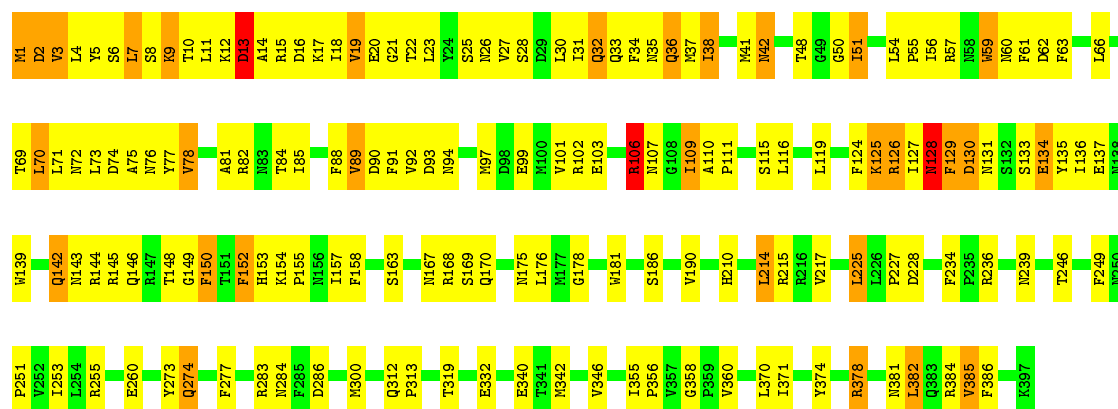
• Molecule 2: Intermediate capsid protein VP6

Chain I: 58% 33% 9%



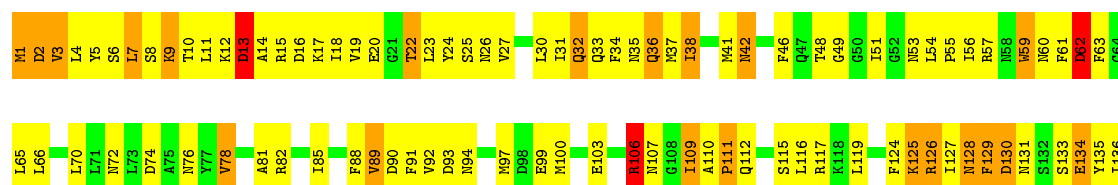
• Molecule 2: Intermediate capsid protein VP6

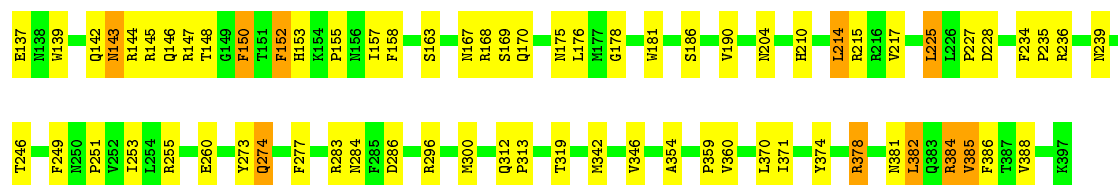
Chain J: 58% 34% 8%



• Molecule 2: Intermediate capsid protein VP6

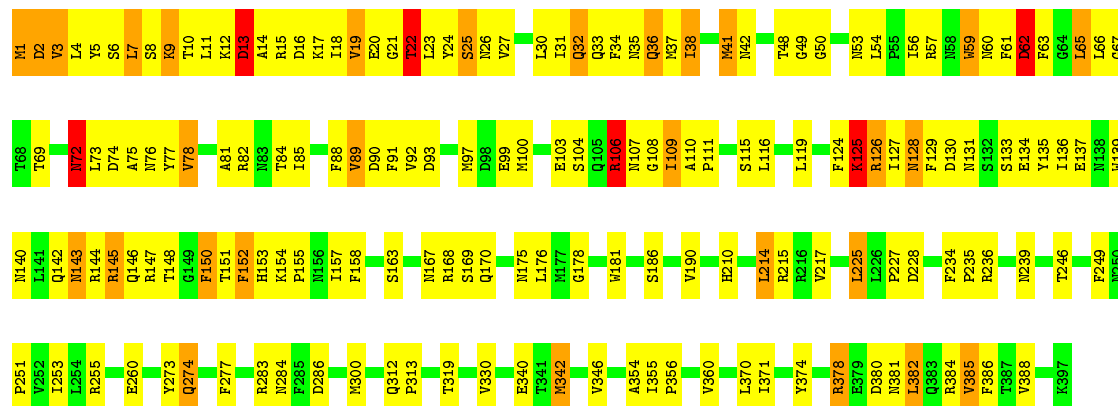
Chain K: 59% 33% 8%





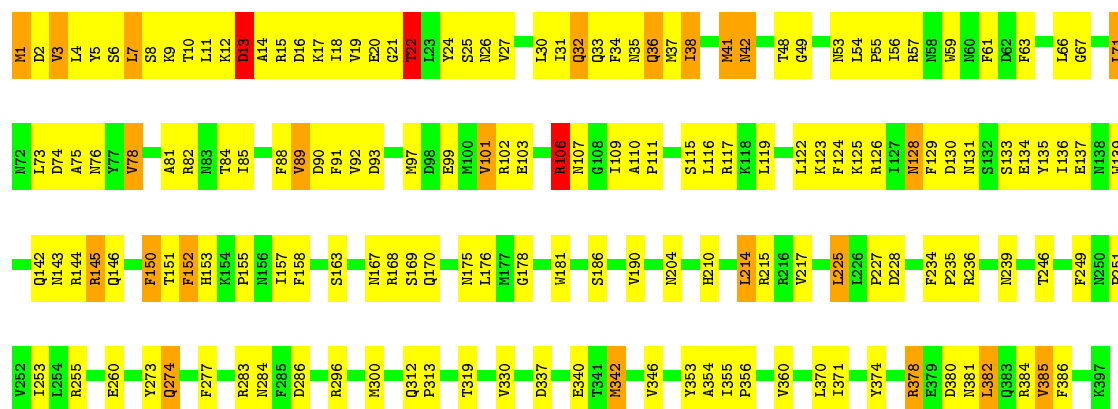
• Molecule 2: Intermediate capsid protein VP6

Chain L: 57% 35% 7% •



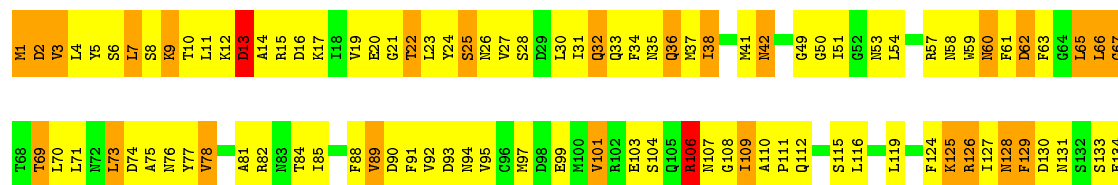
• Molecule 2: Intermediate capsid protein VP6

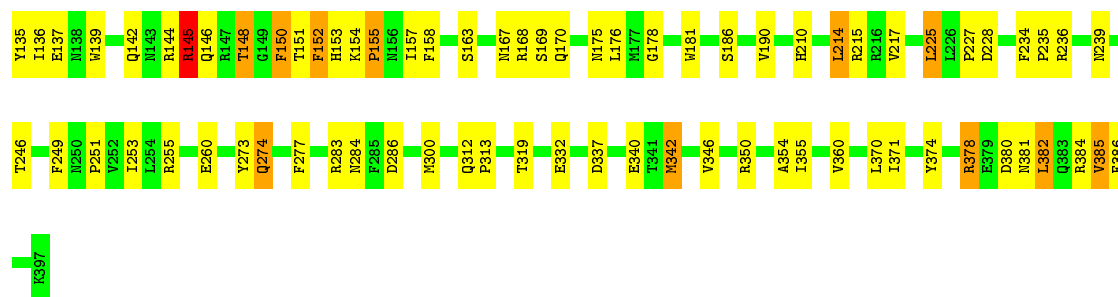
Chain M: 58% 35% 6% •



• Molecule 2: Intermediate capsid protein VP6

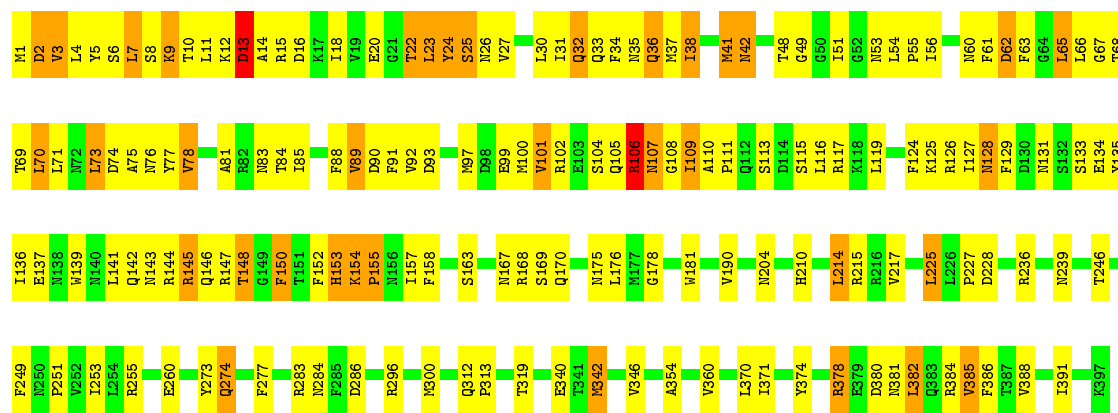
Chain N: 56% 34% 9% •





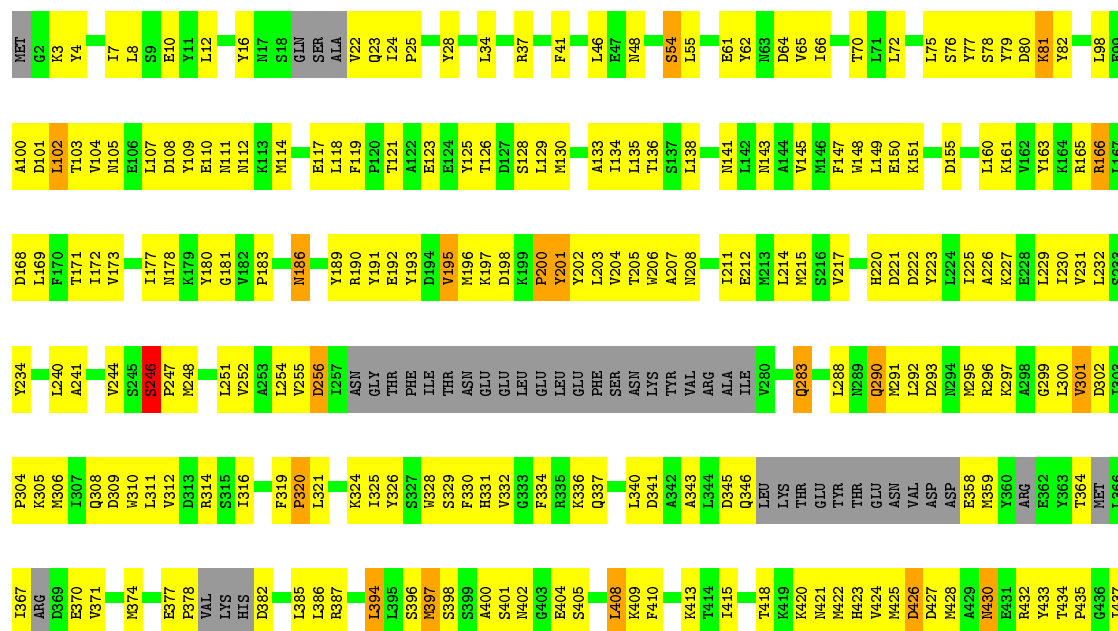
• Molecule 2: Intermediate capsid protein VP6

Chain O: 57% 33% 9%



• Molecule 3: RNA-directed RNA polymerase

Chain W: 40% 44% 5% 10%



L438	P439	V441	D444	F445	P446	I447	L448	G450	R451	R452	R458	T459	R460	I461	F462	F463	I464	L465	P466	Y467	E468	F469	F470	I471	A472	Q473	H474	A475	V476	V477	A478	ASU	K479	M480	R488	E489	Y490	A491	Q496	S497	N498	Q499	L500	L501	S502	Y503	V506	THR	ARG	F509	LEU	SER	GLN	ASN
ASN	THR	MET	V516	L517	Y518	T519	D520	V521	W524	S527	Q528	E529	R530	T531	Q532	P533	F534	R535	K536	G537	I538	I539	M540	G541	L542	ASP	ILE	LEU	ALA	ASN	MET	THR	LYS	ASP	ALA	R553	V554	L555	L558	N559	L560	Y561	Q562	Q563	T564	Q565	I566	N567	L568	S571	Y572	V573	Q574	I575
V580	I581	R582	K583	I584	Q585	Y586	G587	V589	A590	S591	G592	E593	K594	Q595	T596	R597	A598	A599	M600	I602	L605	A606	L607	L612	SER	ARG	ILE	SER	ASN	LYS	H619	SER	PHE	A622	T623	K624	I625	I626	R627	V628	D629	N633	L637	GLN	PHE	ASN	THR	GLU	VAL	THR	LYS	MET		
I648	Q649	D650	V651	D654	V655	Y659	N663	V666	K667	S671	THR	T673	G674	I675	R680	K686	I687	F688	F689	R690	A691	G692	L695	L696	N697	N698	R701	G702	Q703	S704	T705	D708	Q709	I712	Y717	I718	R721	L722	R723	T807	R729	I732	L733	T734	K735									
I736	M737	T740	S741	I744	T745	G746	S747	L748	N750	F751	E754	T758	T759	M760	S761	T762	F766	E769	D770	F771	I772	T777	T778	V779	D780	E781	V782	Y783	I784	Q785	R786	S790	L791	K795	S796	G797	I798	B801	I802	A803	A804	T807	R808	K809	M810	Y811	V812							
T813	R814	L815	S816	L819	L820	K823	N824	N825	I826	V827	S828	R829	G830	I831	A832	E835	K836	A837	K838	L839	N840	A843	P844	I845	S846	L847	E848	Q853	S854	L857	L858	L861	Q862	K863	P864	V865	T866	R867	R868	S869	S870	K871	I872	T873	I874	N875	R879	D880	I881	K882	P883			
F884	F885	T886	V887	A890	H891	L892	P893	I894	Q897	K898	F899	M900	P901	N906	V907	Q908	Q912	R917	T918	Y919	Q920	I921	E922	D923	D924	G925	S926	R927	S928	A929	I930	S931	R932	L933	I934	S935	LYS	TYR	S938	V939	Y940	I944	E945	Y948	I951	S952	L953	H954	E957	I958				
GLN	LEU	Y961	L962	ILE	S964	L965	G966	PRO	LYS	ILE	ASP	ALA	ASP	TYR	VAL	GLY	SER	LYS	ILE	Y981	S982	ARG	D984	K985	Y986	R987	I988	S991	Y992	L996	I999	H1000	Y1001	G1002	C1003	Y1004	Q1005	L1006	F1009	N1010	D1013	L1014	GLU	K1016	L1017	I1018	R1019	ILE	PRO	PHE	LYS	GLY		
LYS	ILE	PRO	ALA	VAL	THR	F1031	H1034	A1037	I1042	M1043	K1047	M1048	G1049	S1050	W1051	I1052	S1053	L1054	Y1058	P1059	M1063	K1068	K1069	H1070	W1071	M1072	I1073	T1074	R1077	S1078	P1079	Y1080	T1081	H1082	A1083	R1084	F1085	F1086	GLN	GLU	PRO													

4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	740.75Å 1198.07Å 1345.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 5.00	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-5.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.49 (at 3.78Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.293 , 0.296	Depositor
Wilson B-factor (Å ²)	167.1	Xtriage
Anisotropy	0.043	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	62014	wwPDB-VP
Average B, all atoms (Å ²)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.48	0/6491	0.84	9/8806 (0.1%)
1	B	0.50	0/6745	0.82	10/9149 (0.1%)
2	C	0.51	0/3232	0.78	5/4397 (0.1%)
2	D	0.51	0/3232	0.78	5/4397 (0.1%)
2	E	0.51	0/3232	0.77	5/4397 (0.1%)
2	F	0.50	0/3232	0.76	5/4397 (0.1%)
2	G	0.50	0/3232	0.77	5/4397 (0.1%)
2	H	0.50	0/3232	0.76	5/4397 (0.1%)
2	I	0.50	0/3232	0.77	5/4397 (0.1%)
2	J	0.51	0/3232	0.78	5/4397 (0.1%)
2	K	0.51	0/3232	0.77	5/4397 (0.1%)
2	L	0.51	0/3232	0.77	5/4397 (0.1%)
2	M	0.51	0/3232	0.77	5/4397 (0.1%)
2	N	0.51	0/3232	0.77	5/4397 (0.1%)
2	O	0.52	0/3232	0.79	7/4397 (0.2%)
3	W	0.41	0/8045	0.62	3/10847 (0.0%)
All	All	0.49	0/63297	0.77	89/85963 (0.1%)

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

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

There are no bond length outliers.

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	TYR	CB-CG-CD2	10.70	127.42	121.00
1	A	273	TYR	CB-CG-CD1	-9.86	115.08	121.00
1	A	273	TYR	CA-CB-CG	9.85	132.12	113.40
1	B	273	TYR	CB-CG-CD1	9.85	126.91	121.00
1	B	273	TYR	CB-CG-CD2	-9.21	115.48	121.00
1	B	273	TYR	CA-CB-CG	9.02	130.53	113.40
1	A	367	LEU	N-CA-C	-7.59	90.51	111.00
1	A	298	TYR	N-CA-C	7.41	131.01	111.00
2	L	384	ARG	NE-CZ-NH2	7.00	123.80	120.30
2	H	384	ARG	NE-CZ-NH2	6.92	123.76	120.30
2	F	384	ARG	NE-CZ-NH2	6.86	123.73	120.30
2	I	384	ARG	NE-CZ-NH2	6.80	123.70	120.30
2	K	384	ARG	NE-CZ-NH2	6.75	123.67	120.30
1	A	639	LYS	N-CA-C	-6.67	92.98	111.00
2	D	236	ARG	NE-CZ-NH2	6.67	123.64	120.30
2	C	384	ARG	NE-CZ-NH2	6.67	123.64	120.30
2	O	384	ARG	NE-CZ-NH2	6.66	123.63	120.30
2	N	384	ARG	NE-CZ-NH2	6.62	123.61	120.30
2	E	384	ARG	NE-CZ-NH2	6.59	123.59	120.30
2	F	236	ARG	NE-CZ-NH2	6.57	123.58	120.30
2	D	384	ARG	NE-CZ-NH2	6.57	123.58	120.30
2	C	283	ARG	NE-CZ-NH2	6.51	123.56	120.30
2	L	236	ARG	NE-CZ-NH2	6.51	123.56	120.30
2	H	236	ARG	NE-CZ-NH2	6.51	123.55	120.30
2	M	283	ARG	NE-CZ-NH2	6.46	123.53	120.30
2	J	283	ARG	NE-CZ-NH2	6.42	123.51	120.30
2	M	236	ARG	NE-CZ-NH2	6.41	123.51	120.30
2	J	384	ARG	NE-CZ-NH2	6.40	123.50	120.30
2	M	384	ARG	NE-CZ-NH2	6.38	123.49	120.30
2	J	236	ARG	NE-CZ-NH2	6.38	123.49	120.30
2	I	236	ARG	NE-CZ-NH2	6.37	123.49	120.30
2	G	236	ARG	NE-CZ-NH2	6.35	123.47	120.30
2	N	236	ARG	NE-CZ-NH2	6.34	123.47	120.30
3	W	1082	ASN	N-CA-C	6.33	128.08	111.00
2	D	283	ARG	NE-CZ-NH2	6.30	123.45	120.30
2	O	283	ARG	NE-CZ-NH2	6.27	123.44	120.30
2	N	283	ARG	NE-CZ-NH2	6.26	123.43	120.30
2	G	384	ARG	NE-CZ-NH2	6.25	123.43	120.30
2	O	236	ARG	NE-CZ-NH2	6.25	123.42	120.30
2	E	236	ARG	NE-CZ-NH2	6.23	123.42	120.30
2	C	236	ARG	NE-CZ-NH2	6.23	123.42	120.30
2	K	236	ARG	NE-CZ-NH2	6.19	123.40	120.30
2	G	283	ARG	NE-CZ-NH2	6.17	123.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	283	ARG	NE-CZ-NH2	6.13	123.37	120.30
2	F	283	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	B	636	LYS	N-CA-C	-6.10	94.53	111.00
2	K	283	ARG	NE-CZ-NH2	6.08	123.34	120.30
2	L	283	ARG	NE-CZ-NH2	6.08	123.34	120.30
2	H	283	ARG	NE-CZ-NH2	6.06	123.33	120.30
2	I	283	ARG	NE-CZ-NH2	6.03	123.31	120.30
2	O	154	LYS	N-CA-C	-5.98	94.86	111.00
2	O	300	MET	CG-SD-CE	5.80	109.48	100.20
2	C	300	MET	CG-SD-CE	5.80	109.47	100.20
2	F	300	MET	CG-SD-CE	5.79	109.47	100.20
2	I	300	MET	CG-SD-CE	5.78	109.44	100.20
2	N	300	MET	CG-SD-CE	5.76	109.42	100.20
2	L	300	MET	CG-SD-CE	5.76	109.41	100.20
1	B	497	ILE	N-CA-C	-5.75	95.47	111.00
2	M	300	MET	CG-SD-CE	5.75	109.41	100.20
2	D	300	MET	CG-SD-CE	5.75	109.39	100.20
2	J	300	MET	CG-SD-CE	5.74	109.39	100.20
2	G	300	MET	CG-SD-CE	5.73	109.37	100.20
2	H	300	MET	CG-SD-CE	5.72	109.36	100.20
2	K	300	MET	CG-SD-CE	5.70	109.31	100.20
1	B	76	LEU	CA-CB-CG	5.69	128.40	115.30
2	E	300	MET	CG-SD-CE	5.63	109.21	100.20
3	W	1077	ARG	N-CA-C	5.57	126.05	111.00
1	B	273	TYR	CB-CA-C	-5.50	99.39	110.40
1	B	811	LEU	N-CA-C	-5.48	96.21	111.00
2	M	342	MET	CG-SD-CE	5.35	108.75	100.20
2	D	342	MET	CG-SD-CE	5.32	108.70	100.20
2	G	342	MET	CG-SD-CE	5.29	108.67	100.20
1	A	317	LEU	CA-CB-CG	-5.27	103.18	115.30
2	J	342	MET	CG-SD-CE	5.27	108.63	100.20
1	B	317	LEU	CA-CB-CG	-5.25	103.24	115.30
2	L	342	MET	CG-SD-CE	5.23	108.57	100.20
2	O	153	HIS	N-CA-C	5.22	125.09	111.00
2	E	342	MET	CG-SD-CE	5.21	108.54	100.20
2	N	342	MET	CG-SD-CE	5.21	108.53	100.20
2	F	342	MET	CG-SD-CE	5.19	108.51	100.20
2	O	342	MET	CG-SD-CE	5.19	108.50	100.20
2	I	342	MET	CG-SD-CE	5.18	108.49	100.20
1	B	82	HIS	N-CA-C	-5.17	97.05	111.00
2	C	342	MET	CG-SD-CE	5.16	108.46	100.20
3	W	1085	PHE	N-CA-C	5.16	124.92	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	342	MET	CG-SD-CE	5.15	108.44	100.20
2	H	342	MET	CG-SD-CE	5.14	108.43	100.20
1	A	842	LEU	CA-CB-CG	-5.07	103.64	115.30
1	A	719	GLY	N-CA-C	-5.06	100.46	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6374	0	6394	1006	0
1	B	6624	0	6652	1133	0
2	C	3162	0	3101	170	0
2	D	3162	0	3101	179	0
2	E	3162	0	3101	164	0
2	F	3162	0	3101	160	0
2	G	3162	0	3101	149	0
2	H	3162	0	3101	175	0
2	I	3162	0	3101	215	0
2	J	3162	0	3101	187	0
2	K	3162	0	3101	166	0
2	L	3162	0	3101	178	0
2	M	3162	0	3101	173	0
2	N	3162	0	3101	191	0
2	O	3162	0	3101	163	0
3	W	7905	0	7966	543	0
4	C	1	0	0	0	0
4	F	1	0	0	0	0
4	I	1	0	0	0	0
4	L	1	0	0	0	0
4	O	1	0	0	0	0
All	All	62014	0	61325	4691	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 38.

All (4691) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:VAL:HG22	3:W:673:VAL:CG1	1.63	1.28
1:B:771:VAL:HB	1:B:809:PHE:HB3	1.23	1.18
1:B:75:VAL:CG2	3:W:673:VAL:HG12	1.72	1.18
1:A:333:VAL:HG11	1:A:380:LYS:HA	1.27	1.15
1:A:428:GLN:OE1	1:A:456:PHE:HB2	1.46	1.13
1:A:563:MET:HA	1:A:563:MET:HE3	1.22	1.12
2:G:145:ARG:HB3	2:G:145:ARG:HH11	1.10	1.12
2:H:83:ASN:ND2	2:I:122:LEU:HB2	1.65	1.11
1:A:451:ASP:HB3	1:A:452:PRO:HD2	1.14	1.11
1:B:432:VAL:HA	1:B:436:ILE:HD11	1.18	1.11
1:B:734:ASN:HB3	1:B:737:GLU:HB2	1.28	1.10
1:B:718:TYR:HB3	1:B:721:VAL:HG21	1.33	1.10
1:A:270:ILE:HD11	1:A:292:LEU:HD11	1.31	1.09
1:B:548:ARG:NH1	1:B:878:ASN:H	1.50	1.09
2:L:22:THR:HG23	2:L:73:LEU:HD12	1.35	1.08
1:A:699:ILE:HG12	1:A:700:ALA:H	1.18	1.07
2:G:145:ARG:HD2	2:I:143:ASN:HA	1.34	1.07
1:B:200:VAL:HG21	1:B:243:SER:HB3	1.13	1.07
1:A:318:TRP:HA	1:A:321:ILE:HD12	1.34	1.07
2:N:106:ARG:H	2:N:106:ARG:HD3	1.17	1.06
1:B:790:ARG:HA	1:B:790:ARG:HE	0.98	1.06
1:B:318:TRP:HA	1:B:321:ILE:HD12	1.37	1.06
1:A:658:PRO:HG2	1:B:348:LYS:HG2	1.38	1.05
1:B:498:ARG:HB2	2:I:32:GLN:HE22	1.15	1.05
1:A:721:VAL:HG12	1:A:722:ASN:H	1.18	1.04
1:B:510:LEU:HD11	1:B:537:SER:HA	1.36	1.04
1:A:199:VAL:HG12	1:A:200:VAL:H	1.20	1.04
1:B:457:GLN:HG3	1:B:458:ILE:H	1.22	1.03
1:B:646:LEU:HA	1:B:649:LEU:HD12	1.40	1.03
1:A:428:GLN:NE2	1:A:455:PRO:HB2	1.73	1.03
1:A:451:ASP:CB	1:A:452:PRO:HD2	1.84	1.03
1:B:274:ILE:HG23	1:B:278:ILE:HD11	1.40	1.03
1:A:510:LEU:HD22	1:A:540:LEU:HD13	1.39	1.02
1:B:444:ARG:HH21	1:B:520:THR:HG23	1.20	1.02
1:A:310:LEU:HD12	1:A:310:LEU:H	1.21	1.02
1:B:457:GLN:HB2	1:B:476:ASN:ND2	1.75	1.02
1:A:513:LEU:HA	1:A:516:GLN:NE2	1.75	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:PHE:O	1:B:228:MET:HG2	1.61	1.01
1:B:573:THR:HG22	1:B:574:GLU:H	0.88	1.01
1:A:521:MET:HB3	1:A:522:PRO:HD3	1.39	1.01
1:B:790:ARG:HE	1:B:790:ARG:CA	1.70	1.00
1:A:506:LEU:HD23	1:A:544:VAL:HA	1.40	1.00
2:C:106:ARG:HD3	2:C:106:ARG:H	1.26	1.00
1:A:367:LEU:HD21	3:W:929:ALA:HA	1.44	0.99
1:B:573:THR:HG22	1:B:574:GLU:N	1.71	0.99
1:A:705:ILE:HA	1:A:823:THR:HG22	1.43	0.99
1:B:674:VAL:HG21	1:B:679:LEU:HD13	1.44	0.99
1:B:510:LEU:HD22	1:B:540:LEU:HD13	1.42	0.99
1:B:573:THR:CG2	1:B:574:GLU:H	1.71	0.99
1:B:473:HIS:HB2	2:I:126:ARG:HH22	1.21	0.99
2:L:42:ASN:HA	2:L:61:PHE:HB2	1.43	0.98
1:B:371:ASN:HD22	1:B:583:SER:HB3	1.28	0.98
1:B:204:THR:HG23	1:B:244:ILE:HG22	1.44	0.98
2:H:106:ARG:H	2:H:106:ARG:HD3	1.26	0.98
1:A:275:PRO:HB2	1:A:278:ILE:HD11	1.45	0.98
1:B:265:LEU:HB3	1:B:296:ALA:HB1	1.46	0.98
1:B:435:ILE:HG22	1:B:436:ILE:H	1.29	0.98
2:J:106:ARG:HD3	2:J:106:ARG:H	1.23	0.97
1:B:743:ASP:C	1:B:744:TYR:HD2	1.67	0.97
1:B:700:ALA:HB2	1:B:827:LYS:HB2	1.45	0.97
1:B:700:ALA:CB	1:B:827:LYS:HB2	1.95	0.97
1:A:540:LEU:O	1:A:544:VAL:HG23	1.64	0.97
1:A:270:ILE:HG23	1:A:854:LEU:HD21	1.46	0.96
3:W:441:VAL:HB	3:W:447:ILE:HD11	1.46	0.96
1:A:192:ASN:O	1:A:193:SER:HB3	1.65	0.96
1:B:200:VAL:HG21	1:B:243:SER:CB	1.96	0.96
2:H:83:ASN:HD21	2:I:122:LEU:HB2	1.30	0.96
1:A:660:ASP:HB3	1:B:539:ARG:HD2	1.43	0.96
1:A:588:ILE:HG22	1:A:589:GLY:H	1.28	0.96
1:B:717:MET:HE1	1:B:830:PRO:HD2	1.48	0.95
1:B:458:ILE:HD12	1:B:459:ALA:N	1.81	0.95
1:B:435:ILE:O	1:B:438:PRO:HD2	1.67	0.95
2:I:145:ARG:NH1	2:I:145:ARG:HB3	1.82	0.95
3:W:385:LEU:HD23	3:W:479:LYS:HE2	1.48	0.95
3:W:651:VAL:O	3:W:655:VAL:HG23	1.66	0.95
1:A:563:MET:HA	1:A:563:MET:CE	1.98	0.94
1:A:510:LEU:HD11	1:A:537:SER:HA	1.46	0.94
1:A:779:ASP:HA	1:A:798:ILE:CD1	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:HIS:O	1:B:447:TYR:HB2	1.68	0.93
2:O:27:VAL:O	2:O:31:ILE:HG12	1.66	0.93
1:B:764:PRO:O	1:B:765:PHE:HB3	1.65	0.93
1:B:518:PHE:HB3	1:B:519:PRO:HD2	1.49	0.93
1:B:790:ARG:HA	1:B:790:ARG:NE	1.84	0.92
1:A:428:GLN:HE21	1:A:455:PRO:HB2	1.30	0.92
2:G:145:ARG:HB3	2:G:145:ARG:NH1	1.84	0.92
1:B:126:PHE:HD2	1:B:126:PHE:H	1.09	0.92
3:W:8:LEU:HD12	3:W:737:MET:HG2	1.49	0.92
1:B:190:ASN:HD21	1:B:193:SER:HB3	1.31	0.92
1:B:722:ASN:HD22	1:B:824:LYS:HA	1.35	0.92
2:G:6:SER:OG	2:G:128:ASN:HA	1.70	0.92
1:A:779:ASP:HA	1:A:798:ILE:HD12	1.50	0.91
1:B:428:GLN:HB2	1:B:456:PHE:CD1	2.05	0.91
1:B:513:LEU:HA	1:B:516:GLN:NE2	1.85	0.91
1:B:803:ASN:H	1:B:807:ASN:HD21	1.17	0.91
1:B:166:PHE:HE2	1:B:689:MET:HA	1.34	0.91
1:A:661:GLN:HE21	1:B:348:LYS:NZ	1.67	0.91
1:B:454:THR:HG21	1:B:476:ASN:ND2	1.86	0.91
1:B:459:ALA:HB1	1:B:463:ILE:HD11	1.51	0.90
1:A:588:ILE:HG22	1:A:589:GLY:N	1.85	0.90
2:L:88:PHE:O	2:L:92:VAL:HG23	1.72	0.90
1:A:126:PHE:N	1:A:126:PHE:HD2	1.68	0.90
1:A:339:LEU:HD22	1:A:588:ILE:HA	1.53	0.90
2:L:106:ARG:H	2:L:106:ARG:HD3	1.37	0.90
2:N:145:ARG:O	2:N:146:GLN:HG3	1.71	0.90
2:C:88:PHE:O	2:C:92:VAL:HG23	1.72	0.89
1:B:509:ALA:O	1:B:513:LEU:HG	1.71	0.89
1:A:169:LEU:O	1:A:173:VAL:HG23	1.73	0.89
1:A:244:ILE:HD13	1:A:835:PHE:HE1	1.38	0.89
1:A:660:ASP:HB3	1:B:539:ARG:HH11	1.38	0.89
1:A:358:LEU:HD21	3:W:986:TYR:CE2	2.08	0.89
2:K:106:ARG:H	2:K:106:ARG:HD3	1.37	0.89
1:A:855:LEU:O	1:A:857:PHE:N	2.06	0.88
1:B:457:GLN:O	1:B:459:ALA:N	2.05	0.88
1:A:371:ASN:C	1:A:373:GLN:H	1.71	0.88
1:A:486:ASP:HB2	1:A:490:ASN:HD22	1.38	0.88
1:B:99:GLU:HB3	1:B:100:PRO:HD3	1.54	0.88
1:B:658:PRO:HB2	1:B:661:GLN:HG2	1.56	0.88
1:B:874:MET:O	1:B:875:ARG:HB2	1.73	0.88
2:M:88:PHE:O	2:M:92:VAL:HG23	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ARG:HH11	1:A:229:ARG:HG2	1.39	0.88
2:J:106:ARG:HD3	2:J:106:ARG:N	1.87	0.88
1:B:803:ASN:H	1:B:807:ASN:ND2	1.72	0.87
3:W:438:ILE:HG22	3:W:468:GLU:HB3	1.55	0.87
1:B:182:LEU:HD11	1:B:847:THR:H	1.38	0.87
1:B:297:ARG:HG3	1:B:848:PHE:HD2	1.40	0.87
1:A:428:GLN:HB2	1:A:456:PHE:CD1	2.09	0.86
1:A:509:ALA:O	1:A:513:LEU:HG	1.75	0.86
1:B:447:TYR:O	1:B:448:ARG:HG2	1.73	0.86
2:D:88:PHE:O	2:D:92:VAL:HG23	1.73	0.86
2:O:88:PHE:O	2:O:92:VAL:HG23	1.72	0.86
2:I:76:ASN:H	2:M:76:ASN:HB2	1.37	0.86
3:W:98:LEU:HD11	3:W:172:ILE:HG23	1.56	0.86
1:B:451:ASP:H	1:B:452:PRO:HD3	1.39	0.86
1:B:513:LEU:HA	1:B:516:GLN:CD	1.95	0.86
3:W:499:GLN:HG3	3:W:1086:PHE:HB2	1.55	0.86
1:B:413:VAL:HG12	1:B:414:VAL:N	1.88	0.86
2:N:88:PHE:O	2:N:92:VAL:HG23	1.74	0.86
1:B:473:HIS:HB2	2:I:126:ARG:NH2	1.91	0.86
1:B:745:ALA:HB1	1:B:748:THR:HB	1.57	0.86
2:H:88:PHE:O	2:H:92:VAL:HG23	1.73	0.86
2:I:24:TYR:O	2:I:27:VAL:HG22	1.74	0.86
1:B:540:LEU:O	1:B:544:VAL:HG23	1.75	0.86
1:B:182:LEU:HD23	1:B:183:LEU:H	1.40	0.86
1:A:275:PRO:HB2	1:A:278:ILE:CD1	2.04	0.86
1:A:150:LEU:HD12	1:A:696:SER:HB2	1.58	0.86
2:E:88:PHE:O	2:E:92:VAL:HG23	1.75	0.86
2:J:88:PHE:O	2:J:92:VAL:HG23	1.75	0.85
1:A:451:ASP:HB3	1:A:452:PRO:CD	2.03	0.85
2:I:88:PHE:O	2:I:92:VAL:HG23	1.76	0.85
1:B:590:ASN:HD22	1:B:590:ASN:N	1.74	0.85
1:B:366:PHE:C	1:B:368:THR:H	1.76	0.85
3:W:605:LEU:HB2	3:W:628:VAL:HG11	1.57	0.85
2:C:150:PHE:HB2	2:C:152:PHE:CE1	2.11	0.85
1:A:366:PHE:C	1:A:368:THR:H	1.76	0.85
2:F:88:PHE:O	2:F:92:VAL:HG23	1.75	0.85
2:M:106:ARG:H	2:M:106:ARG:HD3	1.40	0.85
1:B:126:PHE:HD2	1:B:126:PHE:N	1.73	0.85
2:G:88:PHE:O	2:G:92:VAL:HG23	1.75	0.85
2:H:6:SER:OG	2:H:128:ASN:HA	1.77	0.85
2:M:6:SER:OG	2:M:128:ASN:HA	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:VAL:HG22	1:A:846:LEU:HG	1.58	0.84
1:B:723:ILE:HG22	1:B:724:ALA:H	1.40	0.84
3:W:248:MET:HE3	3:W:248:MET:O	1.77	0.84
1:B:306:ASP:O	1:B:308:LEU:N	2.10	0.84
1:B:518:PHE:HD2	2:H:69:THR:HB	1.40	0.84
2:K:88:PHE:O	2:K:92:VAL:HG23	1.76	0.84
1:B:415:PRO:HG2	1:B:480:PHE:HD1	1.42	0.84
1:A:660:ASP:HB3	1:B:539:ARG:CD	2.05	0.84
1:B:701:GLN:HB2	1:B:826:TYR:HD2	1.40	0.84
1:B:825:VAL:HG12	1:B:826:TYR:N	1.91	0.84
2:L:144:ARG:O	2:L:145:ARG:HB2	1.74	0.84
1:A:125:ILE:HD12	1:A:125:ILE:N	1.92	0.84
1:A:570:THR:HG22	1:A:571:LEU:H	1.42	0.84
1:B:200:VAL:CG2	1:B:243:SER:HB3	2.05	0.84
1:B:735:LEU:HG	1:B:760:VAL:O	1.78	0.84
1:B:498:ARG:NH1	2:J:25:SER:HB3	1.92	0.84
1:B:471:TRP:HB2	1:B:512:GLN:OE1	1.77	0.84
1:A:126:PHE:CD2	1:A:126:PHE:N	2.42	0.84
1:B:503:ILE:HD11	1:B:548:ARG:HG2	1.58	0.84
2:F:82:ARG:NH1	2:H:144:ARG:HD2	1.93	0.84
2:I:76:ASN:HB2	2:M:76:ASN:HB2	1.57	0.84
1:A:771:VAL:HG13	1:A:772:ILE:H	1.43	0.84
1:A:361:GLN:HB2	1:A:528:SER:OG	1.78	0.83
1:B:428:GLN:HG2	1:B:429:LEU:N	1.92	0.83
1:B:435:ILE:HG22	1:B:436:ILE:N	1.93	0.83
2:L:23:LEU:HD21	2:N:36:GLN:OE1	1.76	0.83
3:W:296:ARG:NH2	3:W:308:GLN:HE21	1.75	0.83
3:W:248:MET:HG2	3:W:326:TYR:CD2	2.13	0.83
3:W:520:ASP:HB2	3:W:667:LYS:HE3	1.59	0.83
1:A:158:GLY:H	1:A:762:ALA:HB3	1.43	0.83
1:B:454:THR:HG21	1:B:476:ASN:HD21	1.39	0.83
2:I:23:LEU:HD23	2:I:24:TYR:N	1.94	0.83
3:W:254:LEU:HB3	3:W:314:ARG:HD2	1.58	0.83
3:W:4:TYR:HD1	3:W:733:LEU:HD22	1.41	0.83
1:A:216:GLU:CD	1:A:216:GLU:H	1.81	0.83
1:A:474:PHE:O	1:A:478:ASN:HB2	1.77	0.83
1:B:126:PHE:N	1:B:126:PHE:CD2	2.43	0.83
1:B:457:GLN:HB2	1:B:476:ASN:CG	1.98	0.83
1:B:799:LEU:HD22	1:B:800:TYR:N	1.93	0.83
1:A:471:TRP:HB2	1:A:512:GLN:OE1	1.79	0.83
1:A:524:ASP:O	1:A:526:LYS:N	2.10	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:LYS:HG3	1:A:654:VAL:HG21	1.59	0.83
3:W:539:ILE:HG23	3:W:562:LYS:HG3	1.61	0.82
3:W:750:LEU:HD21	3:W:861:LEU:HD22	1.60	0.82
2:O:6:SER:OG	2:O:128:ASN:HA	1.80	0.82
2:I:38:ILE:HG22	2:I:42:ASN:HD21	1.42	0.82
1:B:516:GLN:HA	1:B:518:PHE:HE1	1.41	0.82
1:B:590:ASN:H	1:B:590:ASN:HD22	1.25	0.82
1:A:461:GLN:HA	2:F:32:GLN:HE22	1.43	0.82
1:B:428:GLN:HA	1:B:431:ILE:HD12	1.61	0.82
2:F:150:PHE:HB2	2:F:152:PHE:CE1	2.15	0.82
1:A:486:ASP:HB2	1:A:490:ASN:ND2	1.94	0.81
1:A:734:ASN:HB3	1:A:737:GLU:HG2	1.61	0.81
1:B:722:ASN:HB2	1:B:824:LYS:HB3	1.62	0.81
2:H:109:ILE:HG13	2:H:109:ILE:O	1.79	0.81
1:B:454:THR:CG2	1:B:476:ASN:HD21	1.92	0.81
1:A:406:SER:O	1:A:409:TRP:HB3	1.81	0.81
2:L:22:THR:HB	2:N:128:ASN:O	1.79	0.81
3:W:367:ILE:O	3:W:371:VAL:HG23	1.80	0.81
1:B:494:ASN:ND2	1:B:495:ASP:H	1.79	0.81
1:B:769:SER:HB3	1:B:807:ASN:OD1	1.80	0.81
1:A:712:LEU:HB3	1:A:721:VAL:O	1.79	0.81
1:B:218:GLU:HG3	1:B:221:VAL:HG23	1.62	0.81
1:B:193:SER:HB2	1:B:226:ALA:HA	1.62	0.81
1:B:725:ARG:H	1:B:725:ARG:HD2	1.44	0.81
1:B:498:ARG:HB2	2:I:32:GLN:NE2	1.94	0.81
1:B:537:SER:O	1:B:540:LEU:HB3	1.81	0.81
2:H:76:ASN:HB2	2:J:76:ASN:HB2	1.60	0.81
1:B:511:MET:CE	2:J:70:LEU:HG	2.09	0.81
1:A:459:ALA:O	1:A:462:GLN:HB2	1.81	0.81
1:B:118:LYS:HG2	1:B:119:GLN:H	1.46	0.81
2:I:76:ASN:CB	2:M:76:ASN:HB2	2.11	0.81
1:A:712:LEU:HG	1:A:819:PRO:HB2	1.61	0.81
1:B:315:GLU:HB3	1:B:571:LEU:HD11	1.61	0.80
2:D:128:ASN:O	2:E:22:THR:HB	1.82	0.80
2:E:24:TYR:O	2:E:27:VAL:HG22	1.82	0.80
2:O:67:GLY:O	2:O:69:THR:N	2.14	0.80
3:W:906:ASN:HD22	3:W:907:VAL:H	1.26	0.80
1:A:660:ASP:O	1:A:662:MET:N	2.14	0.80
1:B:510:LEU:CD1	1:B:537:SER:HA	2.11	0.80
1:A:362:SER:HB2	1:A:365:GLN:NE2	1.97	0.80
1:A:699:ILE:HG12	1:A:700:ALA:N	1.97	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:150:PHE:HB2	2:L:152:PHE:CE1	2.17	0.80
1:A:546:LEU:HD21	1:A:588:ILE:CD1	2.12	0.80
1:A:126:PHE:H	1:A:126:PHE:HD2	1.26	0.80
1:A:270:ILE:CD1	1:A:292:LEU:HD11	2.10	0.80
1:B:239:VAL:HG23	1:B:844:SER:O	1.81	0.80
1:A:370:ILE:HD11	3:W:933:LEU:O	1.81	0.80
1:A:769:SER:HB3	1:A:807:ASN:OD1	1.82	0.80
2:N:144:ARG:O	2:N:145:ARG:HB2	1.81	0.80
1:B:869:VAL:CG1	1:B:873:ASN:HA	2.11	0.80
3:W:78:SER:O	3:W:747:SER:HB2	1.81	0.80
1:A:437:TYR:N	1:A:438:PRO:HD2	1.97	0.79
1:B:393:SER:O	1:B:394:LEU:HD23	1.82	0.79
1:B:506:LEU:HD23	1:B:544:VAL:HA	1.62	0.79
1:B:743:ASP:CG	1:B:745:ALA:H	1.85	0.79
1:A:199:VAL:HG12	1:A:200:VAL:N	1.97	0.79
1:A:303:LEU:HA	1:A:615:ASN:ND2	1.97	0.79
1:A:694:ARG:HG2	1:A:701:GLN:HE22	1.46	0.79
1:B:790:ARG:HG3	1:B:791:LYS:H	1.48	0.79
2:L:104:SER:O	2:L:108:GLY:HA3	1.82	0.79
1:A:869:VAL:HG11	1:A:873:ASN:HA	1.64	0.79
2:I:57:ARG:HH11	2:I:94:ASN:HD21	1.31	0.79
1:B:744:TYR:CD2	1:B:744:TYR:N	2.38	0.79
1:A:721:VAL:HG12	1:A:722:ASN:N	1.98	0.79
2:K:6:SER:OG	2:K:128:ASN:HA	1.82	0.79
3:W:836:LYS:HA	3:W:839:LEU:HD12	1.64	0.79
1:B:457:GLN:HG3	1:B:458:ILE:N	1.98	0.79
1:B:465:ASN:HD22	1:B:468:VAL:HG23	1.47	0.79
1:A:370:ILE:HG13	3:W:933:LEU:CD1	2.13	0.79
1:A:480:PHE:CD2	1:A:493:LEU:HB3	2.18	0.79
1:A:606:VAL:HG23	1:A:607:ASN:H	1.46	0.79
1:B:673:PRO:O	1:B:674:VAL:HG13	1.83	0.79
2:H:2:ASP:HB2	2:H:128:ASN:HD21	1.46	0.79
3:W:1018:ILE:HD12	3:W:1037:ALA:HB1	1.65	0.79
1:B:124:ARG:C	1:B:125:ILE:HD12	2.02	0.79
2:N:50:GLY:O	2:N:51:ILE:HG23	1.83	0.79
1:A:869:VAL:CG1	1:A:873:ASN:HA	2.12	0.79
1:B:277:ARG:O	1:B:278:ILE:HG12	1.83	0.79
3:W:843:ALA:HB3	3:W:844:PRO:HD3	1.64	0.79
1:B:272:ASN:C	1:B:274:ILE:H	1.87	0.78
1:B:743:ASP:C	1:B:744:TYR:CD2	2.54	0.78
1:B:548:ARG:HH11	1:B:878:ASN:H	1.28	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:128:ASN:O	2:K:22:THR:HB	1.83	0.78
1:A:445:MET:C	1:A:447:TYR:H	1.84	0.78
1:B:75:VAL:HG22	3:W:673:VAL:HG12	0.83	0.78
2:M:145:ARG:O	2:M:146:GLN:HG3	1.83	0.78
3:W:296:ARG:HH22	3:W:308:GLN:HE21	1.29	0.78
1:A:305:GLN:O	1:A:307:ARG:HG3	1.82	0.78
1:A:428:GLN:HG2	1:A:429:LEU:N	1.98	0.78
1:B:523:VAL:C	1:B:525:TYR:H	1.85	0.78
1:A:118:LYS:HG2	1:A:119:GLN:N	1.98	0.78
1:A:480:PHE:HD2	1:A:493:LEU:HB3	1.49	0.78
1:B:549:LEU:HD13	1:B:877:MET:HE1	1.64	0.78
1:B:606:VAL:HG23	1:B:607:ASN:H	1.46	0.78
1:A:639:LYS:O	1:A:643:GLU:HG3	1.84	0.78
3:W:1001:TYR:HD1	3:W:1084:ASN:HB3	1.49	0.78
2:I:42:ASN:HA	2:I:61:PHE:HB2	1.66	0.78
1:B:702:GLY:HA3	1:B:759:LEU:O	1.84	0.77
1:B:717:MET:CE	1:B:830:PRO:HD2	2.15	0.77
2:N:144:ARG:NH2	2:N:146:GLN:HE22	1.81	0.77
3:W:212:GLU:HB2	3:W:696:LEU:HD12	1.65	0.77
1:B:374:ALA:HB1	1:B:580:SER:HB3	1.66	0.77
1:B:562:THR:HB	1:B:611:HIS:CD2	2.20	0.77
1:B:779:ASP:HA	1:B:798:ILE:CD1	2.14	0.77
3:W:186:ASN:HD22	3:W:186:ASN:H	1.32	0.77
1:B:406:SER:O	1:B:409:TRP:HB3	1.84	0.77
2:E:93:ASP:O	2:E:97:MET:HG3	1.84	0.77
2:H:106:ARG:CD	2:H:106:ARG:H	1.98	0.77
2:I:128:ASN:HD22	2:J:19:VAL:HB	1.49	0.77
2:K:93:ASP:O	2:K:97:MET:HG3	1.85	0.77
2:M:22:THR:HG23	2:M:73:LEU:HD12	1.66	0.77
1:B:764:PRO:O	1:B:765:PHE:CB	2.33	0.77
3:W:704:SER:HB2	3:W:709:GLN:HE22	1.47	0.77
1:A:471:TRP:O	1:A:475:VAL:HG23	1.85	0.77
1:B:169:LEU:O	1:B:173:VAL:HG23	1.84	0.77
1:B:855:LEU:O	1:B:857:PHE:N	2.17	0.77
1:B:204:THR:CG2	1:B:244:ILE:HG22	2.14	0.77
2:H:93:ASP:O	2:H:97:MET:HG3	1.85	0.77
1:A:371:ASN:C	1:A:373:GLN:N	2.37	0.76
1:B:218:GLU:HG3	1:B:221:VAL:CG2	2.15	0.76
1:B:503:ILE:O	1:B:505:GLN:HG2	1.85	0.76
1:B:573:THR:O	1:B:574:GLU:HG2	1.84	0.76
1:B:166:PHE:CE2	1:B:689:MET:HA	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:744:TYR:HD2	1:B:744:TYR:N	1.77	0.76
2:F:17:LYS:HG2	2:H:130:ASP:HA	1.67	0.76
3:W:217:VAL:HG13	3:W:222:ASP:HB2	1.66	0.76
1:A:405:ILE:HG21	1:A:536:LEU:HG	1.67	0.76
1:A:614:TYR:O	1:A:618:ILE:HG12	1.85	0.76
1:B:200:VAL:HG23	1:B:242:PRO:O	1.86	0.76
1:B:731:GLN:HG2	2:D:62:ASP:HB2	1.67	0.76
1:A:548:ARG:HH12	1:A:878:ASN:H	1.34	0.76
1:A:122:LEU:HG	1:A:201:ASP:OD2	1.84	0.76
1:A:461:GLN:HA	2:F:32:GLN:NE2	2.00	0.76
1:A:588:ILE:CG2	1:A:589:GLY:H	1.99	0.76
1:B:133:ILE:HD12	1:B:145:ARG:HB2	1.66	0.76
1:B:678:ARG:O	1:B:681:ILE:HG22	1.85	0.76
2:C:24:TYR:O	2:C:27:VAL:HG22	1.86	0.76
2:D:67:GLY:O	2:D:68:THR:HG23	1.85	0.76
2:I:110:ALA:HB1	2:I:111:PRO:CD	2.16	0.76
1:A:678:ARG:O	1:A:681:ILE:HG22	1.86	0.76
1:A:158:GLY:H	1:A:762:ALA:CB	1.99	0.76
1:B:199:VAL:HG12	1:B:200:VAL:N	2.00	0.76
1:B:701:GLN:HA	1:B:761:GLY:O	1.85	0.76
2:G:93:ASP:O	2:G:97:MET:HG3	1.85	0.76
1:A:503:ILE:HD13	1:A:547:THR:HB	1.68	0.76
1:B:675:GLU:HB3	1:B:678:ARG:HG2	1.68	0.76
1:A:244:ILE:HD13	1:A:835:PHE:CE1	2.21	0.76
1:A:428:GLN:HA	1:A:431:ILE:HD12	1.68	0.76
1:B:96:PRO:O	1:B:652:PHE:HB3	1.84	0.76
2:I:93:ASP:O	2:I:97:MET:HG3	1.86	0.76
1:B:361:GLN:HE22	3:W:624:LYS:NZ	1.84	0.76
1:A:310:LEU:CD1	1:A:310:LEU:H	1.97	0.75
1:B:518:PHE:CB	1:B:519:PRO:HD2	2.14	0.75
2:C:145:ARG:HB3	2:C:145:ARG:NH1	2.02	0.75
2:F:104:SER:HB3	2:F:108:GLY:CA	2.16	0.75
1:B:781:THR:O	1:B:783:PHE:N	2.19	0.75
1:A:371:ASN:HA	1:A:374:ALA:HB3	1.68	0.75
1:A:457:GLN:HB2	1:A:476:ASN:HD21	1.52	0.75
2:L:19:VAL:HG23	2:N:128:ASN:HB3	1.69	0.75
2:J:93:ASP:O	2:J:97:MET:HG3	1.87	0.75
1:B:251:ALA:HA	2:N:69:THR:HG21	1.69	0.75
1:B:498:ARG:CB	2:I:32:GLN:HE22	1.97	0.75
1:A:694:ARG:HG2	1:A:701:GLN:NE2	2.01	0.74
2:C:38:ILE:HG22	2:C:42:ASN:HD21	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:520:ASP:HB3	3:W:667:LYS:HB3	1.69	0.74
1:B:698:LYS:O	1:B:699:ILE:HB	1.86	0.74
2:I:76:ASN:HB2	2:M:76:ASN:CB	2.17	0.74
1:A:148:TRP:CZ3	1:A:246:HIS:HB2	2.22	0.74
1:A:537:SER:O	1:A:540:LEU:HB3	1.87	0.74
1:B:491:GLN:HG3	1:B:565:MET:H	1.50	0.74
2:J:128:ASN:HB3	2:K:19:VAL:HG23	1.69	0.74
2:N:57:ARG:HH11	2:N:94:ASN:HD21	1.33	0.74
3:W:708:ASP:HB3	3:W:1080:TYR:CE1	2.21	0.74
3:W:820:LEU:HB3	3:W:824:ASN:HD22	1.51	0.74
1:A:492:VAL:HG13	1:A:558:MET:SD	2.27	0.74
1:A:647:LYS:CG	1:A:654:VAL:HG21	2.17	0.74
1:B:482:GLN:HB2	1:B:493:LEU:HD22	1.70	0.74
1:B:675:GLU:HB3	1:B:678:ARG:CG	2.17	0.74
1:B:688:ASN:O	1:B:692:ILE:HD12	1.87	0.74
3:W:825:ASN:HA	3:W:828:SER:HB2	1.69	0.74
1:B:614:TYR:O	1:B:618:ILE:HG12	1.87	0.74
2:O:150:PHE:HB2	2:O:152:PHE:CE1	2.23	0.74
3:W:165:ARG:HD3	3:W:223:TYR:HB2	1.68	0.74
1:B:293:PRO:C	1:B:295:THR:H	1.90	0.74
2:D:23:LEU:HD23	2:D:24:TYR:N	2.03	0.74
2:D:93:ASP:O	2:D:97:MET:HG3	1.87	0.74
2:L:93:ASP:O	2:L:97:MET:HG3	1.88	0.74
2:I:75:ALA:HB3	2:M:76:ASN:HA	1.68	0.74
1:A:286:LEU:HD23	1:A:286:LEU:H	1.52	0.74
1:A:784:ALA:O	1:A:787:VAL:HG23	1.88	0.74
1:A:802:ILE:HA	1:A:807:ASN:HD21	1.52	0.74
1:B:190:ASN:ND2	1:B:193:SER:HB3	2.03	0.74
1:B:783:PHE:HD1	1:B:783:PHE:H	1.33	0.74
2:C:82:ARG:CZ	2:E:144:ARG:HD2	2.18	0.74
2:D:24:TYR:O	2:D:27:VAL:HG22	1.88	0.74
2:H:105:GLN:C	2:H:107:ASN:H	1.91	0.74
1:A:405:ILE:CG2	1:A:536:LEU:HG	2.18	0.74
1:A:428:GLN:HB2	1:A:456:PHE:HD1	1.51	0.74
2:E:54:LEU:HD12	2:E:55:PRO:HD2	1.70	0.74
1:A:164:GLU:O	1:A:167:LEU:HB3	1.87	0.74
1:A:301:PRO:O	1:A:303:LEU:HD23	1.87	0.74
1:A:252:PHE:HD2	1:A:684:LEU:HD21	1.52	0.74
1:B:510:LEU:HD11	1:B:537:SER:CA	2.15	0.74
2:D:6:SER:OG	2:D:128:ASN:HA	1.87	0.74
1:B:368:THR:HG22	1:B:371:ASN:HD21	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:ASN:ND2	1:B:446:HIS:HB3	2.02	0.73
2:J:150:PHE:HB2	2:J:152:PHE:CE1	2.22	0.73
3:W:473:GLN:OE1	3:W:595:GLN:HG2	1.88	0.73
1:A:117:LYS:O	1:A:179:ASP:HB2	1.88	0.73
1:A:275:PRO:CB	1:A:278:ILE:HD11	2.18	0.73
2:G:106:ARG:H	2:G:106:ARG:HD3	1.53	0.73
1:B:254:GLU:HG2	2:N:69:THR:HB	1.68	0.73
1:A:711:GLN:C	1:A:712:LEU:HD23	2.08	0.73
2:M:144:ARG:HD2	2:N:82:ARG:NH1	2.02	0.73
1:A:277:ARG:HD3	1:A:559:ALA:HB2	1.71	0.73
1:B:257:LEU:O	1:B:260:GLN:HG3	1.88	0.73
1:A:660:ASP:CB	1:B:539:ARG:HD2	2.19	0.73
2:C:93:ASP:O	2:C:97:MET:HG3	1.87	0.73
2:F:42:ASN:HA	2:F:61:PHE:HB2	1.70	0.73
2:H:109:ILE:HB	2:H:380:ASP:HB3	1.68	0.73
1:A:310:LEU:HD12	1:A:310:LEU:N	2.00	0.73
1:B:457:GLN:C	1:B:459:ALA:H	1.91	0.73
1:B:540:LEU:HD23	1:B:541:GLY:N	2.03	0.73
2:N:93:ASP:O	2:N:97:MET:HG3	1.87	0.73
3:W:708:ASP:O	3:W:712:ILE:HG13	1.88	0.73
1:A:499:ASN:HA	1:A:505:GLN:NE2	2.04	0.73
1:B:111:ILE:C	1:B:113:PRO:HD3	2.09	0.73
1:B:265:LEU:HB3	1:B:296:ALA:CB	2.17	0.73
2:I:145:ARG:HH11	2:I:145:ARG:HB3	1.50	0.73
2:N:24:TYR:O	2:N:27:VAL:HG22	1.89	0.73
1:A:245:LEU:HB3	1:A:249:ASP:HB2	1.71	0.73
1:A:286:LEU:HD23	1:A:286:LEU:N	2.04	0.73
1:B:703:VAL:HG13	1:B:824:LYS:O	1.89	0.73
2:F:93:ASP:O	2:F:97:MET:HG3	1.87	0.73
2:M:93:ASP:O	2:M:97:MET:HG3	1.88	0.73
3:W:906:ASN:HD22	3:W:907:VAL:N	1.85	0.73
1:A:631:LEU:HB3	1:A:633:LEU:HD13	1.69	0.73
1:A:661:GLN:HE21	1:B:348:LYS:HZ1	1.37	0.73
1:B:491:GLN:CD	1:B:564:ASN:HB3	2.08	0.73
1:B:503:ILE:O	1:B:505:GLN:N	2.22	0.73
1:B:674:VAL:HG23	1:B:679:LEU:HD22	1.69	0.73
1:B:771:VAL:HB	1:B:809:PHE:CB	2.11	0.73
1:B:770:SER:HB2	1:B:773:SER:OG	1.88	0.73
2:F:145:ARG:O	2:F:146:GLN:HG2	1.89	0.73
2:J:11:LEU:O	2:J:14:ALA:HB3	1.89	0.73
1:B:277:ARG:O	1:B:279:ARG:N	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:701:GLN:O	1:B:826:TYR:HB3	1.89	0.73
2:D:63:PHE:CD2	2:D:84:THR:HG23	2.24	0.73
2:F:23:LEU:HD21	2:H:36:GLN:OE1	1.89	0.73
2:H:27:VAL:O	2:H:31:ILE:HG12	1.88	0.73
1:B:436:ILE:HG13	1:B:437:TYR:H	1.54	0.72
1:B:471:TRP:O	1:B:475:VAL:HG23	1.88	0.72
2:H:106:ARG:N	2:H:106:ARG:HD3	2.03	0.72
1:A:643:GLU:HG2	1:A:662:MET:HE3	1.72	0.72
1:B:442:MET:CE	1:B:463:ILE:HG12	2.19	0.72
1:B:498:ARG:HH12	2:J:25:SER:HB3	1.52	0.72
1:B:521:MET:HB2	1:B:522:PRO:CD	2.19	0.72
1:B:712:LEU:CD1	1:B:722:ASN:HB3	2.18	0.72
3:W:394:LEU:HD21	3:W:424:VAL:HG11	1.69	0.72
3:W:473:GLN:HG2	3:W:561:TYR:CE1	2.23	0.72
1:A:510:LEU:CD1	1:A:537:SER:HA	2.20	0.72
1:A:370:ILE:HG13	3:W:933:LEU:HD12	1.71	0.72
1:B:435:ILE:C	1:B:436:ILE:HG12	2.08	0.72
1:B:492:VAL:HG11	1:B:558:MET:HG2	1.71	0.72
1:B:516:GLN:HA	1:B:518:PHE:CE1	2.25	0.72
1:B:630:ARG:O	1:B:631:LEU:HG	1.90	0.72
1:B:799:LEU:HD22	1:B:800:TYR:H	1.52	0.72
2:J:106:ARG:HG2	2:J:107:ASN:H	1.54	0.72
3:W:627:ARG:HH11	3:W:627:ARG:HG2	1.54	0.72
1:A:420:ILE:HG12	1:A:423:SER:HB2	1.69	0.72
1:A:496:ASN:HD22	1:A:498:ARG:HB2	1.53	0.72
1:A:629:ASN:O	1:A:631:LEU:N	2.17	0.72
1:B:615:ASN:O	1:B:618:ILE:HB	1.90	0.72
2:J:144:ARG:HD2	2:K:82:ARG:NH1	2.05	0.72
2:M:122:LEU:HB2	2:O:83:ASN:ND2	2.04	0.72
2:F:22:THR:HB	2:H:128:ASN:O	1.89	0.72
1:B:156:PRO:HB2	1:B:161:ASP:HB3	1.72	0.72
1:B:444:ARG:NH2	1:B:520:THR:HG23	2.03	0.72
3:W:370:GLU:O	3:W:374:MET:HG3	1.88	0.72
1:A:613:ASN:HD22	1:A:649:LEU:CD2	2.03	0.72
1:A:239:VAL:CG2	1:A:846:LEU:HG	2.19	0.72
1:A:605:ASN:O	1:A:608:VAL:HB	1.90	0.72
3:W:430:ASN:HB3	3:W:432:ARG:HG3	1.71	0.72
3:W:447:ILE:HD12	3:W:447:ILE:N	2.05	0.72
3:W:331:HIS:NE2	3:W:692:GLY:HA2	2.05	0.72
1:A:721:VAL:CG1	1:A:722:ASN:H	2.01	0.72
1:A:146:TRP:O	1:A:833:PHE:HB3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:ALA:O	1:B:555:GLU:HB2	1.90	0.72
1:B:825:VAL:HG12	1:B:826:TYR:H	1.53	0.72
2:D:145:ARG:O	2:D:146:GLN:HG3	1.90	0.72
2:I:135:TYR:OH	2:I:340:GLU:OE1	2.06	0.72
1:A:445:MET:O	1:A:447:TYR:N	2.23	0.71
1:B:355:LEU:HG	1:B:356:GLU:N	2.05	0.71
2:D:11:LEU:O	2:D:14:ALA:HB3	1.90	0.71
1:B:473:HIS:HB3	2:I:126:ARG:HH12	1.54	0.71
3:W:101:ASP:O	3:W:104:VAL:HG23	1.90	0.71
1:A:735:LEU:HG	1:A:760:VAL:O	1.89	0.71
1:A:764:PRO:O	1:A:797:PRO:HD2	1.91	0.71
1:B:422:GLU:HA	1:B:425:VAL:HG23	1.72	0.71
1:B:442:MET:HE1	1:B:463:ILE:HG12	1.71	0.71
1:B:480:PHE:CE2	1:B:493:LEU:HB2	2.24	0.71
2:J:130:ASP:HA	2:K:17:LYS:HG2	1.71	0.71
2:O:93:ASP:O	2:O:97:MET:HG3	1.90	0.71
1:B:156:PRO:CB	1:B:161:ASP:HB3	2.20	0.71
2:C:144:ARG:HD2	2:D:82:ARG:CZ	2.20	0.71
2:L:6:SER:OG	2:L:128:ASN:HA	1.91	0.71
1:A:246:HIS:HB3	1:A:249:ASP:OD2	1.90	0.71
1:A:709:ASP:HB3	1:A:820:THR:HG23	1.73	0.71
1:B:194:ARG:O	1:B:196:ALA:N	2.23	0.71
1:B:428:GLN:OE1	1:B:456:PHE:HB2	1.90	0.71
2:I:11:LEU:O	2:I:14:ALA:HB3	1.91	0.71
2:I:150:PHE:HB2	2:I:152:PHE:CE1	2.25	0.71
3:W:22:VAL:HG22	3:W:77:TYR:HB3	1.72	0.71
3:W:293:ASP:HA	3:W:296:ARG:HD2	1.72	0.71
1:A:236:ARG:HB2	1:A:238:VAL:HG23	1.72	0.71
1:B:166:PHE:CE2	1:B:689:MET:HG3	2.24	0.71
1:B:791:LYS:O	1:B:792:VAL:HG22	1.91	0.71
2:K:11:LEU:O	2:K:14:ALA:HB3	1.91	0.71
1:A:530:GLN:HA	1:A:533:ILE:HD12	1.71	0.71
1:B:605:ASN:O	1:B:608:VAL:HB	1.91	0.71
2:K:38:ILE:HG22	2:K:42:ASN:HD21	1.56	0.71
1:A:194:ARG:NH1	1:A:229:ARG:HG2	2.05	0.71
2:N:11:LEU:O	2:N:14:ALA:HB3	1.91	0.71
2:N:38:ILE:HG22	2:N:42:ASN:HD21	1.56	0.71
1:B:277:ARG:HG2	1:B:278:ILE:H	1.54	0.71
2:H:116:LEU:HD12	2:H:119:LEU:HB2	1.73	0.71
2:O:11:LEU:O	2:O:14:ALA:HB3	1.90	0.71
1:A:283:ASN:O	1:A:863:VAL:HG23	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:36:GLN:OE1	2:H:23:LEU:HD21	1.91	0.71
1:A:496:ASN:ND2	1:A:498:ARG:HB2	2.06	0.71
1:A:510:LEU:HD11	1:A:537:SER:CA	2.21	0.71
1:B:712:LEU:HD12	1:B:722:ASN:HB3	1.72	0.71
1:B:548:ARG:HH12	1:B:878:ASN:H	1.35	0.71
2:G:4:LEU:HA	2:G:7:LEU:HD12	1.73	0.71
2:K:53:ASN:HD22	2:K:354:ALA:HB3	1.56	0.71
2:M:11:LEU:O	2:M:14:ALA:HB3	1.91	0.71
1:A:102:GLU:O	3:W:555:LEU:HD11	1.90	0.70
1:A:312:ASP:O	1:A:313:ASN:HB3	1.90	0.70
1:A:415:PRO:HG2	1:A:480:PHE:CD1	2.26	0.70
1:A:501:HIS:C	1:A:503:ILE:HG13	2.11	0.70
1:B:374:ALA:HB1	1:B:580:SER:HA	1.71	0.70
2:L:82:ARG:CZ	2:N:144:ARG:HD2	2.21	0.70
3:W:340:LEU:O	3:W:340:LEU:HD12	1.90	0.70
1:B:164:GLU:O	1:B:167:LEU:HB3	1.90	0.70
2:D:4:LEU:HA	2:D:7:LEU:HD12	1.73	0.70
2:M:150:PHE:HB2	2:M:152:PHE:CE1	2.26	0.70
1:A:615:ASN:O	1:A:618:ILE:HB	1.89	0.70
1:B:518:PHE:CD2	2:H:69:THR:HB	2.24	0.70
1:B:477:ASN:ND2	2:I:39:ILE:HG21	2.06	0.70
2:J:106:ARG:H	2:J:106:ARG:CD	2.03	0.70
2:J:109:ILE:HD12	2:J:109:ILE:O	1.91	0.70
1:B:259:HIS:CD2	1:B:677:ARG:HG3	2.25	0.70
2:C:11:LEU:O	2:C:14:ALA:HB3	1.90	0.70
2:J:12:LYS:C	2:J:14:ALA:H	1.94	0.70
1:B:511:MET:HE1	2:J:70:LEU:HG	1.72	0.70
2:K:54:LEU:HD12	2:K:55:PRO:HD2	1.71	0.70
2:N:4:LEU:HA	2:N:7:LEU:HD12	1.73	0.70
1:A:506:LEU:CD2	1:A:544:VAL:HA	2.18	0.70
1:A:551:ALA:O	1:A:555:GLU:HB2	1.92	0.70
1:B:230:GLN:HA	1:B:242:PRO:HD3	1.73	0.70
1:A:131:LEU:HD12	1:A:132:PRO:HD2	1.74	0.70
1:A:467:GLN:HB2	1:A:515:ARG:HD2	1.72	0.70
1:A:762:ALA:O	1:A:763:LEU:HG	1.92	0.70
1:B:508:GLU:HG2	1:B:512:GLN:NE2	2.07	0.70
1:B:790:ARG:HG3	1:B:791:LYS:N	2.05	0.70
2:J:116:LEU:HD12	2:J:119:LEU:HB2	1.74	0.70
2:N:167:ASN:HD22	2:N:178:GLY:HA2	1.57	0.70
1:A:783:PHE:H	1:A:783:PHE:HD1	1.38	0.70
2:C:167:ASN:HD22	2:C:178:GLY:HA2	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:153:HIS:NE2	2:E:153:HIS:NE2	2.39	0.70
2:G:167:ASN:HD22	2:G:178:GLY:HA2	1.57	0.70
1:A:482:GLN:OE1	1:A:493:LEU:HD22	1.90	0.70
1:A:560:CYS:HB2	1:A:603:TYR:HD2	1.57	0.70
1:B:262:VAL:CG1	1:B:297:ARG:HB3	2.21	0.70
1:B:786:ILE:HG13	1:B:787:VAL:H	1.56	0.70
2:I:12:LYS:C	2:I:14:ALA:H	1.95	0.70
2:K:167:ASN:HD22	2:K:178:GLY:HA2	1.57	0.70
2:O:154:LYS:N	2:O:155:PRO:CD	2.54	0.70
1:B:393:SER:N	1:B:573:THR:HG23	2.06	0.70
1:B:857:PHE:HD1	1:B:857:PHE:H	1.40	0.70
2:C:4:LEU:HA	2:C:7:LEU:HD12	1.74	0.70
2:J:167:ASN:HD22	2:J:178:GLY:HA2	1.57	0.70
2:J:38:ILE:HG22	2:J:42:ASN:HD21	1.56	0.70
2:O:167:ASN:HD22	2:O:178:GLY:HA2	1.57	0.70
1:A:396:PHE:HB3	1:A:578:LEU:CD1	2.22	0.70
1:A:401:TYR:HA	1:A:404:LEU:HD13	1.73	0.70
1:A:436:ILE:HD11	1:A:437:TYR:CD1	2.27	0.70
1:B:721:VAL:CG1	1:B:799:LEU:HD21	2.22	0.70
2:C:6:SER:OG	2:C:128:ASN:HA	1.92	0.70
2:E:38:ILE:HG22	2:E:42:ASN:HD21	1.57	0.70
3:W:999:ILE:HD11	3:W:1009:PHE:CD1	2.27	0.70
1:A:781:THR:O	1:A:783:PHE:N	2.24	0.69
1:B:318:TRP:CA	1:B:321:ILE:HD12	2.19	0.69
1:B:670:ARG:O	1:B:671:LEU:HD23	1.92	0.69
1:B:791:LYS:O	1:B:792:VAL:HG13	1.91	0.69
2:D:239:ASN:HD22	2:D:246:THR:HG22	1.57	0.69
2:O:4:LEU:HA	2:O:7:LEU:HD12	1.74	0.69
1:B:590:ASN:H	1:B:590:ASN:ND2	1.90	0.69
2:C:22:THR:OG1	2:C:26:ASN:ND2	2.25	0.69
2:F:104:SER:HB3	2:F:108:GLY:HA2	1.74	0.69
2:O:106:ARG:HD3	2:O:106:ARG:H	1.56	0.69
3:W:434:THR:HG21	3:W:437:ILE:HD12	1.74	0.69
1:A:437:TYR:H	1:A:438:PRO:HD2	1.56	0.69
1:A:548:ARG:HH11	1:A:877:MET:HA	1.56	0.69
1:B:182:LEU:HD11	1:B:847:THR:N	2.07	0.69
2:C:239:ASN:HD22	2:C:246:THR:HG22	1.58	0.69
2:D:150:PHE:HB2	2:D:152:PHE:CE1	2.27	0.69
2:K:150:PHE:HB2	2:K:152:PHE:CE1	2.27	0.69
2:L:11:LEU:O	2:L:14:ALA:HB3	1.93	0.69
2:L:239:ASN:HD22	2:L:246:THR:HG22	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:106:ARG:N	2:N:106:ARG:HD3	2.01	0.69
3:W:248:MET:HA	3:W:251:LEU:HD12	1.73	0.69
1:A:275:PRO:HB2	1:A:278:ILE:CG1	2.22	0.69
1:A:306:ASP:C	1:A:308:LEU:H	1.95	0.69
2:F:110:ALA:HB1	2:F:111:PRO:CD	2.22	0.69
2:H:12:LYS:C	2:H:14:ALA:H	1.95	0.69
2:I:109:ILE:HD12	2:I:109:ILE:O	1.90	0.69
2:I:167:ASN:HD22	2:I:178:GLY:HA2	1.57	0.69
2:J:22:THR:O	2:J:72:ASN:HA	1.92	0.69
3:W:840:ASN:HA	3:W:845:ILE:CG2	2.23	0.69
2:E:11:LEU:O	2:E:14:ALA:HB3	1.91	0.69
2:G:11:LEU:O	2:G:14:ALA:HB3	1.92	0.69
2:M:167:ASN:HD22	2:M:178:GLY:HA2	1.57	0.69
1:B:366:PHE:C	1:B:368:THR:N	2.46	0.69
1:B:374:ALA:HB1	1:B:580:SER:CB	2.23	0.69
1:A:634:TYR:HB2	1:B:875:ARG:HH22	1.57	0.69
2:E:5:TYR:CE2	2:E:131:ASN:HA	2.27	0.69
2:F:167:ASN:HD22	2:F:178:GLY:HA2	1.57	0.69
2:N:116:LEU:HD12	2:N:119:LEU:HB2	1.74	0.69
3:W:535:ARG:CZ	3:W:568:LEU:HD13	2.22	0.69
1:A:540:LEU:HD23	1:A:541:GLY:N	2.08	0.69
1:A:588:ILE:CG2	1:A:589:GLY:N	2.56	0.69
1:A:666:ARG:CG	1:A:667:ASP:N	2.55	0.69
1:A:803:ASN:HD22	1:A:805:ASP:HB3	1.58	0.69
1:B:772:ILE:HG23	1:B:773:SER:N	2.06	0.69
3:W:519:THR:HG22	3:W:520:ASP:N	2.08	0.69
1:A:664:ARG:HD3	1:B:538:ASN:OD1	1.92	0.69
1:B:368:THR:HA	1:B:579:THR:HG23	1.75	0.69
1:B:563:MET:HA	1:B:563:MET:HE3	1.73	0.69
1:B:783:PHE:N	1:B:783:PHE:CD1	2.60	0.69
2:D:106:ARG:H	2:D:106:ARG:HD3	1.58	0.69
1:A:322:THR:HG22	1:A:390:ARG:HB2	1.75	0.69
1:A:451:ASP:CB	1:A:452:PRO:CD	2.68	0.69
1:A:689:MET:HA	1:A:692:ILE:HD13	1.73	0.69
2:E:109:ILE:HB	2:E:380:ASP:HB3	1.74	0.69
2:E:150:PHE:HB2	2:E:152:PHE:CE1	2.27	0.69
1:A:118:LYS:HG2	1:A:119:GLN:H	1.57	0.69
1:A:546:LEU:HD21	1:A:588:ILE:HD13	1.73	0.69
1:A:757:VAL:HG12	1:A:758:ALA:H	1.57	0.69
1:B:118:LYS:HG2	1:B:119:GLN:N	2.08	0.69
1:B:594:ILE:HD12	1:B:594:ILE:C	2.13	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:752:LEU:C	1:B:754:ASN:H	1.95	0.69
1:B:812:VAL:HG13	1:B:813:ALA:H	1.57	0.69
2:E:116:LEU:HD12	2:E:119:LEU:HB2	1.73	0.69
2:F:11:LEU:O	2:F:14:ALA:HB3	1.93	0.69
2:G:12:LYS:C	2:G:14:ALA:H	1.96	0.69
1:A:100:PRO:HB2	3:W:558:LEU:HD11	1.75	0.69
1:B:457:GLN:CG	1:B:458:ILE:H	1.89	0.69
1:B:633:LEU:O	1:B:633:LEU:HD23	1.92	0.69
2:H:239:ASN:HD22	2:H:246:THR:HG22	1.58	0.69
2:I:6:SER:OG	2:I:128:ASN:HA	1.92	0.69
2:K:106:ARG:HG2	2:K:107:ASN:H	1.56	0.69
2:K:144:ARG:O	2:K:145:ARG:HB2	1.92	0.69
2:L:167:ASN:HD22	2:L:178:GLY:HA2	1.57	0.69
2:M:116:LEU:HD12	2:M:119:LEU:HB2	1.75	0.69
2:M:12:LYS:C	2:M:14:ALA:H	1.96	0.69
2:O:109:ILE:O	2:O:109:ILE:HD12	1.92	0.69
3:W:105:ASN:ND2	3:W:111:ASN:HA	2.08	0.69
3:W:147:PHE:HE1	3:W:151:LYS:HE3	1.58	0.69
3:W:535:ARG:NH2	3:W:568:LEU:HD13	2.07	0.69
1:B:364:THR:CG2	3:W:622:ALA:HA	2.22	0.69
1:A:306:ASP:O	1:A:308:LEU:N	2.25	0.68
1:A:570:THR:HG22	1:A:571:LEU:N	2.07	0.68
1:B:166:PHE:O	1:B:169:LEU:HB2	1.93	0.68
1:A:658:PRO:HG3	1:B:345:GLN:HA	1.75	0.68
1:B:805:ASP:O	1:B:807:ASN:N	2.26	0.68
2:E:12:LYS:C	2:E:14:ALA:H	1.96	0.68
1:A:366:PHE:CD1	1:A:366:PHE:N	2.60	0.68
1:A:807:ASN:O	1:A:809:PHE:N	2.26	0.68
1:B:264:PRO:O	1:B:265:LEU:HB2	1.92	0.68
1:A:661:GLN:NE2	1:B:348:LYS:NZ	2.39	0.68
2:F:6:SER:OG	2:F:128:ASN:HA	1.92	0.68
2:H:106:ARG:O	2:H:107:ASN:HB2	1.93	0.68
2:J:4:LEU:HA	2:J:7:LEU:HD12	1.75	0.68
2:L:116:LEU:HD12	2:L:119:LEU:HB2	1.75	0.68
2:D:12:LYS:C	2:D:14:ALA:H	1.95	0.68
2:E:167:ASN:HD22	2:E:178:GLY:HA2	1.57	0.68
2:F:4:LEU:HA	2:F:7:LEU:HD12	1.75	0.68
2:L:110:ALA:HB1	2:L:111:PRO:CD	2.23	0.68
2:N:12:LYS:C	2:N:14:ALA:H	1.94	0.68
1:B:548:ARG:NH1	1:B:878:ASN:N	2.35	0.68
2:C:116:LEU:HD12	2:C:119:LEU:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:116:LEU:HD12	2:D:119:LEU:HB2	1.75	0.68
2:F:116:LEU:HD12	2:F:119:LEU:HB2	1.75	0.68
2:F:153:HIS:NE2	2:H:153:HIS:NE2	2.41	0.68
2:H:11:LEU:O	2:H:14:ALA:HB3	1.93	0.68
2:N:239:ASN:HD22	2:N:246:THR:HG22	1.58	0.68
1:A:318:TRP:CA	1:A:321:ILE:HD12	2.19	0.68
2:I:116:LEU:HD12	2:I:119:LEU:HB2	1.75	0.68
1:B:180:TYR:HD1	1:B:181:LEU:N	1.91	0.68
2:I:239:ASN:HD22	2:I:246:THR:HG22	1.59	0.68
2:M:153:HIS:NE2	2:N:153:HIS:NE2	2.40	0.68
3:W:186:ASN:HD21	3:W:190:ARG:H	1.39	0.68
1:A:396:PHE:HB3	1:A:578:LEU:HD12	1.76	0.68
1:B:431:ILE:HA	1:B:435:ILE:HD12	1.76	0.68
1:A:660:ASP:CB	1:B:539:ARG:HH11	2.04	0.68
1:B:545:ASP:HB3	1:B:877:MET:SD	2.34	0.68
1:B:855:LEU:O	1:B:858:VAL:HG23	1.94	0.68
2:M:4:LEU:HA	2:M:7:LEU:HD12	1.75	0.68
3:W:691:ALA:HB2	3:W:723:ARG:HB3	1.75	0.68
1:A:659:ASP:O	1:A:662:MET:HB2	1.94	0.68
2:H:4:LEU:HA	2:H:7:LEU:HD12	1.76	0.68
2:I:4:LEU:HA	2:I:7:LEU:HD12	1.74	0.68
2:N:65:LEU:O	2:N:66:LEU:HD23	1.94	0.68
3:W:324:LYS:HG2	3:W:328:TRP:CD1	2.29	0.68
1:B:498:ARG:HB3	1:B:505:GLN:HE22	1.59	0.68
1:B:869:VAL:HG11	1:B:873:ASN:HA	1.74	0.68
2:H:167:ASN:HD22	2:H:178:GLY:HA2	1.57	0.68
2:I:135:TYR:CZ	2:I:342:MET:HE3	2.28	0.68
2:J:239:ASN:HD22	2:J:246:THR:HG22	1.58	0.68
2:O:12:LYS:C	2:O:14:ALA:H	1.96	0.68
1:A:136:ALA:O	1:A:137:ASN:HB3	1.94	0.68
1:A:587:LEU:HD13	1:A:587:LEU:O	1.94	0.68
1:B:143:ARG:HG3	1:B:216:GLU:OE2	1.92	0.68
1:B:246:HIS:CD2	1:B:248:ILE:H	2.11	0.68
1:B:530:GLN:HA	1:B:533:ILE:HD12	1.76	0.68
1:B:492:VAL:HG11	1:B:558:MET:CG	2.22	0.68
2:D:167:ASN:HD22	2:D:178:GLY:HA2	1.57	0.68
2:K:12:LYS:C	2:K:14:ALA:H	1.96	0.68
2:M:239:ASN:HD22	2:M:246:THR:HG22	1.59	0.68
1:A:101:LYS:HZ2	3:W:382:ASP:N	1.92	0.68
1:A:589:GLY:O	1:A:591:ALA:N	2.26	0.67
1:B:499:ASN:O	1:B:500:GLY:C	2.33	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:76:ASN:HB2	2:J:76:ASN:CB	2.23	0.67
2:I:9:LYS:O	2:I:13:ASP:HB2	1.94	0.67
3:W:686:LYS:HB2	3:W:688:PHE:HE2	1.58	0.67
1:A:188:VAL:O	1:A:198:LYS:HA	1.93	0.67
1:B:125:ILE:N	1:B:125:ILE:HD12	2.10	0.67
1:B:721:VAL:HG12	1:B:722:ASN:N	2.08	0.67
2:C:12:LYS:C	2:C:14:ALA:H	1.96	0.67
2:D:144:ARG:O	2:D:145:ARG:HB2	1.94	0.67
2:F:12:LYS:C	2:F:14:ALA:H	1.96	0.67
2:G:239:ASN:HD22	2:G:246:THR:HG22	1.58	0.67
2:K:117:ARG:HH21	2:M:57:ARG:NH1	1.90	0.67
1:B:258:GLN:HB3	2:N:71:LEU:HB2	1.76	0.67
3:W:438:ILE:HD11	3:W:563:GLN:HB3	1.75	0.67
1:A:270:ILE:HG23	1:A:854:LEU:CD2	2.22	0.67
3:W:217:VAL:HG13	3:W:222:ASP:CB	2.25	0.67
1:A:306:ASP:HB3	1:A:310:LEU:CD1	2.24	0.67
1:B:745:ALA:O	1:B:748:THR:N	2.28	0.67
1:B:605:ASN:HD21	1:B:855:LEU:HD12	1.58	0.67
2:D:38:ILE:HD12	2:D:65:LEU:HD23	1.75	0.67
2:E:4:LEU:HA	2:E:7:LEU:HD12	1.75	0.67
2:F:19:VAL:HG23	2:H:128:ASN:HB3	1.77	0.67
2:I:104:SER:O	2:I:108:GLY:HA3	1.94	0.67
2:H:76:ASN:H	2:J:76:ASN:HB2	1.60	0.67
2:K:116:LEU:HD12	2:K:119:LEU:HB2	1.76	0.67
2:L:4:LEU:HA	2:L:7:LEU:HD12	1.75	0.67
2:N:73:LEU:HD23	2:N:73:LEU:N	2.09	0.67
1:A:136:ALA:O	1:A:137:ASN:CB	2.43	0.67
1:A:310:LEU:O	1:A:318:TRP:HD1	1.76	0.67
1:B:183:LEU:HD12	1:B:844:SER:HB3	1.77	0.67
2:I:63:PHE:CD2	2:I:84:THR:HG23	2.28	0.67
2:O:239:ASN:HD22	2:O:246:THR:HG22	1.58	0.67
1:A:571:LEU:O	1:A:571:LEU:HD13	1.94	0.67
1:B:869:VAL:HG22	1:B:875:ARG:HA	1.76	0.67
2:F:239:ASN:HD22	2:F:246:THR:HG22	1.58	0.67
2:K:239:ASN:HD22	2:K:246:THR:HG22	1.58	0.67
1:B:666:ARG:CG	1:B:667:ASP:N	2.57	0.67
1:B:782:VAL:HG11	1:B:796:LYS:O	1.94	0.67
2:O:9:LYS:O	2:O:13:ASP:HB2	1.95	0.67
1:B:361:GLN:HE22	3:W:624:LYS:HZ1	1.42	0.67
1:B:108:LEU:N	1:B:108:LEU:HD22	2.10	0.67
1:B:154:THR:O	1:B:155:LEU:HD23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:4:LEU:HA	2:K:7:LEU:HD12	1.75	0.67
2:I:76:ASN:N	2:M:76:ASN:HB2	2.09	0.67
1:A:219:GLY:O	1:A:221:VAL:N	2.28	0.67
1:A:223:ARG:O	1:A:226:ALA:HB3	1.95	0.67
1:A:839:MET:HG2	1:A:840:HIS:H	1.60	0.67
1:B:371:ASN:ND2	1:B:583:SER:HB3	2.06	0.67
2:G:116:LEU:HD12	2:G:119:LEU:HB2	1.76	0.67
2:K:9:LYS:O	2:K:13:ASP:HB2	1.95	0.67
1:A:367:LEU:CD2	3:W:929:ALA:HA	2.22	0.67
1:A:503:ILE:C	1:A:505:GLN:H	1.98	0.67
1:A:521:MET:HB3	1:A:522:PRO:CD	2.22	0.67
1:A:650:HIS:O	1:A:651:ILE:HB	1.94	0.67
1:B:200:VAL:HG12	1:B:201:ASP:N	2.08	0.67
1:B:700:ALA:HB1	1:B:827:LYS:HB2	1.75	0.67
1:B:771:VAL:HG12	1:B:772:ILE:N	2.09	0.67
3:W:778:THR:O	3:W:782:VAL:HG22	1.93	0.67
1:A:252:PHE:CD2	1:A:684:LEU:HD21	2.30	0.66
1:B:523:VAL:C	1:B:525:TYR:N	2.47	0.66
2:O:116:LEU:HD12	2:O:119:LEU:HB2	1.76	0.66
1:A:524:ASP:OD1	1:A:525:TYR:N	2.27	0.66
1:B:229:ARG:HD2	1:B:230:GLN:HE22	1.60	0.66
1:B:672:LEU:HB3	1:B:673:PRO:HD2	1.77	0.66
2:D:99:GLU:OE1	2:D:116:LEU:HD22	1.94	0.66
2:D:99:GLU:HG2	2:D:99:GLU:O	1.94	0.66
2:O:49:GLY:HA2	2:O:54:LEU:HD23	1.77	0.66
1:A:563:MET:CA	1:A:563:MET:HE3	2.14	0.66
1:B:825:VAL:CG1	1:B:826:TYR:N	2.57	0.66
2:E:239:ASN:HD22	2:E:246:THR:HG22	1.59	0.66
3:W:1006:LEU:HG	3:W:1086:PHE:HE1	1.60	0.66
1:A:246:HIS:CD2	1:A:248:ILE:H	2.14	0.66
1:A:508:GLU:HG2	1:A:512:GLN:NE2	2.10	0.66
1:B:724:ALA:HB2	1:B:824:LYS:HE3	1.77	0.66
2:C:153:HIS:NE2	2:E:153:HIS:NE2	2.43	0.66
2:E:14:ALA:O	2:E:18:ILE:HD12	1.95	0.66
1:A:701:GLN:HG2	1:A:826:TYR:CD2	2.31	0.66
1:B:374:ALA:HB1	1:B:580:SER:CA	2.25	0.66
2:L:153:HIS:NE2	2:M:153:HIS:NE2	2.44	0.66
3:W:296:ARG:NH2	3:W:308:GLN:NE2	2.43	0.66
3:W:440:PRO:HA	3:W:567:ASN:HD22	1.61	0.66
3:W:967:ILE:H	3:W:967:ILE:HD12	1.59	0.66
1:A:454:THR:HB	1:A:457:GLN:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:LEU:O	1:A:516:GLN:OE1	2.14	0.66
1:A:653:ASP:HB3	1:A:656:ARG:HB2	1.77	0.66
1:B:396:PHE:HB2	1:B:578:LEU:HD11	1.77	0.66
2:E:23:LEU:HD23	2:E:24:TYR:N	2.11	0.66
2:N:150:PHE:HB2	2:N:152:PHE:CE1	2.30	0.66
2:N:9:LYS:O	2:N:13:ASP:HB2	1.96	0.66
1:A:277:ARG:HD3	1:A:559:ALA:CB	2.25	0.66
1:B:594:ILE:HB	1:B:595:PRO:CD	2.26	0.66
1:B:825:VAL:CG1	1:B:826:TYR:H	2.08	0.66
1:A:729:GLY:C	1:A:730:PHE:HD1	1.98	0.66
1:B:349:MET:O	1:B:353:LEU:HB2	1.94	0.66
2:C:2:ASP:HB2	2:C:128:ASN:HD21	1.60	0.66
2:J:5:TYR:CE2	2:J:131:ASN:HA	2.31	0.66
2:L:12:LYS:C	2:L:14:ALA:H	1.96	0.66
2:M:9:LYS:O	2:M:13:ASP:HB2	1.96	0.66
2:N:4:LEU:HA	2:N:7:LEU:CD1	2.26	0.66
1:A:521:MET:CE	1:A:521:MET:HA	2.26	0.66
1:B:140:LYS:O	1:B:142:LEU:N	2.29	0.66
1:B:445:MET:O	1:B:447:TYR:N	2.23	0.66
1:B:504:ASN:O	1:B:507:MET:N	2.29	0.66
2:C:22:THR:HG23	2:C:73:LEU:HD12	1.78	0.66
2:G:145:ARG:CB	2:G:145:ARG:HH11	2.00	0.66
2:I:110:ALA:HB1	2:I:111:PRO:HD2	1.77	0.66
1:B:170:TYR:HE1	1:B:681:ILE:HG23	1.60	0.66
1:B:194:ARG:HA	1:B:194:ARG:NE	2.11	0.66
2:O:4:LEU:HA	2:O:7:LEU:CD1	2.26	0.66
1:A:166:PHE:O	1:A:169:LEU:HB2	1.96	0.65
2:C:150:PHE:HB2	2:C:152:PHE:HE1	1.61	0.65
2:D:9:LYS:O	2:D:13:ASP:HB2	1.94	0.65
2:F:26:ASN:OD1	2:H:33:GLN:HB2	1.97	0.65
2:I:109:ILE:HB	2:I:380:ASP:HB3	1.79	0.65
2:N:150:PHE:HB2	2:N:152:PHE:HE1	1.61	0.65
1:A:603:TYR:O	1:A:606:VAL:HG22	1.96	0.65
2:C:4:LEU:HA	2:C:7:LEU:CD1	2.27	0.65
2:C:54:LEU:HD12	2:C:55:PRO:HD2	1.77	0.65
2:G:128:ASN:O	2:H:22:THR:HB	1.95	0.65
3:W:394:LEU:HD22	3:W:815:LEU:HD21	1.77	0.65
1:A:508:GLU:C	1:A:512:GLN:HE21	2.00	0.65
1:A:755:GLN:O	1:A:757:VAL:HG23	1.96	0.65
1:A:849:THR:HB	1:A:851:TYR:HE1	1.61	0.65
1:B:322:THR:HB	1:B:390:ARG:HH11	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:PHE:HE1	1:B:398:THR:HA	1.60	0.65
1:B:642:VAL:O	1:B:646:LEU:HG	1.96	0.65
2:D:109:ILE:HB	2:D:380:ASP:HB3	1.78	0.65
2:G:9:LYS:O	2:G:13:ASP:HB2	1.96	0.65
2:J:12:LYS:HG2	2:J:16:ASP:OD2	1.95	0.65
2:K:46:PHE:HE2	2:K:119:LEU:HD21	1.62	0.65
2:M:144:ARG:HD2	2:N:82:ARG:CZ	2.27	0.65
2:C:9:LYS:O	2:C:13:ASP:HB2	1.96	0.65
3:W:135:LEU:HD13	3:W:709:GLN:OE1	1.96	0.65
1:A:711:GLN:O	1:A:712:LEU:HD23	1.96	0.65
1:A:871:PHE:O	1:A:871:PHE:HD1	1.80	0.65
1:B:708:ARG:O	1:B:709:ASP:C	2.35	0.65
1:A:501:HIS:O	1:A:503:ILE:HG13	1.97	0.65
2:D:22:THR:O	2:D:72:ASN:HA	1.95	0.65
2:G:4:LEU:HA	2:G:7:LEU:CD1	2.26	0.65
2:I:150:PHE:HB2	2:I:152:PHE:CZ	2.32	0.65
1:A:516:GLN:N	1:A:516:GLN:OE1	2.28	0.65
1:A:622:VAL:HG11	1:A:673:PRO:O	1.97	0.65
1:A:642:VAL:O	1:A:646:LEU:HG	1.96	0.65
1:B:805:ASP:C	1:B:807:ASN:H	1.99	0.65
2:H:9:LYS:O	2:H:13:ASP:HB2	1.97	0.65
2:I:130:ASP:HA	2:J:17:LYS:HG2	1.78	0.65
2:I:153:HIS:NE2	2:K:153:HIS:NE2	2.45	0.65
3:W:704:SER:HB2	3:W:709:GLN:NE2	2.12	0.65
1:A:142:LEU:O	1:A:144:ASN:N	2.28	0.65
1:A:589:GLY:C	1:A:591:ALA:H	1.99	0.65
1:A:782:VAL:O	1:A:785:GLN:HG2	1.97	0.65
1:A:658:PRO:CG	1:B:348:LYS:HG2	2.23	0.65
1:B:401:TYR:HA	1:B:404:LEU:HD13	1.79	0.65
1:B:170:TYR:CE1	1:B:681:ILE:HG23	2.31	0.65
1:A:779:ASP:CA	1:A:798:ILE:HD12	2.26	0.65
1:B:236:ARG:O	1:B:237:ASN:HB2	1.97	0.65
1:B:315:GLU:CB	1:B:571:LEU:HD11	2.25	0.65
3:W:207:ALA:O	3:W:211:ILE:HG13	1.96	0.65
1:A:271:PHE:HA	1:A:274:ILE:HD12	1.79	0.65
1:B:298:TYR:HD1	1:B:299:ILE:N	1.94	0.65
1:B:96:PRO:HG2	1:B:657:VAL:HG22	1.79	0.65
2:N:12:LYS:HG2	2:N:16:ASP:OD2	1.96	0.65
1:B:378:CYS:HB2	1:B:580:SER:HB2	1.79	0.64
2:E:9:LYS:O	2:E:13:ASP:HB2	1.97	0.64
2:F:9:LYS:O	2:F:13:ASP:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4:LEU:HA	2:I:7:LEU:CD1	2.27	0.64
2:J:57:ARG:HH11	2:J:94:ASN:HD21	1.46	0.64
1:A:793:ASP:C	1:A:795:LEU:H	2.00	0.64
1:B:603:TYR:O	1:B:606:VAL:HG22	1.97	0.64
1:B:314:PHE:CZ	1:B:664:ARG:HG2	2.32	0.64
2:D:106:ARG:HG2	2:D:107:ASN:H	1.62	0.64
2:D:4:LEU:HA	2:D:7:LEU:CD1	2.27	0.64
2:L:9:LYS:O	2:L:13:ASP:HB2	1.96	0.64
1:A:802:ILE:HA	1:A:807:ASN:ND2	2.12	0.64
2:O:104:SER:HB3	2:O:108:GLY:HA2	1.79	0.64
3:W:191:TYR:CE2	3:W:204:VAL:HG11	2.31	0.64
3:W:777:THR:HG21	3:W:882:LYS:NZ	2.11	0.64
1:A:714:ARG:HA	1:A:720:TYR:HB3	1.78	0.64
1:A:863:VAL:HG12	1:A:864:GLU:H	1.61	0.64
2:D:110:ALA:HB1	2:D:111:PRO:CD	2.28	0.64
2:L:27:VAL:O	2:L:31:ILE:HG12	1.97	0.64
1:A:414:VAL:HB	1:A:419:PHE:HE1	1.62	0.64
1:A:834:ASP:O	1:A:838:SER:HB2	1.97	0.64
1:B:182:LEU:CD2	1:B:183:LEU:H	2.08	0.64
1:B:457:GLN:CG	1:B:458:ILE:N	2.53	0.64
1:B:491:GLN:NE2	1:B:566:GLN:HG2	2.12	0.64
1:B:606:VAL:HG23	1:B:607:ASN:N	2.11	0.64
2:J:144:ARG:NH2	2:J:146:GLN:HE22	1.96	0.64
1:A:246:HIS:O	1:A:249:ASP:N	2.31	0.64
1:A:548:ARG:HB3	1:A:876:ILE:HG23	1.78	0.64
1:B:645:PHE:HD2	1:B:646:LEU:HD23	1.62	0.64
1:B:718:TYR:HB3	1:B:721:VAL:CG2	2.18	0.64
2:F:109:ILE:HB	2:F:380:ASP:HB3	1.79	0.64
2:J:9:LYS:O	2:J:13:ASP:HB2	1.98	0.64
2:J:4:LEU:HA	2:J:7:LEU:CD1	2.28	0.64
2:K:12:LYS:HG2	2:K:16:ASP:OD2	1.97	0.64
2:M:139:TRP:NE1	2:M:143:ASN:ND2	2.46	0.64
3:W:532:GLN:HB2	3:W:533:PRO:HD3	1.78	0.64
3:W:906:ASN:ND2	3:W:907:VAL:N	2.44	0.64
1:A:246:HIS:HD2	1:A:248:ILE:HB	1.63	0.64
1:A:378:CYS:SG	1:A:584:LEU:HD13	2.38	0.64
1:B:703:VAL:HG22	1:B:825:VAL:HG22	1.78	0.64
2:F:38:ILE:HG22	2:F:42:ASN:HD21	1.62	0.64
2:M:42:ASN:HA	2:M:61:PHE:HB3	1.80	0.64
2:N:128:ASN:O	2:N:129:PHE:HB3	1.98	0.64
1:A:606:VAL:HG23	1:A:607:ASN:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:GLN:OE1	1:B:389:GLN:HA	1.98	0.64
1:B:492:VAL:HG13	1:B:565:MET:SD	2.38	0.64
1:B:721:VAL:HG12	1:B:722:ASN:H	1.63	0.64
1:B:182:LEU:HD11	1:B:847:THR:HA	1.78	0.64
2:M:12:LYS:HG2	2:M:16:ASP:OD2	1.98	0.64
3:W:890:ALA:HB2	3:W:1053:SER:HB2	1.79	0.64
1:A:360:ILE:HG23	1:A:363:GLU:HB2	1.78	0.64
2:D:54:LEU:HD12	2:D:55:PRO:HD2	1.79	0.64
2:G:106:ARG:HG2	2:G:107:ASN:H	1.62	0.64
2:D:12:LYS:HG2	2:D:16:ASP:OD2	1.98	0.64
2:E:4:LEU:HA	2:E:7:LEU:CD1	2.28	0.64
2:H:57:ARG:HH11	2:H:94:ASN:HD21	1.44	0.64
2:K:4:LEU:HA	2:K:7:LEU:CD1	2.28	0.64
2:O:14:ALA:O	2:O:18:ILE:HD12	1.97	0.64
3:W:387:ARG:HB3	3:W:387:ARG:HH11	1.63	0.64
3:W:509:PHE:CD2	3:W:624:LYS:HB3	2.32	0.64
1:A:158:GLY:N	1:A:762:ALA:HB3	2.13	0.63
1:A:371:ASN:HB3	1:A:583:SER:HB2	1.80	0.63
1:B:498:ARG:CB	1:B:505:GLN:HE22	2.10	0.63
1:B:491:GLN:HE22	1:B:566:GLN:HG2	1.63	0.63
2:J:110:ALA:HB1	2:J:111:PRO:CD	2.28	0.63
2:I:19:VAL:CG2	2:K:128:ASN:HB3	2.27	0.63
2:L:12:LYS:HG2	2:L:16:ASP:OD2	1.98	0.63
2:M:27:VAL:O	2:M:31:ILE:HG12	1.97	0.63
3:W:741:SER:HB3	3:W:751:PHE:CD1	2.33	0.63
1:A:772:ILE:O	1:A:775:ILE:HG13	1.98	0.63
1:B:346:ILE:O	1:B:349:MET:HB3	1.97	0.63
1:B:442:MET:HG2	1:B:443:GLN:H	1.63	0.63
1:B:645:PHE:CD2	1:B:646:LEU:HD23	2.33	0.63
2:F:4:LEU:HA	2:F:7:LEU:CD1	2.29	0.63
2:J:71:LEU:HG	2:J:72:ASN:OD1	1.98	0.63
2:M:4:LEU:HA	2:M:7:LEU:CD1	2.28	0.63
1:A:491:GLN:OE1	1:A:564:ASN:HB3	1.99	0.63
1:B:396:PHE:CE1	1:B:398:THR:HA	2.33	0.63
1:B:730:PHE:N	1:B:730:PHE:CD1	2.67	0.63
1:B:772:ILE:O	1:B:775:ILE:HB	1.98	0.63
2:F:110:ALA:HB1	2:F:111:PRO:HD2	1.80	0.63
2:I:145:ARG:HH11	2:I:145:ARG:CB	2.12	0.63
1:A:560:CYS:HB2	1:A:603:TYR:CD2	2.33	0.63
1:A:721:VAL:HG11	1:A:799:LEU:HD22	1.81	0.63
1:A:839:MET:HE2	1:A:839:MET:C	2.19	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:GLN:HG3	1:B:564:ASN:HD21	1.62	0.63
1:B:415:PRO:CB	1:B:480:PHE:HB2	2.28	0.63
1:B:503:ILE:HD11	1:B:548:ARG:CG	2.26	0.63
1:B:722:ASN:ND2	1:B:824:LYS:HA	2.10	0.63
2:D:109:ILE:HD12	2:D:109:ILE:O	1.99	0.63
2:F:12:LYS:HG2	2:F:16:ASP:OD2	1.99	0.63
2:O:141:LEU:HD12	2:O:148:THR:HG21	1.80	0.63
3:W:872:ILE:HD11	3:W:1072:ASN:HB2	1.80	0.63
1:A:262:VAL:HG12	1:A:297:ARG:HB3	1.80	0.63
1:B:498:ARG:HD3	2:I:32:GLN:HE21	1.63	0.63
2:F:104:SER:O	2:F:105:GLN:HB2	1.98	0.63
2:L:346:VAL:HG21	2:L:385:VAL:HG13	1.81	0.63
3:W:324:LYS:O	3:W:328:TRP:HD1	1.82	0.63
3:W:729:ARG:NH1	3:W:770:ASP:OD1	2.31	0.63
1:B:231:ARG:HB3	1:B:240:ASN:HB2	1.80	0.63
1:B:422:GLU:HA	1:B:425:VAL:CG2	2.29	0.63
1:B:492:VAL:HG11	1:B:558:MET:SD	2.38	0.63
1:B:587:LEU:HG	1:B:587:LEU:O	1.97	0.63
1:B:701:GLN:HB2	1:B:826:TYR:CD2	2.29	0.63
1:B:735:LEU:HD21	1:B:759:LEU:HB3	1.80	0.63
1:A:513:LEU:HA	1:A:516:GLN:HE22	1.64	0.63
2:C:12:LYS:HG2	2:C:16:ASP:OD2	1.99	0.63
2:L:24:TYR:O	2:L:27:VAL:HG22	1.98	0.63
2:L:85:ILE:O	2:L:89:VAL:HG23	1.99	0.63
2:O:12:LYS:HG2	2:O:16:ASP:OD2	1.99	0.63
2:O:85:ILE:O	2:O:89:VAL:HG23	1.99	0.63
3:W:470:PHE:HE1	3:W:594:LYS:HD3	1.64	0.63
1:A:795:LEU:O	1:A:797:PRO:HD3	1.98	0.63
1:B:127:GLU:OE1	1:B:151:LYS:HE2	1.98	0.63
1:B:549:LEU:HD13	1:B:877:MET:CE	2.28	0.63
1:B:818:VAL:HG12	1:B:819:PRO:HD2	1.80	0.63
2:K:346:VAL:HG21	2:K:385:VAL:HG13	1.81	0.63
2:N:106:ARG:H	2:N:106:ARG:CD	1.99	0.63
2:O:147:ARG:HG2	2:O:148:THR:N	2.13	0.63
1:A:436:ILE:HD12	1:A:436:ILE:C	2.18	0.63
1:A:601:PHE:HD1	1:A:601:PHE:H	1.46	0.63
1:A:328:LEU:HD11	1:A:606:VAL:HG21	1.80	0.62
1:A:416:ASN:HB3	1:A:424:LEU:CD2	2.29	0.62
1:B:274:ILE:HG23	1:B:278:ILE:CD1	2.24	0.62
2:I:12:LYS:HG2	2:I:16:ASP:OD2	1.99	0.62
2:I:85:ILE:O	2:I:89:VAL:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:346:VAL:HG21	2:N:385:VAL:HG13	1.81	0.62
2:N:49:GLY:HA2	2:N:54:LEU:HD23	1.81	0.62
3:W:147:PHE:CE1	3:W:151:LYS:HE3	2.33	0.62
3:W:161:LYS:O	3:W:165:ARG:HG3	1.98	0.62
1:A:721:VAL:HG13	1:A:800:TYR:O	1.98	0.62
1:A:810:TYR:O	1:A:812:VAL:N	2.32	0.62
1:B:199:VAL:CG1	1:B:200:VAL:N	2.62	0.62
1:B:451:ASP:N	1:B:452:PRO:HD3	2.13	0.62
1:B:494:ASN:ND2	1:B:495:ASP:N	2.46	0.62
1:B:305:GLN:HE21	1:B:564:ASN:CG	2.03	0.62
1:B:704:ILE:O	1:B:823:THR:OG1	2.17	0.62
1:B:812:VAL:HG22	1:B:813:ALA:N	2.13	0.62
1:B:95:ILE:HG22	1:B:97:THR:OG1	1.99	0.62
2:J:346:VAL:HG21	2:J:385:VAL:HG13	1.81	0.62
2:O:346:VAL:HG21	2:O:385:VAL:HG13	1.81	0.62
1:A:360:ILE:CG2	1:A:363:GLU:HB2	2.29	0.62
1:A:472:LEU:O	1:A:476:ASN:HB2	1.99	0.62
1:A:545:ASP:HA	1:A:548:ARG:HD2	1.80	0.62
1:B:596:SER:HB2	1:B:599:THR:OG1	1.99	0.62
2:H:346:VAL:HG21	2:H:385:VAL:HG13	1.81	0.62
2:K:48:THR:HG22	2:K:115:SER:OG	1.98	0.62
2:J:144:ARG:HD2	2:K:82:ARG:CZ	2.28	0.62
2:O:135:TYR:OH	2:O:340:GLU:OE1	2.17	0.62
3:W:408:LEU:HD13	3:W:415:ILE:HG13	1.79	0.62
3:W:781:GLU:O	3:W:785:GLN:HB2	1.98	0.62
1:A:503:ILE:CD1	1:A:547:THR:HB	2.29	0.62
1:B:122:LEU:HD11	1:B:200:VAL:CG1	2.29	0.62
1:B:681:ILE:O	1:B:684:LEU:HB3	1.99	0.62
1:B:723:ILE:O	1:B:824:LYS:HD2	2.00	0.62
2:C:21:GLY:O	2:C:22:THR:O	2.17	0.62
1:B:497:ILE:HG12	2:I:68:THR:HG23	1.82	0.62
1:B:394:LEU:C	1:B:396:PHE:H	2.02	0.62
1:B:791:LYS:C	1:B:792:VAL:HG13	2.20	0.62
2:C:8:SER:O	2:C:11:LEU:N	2.33	0.62
2:E:116:LEU:HA	2:E:119:LEU:HD12	1.81	0.62
2:H:109:ILE:CG1	2:H:109:ILE:O	2.48	0.62
2:I:346:VAL:HG21	2:I:385:VAL:HG13	1.81	0.62
2:L:4:LEU:HA	2:L:7:LEU:CD1	2.28	0.62
1:A:763:LEU:HD23	1:A:764:PRO:HD3	1.80	0.62
1:B:432:VAL:HA	1:B:436:ILE:CD1	2.12	0.62
1:B:692:ILE:H	1:B:692:ILE:HD12	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:85:ILE:O	2:J:89:VAL:HG23	1.99	0.62
3:W:1001:TYR:CD1	3:W:1084:ASN:HB3	2.33	0.62
3:W:463:PHE:HD2	3:W:465:LEU:HD21	1.65	0.62
3:W:906:ASN:ND2	3:W:907:VAL:H	1.95	0.62
1:A:738:LEU:C	1:A:740:ARG:H	2.02	0.62
1:B:371:ASN:HA	1:B:374:ALA:HB3	1.82	0.62
1:B:435:ILE:O	1:B:436:ILE:HG12	2.00	0.62
3:W:161:LYS:HB3	3:W:165:ARG:HH12	1.64	0.62
3:W:324:LYS:O	3:W:328:TRP:CD1	2.53	0.62
1:A:556:THR:O	1:A:557:LEU:C	2.38	0.62
1:A:596:SER:O	1:A:600:LEU:HD12	1.99	0.62
2:F:346:VAL:HG21	2:F:385:VAL:HG13	1.81	0.62
2:H:4:LEU:HA	2:H:7:LEU:CD1	2.28	0.62
2:I:23:LEU:HD23	2:I:24:TYR:H	1.65	0.62
2:J:22:THR:HG22	2:J:73:LEU:HD12	1.81	0.62
2:H:76:ASN:CB	2:J:76:ASN:HB2	2.30	0.62
2:L:38:ILE:HD12	2:L:65:LEU:CD2	2.29	0.62
2:N:8:SER:O	2:N:11:LEU:N	2.33	0.62
1:B:634:TYR:O	1:B:635:GLN:HG2	1.99	0.62
2:G:46:PHE:HE2	2:G:119:LEU:HD21	1.63	0.62
2:H:12:LYS:HG2	2:H:16:ASP:OD2	2.00	0.62
2:L:62:ASP:CG	2:L:62:ASP:O	2.37	0.62
2:M:346:VAL:HG21	2:M:385:VAL:HG13	1.81	0.62
2:O:23:LEU:HD23	2:O:24:TYR:N	2.14	0.62
3:W:758:THR:HG22	3:W:766:PHE:O	2.00	0.62
1:A:692:ILE:H	1:A:692:ILE:HD12	1.64	0.62
1:B:240:ASN:HA	1:B:842:LEU:O	2.00	0.62
1:B:722:ASN:O	1:B:824:LYS:HB2	1.99	0.62
2:D:27:VAL:O	2:D:31:ILE:HG12	1.99	0.62
2:L:109:ILE:HD12	2:L:109:ILE:O	1.99	0.62
3:W:247:PRO:HG3	3:W:291:MET:HB3	1.81	0.62
1:B:503:ILE:HG21	1:B:544:VAL:HG13	1.80	0.61
2:E:12:LYS:HG2	2:E:16:ASP:OD2	1.99	0.61
3:W:225:ILE:HD13	3:W:325:ILE:HD13	1.81	0.61
3:W:928:SER:HB2	3:W:984:ASP:OD1	2.00	0.61
1:A:568:VAL:HG12	1:A:569:GLN:N	2.14	0.61
1:B:508:GLU:CD	2:J:71:LEU:HB3	2.20	0.61
1:B:863:VAL:HG12	1:B:864:GLU:H	1.65	0.61
2:G:27:VAL:O	2:G:31:ILE:HG12	2.01	0.61
2:L:22:THR:HG23	2:L:73:LEU:CD1	2.23	0.61
2:M:116:LEU:HA	2:M:119:LEU:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:145:ARG:CZ	2:M:145:ARG:HB3	2.31	0.61
2:N:66:LEU:HD13	2:N:77:TYR:OH	2.00	0.61
1:A:225:ILE:HA	1:A:228:MET:HE1	1.83	0.61
1:A:362:SER:CB	1:A:365:GLN:NE2	2.63	0.61
1:A:447:TYR:OH	1:A:458:ILE:HG23	2.01	0.61
1:B:194:ARG:HA	1:B:194:ARG:CZ	2.30	0.61
1:B:415:PRO:HG2	1:B:480:PHE:CD1	2.30	0.61
1:B:428:GLN:HB2	1:B:456:PHE:HD1	1.61	0.61
1:B:182:LEU:HD21	1:B:846:LEU:HA	1.82	0.61
1:B:94:THR:O	1:B:316:SER:HB3	2.01	0.61
2:D:23:LEU:HD23	2:D:24:TYR:H	1.62	0.61
2:D:346:VAL:HG21	2:D:385:VAL:HG13	1.81	0.61
2:E:8:SER:O	2:E:11:LEU:N	2.34	0.61
2:E:346:VAL:HG21	2:E:385:VAL:HG13	1.81	0.61
1:B:744:TYR:O	1:B:745:ALA:HB3	2.00	0.61
2:G:12:LYS:HG2	2:G:16:ASP:OD2	1.99	0.61
2:J:116:LEU:HA	2:J:119:LEU:HD12	1.82	0.61
2:K:8:SER:O	2:K:11:LEU:N	2.34	0.61
2:O:38:ILE:HG22	2:O:42:ASN:HD21	1.64	0.61
1:A:389:GLN:O	1:A:389:GLN:HG3	2.00	0.61
1:B:521:MET:HB2	1:B:522:PRO:HD2	1.81	0.61
2:G:38:ILE:HG22	2:G:42:ASN:HD21	1.64	0.61
2:G:128:ASN:HB3	2:H:19:VAL:HG23	1.81	0.61
2:I:116:LEU:HA	2:I:119:LEU:HD12	1.82	0.61
2:L:8:SER:O	2:L:11:LEU:N	2.33	0.61
2:M:63:PHE:CD2	2:M:84:THR:HG23	2.35	0.61
2:O:8:SER:O	2:O:11:LEU:N	2.34	0.61
1:A:506:LEU:HD21	1:A:543:LEU:C	2.20	0.61
1:B:297:ARG:HG3	1:B:848:PHE:CD2	2.29	0.61
2:D:85:ILE:O	2:D:89:VAL:HG23	2.01	0.61
3:W:292:LEU:O	3:W:296:ARG:HG3	2.00	0.61
3:W:463:PHE:CD1	3:W:590:ALA:HB3	2.35	0.61
1:A:443:GLN:CD	1:A:521:MET:HG2	2.21	0.61
1:B:545:ASP:HA	1:B:548:ARG:HD2	1.82	0.61
3:W:779:VAL:O	3:W:782:VAL:HG23	2.00	0.61
3:W:917:ARG:HD2	3:W:919:TYR:CE1	2.36	0.61
1:A:282:VAL:O	1:A:284:TYR:N	2.34	0.61
1:A:443:GLN:O	1:A:445:MET:N	2.34	0.61
1:A:450:GLY:O	1:A:451:ASP:HB2	2.01	0.61
1:A:257:LEU:HD13	1:A:843:THR:O	2.01	0.61
1:B:496:ASN:HB3	1:B:498:ARG:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:147:ARG:O	2:O:148:THR:HB	1.99	0.61
2:O:150:PHE:CD1	2:O:150:PHE:N	2.69	0.61
3:W:967:ILE:HD12	3:W:967:ILE:N	2.15	0.61
1:A:125:ILE:HD13	1:A:126:PHE:HE2	1.66	0.61
2:J:6:SER:OG	2:J:128:ASN:HA	2.00	0.61
2:L:72:ASN:ND2	2:N:126:ARG:HH11	1.99	0.61
2:O:116:LEU:HA	2:O:119:LEU:HD12	1.82	0.61
3:W:145:VAL:HG21	3:W:211:ILE:HG23	1.82	0.61
1:A:701:GLN:HB3	1:A:826:TYR:HD2	1.66	0.61
1:B:523:VAL:O	1:B:525:TYR:N	2.34	0.61
1:B:96:PRO:O	1:B:320:THR:HG21	1.99	0.61
2:E:135:TYR:CZ	2:E:342:MET:HE3	2.36	0.61
2:G:346:VAL:HG21	2:G:385:VAL:HG13	1.81	0.61
2:J:8:SER:O	2:J:11:LEU:N	2.34	0.61
2:I:19:VAL:HG23	2:K:128:ASN:HB3	1.83	0.61
2:K:152:PHE:N	2:K:152:PHE:CD1	2.69	0.61
2:N:116:LEU:HA	2:N:119:LEU:HD12	1.82	0.61
3:W:98:LEU:CD1	3:W:172:ILE:HG23	2.30	0.61
3:W:573:VAL:HG21	3:W:586:TYR:CD1	2.36	0.61
1:A:434:THR:HG22	1:A:434:THR:O	2.00	0.60
1:A:570:THR:CG2	1:A:571:LEU:H	2.12	0.60
1:A:660:ASP:O	1:A:661:GLN:C	2.38	0.60
1:A:817:TRP:CG	1:A:818:VAL:N	2.65	0.60
1:B:133:ILE:CD1	1:B:145:ARG:HB2	2.31	0.60
1:B:180:TYR:CD1	1:B:181:LEU:N	2.68	0.60
1:B:333:VAL:HG11	1:B:380:LYS:HA	1.83	0.60
1:B:482:GLN:CB	1:B:493:LEU:HD22	2.30	0.60
2:E:150:PHE:HB2	2:E:152:PHE:CZ	2.37	0.60
2:N:109:ILE:HB	2:N:380:ASP:HB3	1.82	0.60
1:A:319:ASP:OD2	1:A:571:LEU:HB3	2.00	0.60
1:A:403:SER:HA	1:A:582:THR:OG1	2.00	0.60
1:A:631:LEU:HB3	1:A:633:LEU:CD1	2.31	0.60
1:A:817:TRP:CH2	1:A:819:PRO:HA	2.36	0.60
1:B:156:PRO:HB2	1:B:161:ASP:CB	2.30	0.60
1:B:503:ILE:HD13	1:B:544:VAL:CG1	2.31	0.60
1:B:527:ARG:O	1:B:531:ARG:CG	2.49	0.60
1:B:779:ASP:HA	1:B:798:ILE:HD11	1.82	0.60
2:C:346:VAL:HG21	2:C:385:VAL:HG13	1.81	0.60
2:F:109:ILE:O	2:F:109:ILE:HD12	2.01	0.60
2:H:142:GLN:HE21	2:H:143:ASN:N	1.98	0.60
2:L:150:PHE:HB2	2:L:152:PHE:HE1	1.60	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:49:GLY:HA2	2:M:54:LEU:CD2	2.31	0.60
1:B:364:THR:HG21	3:W:622:ALA:HA	1.83	0.60
1:A:122:LEU:HD11	1:A:200:VAL:HG12	1.82	0.60
1:A:308:LEU:O	1:A:309:ASN:C	2.39	0.60
1:A:625:ILE:O	1:A:628:ALA:HB3	2.00	0.60
1:A:757:VAL:HG12	1:A:758:ALA:N	2.17	0.60
1:A:779:ASP:HA	1:A:798:ILE:HD11	1.80	0.60
1:B:118:LYS:CG	1:B:119:GLN:H	2.13	0.60
1:B:684:LEU:O	1:B:687:MET:HG2	2.02	0.60
2:D:133:SER:O	2:D:135:TYR:N	2.35	0.60
1:A:355:LEU:HD13	1:A:363:GLU:HG2	1.83	0.60
1:B:424:LEU:O	1:B:424:LEU:HD12	2.01	0.60
2:E:57:ARG:HH11	2:E:94:ASN:HD21	1.49	0.60
2:I:153:HIS:NE2	2:J:153:HIS:NE2	2.50	0.60
2:M:8:SER:O	2:M:11:LEU:N	2.34	0.60
2:M:5:TYR:CE2	2:M:131:ASN:HA	2.37	0.60
2:N:12:LYS:C	2:N:14:ALA:N	2.54	0.60
3:W:100:ALA:O	3:W:102:LEU:HD13	2.02	0.60
1:B:275:PRO:HD2	1:B:278:ILE:HD11	1.83	0.60
1:B:492:VAL:O	1:B:493:LEU:C	2.40	0.60
1:B:875:ARG:HD3	1:B:878:ASN:HD22	1.66	0.60
2:E:133:SER:O	2:E:135:TYR:N	2.35	0.60
2:L:116:LEU:HA	2:L:119:LEU:HD12	1.83	0.60
2:O:24:TYR:HB2	2:O:71:LEU:HD12	1.83	0.60
1:A:437:TYR:CD2	1:A:442:MET:HG3	2.36	0.60
1:A:803:ASN:C	1:A:805:ASP:H	2.05	0.60
1:B:389:GLN:NE2	1:B:567:HIS:HA	2.17	0.60
1:B:604:TYR:O	1:B:608:VAL:HG23	2.00	0.60
2:D:8:SER:O	2:D:11:LEU:N	2.34	0.60
2:H:8:SER:O	2:H:11:LEU:N	2.34	0.60
2:N:157:ILE:HG12	2:N:214:LEU:HD13	1.84	0.60
2:N:27:VAL:O	2:N:30:LEU:N	2.34	0.60
1:A:203:GLU:O	1:A:207:ILE:HG13	2.02	0.60
1:B:371:ASN:HD22	1:B:583:SER:CB	2.10	0.60
1:B:674:VAL:CG2	1:B:679:LEU:HD13	2.27	0.60
1:B:745:ALA:O	1:B:746:GLN:C	2.40	0.60
1:B:874:MET:O	1:B:875:ARG:CB	2.50	0.60
2:E:85:ILE:O	2:E:89:VAL:HG23	2.01	0.60
2:F:104:SER:HB3	2:F:108:GLY:HA3	1.84	0.60
2:H:23:LEU:H	2:H:26:ASN:ND2	2.00	0.60
2:I:68:THR:HG22	2:I:69:THR:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:73:LEU:HD22	2:L:77:TYR:CD2	2.36	0.60
2:M:145:ARG:NH1	2:M:145:ARG:HB3	2.16	0.60
1:A:225:ILE:HA	1:A:228:MET:CE	2.32	0.60
1:A:237:ASN:O	1:A:237:ASN:OD1	2.20	0.60
1:A:326:TYR:CD1	1:A:384:ALA:HB1	2.36	0.60
1:A:492:VAL:CG1	1:A:558:MET:SD	2.90	0.60
1:A:546:LEU:CD1	1:A:584:LEU:HD23	2.32	0.60
1:A:666:ARG:HG3	1:A:667:ASP:N	2.14	0.60
1:A:727:LEU:O	1:A:727:LEU:HD12	2.02	0.60
1:B:274:ILE:CG2	1:B:278:ILE:HD11	2.25	0.60
1:B:371:ASN:C	1:B:373:GLN:N	2.52	0.60
1:B:508:GLU:C	1:B:512:GLN:HE21	2.05	0.60
1:B:387:LEU:HD23	1:B:554:TYR:CE1	2.36	0.60
1:B:743:ASP:OD2	1:B:745:ALA:HA	2.01	0.60
2:C:133:SER:O	2:C:135:TYR:N	2.34	0.60
2:D:116:LEU:HA	2:D:119:LEU:HD12	1.82	0.60
2:F:133:SER:O	2:F:135:TYR:N	2.35	0.60
2:G:157:ILE:HG12	2:G:214:LEU:HD13	1.84	0.60
2:J:110:ALA:HB1	2:J:111:PRO:HD2	1.83	0.60
2:K:116:LEU:HA	2:K:119:LEU:HD12	1.84	0.60
2:K:5:TYR:CE2	2:K:131:ASN:HA	2.37	0.60
2:M:274:GLN:N	2:M:274:GLN:HE21	2.00	0.60
3:W:473:GLN:HE22	3:W:593:GLU:HB3	1.66	0.60
1:B:180:TYR:CD1	1:B:180:TYR:C	2.75	0.60
1:B:435:ILE:CG2	1:B:436:ILE:H	2.09	0.60
1:B:502:VAL:O	1:B:504:ASN:N	2.35	0.60
1:B:723:ILE:O	1:B:724:ALA:HB2	2.01	0.60
2:D:38:ILE:HG22	2:D:42:ASN:HD21	1.67	0.60
2:E:157:ILE:HG12	2:E:214:LEU:HD13	1.84	0.60
2:J:133:SER:O	2:J:135:TYR:N	2.35	0.60
2:J:274:GLN:N	2:J:274:GLN:HE21	2.00	0.60
1:A:535:LEU:O	1:A:539:ARG:HG2	2.02	0.60
1:B:601:PHE:H	1:B:601:PHE:HD1	1.47	0.60
1:B:555:GLU:OE2	1:B:871:PHE:HE2	1.85	0.60
2:F:157:ILE:HG12	2:F:214:LEU:HD13	1.84	0.60
2:G:73:LEU:HD22	2:G:77:TYR:CD2	2.37	0.60
2:H:5:TYR:CE2	2:H:131:ASN:HA	2.37	0.60
2:K:133:SER:O	2:K:135:TYR:N	2.35	0.60
2:M:152:PHE:CD1	2:M:152:PHE:N	2.70	0.60
2:O:8:SER:C	2:O:10:THR:N	2.55	0.60
3:W:708:ASP:HB3	3:W:1080:TYR:CZ	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:165:ARG:HE	3:W:220:HIS:HA	1.67	0.60
3:W:463:PHE:CE1	3:W:590:ALA:HB3	2.37	0.60
3:W:933:LEU:HD23	3:W:962:LEU:HD22	1.84	0.60
1:A:445:MET:C	1:A:447:TYR:N	2.54	0.59
1:A:604:TYR:O	1:A:608:VAL:HG23	2.01	0.59
1:B:482:GLN:O	1:B:482:GLN:HG3	2.02	0.59
1:B:508:GLU:OE2	2:J:71:LEU:HB3	2.02	0.59
1:B:535:LEU:O	1:B:539:ARG:HG2	2.01	0.59
2:C:274:GLN:HE21	2:C:274:GLN:N	2.00	0.59
2:C:85:ILE:O	2:C:89:VAL:HG23	2.01	0.59
2:D:128:ASN:ND2	2:E:19:VAL:HG21	2.17	0.59
2:G:111:PRO:HB3	2:G:116:LEU:HD23	1.83	0.59
2:H:133:SER:O	2:H:135:TYR:N	2.35	0.59
1:A:366:PHE:C	1:A:368:THR:N	2.48	0.59
1:A:577:GLN:O	1:A:581:VAL:HG23	2.01	0.59
1:B:513:LEU:HA	1:B:516:GLN:OE1	2.01	0.59
2:D:76:ASN:HB2	2:L:76:ASN:HB2	1.83	0.59
2:H:152:PHE:N	2:H:152:PHE:CD1	2.69	0.59
2:I:157:ILE:HG12	2:I:214:LEU:HD13	1.84	0.59
2:M:24:TYR:O	2:M:27:VAL:HG22	2.02	0.59
2:L:19:VAL:CG2	2:N:128:ASN:HB3	2.32	0.59
1:A:246:HIS:CD2	1:A:248:ILE:HB	2.36	0.59
1:A:744:TYR:O	1:A:746:GLN:N	2.35	0.59
1:A:747:ILE:HD11	1:A:786:ILE:HG21	1.85	0.59
1:A:548:ARG:HH11	1:A:877:MET:CA	2.14	0.59
1:B:112:LYS:N	1:B:113:PRO:HD3	2.18	0.59
1:B:124:ARG:HB2	1:B:249:ASP:CG	2.22	0.59
1:B:363:GLU:HA	1:B:363:GLU:OE1	2.02	0.59
1:B:401:TYR:O	1:B:404:LEU:HB2	2.02	0.59
1:B:863:VAL:HG12	1:B:864:GLU:N	2.17	0.59
2:C:131:ASN:HD22	2:C:131:ASN:N	1.99	0.59
2:G:85:ILE:O	2:G:89:VAL:HG23	2.01	0.59
2:H:274:GLN:HE21	2:H:274:GLN:N	2.00	0.59
2:M:133:SER:O	2:M:135:TYR:N	2.35	0.59
2:N:274:GLN:HE21	2:N:274:GLN:N	2.00	0.59
2:N:85:ILE:O	2:N:89:VAL:HG23	2.02	0.59
3:W:816:SER:HB3	3:W:820:LEU:HD11	1.82	0.59
1:A:703:VAL:HG21	1:A:797:PRO:HB3	1.84	0.59
1:B:543:LEU:HD23	1:B:546:LEU:HD12	1.84	0.59
2:F:23:LEU:HD11	2:H:36:GLN:HB2	1.85	0.59
2:J:8:SER:C	2:J:10:THR:N	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:PRO:HB3	1:A:479:GLN:HA	1.84	0.59
1:A:521:MET:HA	1:A:521:MET:HE2	1.84	0.59
1:A:545:ASP:O	1:A:548:ARG:N	2.35	0.59
1:A:700:ALA:O	1:A:701:GLN:HB2	2.02	0.59
1:A:839:MET:HG2	1:A:840:HIS:N	2.16	0.59
1:B:383:ILE:HD11	1:B:550:LEU:CD2	2.32	0.59
2:D:70:LEU:HD12	2:D:71:LEU:N	2.17	0.59
2:L:157:ILE:HG12	2:L:214:LEU:HD13	1.84	0.59
2:L:53:ASN:HD22	2:L:354:ALA:HB3	1.66	0.59
1:A:371:ASN:O	1:A:373:GLN:N	2.36	0.59
1:A:548:ARG:NH1	1:A:877:MET:HA	2.17	0.59
1:A:770:SER:O	1:A:771:VAL:C	2.40	0.59
1:B:141:GLU:O	1:B:142:LEU:HB2	2.03	0.59
1:B:368:THR:O	1:B:371:ASN:ND2	2.36	0.59
1:B:393:SER:HB3	1:B:573:THR:HG21	1.84	0.59
2:C:8:SER:C	2:C:10:THR:N	2.55	0.59
2:D:104:SER:O	2:D:108:GLY:HA3	2.02	0.59
2:H:135:TYR:CZ	2:H:342:MET:HE3	2.38	0.59
2:M:135:TYR:OH	2:M:340:GLU:OE1	2.20	0.59
2:M:74:ASP:OD2	2:M:76:ASN:HB3	2.03	0.59
2:O:274:GLN:N	2:O:274:GLN:HE21	2.00	0.59
3:W:791:LEU:HD23	3:W:791:LEU:H	1.65	0.59
1:A:160:TYR:CZ	1:A:635:GLN:HB2	2.38	0.59
1:A:803:ASN:H	1:A:807:ASN:ND2	2.00	0.59
1:B:190:ASN:HD21	1:B:193:SER:CB	2.10	0.59
2:C:5:TYR:CE2	2:C:131:ASN:HA	2.36	0.59
2:D:157:ILE:HG12	2:D:214:LEU:HD13	1.84	0.59
2:J:157:ILE:HG12	2:J:214:LEU:HD13	1.84	0.59
1:B:498:ARG:HH22	2:J:25:SER:H	1.49	0.59
2:K:157:ILE:HG12	2:K:214:LEU:HD13	1.84	0.59
2:L:130:ASP:HA	2:M:17:LYS:HG2	1.83	0.59
3:W:134:ILE:HG23	3:W:136:THR:HG22	1.85	0.59
1:A:413:VAL:HG12	1:A:414:VAL:N	2.17	0.59
1:A:464:GLN:HG3	2:F:39:ILE:HD11	1.84	0.59
1:A:368:THR:HG21	1:A:582:THR:HB	1.83	0.59
2:E:274:GLN:HE21	2:E:274:GLN:N	2.00	0.59
2:G:8:SER:C	2:G:10:THR:N	2.56	0.59
2:H:157:ILE:HG12	2:H:214:LEU:HD13	1.84	0.59
2:J:124:PHE:O	2:J:127:ILE:HG13	2.03	0.59
2:D:76:ASN:H	2:L:76:ASN:HB2	1.67	0.59
3:W:687:ILE:CG2	3:W:900:MET:HG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:GLU:CD	1:A:216:GLU:N	2.55	0.59
1:A:322:THR:HG21	1:A:390:ARG:HA	1.83	0.59
1:A:409:TRP:HH2	1:A:547:THR:HG1	1.50	0.59
1:A:467:GLN:HE21	1:A:511:MET:HG2	1.67	0.59
1:A:520:THR:HG21	1:A:526:LYS:HD3	1.85	0.59
1:A:545:ASP:HA	1:A:548:ARG:CD	2.33	0.59
1:A:771:VAL:HG22	1:A:772:ILE:N	2.18	0.59
1:A:784:ALA:O	1:A:785:GLN:C	2.41	0.59
1:B:833:PHE:CZ	1:B:835:PHE:HA	2.38	0.59
2:F:8:SER:O	2:F:11:LEU:N	2.36	0.59
2:F:274:GLN:N	2:F:274:GLN:HE21	2.00	0.59
2:G:152:PHE:N	2:G:152:PHE:CD1	2.71	0.59
2:G:71:LEU:HG	2:G:72:ASN:N	2.17	0.59
2:H:85:ILE:O	2:H:89:VAL:HG23	2.03	0.59
2:J:12:LYS:C	2:J:14:ALA:N	2.55	0.59
2:L:274:GLN:HE21	2:L:274:GLN:N	2.00	0.59
2:O:4:LEU:HG	2:O:391:ILE:HG21	1.85	0.59
3:W:460:ARG:HH11	3:W:460:ARG:HG3	1.67	0.59
3:W:586:TYR:CE2	3:W:588:ALA:HB3	2.37	0.59
1:A:242:PRO:HA	1:A:841:MET:SD	2.42	0.59
1:A:401:TYR:O	1:A:404:LEU:HB2	2.02	0.59
1:A:546:LEU:HD11	1:A:588:ILE:HD12	1.83	0.59
1:A:629:ASN:C	1:A:631:LEU:H	2.02	0.59
1:A:810:TYR:CD1	1:A:811:LEU:N	2.71	0.59
1:A:722:ASN:HD22	1:A:824:LYS:HA	1.68	0.59
1:B:803:ASN:N	1:B:807:ASN:ND2	2.48	0.59
2:I:152:PHE:N	2:I:152:PHE:CD1	2.70	0.59
2:K:8:SER:C	2:K:10:THR:N	2.55	0.59
2:M:135:TYR:CZ	2:M:342:MET:HE3	2.37	0.59
2:M:38:ILE:HG22	2:M:42:ASN:HD21	1.67	0.59
2:N:109:ILE:O	2:N:109:ILE:HD12	2.03	0.59
2:O:100:MET:HG3	2:O:388:VAL:HG11	1.85	0.59
2:O:12:LYS:C	2:O:14:ALA:N	2.57	0.59
3:W:105:ASN:HB3	3:W:110:GLU:HB2	1.85	0.59
1:A:437:TYR:CE2	1:A:442:MET:HG3	2.37	0.58
1:A:484:VAL:HG12	1:A:485:ILE:H	1.68	0.58
1:A:571:LEU:HD23	1:B:531:ARG:NH2	2.17	0.58
1:A:803:ASN:O	1:A:805:ASP:N	2.36	0.58
1:B:285:ILE:C	1:B:286:LEU:HD13	2.22	0.58
1:B:326:TYR:CD1	1:B:384:ALA:HB1	2.37	0.58
1:B:745:ALA:HB1	1:B:748:THR:CB	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:116:LEU:HA	2:F:119:LEU:HD12	1.85	0.58
2:G:153:HIS:NE2	2:H:153:HIS:NE2	2.51	0.58
2:H:116:LEU:HA	2:H:119:LEU:HD12	1.84	0.58
3:W:319:PHE:N	3:W:320:PRO:CD	2.66	0.58
3:W:343:ALA:O	3:W:346:GLN:HG3	2.03	0.58
1:A:428:GLN:NE2	1:A:455:PRO:CB	2.59	0.58
1:A:508:GLU:O	1:A:512:GLN:HG3	2.02	0.58
1:B:437:TYR:CD2	1:B:443:GLN:HB3	2.38	0.58
1:B:463:ILE:HG21	1:B:468:VAL:HG11	1.84	0.58
1:A:571:LEU:HD23	1:B:531:ARG:CZ	2.32	0.58
1:B:875:ARG:HD3	1:B:878:ASN:ND2	2.18	0.58
2:C:12:LYS:C	2:C:14:ALA:N	2.56	0.58
2:C:157:ILE:HG12	2:C:214:LEU:HD13	1.84	0.58
2:G:274:GLN:HE21	2:G:274:GLN:N	2.00	0.58
2:H:22:THR:HG23	2:H:73:LEU:HD12	1.83	0.58
1:A:420:ILE:CD1	1:A:422:GLU:HG3	2.33	0.58
1:A:503:ILE:C	1:A:505:GLN:N	2.55	0.58
1:A:661:GLN:HG3	1:B:348:LYS:HZ1	1.67	0.58
1:B:111:ILE:HG22	1:B:113:PRO:HD3	1.84	0.58
1:B:190:ASN:O	1:B:192:ASN:N	2.37	0.58
1:B:223:ARG:O	1:B:226:ALA:HB3	2.03	0.58
1:B:421:ARG:O	1:B:425:VAL:HG23	2.02	0.58
2:D:274:GLN:N	2:D:274:GLN:HE21	2.00	0.58
2:E:152:PHE:N	2:E:152:PHE:CD1	2.71	0.58
2:K:260:GLU:HG2	2:K:274:GLN:HG3	1.85	0.58
2:L:5:TYR:CE2	2:L:131:ASN:HA	2.37	0.58
2:M:157:ILE:HG12	2:M:214:LEU:HD13	1.84	0.58
2:M:85:ILE:O	2:M:89:VAL:HG23	2.02	0.58
1:A:197:GLY:O	1:A:198:LYS:C	2.42	0.58
2:D:130:ASP:HA	2:E:17:LYS:HG2	1.84	0.58
2:F:5:TYR:CE2	2:F:131:ASN:HA	2.38	0.58
2:G:133:SER:O	2:G:135:TYR:N	2.35	0.58
2:I:10:THR:O	2:I:14:ALA:HB2	2.04	0.58
2:K:145:ARG:O	2:K:146:GLN:HG2	2.02	0.58
2:L:17:LYS:HG2	2:N:130:ASP:HA	1.84	0.58
3:W:105:ASN:HB2	3:W:111:ASN:CG	2.23	0.58
1:A:244:ILE:O	1:A:245:LEU:HD23	2.03	0.58
1:A:259:HIS:CD2	1:A:677:ARG:HG3	2.38	0.58
1:B:218:GLU:O	1:B:221:VAL:HG23	2.03	0.58
2:G:116:LEU:HA	2:G:119:LEU:HD12	1.84	0.58
2:G:12:LYS:C	2:G:14:ALA:N	2.57	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:130:ASP:HA	2:G:17:LYS:HG2	1.85	0.58
2:L:74:ASP:OD2	2:L:76:ASN:HB3	2.03	0.58
2:O:157:ILE:HG12	2:O:214:LEU:HD13	1.84	0.58
3:W:470:PHE:CE1	3:W:594:LYS:HD3	2.39	0.58
1:A:180:TYR:CD1	1:A:180:TYR:C	2.75	0.58
1:A:188:VAL:HG12	1:A:189:GLU:N	2.17	0.58
1:A:160:TYR:OH	1:A:635:GLN:HB2	2.04	0.58
1:B:508:GLU:O	1:B:512:GLN:HG3	2.04	0.58
2:E:22:THR:HG23	2:E:73:LEU:HD12	1.86	0.58
2:H:8:SER:C	2:H:10:THR:N	2.56	0.58
2:K:49:GLY:HA3	2:K:55:PRO:O	2.03	0.58
2:M:128:ASN:O	2:N:22:THR:HB	2.03	0.58
2:N:133:SER:O	2:N:135:TYR:N	2.36	0.58
3:W:126:THR:O	3:W:126:THR:HG23	2.03	0.58
1:A:744:TYR:C	1:A:746:GLN:H	2.07	0.58
1:B:371:ASN:HB3	1:B:583:SER:HB2	1.86	0.58
1:B:772:ILE:CG2	1:B:773:SER:N	2.66	0.58
2:C:116:LEU:HA	2:C:119:LEU:HD12	1.84	0.58
2:F:85:ILE:O	2:F:89:VAL:HG23	2.04	0.58
2:I:260:GLU:HG2	2:I:274:GLN:HG3	1.86	0.58
2:J:5:TYR:HE2	2:J:131:ASN:HA	1.69	0.58
2:K:85:ILE:O	2:K:89:VAL:HG23	2.02	0.58
2:O:260:GLU:HG2	2:O:274:GLN:HG3	1.86	0.58
3:W:22:VAL:CG2	3:W:77:TYR:HB3	2.34	0.58
3:W:744:ILE:HG13	3:W:858:LEU:HD13	1.85	0.58
1:A:613:ASN:HD22	1:A:649:LEU:HD23	1.69	0.58
1:B:340:VAL:HB	1:B:587:LEU:HD12	1.84	0.58
1:B:416:ASN:O	1:B:418:MET:N	2.36	0.58
2:E:8:SER:C	2:E:10:THR:N	2.55	0.58
2:F:260:GLU:HG2	2:F:274:GLN:HG3	1.86	0.58
2:G:8:SER:O	2:G:11:LEU:N	2.36	0.58
2:J:116:LEU:HD12	2:J:119:LEU:HD12	1.86	0.58
2:L:133:SER:O	2:L:135:TYR:N	2.36	0.58
2:M:12:LYS:C	2:M:14:ALA:N	2.57	0.58
2:N:116:LEU:HD12	2:N:119:LEU:HD12	1.86	0.58
3:W:28:TYR:CD2	3:W:72:LEU:HD13	2.37	0.58
3:W:542:LEU:HD23	3:W:558:LEU:HD23	1.86	0.58
3:W:623:THR:HG21	3:W:626:ILE:HD11	1.86	0.58
1:A:303:LEU:HA	1:A:615:ASN:HD22	1.67	0.58
1:A:365:GLN:HB2	1:A:366:PHE:CZ	2.39	0.58
1:A:420:ILE:CG1	1:A:423:SER:HB2	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:VAL:HG12	1:A:569:GLN:H	1.68	0.58
1:A:304:LEU:N	1:A:615:ASN:HD21	2.02	0.58
1:B:190:ASN:HB2	1:B:199:VAL:HG23	1.85	0.58
1:B:459:ALA:O	1:B:463:ILE:HG13	2.03	0.58
1:B:696:SER:O	1:B:827:LYS:HE3	2.04	0.58
2:C:7:LEU:O	2:C:11:LEU:HG	2.04	0.58
2:C:260:GLU:HG2	2:C:274:GLN:HG3	1.86	0.58
2:D:68:THR:O	2:D:69:THR:C	2.41	0.58
2:J:10:THR:O	2:J:14:ALA:HB2	2.04	0.58
2:K:12:LYS:C	2:K:14:ALA:N	2.56	0.58
2:O:133:SER:O	2:O:135:TYR:N	2.36	0.58
3:W:906:ASN:ND2	3:W:907:VAL:HG23	2.18	0.58
1:A:390:ARG:HD2	1:A:570:THR:HG21	1.84	0.58
1:A:803:ASN:H	1:A:807:ASN:HD22	1.50	0.58
1:B:491:GLN:HE22	1:B:566:GLN:CG	2.16	0.58
3:W:292:LEU:HD23	3:W:295:MET:CE	2.34	0.58
3:W:519:THR:CG2	3:W:520:ASP:N	2.67	0.58
2:I:274:GLN:HE21	2:I:274:GLN:N	2.00	0.57
2:I:38:ILE:HG22	2:I:42:ASN:ND2	2.16	0.57
2:K:274:GLN:HE21	2:K:274:GLN:N	2.01	0.57
2:K:53:ASN:HD22	2:K:354:ALA:CB	2.17	0.57
2:L:104:SER:HB3	2:L:108:GLY:HA2	1.86	0.57
2:L:12:LYS:C	2:L:14:ALA:N	2.56	0.57
3:W:449:LEU:HD13	3:W:573:VAL:HG13	1.85	0.57
1:A:527:ARG:O	1:A:531:ARG:CG	2.51	0.57
1:A:681:ILE:O	1:A:684:LEU:HB3	2.03	0.57
1:B:140:LYS:C	1:B:142:LEU:H	2.06	0.57
1:B:199:VAL:CG1	1:B:200:VAL:H	2.17	0.57
2:D:260:GLU:HG2	2:D:274:GLN:HG3	1.86	0.57
2:F:12:LYS:C	2:F:14:ALA:N	2.56	0.57
2:I:8:SER:O	2:I:11:LEU:N	2.36	0.57
2:I:133:SER:O	2:I:135:TYR:N	2.36	0.57
2:M:260:GLU:HG2	2:M:274:GLN:HG3	1.86	0.57
1:A:548:ARG:NH1	1:A:878:ASN:H	2.01	0.57
1:B:434:THR:HG22	1:B:434:THR:O	2.04	0.57
1:B:472:LEU:O	1:B:476:ASN:HB2	2.04	0.57
1:B:415:PRO:HB2	1:B:480:PHE:HB2	1.86	0.57
1:B:494:ASN:CG	1:B:495:ASP:H	2.07	0.57
2:E:260:GLU:HG2	2:E:274:GLN:HG3	1.86	0.57
2:F:144:ARG:HD2	2:G:82:ARG:NH1	2.19	0.57
2:G:10:THR:O	2:G:14:ALA:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:12:LYS:C	2:I:14:ALA:N	2.56	0.57
2:K:10:THR:O	2:K:14:ALA:HB2	2.05	0.57
2:K:62:ASP:O	2:K:62:ASP:CG	2.42	0.57
2:K:8:SER:O	2:K:10:THR:N	2.38	0.57
2:M:8:SER:C	2:M:10:THR:N	2.55	0.57
1:B:254:GLU:HG2	2:N:69:THR:CB	2.34	0.57
2:N:76:ASN:HB2	2:O:76:ASN:H	1.69	0.57
2:F:8:SER:C	2:F:10:THR:N	2.55	0.57
2:I:8:SER:C	2:I:10:THR:N	2.56	0.57
2:L:144:ARG:O	2:L:145:ARG:CB	2.48	0.57
3:W:690:ARG:HB3	3:W:690:ARG:HH11	1.68	0.57
1:A:127:GLU:OE2	1:A:151:LYS:HG2	2.03	0.57
1:A:342:THR:HG21	3:W:967:ILE:HG22	1.87	0.57
1:A:503:ILE:HG22	1:A:506:LEU:HB2	1.86	0.57
1:A:738:LEU:O	1:A:740:ARG:N	2.37	0.57
1:A:771:VAL:CG1	1:A:809:PHE:HB3	2.34	0.57
2:C:116:LEU:HD12	2:C:119:LEU:HD12	1.86	0.57
2:K:7:LEU:O	2:K:11:LEU:HG	2.04	0.57
2:L:7:LEU:O	2:L:11:LEU:HG	2.05	0.57
2:L:145:ARG:O	2:L:146:GLN:HG3	2.04	0.57
1:A:783:PHE:O	1:A:786:ILE:HD12	2.05	0.57
1:B:117:LYS:HB2	1:B:179:ASP:OD2	2.04	0.57
1:B:786:ILE:HG13	1:B:787:VAL:HG23	1.87	0.57
1:B:817:TRP:CD1	1:B:818:VAL:N	2.73	0.57
2:E:149:GLY:C	2:E:150:PHE:CD1	2.77	0.57
2:N:5:TYR:CE2	2:N:131:ASN:HA	2.39	0.57
3:W:561:TYR:OH	3:W:595:GLN:HB3	2.04	0.57
3:W:208:ASN:HB2	3:W:697:ASN:HD21	1.68	0.57
1:A:131:LEU:HD12	1:A:132:PRO:CD	2.35	0.57
1:A:259:HIS:ND1	1:A:260:GLN:N	2.52	0.57
1:B:246:HIS:HB3	1:B:249:ASP:OD2	2.05	0.57
1:B:477:ASN:O	1:B:478:ASN:C	2.43	0.57
1:B:518:PHE:N	1:B:518:PHE:CD1	2.72	0.57
1:B:535:LEU:O	1:B:539:ARG:CG	2.52	0.57
1:B:703:VAL:HG12	1:B:704:ILE:N	2.20	0.57
2:C:128:ASN:HB3	2:D:19:VAL:CG2	2.35	0.57
2:G:116:LEU:HD12	2:G:119:LEU:HD12	1.87	0.57
2:G:260:GLU:HG2	2:G:274:GLN:HG3	1.86	0.57
3:W:951:ILE:HG12	3:W:985:LYS:HA	1.85	0.57
1:A:163:ARG:HH22	1:A:736:GLU:CD	2.07	0.57
1:B:340:VAL:HB	1:B:587:LEU:CD1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:701:GLN:O	1:B:702:GLY:O	2.23	0.57
1:B:839:MET:C	1:B:839:MET:SD	2.83	0.57
2:I:116:LEU:HD12	2:I:119:LEU:HD12	1.86	0.57
1:B:473:HIS:CB	2:I:126:ARG:HH22	2.08	0.57
2:I:145:ARG:O	2:I:146:GLN:HG3	2.04	0.57
2:M:106:ARG:H	2:M:106:ARG:CD	2.14	0.57
2:O:150:PHE:HB2	2:O:152:PHE:HE1	1.70	0.57
3:W:853:GLN:HE21	3:W:857:LEU:HB2	1.69	0.57
1:A:187:ALA:O	1:A:188:VAL:HG23	2.04	0.57
1:A:122:LEU:HD11	1:A:201:ASP:HB2	1.85	0.57
1:A:420:ILE:CD1	1:A:423:SER:HB2	2.35	0.57
1:A:512:GLN:O	1:A:516:GLN:HG3	2.05	0.57
1:A:710:MET:CE	1:A:824:LYS:HE2	2.35	0.57
1:B:277:ARG:C	1:B:278:ILE:HG12	2.23	0.57
1:B:492:VAL:CG1	1:B:558:MET:SD	2.93	0.57
2:J:260:GLU:HG2	2:J:274:GLN:HG3	1.86	0.57
2:N:260:GLU:HG2	2:N:274:GLN:HG3	1.85	0.57
3:W:872:ILE:O	3:W:1073:ILE:HA	2.05	0.57
3:W:572:TYR:CE1	3:W:585:GLN:HG3	2.40	0.57
1:A:370:ILE:H	3:W:933:LEU:HD11	1.70	0.57
1:B:271:PHE:O	1:B:274:ILE:HB	2.05	0.57
1:B:312:ASP:O	1:B:313:ASN:HB2	2.05	0.57
1:B:673:PRO:C	1:B:674:VAL:HG22	2.26	0.57
2:C:150:PHE:HB2	2:C:152:PHE:CZ	2.40	0.57
2:E:27:VAL:O	2:E:31:ILE:HG12	2.05	0.57
2:E:35:ASN:HA	2:E:38:ILE:HD12	1.87	0.57
2:G:24:TYR:O	2:G:27:VAL:HG22	2.03	0.57
2:G:5:TYR:CE2	2:G:131:ASN:HA	2.40	0.57
2:H:7:LEU:O	2:H:11:LEU:HG	2.05	0.57
2:L:144:ARG:HD2	2:M:82:ARG:NH1	2.20	0.57
3:W:226:ALA:O	3:W:230:ILE:HG13	2.04	0.57
3:W:225:ILE:CD1	3:W:325:ILE:HD13	2.33	0.57
3:W:491:ALA:HB3	3:W:629:ASP:OD1	2.05	0.57
1:A:180:TYR:HD1	1:A:181:LEU:N	2.03	0.56
1:A:597:PRO:HB3	1:A:860:ALA:CB	2.35	0.56
1:B:137:ASN:OD1	1:B:137:ASN:O	2.22	0.56
1:B:272:ASN:C	1:B:274:ILE:N	2.54	0.56
1:B:775:ILE:HD12	1:B:775:ILE:N	2.20	0.56
1:B:790:ARG:CA	1:B:790:ARG:NE	2.47	0.56
2:D:8:SER:C	2:D:10:THR:N	2.54	0.56
2:D:116:LEU:HD12	2:D:119:LEU:HD12	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:128:ASN:HB3	2:E:19:VAL:HG23	1.87	0.56
2:G:135:TYR:OH	2:G:340:GLU:OE1	2.23	0.56
2:G:61:PHE:HA	2:G:63:PHE:HE1	1.70	0.56
2:H:42:ASN:OD1	2:H:62:ASP:HA	2.05	0.56
2:K:14:ALA:O	2:K:18:ILE:HD12	2.05	0.56
1:B:254:GLU:CG	2:N:69:THR:HB	2.35	0.56
2:N:74:ASP:OD2	2:N:76:ASN:HB3	2.05	0.56
3:W:440:PRO:HA	3:W:567:ASN:ND2	2.19	0.56
1:A:226:ALA:O	1:A:228:MET:N	2.32	0.56
1:A:332:VAL:HG13	1:A:599:THR:CG2	2.36	0.56
1:A:703:VAL:HG22	1:A:825:VAL:HG22	1.87	0.56
1:B:97:THR:HA	1:B:320:THR:HG23	1.86	0.56
2:E:12:LYS:C	2:E:14:ALA:N	2.56	0.56
2:M:139:TRP:HE1	2:M:143:ASN:HD21	1.52	0.56
2:O:110:ALA:HB1	2:O:111:PRO:CD	2.35	0.56
1:A:305:GLN:O	1:A:307:ARG:N	2.38	0.56
1:A:765:PHE:CD1	1:A:765:PHE:C	2.79	0.56
1:B:393:SER:N	1:B:573:THR:CG2	2.68	0.56
2:D:8:SER:O	2:D:10:THR:N	2.38	0.56
2:D:10:THR:O	2:D:14:ALA:HB2	2.05	0.56
2:I:116:LEU:CD1	2:I:119:LEU:HD12	2.36	0.56
2:J:152:PHE:CD1	2:J:152:PHE:N	2.71	0.56
2:K:35:ASN:HA	2:K:38:ILE:HD12	1.87	0.56
2:N:24:TYR:O	2:N:26:ASN:N	2.38	0.56
3:W:477:VAL:HA	3:W:480:MET:CE	2.35	0.56
3:W:984:ASP:O	3:W:988:ILE:HG12	2.05	0.56
1:A:135:ARG:O	1:A:136:ALA:C	2.44	0.56
1:A:275:PRO:O	1:A:278:ILE:HG13	2.05	0.56
1:A:420:ILE:HD12	1:A:422:GLU:HG3	1.87	0.56
1:A:649:LEU:O	1:A:650:HIS:O	2.24	0.56
1:B:368:THR:O	1:B:369:GLY:O	2.23	0.56
1:B:390:ARG:HG3	1:B:391:THR:H	1.69	0.56
1:B:409:TRP:CH2	1:B:413:VAL:HG21	2.40	0.56
1:B:556:THR:O	1:B:557:LEU:C	2.44	0.56
2:H:260:GLU:HG2	2:H:274:GLN:HG3	1.85	0.56
3:W:329:SER:O	3:W:332:VAL:HG22	2.05	0.56
1:A:209:ASP:O	1:A:213:GLN:HG3	2.05	0.56
1:A:410:LEU:O	1:A:413:VAL:HB	2.05	0.56
1:A:587:LEU:C	1:A:588:ILE:HG13	2.24	0.56
1:A:308:LEU:HB2	1:A:614:TYR:OH	2.06	0.56
1:A:729:GLY:C	1:A:730:PHE:CD1	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ASP:OD1	1:B:153:ASP:O	2.22	0.56
1:B:870:ALA:C	1:B:872:ASP:N	2.56	0.56
2:D:12:LYS:C	2:D:14:ALA:N	2.56	0.56
2:G:2:ASP:HB2	2:G:128:ASN:HD21	1.71	0.56
2:H:10:THR:O	2:H:14:ALA:HB2	2.06	0.56
2:H:27:VAL:CG2	2:H:31:ILE:HD11	2.35	0.56
2:J:74:ASP:OD2	2:J:76:ASN:HB3	2.04	0.56
2:M:110:ALA:HB1	2:M:111:PRO:CD	2.36	0.56
2:M:150:PHE:CD1	2:M:150:PHE:N	2.74	0.56
3:W:112:ASN:ND2	3:W:234:TYR:CE1	2.74	0.56
3:W:334:PHE:HB2	3:W:336:LYS:HE3	1.87	0.56
3:W:948:TYR:O	3:W:951:ILE:HG22	2.05	0.56
1:A:190:ASN:OD1	1:A:192:ASN:N	2.38	0.56
1:B:303:LEU:HD13	1:B:562:THR:HG21	1.88	0.56
1:B:618:ILE:O	1:B:622:VAL:HG23	2.06	0.56
2:H:108:GLY:C	2:H:110:ALA:H	2.09	0.56
2:L:38:ILE:HD12	2:L:65:LEU:HD23	1.86	0.56
2:M:10:THR:O	2:M:14:ALA:HB2	2.05	0.56
2:M:7:LEU:O	2:M:11:LEU:HG	2.06	0.56
2:N:144:ARG:O	2:N:145:ARG:CB	2.52	0.56
2:O:116:LEU:HD12	2:O:119:LEU:HD12	1.87	0.56
3:W:1059:PRO:O	3:W:1063:MET:HG3	2.06	0.56
3:W:208:ASN:HB2	3:W:697:ASN:ND2	2.20	0.56
3:W:528:GLN:O	3:W:531:THR:HG22	2.06	0.56
1:A:245:LEU:HB3	1:A:249:ASP:CB	2.34	0.56
1:B:203:GLU:O	1:B:207:ILE:HG13	2.05	0.56
1:B:246:HIS:ND1	1:B:247:PRO:HD2	2.20	0.56
2:E:109:ILE:O	2:E:109:ILE:HD12	2.05	0.56
2:E:5:TYR:HE2	2:E:131:ASN:HA	1.69	0.56
2:F:150:PHE:HB2	2:F:152:PHE:HE1	1.70	0.56
2:I:76:ASN:H	2:M:76:ASN:CB	2.13	0.56
2:L:8:SER:C	2:L:10:THR:N	2.55	0.56
2:L:260:GLU:HG2	2:L:274:GLN:HG3	1.86	0.56
3:W:385:LEU:CD2	3:W:479:LYS:HE2	2.31	0.56
3:W:499:GLN:NE2	3:W:680:ARG:HH11	2.02	0.56
1:B:392:MET:HA	1:B:573:THR:HG23	1.87	0.56
2:C:35:ASN:HA	2:C:38:ILE:HD12	1.88	0.56
2:D:38:ILE:HD12	2:D:65:LEU:CD2	2.35	0.56
2:E:8:SER:O	2:E:10:THR:N	2.39	0.56
2:F:116:LEU:HD12	2:F:119:LEU:HD12	1.88	0.56
2:F:7:LEU:O	2:F:11:LEU:HG	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:99:GLU:O	2:K:384:ARG:NH1	2.39	0.56
2:M:150:PHE:HB2	2:M:152:PHE:CZ	2.41	0.56
2:N:10:THR:O	2:N:14:ALA:HB2	2.06	0.56
3:W:781:GLU:O	3:W:784:ILE:HG22	2.05	0.56
3:W:930:ILE:O	3:W:934:ILE:HG13	2.06	0.56
1:A:319:ASP:OD2	1:A:571:LEU:CB	2.53	0.56
1:A:857:PHE:H	1:A:857:PHE:HD1	1.52	0.56
1:B:153:ASP:CG	1:B:153:ASP:O	2.43	0.56
1:B:496:ASN:HB3	1:B:498:ARG:CB	2.35	0.56
1:B:305:GLN:HE21	1:B:564:ASN:ND2	2.04	0.56
2:E:99:GLU:O	2:E:99:GLU:HG3	2.05	0.56
2:K:57:ARG:NH1	2:K:94:ASN:HD21	2.03	0.56
2:M:116:LEU:HD12	2:M:119:LEU:HD12	1.86	0.56
2:M:35:ASN:HA	2:M:38:ILE:HD12	1.86	0.56
2:O:35:ASN:HA	2:O:38:ILE:HD12	1.88	0.56
2:O:7:LEU:O	2:O:11:LEU:HG	2.06	0.56
3:W:119:PHE:CG	3:W:125:TYR:HA	2.40	0.56
1:A:389:GLN:O	1:A:389:GLN:CG	2.54	0.56
1:A:389:GLN:NE2	1:A:568:VAL:H	2.04	0.56
1:A:404:LEU:CD2	1:A:435:ILE:HD11	2.36	0.56
1:A:852:SER:O	1:A:853:ASP:HB3	2.04	0.56
2:D:128:ASN:HB3	2:E:19:VAL:CG2	2.36	0.56
2:E:38:ILE:HG22	2:E:42:ASN:ND2	2.19	0.56
1:A:461:GLN:HB3	2:F:32:GLN:NE2	2.20	0.56
2:J:8:SER:O	2:J:10:THR:N	2.39	0.56
2:J:35:ASN:HA	2:J:38:ILE:HD12	1.87	0.56
2:J:50:GLY:O	2:J:51:ILE:HB	2.05	0.56
3:W:1009:PHE:C	3:W:1010:ASN:HD22	2.09	0.56
3:W:563:GLN:OE1	3:W:566:ILE:HB	2.06	0.56
1:B:364:THR:HG23	3:W:622:ALA:HA	1.87	0.56
1:A:503:ILE:CG2	1:A:506:LEU:HB2	2.36	0.56
1:B:325:ASN:O	1:B:328:LEU:HB3	2.05	0.56
1:B:498:ARG:HG3	1:B:505:GLN:OE1	2.05	0.56
1:B:516:GLN:O	1:B:517:GLN:NE2	2.39	0.56
2:D:7:LEU:O	2:D:11:LEU:HG	2.06	0.56
2:N:7:LEU:O	2:N:11:LEU:HG	2.06	0.56
3:W:223:TYR:O	3:W:227:LYS:HB2	2.06	0.56
1:A:440:PHE:O	1:A:442:MET:N	2.38	0.55
1:A:490:ASN:HB3	1:A:492:VAL:HG23	1.88	0.55
1:A:332:VAL:HG13	1:A:599:THR:HG22	1.87	0.55
1:B:266:ASN:O	1:B:267:ASN:C	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:MET:SD	1:B:611:HIS:CD2	2.99	0.55
1:B:707:TYR:HE2	1:B:754:ASN:OD1	1.89	0.55
1:B:712:LEU:CB	1:B:819:PRO:HB2	2.36	0.55
1:B:763:LEU:HD22	1:B:764:PRO:CD	2.36	0.55
2:D:152:PHE:CD1	2:D:152:PHE:N	2.73	0.55
2:F:10:THR:O	2:F:14:ALA:HB2	2.05	0.55
2:I:145:ARG:CZ	2:I:145:ARG:HB3	2.35	0.55
2:I:57:ARG:NH1	2:I:94:ASN:HD21	2.02	0.55
3:W:441:VAL:HG22	3:W:567:ASN:HB3	1.86	0.55
1:A:314:PHE:O	1:A:316:SER:N	2.38	0.55
1:A:346:ILE:O	1:A:349:MET:HB3	2.06	0.55
1:A:414:VAL:O	1:A:416:ASN:N	2.38	0.55
1:A:738:LEU:HA	1:A:741:THR:HG22	1.88	0.55
1:B:260:GLN:O	1:B:262:VAL:N	2.39	0.55
1:B:363:GLU:O	1:B:363:GLU:HG3	2.05	0.55
2:E:129:PHE:CD1	2:E:129:PHE:C	2.80	0.55
2:F:53:ASN:HD22	2:F:354:ALA:HB3	1.71	0.55
3:W:255:VAL:O	3:W:673:VAL:HG21	2.06	0.55
3:W:309:ASP:O	3:W:312:VAL:HG22	2.06	0.55
3:W:524:TRP:NE1	3:W:607:LEU:HD13	2.21	0.55
1:A:535:LEU:O	1:A:539:ARG:CG	2.55	0.55
1:A:396:PHE:CB	1:A:578:LEU:HD12	2.37	0.55
1:B:127:GLU:HB3	1:B:151:LYS:HE3	1.87	0.55
1:B:433:ASN:HD21	1:B:446:HIS:HB3	1.71	0.55
2:C:153:HIS:CD2	2:E:153:HIS:NE2	2.75	0.55
2:F:144:ARG:O	2:F:145:ARG:HB2	2.06	0.55
2:N:8:SER:C	2:N:10:THR:N	2.55	0.55
2:N:116:LEU:CD1	2:N:119:LEU:HD12	2.36	0.55
2:N:99:GLU:O	2:N:99:GLU:HG3	2.06	0.55
2:O:8:SER:O	2:O:10:THR:N	2.40	0.55
3:W:573:VAL:HG23	3:W:586:TYR:HB2	1.88	0.55
3:W:750:LEU:HD21	3:W:861:LEU:CD2	2.34	0.55
3:W:761:SER:OG	3:W:762:THR:N	2.38	0.55
1:A:275:PRO:HB2	1:A:278:ILE:HG13	1.87	0.55
1:A:725:ARG:HB3	1:A:828:GLN:OE1	2.06	0.55
1:A:804:SER:HB2	1:A:810:TYR:CB	2.35	0.55
1:B:428:GLN:HG3	1:B:456:PHE:HD1	1.70	0.55
2:C:99:GLU:HG3	2:C:99:GLU:O	2.07	0.55
2:H:12:LYS:C	2:H:14:ALA:N	2.56	0.55
2:I:35:ASN:HA	2:I:38:ILE:HD12	1.87	0.55
2:J:116:LEU:CD1	2:J:119:LEU:HD12	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:301:VAL:C	3:W:304:PRO:HD2	2.26	0.55
3:W:530:ASN:O	3:W:533:PRO:HD2	2.06	0.55
1:A:150:LEU:HD12	1:A:696:SER:CB	2.34	0.55
1:A:822:THR:C	1:A:823:THR:HG23	2.26	0.55
1:B:413:VAL:HG12	1:B:414:VAL:H	1.69	0.55
1:B:868:ALA:C	1:B:876:ILE:HG23	2.26	0.55
2:G:106:ARG:N	2:G:106:ARG:HD3	2.22	0.55
2:J:14:ALA:C	2:J:16:ASP:H	2.10	0.55
2:J:128:ASN:HB3	2:K:19:VAL:CG2	2.36	0.55
2:N:6:SER:OG	2:N:128:ASN:HA	2.05	0.55
3:W:109:TYR:HD1	3:W:129:LEU:HD13	1.70	0.55
1:A:383:ILE:HD11	1:A:550:LEU:HD23	1.89	0.55
1:A:744:TYR:C	1:A:746:GLN:N	2.60	0.55
1:B:508:GLU:HG2	1:B:512:GLN:HE21	1.71	0.55
1:B:625:ILE:O	1:B:628:ALA:HB3	2.06	0.55
1:B:650:HIS:O	1:B:652:PHE:N	2.39	0.55
1:B:675:GLU:O	1:B:676:VAL:C	2.44	0.55
1:B:675:GLU:HB3	1:B:678:ARG:HG3	1.88	0.55
1:B:723:ILE:HG22	1:B:724:ALA:N	2.16	0.55
1:B:804:SER:HA	1:B:810:TYR:CZ	2.42	0.55
2:C:144:ARG:HD2	2:D:82:ARG:NH1	2.20	0.55
2:C:145:ARG:O	2:C:146:GLN:HG3	2.06	0.55
2:D:116:LEU:CD1	2:D:119:LEU:HD12	2.36	0.55
2:F:8:SER:O	2:F:10:THR:N	2.39	0.55
2:G:63:PHE:N	2:G:63:PHE:CD1	2.74	0.55
2:H:116:LEU:HD12	2:H:119:LEU:HD12	1.89	0.55
2:L:116:LEU:HD12	2:L:119:LEU:HD12	1.87	0.55
2:L:35:ASN:HA	2:L:38:ILE:HD12	1.87	0.55
2:O:144:ARG:O	2:O:145:ARG:HG2	2.07	0.55
2:O:10:THR:O	2:O:14:ALA:HB2	2.06	0.55
3:W:451:ARG:HH21	3:W:459:THR:HG21	1.72	0.55
3:W:882:LYS:HB3	3:W:883:PRO:HD3	1.89	0.55
1:A:732:GLN:O	1:A:733:ILE:HG23	2.06	0.55
1:B:371:ASN:O	1:B:373:GLN:N	2.39	0.55
1:B:784:ALA:O	1:B:785:GLN:O	2.25	0.55
2:C:10:THR:O	2:C:14:ALA:HB2	2.06	0.55
2:C:82:ARG:NH1	2:E:144:ARG:HD2	2.21	0.55
2:H:99:GLU:HG3	2:H:99:GLU:O	2.07	0.55
2:I:89:VAL:O	2:I:91:PHE:N	2.40	0.55
2:L:8:SER:O	2:L:10:THR:N	2.39	0.55
2:O:49:GLY:HA2	2:O:54:LEU:CD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:473:GLN:O	3:W:477:VAL:HG23	2.06	0.55
3:W:584:ILE:HG13	3:W:585:GLN:O	2.06	0.55
1:A:510:LEU:HD22	1:A:540:LEU:CD1	2.26	0.55
1:A:563:MET:O	1:A:565:MET:N	2.40	0.55
1:B:113:PRO:HG2	1:B:609:ASN:HB3	1.89	0.55
1:B:122:LEU:HG	1:B:201:ASP:CG	2.27	0.55
1:B:160:TYR:OH	1:B:635:GLN:HG3	2.07	0.55
1:B:763:LEU:O	1:B:764:PRO:O	2.25	0.55
2:C:152:PHE:N	2:C:152:PHE:CD1	2.74	0.55
2:H:8:SER:O	2:H:10:THR:N	2.40	0.55
2:I:101:VAL:HB	2:I:355:ILE:HG21	1.88	0.55
2:I:153:HIS:NE2	2:J:153:HIS:CD2	2.75	0.55
2:I:60:ASN:C	2:I:61:PHE:CD1	2.80	0.55
2:J:38:ILE:HG22	2:J:42:ASN:ND2	2.22	0.55
2:K:35:ASN:HA	2:K:38:ILE:CD1	2.37	0.55
3:W:559:ASN:HA	3:W:562:LYS:NZ	2.22	0.55
3:W:952:SER:OG	3:W:1071:TRP:HE3	1.90	0.55
1:B:787:VAL:O	1:B:788:LYS:C	2.46	0.55
2:G:8:SER:O	2:G:10:THR:N	2.40	0.55
2:L:116:LEU:CD1	2:L:119:LEU:HD12	2.37	0.55
2:L:10:THR:O	2:L:14:ALA:HB2	2.06	0.55
2:M:99:GLU:HG3	2:M:99:GLU:O	2.07	0.55
3:W:449:LEU:HD21	3:W:461:ILE:CD1	2.37	0.55
1:A:500:GLY:O	1:A:502:VAL:N	2.36	0.55
1:B:360:ILE:HD12	1:B:360:ILE:N	2.22	0.55
1:B:654:VAL:O	1:B:656:ARG:N	2.39	0.55
1:B:698:LYS:O	1:B:699:ILE:CB	2.53	0.55
2:C:109:ILE:HG23	2:C:110:ALA:H	1.70	0.55
2:C:116:LEU:CD1	2:C:119:LEU:HD12	2.36	0.55
2:C:167:ASN:ND2	2:C:178:GLY:HA2	2.23	0.55
2:E:7:LEU:O	2:E:11:LEU:HG	2.07	0.55
2:F:144:ARG:O	2:F:145:ARG:CB	2.55	0.55
2:F:152:PHE:CD1	2:F:152:PHE:N	2.74	0.55
2:N:35:ASN:HA	2:N:38:ILE:HD12	1.89	0.55
3:W:864:PRO:O	3:W:865:VAL:HG12	2.07	0.55
1:A:142:LEU:O	1:A:143:ARG:HG2	2.08	0.54
1:A:525:TYR:O	1:A:529:ILE:HG13	2.05	0.54
1:A:705:ILE:HG22	1:A:757:VAL:O	2.07	0.54
1:A:717:MET:HE1	1:A:830:PRO:O	2.07	0.54
1:B:195:ASP:O	1:B:197:GLY:N	2.39	0.54
1:B:245:LEU:HD12	1:B:250:TYR:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:116:LEU:HD12	2:E:119:LEU:HD12	1.88	0.54
2:J:131:ASN:N	2:J:131:ASN:HD22	2.04	0.54
2:L:82:ARG:NH1	2:N:144:ARG:HD2	2.22	0.54
2:N:8:SER:O	2:N:10:THR:N	2.40	0.54
3:W:536:LYS:O	3:W:540:MET:HG3	2.07	0.54
1:A:742:GLY:HA3	1:B:285:ILE:HD11	1.89	0.54
1:B:388:SER:O	1:B:389:GLN:HB2	2.07	0.54
1:B:779:ASP:HA	1:B:798:ILE:HG13	1.89	0.54
2:C:135:TYR:OH	2:C:340:GLU:OE1	2.24	0.54
2:C:22:THR:HB	2:E:128:ASN:O	2.08	0.54
2:D:144:ARG:HD2	2:E:82:ARG:CZ	2.36	0.54
2:G:35:ASN:HA	2:G:38:ILE:HD12	1.89	0.54
2:I:8:SER:O	2:I:10:THR:N	2.40	0.54
2:I:124:PHE:O	2:I:126:ARG:N	2.39	0.54
2:J:35:ASN:HA	2:J:38:ILE:CD1	2.37	0.54
2:I:153:HIS:CD2	2:K:153:HIS:NE2	2.75	0.54
2:O:35:ASN:HA	2:O:38:ILE:CD1	2.37	0.54
3:W:186:ASN:ND2	3:W:190:ARG:H	2.06	0.54
3:W:346:GLN:HG2	3:W:586:TYR:CZ	2.42	0.54
3:W:476:VAL:O	3:W:480:MET:HG3	2.07	0.54
3:W:582:LYS:HG2	3:W:583:LYS:H	1.71	0.54
3:W:398:SER:HA	3:W:838:LYS:HE2	1.90	0.54
1:A:120:THR:HA	1:A:186:MET:HE1	1.88	0.54
1:A:151:LYS:O	1:A:152:LYS:HB2	2.06	0.54
1:A:166:PHE:CE2	1:A:689:MET:HG3	2.42	0.54
1:A:393:SER:HB2	1:A:573:THR:HG21	1.90	0.54
1:A:717:MET:SD	1:A:829:VAL:HG22	2.47	0.54
1:A:730:PHE:CD1	1:A:730:PHE:N	2.75	0.54
1:A:863:VAL:HG12	1:A:864:GLU:N	2.22	0.54
1:A:871:PHE:O	1:A:871:PHE:CD1	2.60	0.54
2:E:35:ASN:HA	2:E:38:ILE:CD1	2.37	0.54
2:H:116:LEU:CD1	2:H:119:LEU:HD12	2.38	0.54
2:H:150:PHE:HB2	2:H:152:PHE:CE1	2.43	0.54
2:I:49:GLY:HA2	2:I:54:LEU:HD21	1.90	0.54
2:M:8:SER:O	2:M:10:THR:N	2.40	0.54
2:O:116:LEU:CD1	2:O:119:LEU:HD12	2.37	0.54
2:O:144:ARG:O	2:O:146:GLN:N	2.41	0.54
3:W:166:ARG:HH11	3:W:166:ARG:HG2	1.72	0.54
3:W:449:LEU:HD11	3:W:461:ILE:HD12	1.89	0.54
3:W:8:LEU:HD12	3:W:737:MET:CG	2.31	0.54
1:A:111:ILE:HG23	1:A:111:ILE:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:GLU:HG2	1:A:662:MET:CE	2.37	0.54
1:B:404:LEU:O	1:B:407:GLY:N	2.40	0.54
2:C:8:SER:O	2:C:10:THR:N	2.40	0.54
2:D:110:ALA:HB1	2:D:111:PRO:HD2	1.89	0.54
2:C:16:ASP:HB3	2:E:131:ASN:O	2.06	0.54
2:F:65:LEU:O	2:F:66:LEU:HD23	2.08	0.54
2:N:42:ASN:HA	2:N:61:PHE:HB2	1.88	0.54
3:W:186:ASN:HD22	3:W:186:ASN:N	1.96	0.54
3:W:491:ALA:HB2	3:W:627:ARG:HD2	1.88	0.54
1:A:530:GLN:HA	1:A:533:ILE:CD1	2.37	0.54
1:A:633:LEU:C	1:A:635:GLN:H	2.11	0.54
1:A:663:TYR:O	1:A:666:ARG:HG2	2.08	0.54
1:B:323:THR:O	1:B:326:TYR:HB3	2.08	0.54
1:B:326:TYR:CD1	1:B:384:ALA:CB	2.91	0.54
1:B:370:ILE:O	1:B:373:GLN:HB3	2.08	0.54
1:B:506:LEU:HD21	1:B:543:LEU:C	2.27	0.54
2:E:10:THR:O	2:E:14:ALA:HB2	2.07	0.54
2:F:35:ASN:HA	2:F:38:ILE:HD12	1.90	0.54
2:H:74:ASP:OD2	2:H:76:ASN:HB3	2.07	0.54
1:B:481:ARG:HG2	2:I:65:LEU:HD12	1.89	0.54
3:W:772:ILE:CD1	3:W:1047:LYS:HB2	2.37	0.54
3:W:134:ILE:HG13	3:W:698:ASN:OD1	2.08	0.54
1:B:666:ARG:HG3	1:B:667:ASP:N	2.20	0.54
2:E:116:LEU:CD1	2:E:119:LEU:HD12	2.38	0.54
2:E:167:ASN:ND2	2:E:178:GLY:HA2	2.22	0.54
2:I:167:ASN:ND2	2:I:178:GLY:HA2	2.22	0.54
2:J:7:LEU:O	2:J:11:LEU:HG	2.06	0.54
2:N:110:ALA:HB1	2:N:111:PRO:CD	2.37	0.54
2:O:158:PHE:HE2	2:O:214:LEU:HD22	1.73	0.54
3:W:248:MET:HE2	3:W:252:VAL:HG12	1.89	0.54
3:W:364:THR:OG1	3:W:533:PRO:HB3	2.07	0.54
1:A:217:THR:O	1:A:217:THR:HG22	2.07	0.54
1:A:501:HIS:C	1:A:503:ILE:H	2.09	0.54
1:B:428:GLN:HG2	1:B:429:LEU:H	1.71	0.54
1:B:875:ARG:CD	1:B:878:ASN:HD22	2.20	0.54
2:C:14:ALA:C	2:C:16:ASP:H	2.10	0.54
2:C:35:ASN:HA	2:C:38:ILE:CD1	2.38	0.54
2:D:14:ALA:C	2:D:16:ASP:H	2.11	0.54
2:H:35:ASN:HA	2:H:38:ILE:HD12	1.89	0.54
2:I:106:ARG:HD3	2:I:106:ARG:H	1.72	0.54
2:J:99:GLU:HG3	2:J:99:GLU:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:139:TRP:HE1	2:M:143:ASN:ND2	2.04	0.54
2:O:14:ALA:C	2:O:16:ASP:H	2.11	0.54
3:W:1082:ASN:O	3:W:1084:ASN:N	2.40	0.54
3:W:195:VAL:HG23	3:W:196:MET:H	1.73	0.54
3:W:473:GLN:HB3	3:W:594:LYS:HB3	1.90	0.54
3:W:816:SER:HB3	3:W:820:LEU:CD1	2.38	0.54
1:A:311:HIS:HB3	1:A:318:TRP:NE1	2.23	0.54
1:A:645:PHE:HD2	1:A:646:LEU:HD23	1.72	0.54
1:A:650:HIS:O	1:A:651:ILE:CB	2.56	0.54
1:A:701:GLN:HG2	1:A:826:TYR:CE2	2.43	0.54
1:A:738:LEU:C	1:A:740:ARG:N	2.62	0.54
1:B:501:HIS:C	1:B:503:ILE:N	2.60	0.54
2:F:158:PHE:HE2	2:F:214:LEU:HD22	1.73	0.54
2:K:14:ALA:C	2:K:16:ASP:H	2.11	0.54
2:M:167:ASN:ND2	2:M:178:GLY:HA2	2.23	0.54
3:W:573:VAL:CG1	3:W:575:ILE:HG13	2.38	0.54
3:W:736:ILE:O	3:W:740:THR:HG23	2.07	0.54
1:A:178:PRO:HD2	1:A:256:PHE:CE2	2.43	0.54
1:B:427:CYS:O	1:B:431:ILE:HG13	2.08	0.54
1:B:771:VAL:CG1	1:B:772:ILE:N	2.71	0.54
2:D:167:ASN:ND2	2:D:178:GLY:HA2	2.23	0.54
2:G:116:LEU:CD1	2:G:119:LEU:HD12	2.38	0.54
2:K:158:PHE:HE2	2:K:214:LEU:HD22	1.73	0.54
2:L:128:ASN:O	2:M:22:THR:HB	2.08	0.54
2:L:72:ASN:ND2	2:N:126:ARG:NH1	2.56	0.54
1:A:273:TYR:O	1:A:273:TYR:CD2	2.61	0.54
1:A:298:TYR:O	1:A:299:ILE:HB	2.06	0.54
1:B:457:GLN:CB	1:B:476:ASN:ND2	2.63	0.54
1:B:653:ASP:O	1:B:654:VAL:C	2.46	0.54
2:C:67:GLY:C	2:C:69:THR:H	2.09	0.54
2:D:35:ASN:HA	2:D:38:ILE:HD12	1.89	0.54
2:I:7:LEU:O	2:I:11:LEU:HG	2.08	0.54
2:J:27:VAL:O	2:J:30:LEU:N	2.40	0.54
2:M:116:LEU:CD1	2:M:119:LEU:HD12	2.37	0.54
2:N:167:ASN:ND2	2:N:178:GLY:HA2	2.22	0.54
1:A:804:SER:HB2	1:A:810:TYR:HA	1.89	0.53
1:B:125:ILE:HB	1:B:126:PHE:CD2	2.43	0.53
1:B:125:ILE:CD1	1:B:125:ILE:N	2.71	0.53
1:B:457:GLN:O	1:B:458:ILE:HG13	2.08	0.53
1:B:503:ILE:HD13	1:B:544:VAL:HG12	1.88	0.53
1:B:393:SER:CB	1:B:573:THR:HG21	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:862:THR:HG22	1:B:863:VAL:O	2.09	0.53
2:E:74:ASP:OD2	2:E:76:ASN:HB3	2.08	0.53
2:F:116:LEU:CD1	2:F:119:LEU:HD12	2.38	0.53
2:G:150:PHE:HB2	2:G:152:PHE:CE1	2.43	0.53
2:G:22:THR:OG1	2:G:26:ASN:ND2	2.41	0.53
2:H:23:LEU:N	2:H:26:ASN:ND2	2.57	0.53
2:H:135:TYR:OH	2:H:340:GLU:OE1	2.25	0.53
2:I:158:PHE:HE2	2:I:214:LEU:HD22	1.73	0.53
2:K:116:LEU:HD12	2:K:119:LEU:HD12	1.89	0.53
2:M:35:ASN:HA	2:M:38:ILE:CD1	2.38	0.53
3:W:186:ASN:HD21	3:W:190:ARG:N	2.05	0.53
3:W:410:PHE:HD1	3:W:807:THR:HG21	1.73	0.53
1:A:306:ASP:C	1:A:308:LEU:N	2.56	0.53
1:B:252:PHE:O	1:B:254:GLU:N	2.40	0.53
1:B:467:GLN:HB3	1:B:512:GLN:HG2	1.90	0.53
2:G:128:ASN:HB3	2:H:19:VAL:CG2	2.37	0.53
2:G:46:PHE:CE2	2:G:119:LEU:HD21	2.43	0.53
2:K:150:PHE:HB2	2:K:152:PHE:CZ	2.42	0.53
2:K:167:ASN:ND2	2:K:178:GLY:HA2	2.22	0.53
2:L:153:HIS:NE2	2:N:153:HIS:NE2	2.55	0.53
2:N:14:ALA:C	2:N:16:ASP:H	2.10	0.53
2:N:89:VAL:O	2:N:91:PHE:N	2.41	0.53
3:W:222:ASP:OD1	3:W:324:LYS:HD3	2.08	0.53
3:W:796:SER:OG	3:W:845:ILE:HG23	2.09	0.53
1:B:140:LYS:C	1:B:142:LEU:N	2.60	0.53
1:B:449:ASN:HD21	1:B:455:PRO:CG	2.21	0.53
2:C:158:PHE:HE2	2:C:214:LEU:HD22	1.73	0.53
2:D:70:LEU:HD12	2:D:71:LEU:H	1.74	0.53
2:G:130:ASP:HA	2:H:17:LYS:HG2	1.90	0.53
2:K:215:ARG:HG3	2:K:371:ILE:O	2.09	0.53
2:N:158:PHE:HE2	2:N:214:LEU:HD22	1.73	0.53
2:N:49:GLY:HA2	2:N:54:LEU:CD2	2.39	0.53
2:O:24:TYR:O	2:O:27:VAL:HG22	2.09	0.53
1:A:503:ILE:HG22	1:A:506:LEU:H	1.73	0.53
1:A:705:ILE:HG12	1:A:705:ILE:O	2.07	0.53
1:B:211:ILE:O	1:B:213:GLN:N	2.41	0.53
2:D:99:GLU:CD	2:D:116:LEU:HD22	2.28	0.53
2:E:116:LEU:HA	2:E:119:LEU:CD1	2.38	0.53
2:F:99:GLU:HG3	2:F:99:GLU:O	2.08	0.53
2:I:35:ASN:HA	2:I:38:ILE:CD1	2.38	0.53
2:J:150:PHE:HB2	2:J:152:PHE:CZ	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:38:ILE:O	2:L:42:ASN:OD1	2.27	0.53
2:O:215:ARG:HG3	2:O:371:ILE:O	2.09	0.53
3:W:221:ASP:O	3:W:225:ILE:HG13	2.09	0.53
3:W:240:LEU:O	3:W:244:VAL:HG23	2.09	0.53
1:A:542:GLN:O	1:A:545:ASP:HB2	2.08	0.53
1:A:771:VAL:O	1:A:772:ILE:C	2.46	0.53
1:B:182:LEU:HD23	1:B:183:LEU:N	2.15	0.53
1:B:199:VAL:HG12	1:B:200:VAL:H	1.70	0.53
1:B:122:LEU:HD11	1:B:200:VAL:HG12	1.88	0.53
1:B:246:HIS:CE1	1:B:247:PRO:HD2	2.44	0.53
1:B:497:ILE:HG23	2:I:68:THR:HG23	1.89	0.53
1:B:170:TYR:CE1	1:B:681:ILE:CG2	2.92	0.53
1:B:94:THR:HG23	1:B:658:PRO:HG3	1.90	0.53
2:D:144:ARG:HD2	2:E:82:ARG:NH1	2.23	0.53
2:G:99:GLU:O	2:G:99:GLU:HG3	2.09	0.53
2:H:158:PHE:HE2	2:H:214:LEU:HD22	1.73	0.53
2:I:215:ARG:HG3	2:I:371:ILE:O	2.09	0.53
2:J:116:LEU:HA	2:J:119:LEU:CD1	2.38	0.53
2:L:158:PHE:HE2	2:L:214:LEU:HD22	1.73	0.53
2:L:63:PHE:N	2:L:63:PHE:CD1	2.75	0.53
2:N:215:ARG:HG3	2:N:371:ILE:O	2.09	0.53
3:W:293:ASP:O	3:W:297:LYS:HG2	2.08	0.53
3:W:387:ARG:HB3	3:W:387:ARG:NH1	2.22	0.53
1:B:361:GLN:NE2	3:W:624:LYS:NZ	2.54	0.53
3:W:873:THR:HA	3:W:1073:ILE:HG23	1.89	0.53
1:A:311:HIS:NE2	1:A:566:GLN:NE2	2.54	0.53
1:A:546:LEU:HD22	1:A:584:LEU:HD21	1.90	0.53
1:A:560:CYS:CB	1:A:603:TYR:HD2	2.21	0.53
1:B:133:ILE:HD11	1:B:147:TYR:CE1	2.43	0.53
1:B:200:VAL:HB	1:B:204:THR:HG21	1.89	0.53
1:B:298:TYR:CD1	1:B:299:ILE:N	2.75	0.53
1:B:428:GLN:CG	1:B:456:PHE:HD1	2.21	0.53
1:B:498:ARG:HG3	1:B:505:GLN:HE22	1.73	0.53
1:B:770:SER:HB3	1:B:772:ILE:HG22	1.90	0.53
3:W:12:LEU:HD22	3:W:16:TYR:HE2	1.73	0.53
3:W:864:PRO:HB3	3:W:867:PHE:HE2	1.73	0.53
1:A:642:VAL:HG13	1:A:665:LEU:HD23	1.90	0.53
2:D:116:LEU:HA	2:D:119:LEU:CD1	2.39	0.53
2:E:158:PHE:HE2	2:E:214:LEU:HD22	1.73	0.53
2:G:158:PHE:HE2	2:G:214:LEU:HD22	1.73	0.53
2:J:158:PHE:HE2	2:J:214:LEU:HD22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:131:ASN:HD22	2:K:131:ASN:N	2.05	0.53
2:L:215:ARG:HG3	2:L:371:ILE:O	2.09	0.53
2:N:35:ASN:HA	2:N:38:ILE:CD1	2.38	0.53
2:O:167:ASN:ND2	2:O:178:GLY:HA2	2.22	0.53
3:W:426:ASP:HB3	3:W:432:ARG:NH2	2.24	0.53
3:W:345:ASP:HB2	3:W:458:ARG:CZ	2.39	0.53
1:A:238:VAL:HG12	1:A:239:VAL:N	2.24	0.53
1:A:487:GLY:O	1:A:488:VAL:HG23	2.08	0.53
1:A:491:GLN:HB3	1:A:564:ASN:HB3	1.90	0.53
1:A:647:LYS:C	1:A:649:LEU:H	2.12	0.53
1:B:400:ASN:ND2	1:B:403:SER:OG	2.41	0.53
1:B:436:ILE:O	1:B:438:PRO:N	2.42	0.53
1:B:458:ILE:HD12	1:B:458:ILE:C	2.29	0.53
1:B:577:GLN:C	1:B:579:THR:N	2.60	0.53
2:E:110:ALA:HB1	2:E:111:PRO:CD	2.39	0.53
2:F:14:ALA:C	2:F:16:ASP:H	2.11	0.53
2:F:144:ARG:HD2	2:G:82:ARG:CZ	2.38	0.53
2:I:116:LEU:HA	2:I:119:LEU:CD1	2.38	0.53
2:I:144:ARG:HD2	2:J:82:ARG:NH1	2.24	0.53
1:B:498:ARG:CB	2:I:32:GLN:NE2	2.66	0.53
2:I:99:GLU:O	2:I:99:GLU:HG3	2.09	0.53
2:O:74:ASP:OD2	2:O:76:ASN:HB3	2.09	0.53
3:W:7:ILE:HA	3:W:10:GLU:OE1	2.08	0.53
3:W:985:LYS:HB3	3:W:985:LYS:NZ	2.24	0.53
1:A:271:PHE:O	1:A:274:ILE:HD12	2.08	0.53
1:A:325:ASN:O	1:A:328:LEU:HB3	2.09	0.53
1:A:550:LEU:O	1:A:551:ALA:C	2.47	0.53
1:A:771:VAL:HA	1:A:802:ILE:HD11	1.91	0.53
1:A:853:ASP:O	1:A:854:LEU:CB	2.56	0.53
1:A:876:ILE:HG22	1:A:877:MET:HG2	1.89	0.53
1:B:371:ASN:C	1:B:373:GLN:H	2.11	0.53
1:B:755:GLN:O	1:B:757:VAL:HG23	2.08	0.53
1:B:786:ILE:O	1:B:788:LYS:N	2.41	0.53
1:B:548:ARG:HD3	1:B:877:MET:H	1.73	0.53
2:C:215:ARG:HG3	2:C:371:ILE:O	2.09	0.53
2:H:167:ASN:ND2	2:H:178:GLY:HA2	2.23	0.53
2:H:215:ARG:HG3	2:H:371:ILE:O	2.09	0.53
2:K:116:LEU:CD1	2:K:119:LEU:HD12	2.39	0.53
2:K:46:PHE:CE2	2:K:119:LEU:HD21	2.41	0.53
2:K:65:LEU:C	2:K:66:LEU:HG	2.29	0.53
2:M:145:ARG:NH1	2:M:145:ARG:CB	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:158:PHE:HE2	2:M:214:LEU:HD22	1.74	0.53
2:N:31:ILE:O	2:N:34:PHE:HB3	2.09	0.53
2:O:89:VAL:O	2:O:91:PHE:N	2.42	0.53
3:W:161:LYS:CB	3:W:165:ARG:HH12	2.21	0.53
3:W:232:LEU:HD21	3:W:299:GLY:HA3	1.90	0.53
3:W:519:THR:CG2	3:W:520:ASP:H	2.21	0.53
3:W:627:ARG:HG2	3:W:627:ARG:NH1	2.16	0.53
1:B:182:LEU:CD2	1:B:183:LEU:N	2.71	0.53
1:A:661:GLN:NE2	1:B:348:LYS:HZ2	2.06	0.53
1:B:387:LEU:O	1:B:389:GLN:N	2.42	0.53
1:B:508:GLU:OE2	2:J:70:LEU:HD23	2.09	0.53
1:B:501:HIS:ND1	1:B:548:ARG:HG2	2.24	0.53
1:B:642:VAL:O	1:B:645:PHE:HB3	2.09	0.53
1:B:654:VAL:HG12	1:B:655:ALA:N	2.24	0.53
1:B:708:ARG:O	1:B:710:MET:N	2.42	0.53
2:D:35:ASN:HA	2:D:38:ILE:CD1	2.39	0.53
2:F:167:ASN:ND2	2:F:178:GLY:HA2	2.22	0.53
2:G:215:ARG:HG3	2:G:371:ILE:O	2.09	0.53
2:J:215:ARG:HG3	2:J:371:ILE:O	2.09	0.53
2:M:215:ARG:HG3	2:M:371:ILE:O	2.09	0.53
2:O:99:GLU:O	2:O:99:GLU:HG3	2.09	0.53
3:W:109:TYR:HA	3:W:118:LEU:CD2	2.39	0.53
3:W:421:ASN:OD1	3:W:422:MET:N	2.42	0.53
1:A:323:THR:O	1:A:326:TYR:HB3	2.08	0.52
1:A:401:TYR:N	1:A:401:TYR:CD1	2.75	0.52
1:A:428:GLN:CD	1:A:456:PHE:HB2	2.27	0.52
1:A:606:VAL:O	1:A:607:ASN:C	2.46	0.52
1:A:721:VAL:CG1	1:A:799:LEU:HD22	2.39	0.52
1:A:794:THR:HG22	1:A:794:THR:O	2.08	0.52
1:A:297:ARG:HG3	1:A:848:PHE:CE2	2.43	0.52
1:B:437:TYR:HD2	1:B:443:GLN:HB3	1.73	0.52
1:B:499:ASN:O	1:B:500:GLY:O	2.27	0.52
1:B:504:ASN:O	1:B:505:GLN:C	2.46	0.52
1:B:654:VAL:O	1:B:657:VAL:HG23	2.08	0.52
1:B:742:GLY:O	1:B:744:TYR:CE2	2.62	0.52
2:I:14:ALA:C	2:I:16:ASP:H	2.11	0.52
2:J:129:PHE:CD1	2:J:129:PHE:C	2.82	0.52
2:J:139:TRP:C	2:J:139:TRP:CD1	2.83	0.52
2:K:89:VAL:O	2:K:91:PHE:N	2.43	0.52
2:L:152:PHE:N	2:L:152:PHE:CD1	2.77	0.52
3:W:168:ASP:O	3:W:171:THR:HB	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:TYR:O	1:A:259:HIS:HB3	2.08	0.52
1:A:424:LEU:HD12	1:A:424:LEU:O	2.08	0.52
1:A:618:ILE:HD13	1:A:645:PHE:CZ	2.44	0.52
1:A:722:ASN:C	1:A:723:ILE:HG13	2.29	0.52
1:B:135:ARG:O	1:B:138:GLY:N	2.43	0.52
1:B:326:TYR:CE1	1:B:384:ALA:HB3	2.44	0.52
1:B:466:PHE:O	1:B:467:GLN:C	2.47	0.52
1:B:663:TYR:O	1:B:666:ARG:HG2	2.09	0.52
2:L:61:PHE:O	2:L:62:ASP:HB3	2.07	0.52
2:M:48:THR:O	2:M:56:ILE:HA	2.10	0.52
3:W:420:LYS:HA	3:W:423:HIS:CD2	2.44	0.52
1:A:329:ALA:O	1:A:333:VAL:HG23	2.10	0.52
1:A:340:VAL:HB	1:A:587:LEU:CD2	2.39	0.52
1:A:658:PRO:HB2	1:A:660:ASP:OD1	2.09	0.52
1:B:311:HIS:CD2	1:B:566:GLN:OE1	2.62	0.52
1:B:525:TYR:O	1:B:529:ILE:HG13	2.08	0.52
2:C:381:ASN:O	2:C:385:VAL:HB	2.10	0.52
2:D:158:PHE:HE2	2:D:214:LEU:HD22	1.74	0.52
2:D:215:ARG:HG3	2:D:371:ILE:O	2.09	0.52
2:D:42:ASN:HA	2:D:61:PHE:HB2	1.92	0.52
2:E:14:ALA:C	2:E:16:ASP:H	2.11	0.52
2:H:150:PHE:HB2	2:H:152:PHE:CZ	2.44	0.52
2:M:101:VAL:HG23	2:M:102:ARG:N	2.24	0.52
2:M:116:LEU:HA	2:M:119:LEU:CD1	2.38	0.52
2:O:110:ALA:HB1	2:O:111:PRO:HD2	1.90	0.52
2:O:116:LEU:HA	2:O:119:LEU:CD1	2.39	0.52
3:W:823:LYS:HE2	3:W:825:ASN:OD1	2.09	0.52
3:W:496:GLN:HB3	3:W:920:GLN:HB2	1.91	0.52
1:A:200:VAL:O	1:A:204:THR:OG1	2.17	0.52
1:A:361:GLN:HG3	1:A:362:SER:H	1.75	0.52
1:A:326:TYR:CD1	1:A:384:ALA:CB	2.92	0.52
1:A:555:GLU:OE2	1:A:871:PHE:CE2	2.63	0.52
1:B:418:MET:HB3	1:B:567:HIS:NE2	2.24	0.52
1:B:431:ILE:O	1:B:435:ILE:HB	2.09	0.52
1:B:689:MET:HA	1:B:692:ILE:HD13	1.91	0.52
2:D:24:TYR:CZ	2:D:68:THR:HG22	2.44	0.52
2:G:35:ASN:HA	2:G:38:ILE:CD1	2.39	0.52
2:I:74:ASP:OD2	2:I:76:ASN:HB3	2.08	0.52
2:J:150:PHE:HB2	2:J:152:PHE:HE1	1.73	0.52
2:L:167:ASN:ND2	2:L:178:GLY:HA2	2.22	0.52
2:M:31:ILE:O	2:M:34:PHE:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:23:LEU:HB3	2:O:26:ASN:HD21	1.73	0.52
3:W:879:ARG:HG3	3:W:879:ARG:HH11	1.75	0.52
1:A:314:PHE:O	1:A:315:GLU:C	2.48	0.52
1:A:421:ARG:O	1:A:425:VAL:HG23	2.10	0.52
1:A:742:GLY:O	1:A:743:ASP:O	2.28	0.52
1:A:872:ASP:OD2	1:A:874:MET:HB2	2.10	0.52
1:B:277:ARG:NH1	1:B:559:ALA:HB2	2.25	0.52
1:B:340:VAL:O	1:B:587:LEU:HD11	2.09	0.52
2:D:74:ASP:OD2	2:D:76:ASN:HB3	2.09	0.52
2:F:150:PHE:HB2	2:F:152:PHE:CZ	2.44	0.52
2:F:381:ASN:O	2:F:385:VAL:HB	2.10	0.52
2:G:381:ASN:O	2:G:385:VAL:HB	2.10	0.52
2:K:53:ASN:ND2	2:K:354:ALA:HB3	2.25	0.52
2:L:8:SER:C	2:L:10:THR:H	2.13	0.52
2:N:116:LEU:HA	2:N:119:LEU:CD1	2.39	0.52
3:W:321:LEU:O	3:W:325:ILE:HG12	2.10	0.52
3:W:573:VAL:HG12	3:W:575:ILE:HG13	1.91	0.52
3:W:967:ILE:H	3:W:967:ILE:CD1	2.23	0.52
1:A:286:LEU:O	1:A:287:ASN:HB2	2.09	0.52
1:A:464:GLN:O	1:A:465:ASN:HB2	2.08	0.52
1:B:396:PHE:C	1:B:396:PHE:CD1	2.83	0.52
1:B:527:ARG:HH11	1:B:527:ARG:HG3	1.74	0.52
1:B:527:ARG:O	1:B:531:ARG:HG2	2.08	0.52
1:B:558:MET:O	1:B:561:VAL:HG23	2.09	0.52
1:B:763:LEU:HD22	1:B:764:PRO:HD2	1.92	0.52
1:B:811:LEU:HD23	1:B:811:LEU:N	2.24	0.52
2:E:215:ARG:HG3	2:E:371:ILE:O	2.09	0.52
2:F:215:ARG:HG3	2:F:371:ILE:O	2.09	0.52
2:G:7:LEU:O	2:G:11:LEU:HG	2.09	0.52
2:H:57:ARG:NH1	2:H:94:ASN:HD21	2.07	0.52
2:M:21:GLY:O	2:M:22:THR:O	2.28	0.52
2:O:107:ASN:CG	2:O:107:ASN:O	2.48	0.52
3:W:538:ILE:HD13	3:W:595:GLN:OE1	2.10	0.52
3:W:744:ILE:N	3:W:744:ILE:HD12	2.24	0.52
3:W:820:LEU:HD13	3:W:824:ASN:HB2	1.91	0.52
1:A:721:VAL:HG13	1:A:800:TYR:C	2.29	0.52
1:A:803:ASN:C	1:A:805:ASP:N	2.63	0.52
1:B:211:ILE:O	1:B:212:PHE:C	2.48	0.52
1:B:326:TYR:HD1	1:B:384:ALA:HB1	1.75	0.52
1:B:570:THR:HG22	1:B:571:LEU:H	1.75	0.52
1:B:632:ASN:O	1:B:634:TYR:N	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:SER:C	2:D:10:THR:H	2.13	0.52
2:F:129:PHE:C	2:F:129:PHE:CD1	2.83	0.52
2:F:5:TYR:HE2	2:F:131:ASN:HA	1.75	0.52
2:G:14:ALA:C	2:G:16:ASP:H	2.11	0.52
2:I:14:ALA:O	2:I:18:ILE:HD12	2.10	0.52
2:J:167:ASN:ND2	2:J:178:GLY:HA2	2.23	0.52
2:J:381:ASN:O	2:J:385:VAL:HB	2.10	0.52
2:K:381:ASN:O	2:K:385:VAL:HB	2.10	0.52
2:L:381:ASN:O	2:L:385:VAL:HB	2.10	0.52
2:N:12:LYS:O	2:N:14:ALA:N	2.43	0.52
2:N:381:ASN:O	2:N:385:VAL:HB	2.10	0.52
2:O:381:ASN:O	2:O:385:VAL:HB	2.10	0.52
3:W:114:MET:HB2	3:W:117:GLU:HG2	1.92	0.52
3:W:428:MET:SD	3:W:811:TYR:HD1	2.32	0.52
3:W:564:THR:O	3:W:568:LEU:HG	2.09	0.52
1:A:786:ILE:O	1:A:789:LEU:N	2.43	0.52
1:B:550:LEU:O	1:B:551:ALA:C	2.49	0.52
1:B:812:VAL:HG23	1:B:817:TRP:CZ3	2.45	0.52
2:D:23:LEU:HD22	2:D:25:SER:OG	2.10	0.52
2:D:41:MET:O	2:D:42:ASN:C	2.47	0.52
2:L:31:ILE:O	2:L:34:PHE:HB3	2.10	0.52
2:M:89:VAL:O	2:M:91:PHE:N	2.43	0.52
1:A:323:THR:OG1	1:A:390:ARG:NH1	2.43	0.52
1:A:467:GLN:HB3	1:A:512:GLN:HG2	1.92	0.52
1:A:163:ARG:NH2	1:A:736:GLU:OE2	2.42	0.52
1:B:314:PHE:N	1:B:314:PHE:CD1	2.77	0.52
1:B:444:ARG:HH22	1:B:520:THR:HA	1.75	0.52
1:B:540:LEU:HA	1:B:543:LEU:HB2	1.92	0.52
1:B:723:ILE:CG2	1:B:724:ALA:H	2.13	0.52
2:H:139:TRP:CD1	2:H:139:TRP:C	2.83	0.52
2:H:14:ALA:C	2:H:16:ASP:H	2.11	0.52
2:K:99:GLU:O	2:K:99:GLU:HG3	2.10	0.52
2:L:106:ARG:N	2:L:106:ARG:HD3	2.17	0.52
2:L:110:ALA:HB1	2:L:111:PRO:HD2	1.92	0.52
2:L:35:ASN:HA	2:L:38:ILE:CD1	2.39	0.52
2:M:14:ALA:C	2:M:16:ASP:H	2.11	0.52
2:M:8:SER:C	2:M:10:THR:H	2.13	0.52
3:W:772:ILE:HG23	3:W:1043:ASN:HD22	1.75	0.52
1:B:293:PRO:C	1:B:295:THR:N	2.60	0.52
2:F:135:TYR:OH	2:F:340:GLU:OE1	2.28	0.52
2:F:35:ASN:HA	2:F:38:ILE:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:128:ASN:O	2:H:129:PHE:HB3	2.09	0.52
2:M:131:ASN:N	2:M:131:ASN:HD22	2.07	0.52
1:A:310:LEU:O	1:A:318:TRP:CD1	2.62	0.51
1:A:540:LEU:C	1:A:540:LEU:HD23	2.30	0.51
1:A:769:SER:O	1:A:771:VAL:N	2.43	0.51
1:B:235:ASP:O	1:B:236:ARG:HB2	2.10	0.51
1:B:286:LEU:N	1:B:286:LEU:HD22	2.25	0.51
1:B:322:THR:O	1:B:323:THR:C	2.48	0.51
1:B:530:GLN:HA	1:B:533:ILE:CD1	2.40	0.51
1:B:563:MET:HA	1:B:563:MET:CE	2.39	0.51
1:B:606:VAL:O	1:B:607:ASN:C	2.47	0.51
2:C:116:LEU:HA	2:C:119:LEU:CD1	2.40	0.51
2:J:89:VAL:O	2:J:91:PHE:N	2.43	0.51
2:M:27:VAL:CG2	2:M:31:ILE:HD11	2.40	0.51
2:O:133:SER:O	2:O:136:ILE:HG22	2.10	0.51
3:W:101:ASP:C	3:W:103:THR:H	2.13	0.51
3:W:880:ASP:O	3:W:883:PRO:HD2	2.10	0.51
1:A:125:ILE:CD1	1:A:125:ILE:N	2.63	0.51
1:A:269:ILE:HG21	1:A:298:TYR:HE2	1.76	0.51
1:A:431:ILE:HG23	1:A:435:ILE:HD12	1.91	0.51
1:B:422:GLU:O	1:B:425:VAL:N	2.43	0.51
1:B:378:CYS:SG	1:B:581:VAL:HA	2.50	0.51
2:C:27:VAL:O	2:C:30:LEU:N	2.38	0.51
2:D:105:GLN:NE2	2:D:359:PRO:O	2.43	0.51
2:H:145:ARG:O	2:H:146:GLN:HG3	2.10	0.51
2:I:139:TRP:CD1	2:I:139:TRP:C	2.84	0.51
2:J:11:LEU:O	2:J:15:ARG:N	2.39	0.51
2:K:74:ASP:OD2	2:K:76:ASN:HB3	2.10	0.51
3:W:177:ILE:HD13	3:W:203:LEU:HD11	1.90	0.51
3:W:227:LYS:O	3:W:231:VAL:HG23	2.10	0.51
3:W:408:LEU:N	3:W:408:LEU:HD12	2.24	0.51
3:W:808:PHE:O	3:W:812:VAL:HG23	2.09	0.51
1:A:259:HIS:HD1	1:A:260:GLN:N	2.07	0.51
1:A:326:TYR:CE1	1:A:384:ALA:HB3	2.45	0.51
1:A:647:LYS:O	1:A:649:LEU:N	2.43	0.51
1:B:133:ILE:HD11	1:B:147:TYR:HE1	1.76	0.51
2:C:24:TYR:OH	2:C:68:THR:HG22	2.10	0.51
2:D:6:SER:O	2:D:8:SER:N	2.44	0.51
2:E:135:TYR:OH	2:E:340:GLU:OE1	2.28	0.51
2:G:6:SER:HG	2:G:128:ASN:HA	1.72	0.51
2:H:148:THR:OG1	2:H:332:GLU:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:128:ASN:HD22	2:J:19:VAL:CB	2.21	0.51
2:H:76:ASN:N	2:J:76:ASN:HB2	2.24	0.51
2:K:41:MET:O	2:K:42:ASN:C	2.49	0.51
2:L:116:LEU:HA	2:L:119:LEU:CD1	2.40	0.51
2:M:381:ASN:O	2:M:385:VAL:HB	2.10	0.51
3:W:803:ALA:HA	3:W:808:PHE:CD2	2.46	0.51
1:A:420:ILE:HG12	1:A:423:SER:CB	2.38	0.51
1:A:519:PRO:O	1:A:520:THR:HG23	2.10	0.51
1:A:645:PHE:CD2	1:A:646:LEU:HD23	2.44	0.51
1:B:442:MET:SD	1:B:463:ILE:HA	2.49	0.51
1:B:460:GLU:HG3	1:B:473:HIS:HD2	1.76	0.51
1:B:498:ARG:CG	1:B:505:GLN:HE22	2.23	0.51
1:B:498:ARG:HG3	1:B:505:GLN:NE2	2.26	0.51
1:B:639:LYS:O	1:B:642:VAL:HG23	2.10	0.51
1:B:699:ILE:HG13	1:B:763:LEU:O	2.10	0.51
1:B:779:ASP:HA	1:B:798:ILE:CG1	2.39	0.51
1:B:89:GLU:C	1:B:91:LEU:N	2.61	0.51
2:C:74:ASP:OD2	2:C:76:ASN:HB3	2.11	0.51
2:D:381:ASN:O	2:D:385:VAL:HB	2.10	0.51
2:E:6:SER:O	2:E:8:SER:N	2.44	0.51
2:E:89:VAL:O	2:E:91:PHE:N	2.44	0.51
2:G:89:VAL:O	2:G:91:PHE:N	2.44	0.51
2:H:5:TYR:HE2	2:H:131:ASN:HA	1.75	0.51
3:W:1005:GLN:CG	3:W:1006:LEU:HD12	2.41	0.51
1:A:631:LEU:O	1:A:633:LEU:HD12	2.10	0.51
1:A:661:GLN:HG3	1:B:348:LYS:NZ	2.26	0.51
1:A:773:SER:HB3	1:A:778:LEU:HD12	1.91	0.51
1:B:104:ILE:HD12	1:B:327:ILE:HD12	1.92	0.51
1:B:548:ARG:HH11	1:B:878:ASN:N	2.04	0.51
1:B:594:ILE:C	1:B:594:ILE:CD1	2.79	0.51
1:B:705:ILE:HG22	1:B:707:TYR:CE1	2.45	0.51
2:D:139:TRP:C	2:D:139:TRP:CD1	2.84	0.51
2:D:89:VAL:O	2:D:91:PHE:N	2.43	0.51
2:H:31:ILE:O	2:H:34:PHE:HB3	2.11	0.51
2:K:155:PRO:O	2:K:186:SER:HB3	2.10	0.51
2:M:253:ILE:HD13	2:M:319:THR:HB	1.93	0.51
2:N:133:SER:O	2:N:136:ILE:HG22	2.11	0.51
2:N:41:MET:O	2:N:42:ASN:C	2.49	0.51
2:O:106:ARG:HD3	2:O:106:ARG:N	2.23	0.51
3:W:126:THR:OG1	3:W:128:SER:HB3	2.11	0.51
3:W:820:LEU:HD13	3:W:824:ASN:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:PHE:O	1:A:254:GLU:N	2.44	0.51
1:A:427:CYS:O	1:A:431:ILE:HG13	2.11	0.51
1:A:496:ASN:O	1:A:497:ILE:C	2.49	0.51
1:A:443:GLN:NE2	1:A:521:MET:HB3	2.25	0.51
1:B:178:PRO:HD2	1:B:256:PHE:CE2	2.45	0.51
1:B:272:ASN:O	1:B:274:ILE:N	2.43	0.51
1:B:431:ILE:HG23	1:B:435:ILE:HD12	1.93	0.51
1:B:481:ARG:NH2	1:B:496:ASN:HD21	2.08	0.51
2:E:31:ILE:O	2:E:34:PHE:HB3	2.09	0.51
2:K:116:LEU:HA	2:K:119:LEU:CD1	2.41	0.51
2:L:89:VAL:O	2:L:91:PHE:N	2.43	0.51
3:W:1005:GLN:HG3	3:W:1006:LEU:HD12	1.92	0.51
3:W:582:LYS:CG	3:W:583:LYS:H	2.24	0.51
3:W:596:THR:O	3:W:600:ASN:HB2	2.10	0.51
1:A:158:GLY:O	1:A:162:VAL:HG23	2.09	0.51
1:A:159:ASP:O	1:A:162:VAL:HB	2.11	0.51
1:A:814:ASN:O	1:A:815:TYR:C	2.48	0.51
1:B:302:ASN:O	1:B:303:LEU:HD23	2.11	0.51
1:B:305:GLN:NE2	1:B:564:ASN:ND2	2.58	0.51
2:C:110:ALA:HB1	2:C:111:PRO:CD	2.41	0.51
2:D:360:VAL:O	2:D:378:ARG:HD3	2.11	0.51
2:F:109:ILE:CB	2:F:380:ASP:HB3	2.40	0.51
2:F:8:SER:C	2:F:10:THR:H	2.14	0.51
2:H:105:GLN:C	2:H:107:ASN:N	2.58	0.51
2:H:381:ASN:O	2:H:385:VAL:HB	2.10	0.51
2:J:253:ILE:HD13	2:J:319:THR:HB	1.92	0.51
2:K:106:ARG:HD3	2:K:106:ARG:N	2.17	0.51
2:K:253:ILE:HD13	2:K:319:THR:HB	1.93	0.51
2:O:253:ILE:HD13	2:O:319:THR:HB	1.93	0.51
2:O:31:ILE:O	2:O:34:PHE:HB3	2.11	0.51
2:O:54:LEU:HD12	2:O:55:PRO:HD2	1.93	0.51
3:W:166:ARG:HG2	3:W:166:ARG:NH1	2.25	0.51
3:W:410:PHE:HE2	3:W:415:ILE:HD11	1.76	0.51
3:W:41:PHE:HB2	3:W:62:TYR:CD1	2.45	0.51
1:A:326:TYR:HD1	1:A:384:ALA:HB1	1.75	0.51
1:A:793:ASP:C	1:A:795:LEU:N	2.63	0.51
1:B:481:ARG:CZ	1:B:496:ASN:OD1	2.59	0.51
1:B:491:GLN:O	1:B:491:GLN:HG3	2.10	0.51
1:B:658:PRO:HD2	1:B:661:GLN:HG3	1.93	0.51
2:C:139:TRP:CD1	2:C:139:TRP:C	2.83	0.51
2:C:42:ASN:HA	2:C:61:PHE:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:381:ASN:O	2:E:385:VAL:HB	2.10	0.51
2:F:360:VAL:O	2:F:378:ARG:HD3	2.11	0.51
2:G:111:PRO:HB3	2:G:116:LEU:CD2	2.41	0.51
2:H:35:ASN:HA	2:H:38:ILE:CD1	2.41	0.51
2:F:23:LEU:HD11	2:H:36:GLN:OE1	2.10	0.51
2:I:381:ASN:O	2:I:385:VAL:HB	2.10	0.51
2:J:12:LYS:O	2:J:14:ALA:N	2.43	0.51
2:J:360:VAL:O	2:J:378:ARG:HD3	2.11	0.51
2:L:14:ALA:C	2:L:16:ASP:H	2.12	0.51
2:L:99:GLU:HG3	2:L:99:GLU:O	2.10	0.51
2:M:106:ARG:HG2	2:M:107:ASN:H	1.75	0.51
2:M:109:ILE:HB	2:M:380:ASP:HB3	1.93	0.51
2:M:24:TYR:O	2:M:26:ASN:N	2.44	0.51
2:M:360:VAL:O	2:M:378:ARG:HD3	2.11	0.51
2:O:41:MET:O	2:O:42:ASN:C	2.49	0.51
3:W:343:ALA:CB	3:W:575:ILE:HD13	2.41	0.51
1:A:130:GLN:O	1:A:131:LEU:HB3	2.10	0.51
1:A:368:THR:HG22	1:A:368:THR:O	2.09	0.51
1:A:631:LEU:CB	1:A:633:LEU:HD13	2.38	0.51
1:B:577:GLN:C	1:B:579:THR:H	2.14	0.51
1:B:712:LEU:HD11	1:B:722:ASN:HB3	1.93	0.51
1:B:869:VAL:N	1:B:876:ILE:HG23	2.26	0.51
2:C:89:VAL:O	2:C:91:PHE:N	2.43	0.51
2:C:17:LYS:HG2	2:E:130:ASP:HA	1.92	0.51
2:F:89:VAL:O	2:F:91:PHE:N	2.44	0.51
2:G:253:ILE:HD13	2:G:319:THR:HB	1.93	0.51
2:G:360:VAL:O	2:G:378:ARG:HD3	2.11	0.51
2:L:139:TRP:C	2:L:139:TRP:CD1	2.84	0.51
3:W:330:PHE:CE1	3:W:690:ARG:NE	2.79	0.51
3:W:899:PHE:C	3:W:901:PRO:HD3	2.31	0.51
3:W:962:LEU:O	3:W:967:ILE:HD13	2.11	0.51
1:A:362:SER:HB2	1:A:365:GLN:HE22	1.72	0.51
1:A:501:HIS:C	1:A:503:ILE:N	2.62	0.51
1:A:527:ARG:O	1:A:531:ARG:HG2	2.10	0.51
1:A:546:LEU:HD11	1:A:584:LEU:HD23	1.93	0.51
1:A:618:ILE:O	1:A:622:VAL:HG23	2.11	0.51
1:A:701:GLN:O	1:A:761:GLY:O	2.29	0.51
1:B:140:LYS:HE2	1:B:805:ASP:OD2	2.10	0.51
2:C:128:ASN:HB3	2:D:19:VAL:HG23	1.93	0.51
2:F:74:ASP:OD2	2:F:76:ASN:HB3	2.11	0.51
2:F:63:PHE:CD2	2:F:84:THR:HG23	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:103:GLU:HG3	2:G:359:PRO:HD2	1.93	0.51
2:G:116:LEU:HA	2:G:119:LEU:CD1	2.40	0.51
2:J:153:HIS:NE2	2:K:153:HIS:NE2	2.59	0.51
2:N:60:ASN:C	2:N:61:PHE:CD1	2.84	0.51
2:O:23:LEU:C	2:O:23:LEU:HD23	2.31	0.51
2:O:8:SER:C	2:O:10:THR:H	2.14	0.51
3:W:659:TYR:CG	3:W:666:VAL:HG21	2.46	0.51
3:W:687:ILE:HG23	3:W:687:ILE:O	2.11	0.51
1:A:508:GLU:O	1:A:512:GLN:NE2	2.45	0.50
1:A:555:GLU:OE1	1:A:871:PHE:HD2	1.93	0.50
1:A:676:VAL:O	1:A:680:ASP:HB2	2.10	0.50
1:B:178:PRO:HD2	1:B:256:PHE:CD2	2.45	0.50
1:B:509:ALA:O	1:B:513:LEU:CG	2.50	0.50
1:B:539:ARG:O	1:B:542:GLN:N	2.44	0.50
1:B:805:ASP:C	1:B:807:ASN:N	2.65	0.50
2:C:129:PHE:C	2:C:129:PHE:CD1	2.85	0.50
2:C:49:GLY:HA2	2:C:54:LEU:HD23	1.93	0.50
2:F:253:ILE:HD13	2:F:319:THR:HB	1.93	0.50
2:H:116:LEU:HA	2:H:119:LEU:CD1	2.40	0.50
2:H:12:LYS:O	2:H:14:ALA:N	2.44	0.50
2:K:11:LEU:O	2:K:15:ARG:N	2.38	0.50
2:L:135:TYR:CZ	2:L:342:MET:HE3	2.45	0.50
2:N:135:TYR:OH	2:N:340:GLU:OE1	2.25	0.50
3:W:330:PHE:CZ	3:W:690:ARG:CZ	2.94	0.50
3:W:358:GLU:HG3	3:W:359:MET:H	1.76	0.50
1:A:452:PRO:O	1:A:453:GLN:CB	2.58	0.50
1:A:467:GLN:NE2	1:A:511:MET:HG2	2.25	0.50
1:B:182:LEU:HD11	1:B:847:THR:CA	2.40	0.50
1:B:392:MET:C	1:B:573:THR:HG23	2.32	0.50
1:B:449:ASN:ND2	1:B:455:PRO:CG	2.75	0.50
1:B:527:ARG:O	1:B:531:ARG:HG3	2.10	0.50
1:B:671:LEU:O	1:B:672:LEU:HD23	2.10	0.50
2:C:133:SER:O	2:C:136:ILE:HG22	2.12	0.50
2:D:155:PRO:O	2:D:186:SER:HB3	2.11	0.50
2:G:8:SER:C	2:G:10:THR:H	2.14	0.50
2:I:133:SER:O	2:I:136:ILE:HG22	2.11	0.50
2:K:360:VAL:O	2:K:378:ARG:HD3	2.11	0.50
2:L:23:LEU:HD11	2:N:36:GLN:HB2	1.92	0.50
3:W:703:GLN:H	3:W:703:GLN:NE2	2.08	0.50
1:A:520:THR:O	1:A:521:MET:HE3	2.11	0.50
1:B:298:TYR:HE1	1:B:300:ARG:HA	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:PHE:CB	1:B:519:PRO:CD	2.89	0.50
1:B:878:ASN:OD1	1:B:878:ASN:O	2.29	0.50
2:D:253:ILE:HD13	2:D:319:THR:HB	1.93	0.50
2:E:56:ILE:HG22	2:E:56:ILE:O	2.11	0.50
2:E:8:SER:C	2:E:10:THR:H	2.14	0.50
2:F:61:PHE:N	2:F:61:PHE:CD1	2.79	0.50
2:H:89:VAL:O	2:H:91:PHE:N	2.44	0.50
2:K:60:ASN:C	2:K:61:PHE:CD1	2.85	0.50
2:L:150:PHE:CD1	2:L:150:PHE:N	2.78	0.50
2:L:155:PRO:O	2:L:186:SER:HB3	2.11	0.50
2:L:6:SER:O	2:L:8:SER:N	2.44	0.50
2:N:8:SER:C	2:N:10:THR:H	2.14	0.50
2:N:23:LEU:O	2:N:26:ASN:ND2	2.43	0.50
3:W:892:LEU:HB2	3:W:1051:TRP:CD1	2.47	0.50
1:A:199:VAL:CG1	1:A:200:VAL:H	2.07	0.50
1:A:436:ILE:CD1	1:A:437:TYR:CD1	2.94	0.50
1:A:822:THR:O	1:A:823:THR:HG23	2.12	0.50
1:A:545:ASP:OD1	1:A:877:MET:HA	2.11	0.50
1:B:457:GLN:C	1:B:458:ILE:HG13	2.31	0.50
1:B:498:ARG:HD3	2:I:32:GLN:NE2	2.26	0.50
1:B:596:SER:O	1:B:599:THR:HB	2.11	0.50
1:B:712:LEU:HB2	1:B:819:PRO:HB2	1.94	0.50
2:C:12:LYS:O	2:C:14:ALA:N	2.45	0.50
2:G:31:ILE:O	2:G:34:PHE:HB3	2.11	0.50
2:G:6:SER:O	2:G:8:SER:N	2.44	0.50
2:H:253:ILE:HD13	2:H:319:THR:HB	1.93	0.50
2:I:31:ILE:O	2:I:34:PHE:HB3	2.11	0.50
2:L:133:SER:O	2:L:136:ILE:HG22	2.12	0.50
2:L:253:ILE:HD13	2:L:319:THR:HB	1.93	0.50
2:N:106:ARG:HG2	2:N:107:ASN:H	1.77	0.50
2:N:139:TRP:C	2:N:139:TRP:CD1	2.84	0.50
2:N:66:LEU:HD13	2:N:77:TYR:CZ	2.46	0.50
3:W:54:SER:OG	3:W:55:LEU:N	2.44	0.50
3:W:8:LEU:HA	3:W:737:MET:SD	2.52	0.50
3:W:385:LEU:HD13	3:W:939:VAL:CG2	2.42	0.50
1:A:389:GLN:OE1	1:A:567:HIS:HA	2.11	0.50
1:A:634:TYR:HD1	1:A:635:GLN:HG3	1.76	0.50
1:B:428:GLN:NE2	1:B:455:PRO:HB2	2.26	0.50
1:B:826:TYR:O	1:B:827:LYS:C	2.50	0.50
2:C:360:VAL:O	2:C:378:ARG:HD3	2.11	0.50
2:C:46:PHE:HE2	2:C:119:LEU:HD21	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:MET:HG3	2:D:388:VAL:HG11	1.93	0.50
2:D:124:PHE:O	2:D:127:ILE:HG13	2.11	0.50
2:D:12:LYS:O	2:D:14:ALA:N	2.45	0.50
2:F:139:TRP:CD1	2:F:139:TRP:C	2.85	0.50
2:G:124:PHE:O	2:G:127:ILE:HG13	2.11	0.50
2:I:124:PHE:C	2:I:126:ARG:H	2.14	0.50
2:J:8:SER:C	2:J:10:THR:H	2.14	0.50
2:L:125:LYS:O	2:L:127:ILE:N	2.42	0.50
2:L:360:VAL:O	2:L:378:ARG:HD3	2.11	0.50
3:W:397:MET:HA	3:W:400:ALA:HB2	1.93	0.50
1:A:214:ASP:O	1:A:215:GLU:C	2.50	0.50
1:B:176:GLU:O	1:B:178:PRO:HD3	2.11	0.50
1:B:387:LEU:HD23	1:B:554:TYR:HE1	1.74	0.50
1:B:578:LEU:HA	1:B:581:VAL:CG2	2.42	0.50
2:C:14:ALA:C	2:C:16:ASP:N	2.65	0.50
2:E:139:TRP:C	2:E:139:TRP:CD1	2.84	0.50
2:E:150:PHE:CD1	2:E:150:PHE:N	2.80	0.50
2:E:151:THR:C	2:E:152:PHE:CD1	2.84	0.50
2:E:253:ILE:HD13	2:E:319:THR:HB	1.93	0.50
2:F:73:LEU:HD22	2:F:77:TYR:CD2	2.46	0.50
2:G:139:TRP:C	2:G:139:TRP:CD1	2.85	0.50
2:G:167:ASN:ND2	2:G:178:GLY:HA2	2.22	0.50
2:I:6:SER:O	2:I:8:SER:N	2.44	0.50
2:J:6:SER:O	2:J:8:SER:N	2.45	0.50
2:L:11:LEU:O	2:L:15:ARG:N	2.39	0.50
2:O:11:LEU:O	2:O:15:ARG:N	2.40	0.50
3:W:898:LYS:HE2	3:W:908:GLN:HG2	1.94	0.50
1:A:229:ARG:O	1:A:242:PRO:CG	2.60	0.50
1:A:332:VAL:HG11	1:A:557:LEU:HD21	1.93	0.50
1:A:675:GLU:O	1:A:676:VAL:C	2.50	0.50
1:B:170:TYR:CE1	1:B:682:PHE:HB2	2.47	0.50
1:B:364:THR:O	1:B:364:THR:HG22	2.12	0.50
1:B:463:ILE:HG21	1:B:468:VAL:CG1	2.41	0.50
1:B:499:ASN:N	1:B:505:GLN:NE2	2.60	0.50
1:B:536:LEU:HD22	1:B:536:LEU:N	2.27	0.50
1:B:618:ILE:HD13	1:B:645:PHE:CZ	2.47	0.50
1:B:810:TYR:HA	1:B:812:VAL:HG12	1.92	0.50
2:C:31:ILE:O	2:C:34:PHE:HB3	2.12	0.50
2:D:133:SER:O	2:D:136:ILE:HG22	2.11	0.50
2:F:6:SER:O	2:F:8:SER:N	2.45	0.50
2:I:360:VAL:O	2:I:378:ARG:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:8:SER:C	2:I:10:THR:H	2.14	0.50
2:K:124:PHE:O	2:K:126:ARG:N	2.45	0.50
2:L:35:ASN:O	2:L:36:GLN:C	2.50	0.50
2:N:104:SER:O	2:N:108:GLY:HA3	2.12	0.50
3:W:607:LEU:HD21	3:W:659:TYR:HE1	1.75	0.50
1:A:289:ASP:C	1:A:290:ARG:HG2	2.32	0.50
1:A:297:ARG:HG3	1:A:848:PHE:CD2	2.46	0.50
1:A:309:ASN:HA	1:A:311:HIS:CE1	2.47	0.50
1:A:603:TYR:O	1:A:606:VAL:CG2	2.60	0.50
1:A:660:ASP:CA	1:B:539:ARG:HH11	2.24	0.50
1:A:704:ILE:HG23	1:A:758:ALA:HB2	1.94	0.50
1:B:141:GLU:O	1:B:142:LEU:CB	2.60	0.50
1:B:392:MET:HB3	1:B:574:GLU:O	2.10	0.50
1:B:477:ASN:O	1:B:479:GLN:N	2.44	0.50
1:B:510:LEU:HD12	1:B:513:LEU:HD12	1.94	0.50
1:B:113:PRO:HD2	1:B:609:ASN:HB3	1.94	0.50
2:E:101:VAL:HG23	2:E:102:ARG:N	2.27	0.50
2:I:12:LYS:O	2:I:14:ALA:N	2.45	0.50
2:I:150:PHE:N	2:I:150:PHE:CD1	2.79	0.50
2:J:23:LEU:O	2:J:26:ASN:ND2	2.45	0.50
2:N:360:VAL:O	2:N:378:ARG:HD3	2.11	0.50
3:W:452:ARG:HG3	3:W:452:ARG:HH11	1.76	0.50
3:W:4:TYR:C	3:W:4:TYR:CD2	2.84	0.50
3:W:777:THR:HG21	3:W:882:LYS:HZ1	1.74	0.50
1:A:369:GLY:O	1:A:370:ILE:C	2.49	0.50
1:A:503:ILE:O	1:A:503:ILE:HG22	2.12	0.50
1:A:613:ASN:HD22	1:A:649:LEU:HD21	1.75	0.50
1:B:306:ASP:C	1:B:308:LEU:H	2.08	0.50
1:B:436:ILE:CG1	1:B:437:TYR:H	2.21	0.50
1:B:444:ARG:HH21	1:B:520:THR:CG2	2.09	0.50
2:C:253:ILE:HD13	2:C:319:THR:HB	1.93	0.50
2:E:24:TYR:O	2:E:26:ASN:N	2.43	0.50
2:E:360:VAL:O	2:E:378:ARG:HD3	2.11	0.50
2:F:153:HIS:NE2	2:G:153:HIS:CD2	2.80	0.50
2:G:124:PHE:O	2:G:126:ARG:N	2.45	0.50
2:G:155:PRO:O	2:G:186:SER:HB3	2.12	0.50
2:G:74:ASP:OD2	2:G:76:ASN:HB3	2.12	0.50
2:J:144:ARG:O	2:J:145:ARG:HB2	2.12	0.50
2:J:63:PHE:N	2:J:63:PHE:CD1	2.80	0.50
2:K:8:SER:C	2:K:10:THR:H	2.14	0.50
2:N:253:ILE:HD13	2:N:319:THR:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:30:LEU:O	2:O:31:ILE:C	2.51	0.50
3:W:255:VAL:HG12	3:W:256:ASP:O	2.12	0.50
1:A:310:LEU:CD1	1:A:310:LEU:N	2.69	0.49
1:A:311:HIS:HA	1:A:318:TRP:CD1	2.47	0.49
1:A:392:MET:O	1:A:420:ILE:HG23	2.11	0.49
1:A:465:ASN:HB3	1:A:468:VAL:HB	1.94	0.49
1:A:284:TYR:OH	1:A:594:ILE:HG23	2.12	0.49
1:A:674:VAL:HG12	1:A:678:ARG:HB2	1.93	0.49
1:A:774:LEU:HD12	1:A:774:LEU:O	2.11	0.49
1:A:555:GLU:OE1	1:A:871:PHE:CD2	2.66	0.49
1:B:394:LEU:C	1:B:396:PHE:N	2.65	0.49
1:B:305:GLN:NE2	1:B:564:ASN:CG	2.65	0.49
2:J:14:ALA:C	2:J:16:ASP:N	2.65	0.49
2:K:133:SER:O	2:K:136:ILE:HG22	2.12	0.49
2:O:6:SER:O	2:O:8:SER:N	2.45	0.49
3:W:145:VAL:CG2	3:W:211:ILE:HG23	2.42	0.49
3:W:466:PRO:HD2	3:W:469:TYR:CD2	2.46	0.49
3:W:532:GLN:O	3:W:536:LYS:HG3	2.12	0.49
1:A:141:GLU:O	1:A:142:LEU:HB2	2.11	0.49
1:A:230:GLN:NE2	1:A:230:GLN:O	2.45	0.49
1:A:390:ARG:HG3	1:A:391:THR:N	2.26	0.49
1:A:404:LEU:O	1:A:405:ILE:C	2.50	0.49
1:A:503:ILE:HG22	1:A:506:LEU:CB	2.42	0.49
1:A:779:ASP:N	1:A:779:ASP:OD1	2.43	0.49
1:B:267:ASN:N	1:B:292:LEU:HD12	2.27	0.49
1:B:322:THR:HG21	1:B:390:ARG:HA	1.94	0.49
1:B:639:LYS:O	1:B:642:VAL:N	2.44	0.49
1:B:134:TYR:CD2	1:B:803:ASN:HB2	2.47	0.49
2:C:106:ARG:HD3	2:C:106:ARG:N	2.10	0.49
2:C:60:ASN:C	2:C:61:PHE:CD1	2.85	0.49
2:F:116:LEU:HA	2:F:119:LEU:CD1	2.42	0.49
2:G:133:SER:O	2:G:136:ILE:HG22	2.12	0.49
2:H:101:VAL:HB	2:H:355:ILE:HG21	1.94	0.49
2:H:360:VAL:O	2:H:378:ARG:HD3	2.11	0.49
2:M:139:TRP:C	2:M:139:TRP:CD1	2.84	0.49
2:O:14:ALA:C	2:O:16:ASP:N	2.66	0.49
2:O:35:ASN:HD21	2:O:66:LEU:HD12	1.77	0.49
3:W:531:THR:HG23	3:W:532:GLN:N	2.27	0.49
1:A:415:PRO:HD2	1:A:480:PHE:HE1	1.76	0.49
1:A:501:HIS:O	1:A:503:ILE:N	2.37	0.49
1:A:527:ARG:HH11	1:A:527:ARG:HG3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ASP:OD2	1:B:761:GLY:HA3	2.11	0.49
1:B:277:ARG:CB	1:B:277:ARG:NH1	2.75	0.49
1:B:428:GLN:HE22	1:B:455:PRO:HB2	1.77	0.49
1:B:480:PHE:O	1:B:481:ARG:C	2.49	0.49
1:B:501:HIS:C	1:B:503:ILE:H	2.15	0.49
1:B:590:ASN:ND2	1:B:590:ASN:N	2.46	0.49
1:B:735:LEU:CD2	1:B:759:LEU:HB3	2.42	0.49
2:C:8:SER:C	2:C:10:THR:H	2.14	0.49
2:E:12:LYS:O	2:E:14:ALA:N	2.45	0.49
2:E:22:THR:CG2	2:E:73:LEU:HD12	2.42	0.49
2:K:31:ILE:O	2:K:34:PHE:HB3	2.11	0.49
3:W:126:THR:C	3:W:128:SER:H	2.15	0.49
3:W:246:SER:OG	3:W:247:PRO:HD3	2.12	0.49
1:A:149:LYS:NZ	1:A:697:ASP:OD1	2.45	0.49
1:A:688:ASN:O	1:A:689:MET:C	2.51	0.49
1:A:771:VAL:HG12	1:A:809:PHE:HB3	1.93	0.49
1:B:450:GLY:O	1:B:451:ASP:HB2	2.11	0.49
1:B:428:GLN:CB	1:B:456:PHE:HD1	2.24	0.49
1:B:498:ARG:HH12	2:J:25:SER:CB	2.23	0.49
1:B:698:LYS:C	1:B:699:ILE:HD13	2.33	0.49
1:B:698:LYS:O	1:B:699:ILE:HD13	2.12	0.49
1:B:869:VAL:HG13	1:B:873:ASN:HA	1.92	0.49
2:G:14:ALA:C	2:G:16:ASP:N	2.66	0.49
2:H:8:SER:C	2:H:10:THR:H	2.14	0.49
2:M:133:SER:O	2:M:136:ILE:HG22	2.13	0.49
2:O:139:TRP:CD1	2:O:139:TRP:C	2.85	0.49
1:A:178:PRO:HD2	1:A:256:PHE:HE2	1.77	0.49
1:A:333:VAL:CG1	1:A:380:LYS:HA	2.19	0.49
1:A:415:PRO:HG2	1:A:480:PHE:HD1	1.73	0.49
1:A:718:TYR:CD1	1:A:718:TYR:N	2.80	0.49
1:B:122:LEU:O	1:B:123:PHE:HB3	2.12	0.49
1:B:174:LEU:O	1:B:177:MET:HB2	2.12	0.49
1:B:305:GLN:O	1:B:307:ARG:N	2.46	0.49
1:B:812:VAL:HA	1:B:817:TRP:HZ3	1.78	0.49
2:J:144:ARG:NH2	2:J:146:GLN:NE2	2.61	0.49
2:K:12:LYS:O	2:K:14:ALA:N	2.45	0.49
2:K:14:ALA:C	2:K:16:ASP:N	2.65	0.49
2:N:22:THR:OG1	2:N:26:ASN:ND2	2.40	0.49
2:O:63:PHE:CD1	2:O:63:PHE:N	2.81	0.49
3:W:345:ASP:HB2	3:W:458:ARG:NH1	2.25	0.49
3:W:759:THR:HG23	3:W:759:THR:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:TYR:O	1:B:606:VAL:CG2	2.61	0.49
1:B:150:LEU:HD12	1:B:696:SER:HA	1.93	0.49
1:B:856:ALA:C	1:B:858:VAL:H	2.14	0.49
2:C:6:SER:O	2:C:8:SER:N	2.45	0.49
2:C:153:HIS:CE1	2:D:153:HIS:CD2	3.01	0.49
2:F:12:LYS:O	2:F:14:ALA:N	2.45	0.49
2:H:155:PRO:O	2:H:186:SER:HB3	2.13	0.49
2:J:115:SER:O	2:J:119:LEU:HG	2.13	0.49
2:J:30:LEU:O	2:J:31:ILE:C	2.51	0.49
2:J:31:ILE:O	2:J:34:PHE:HB3	2.13	0.49
2:O:360:VAL:O	2:O:378:ARG:HD3	2.11	0.49
3:W:803:ALA:HA	3:W:808:PHE:CG	2.47	0.49
1:A:147:TYR:CD1	1:A:147:TYR:N	2.80	0.49
1:A:389:GLN:HE22	1:A:568:VAL:H	1.60	0.49
1:A:452:PRO:O	1:A:453:GLN:HB3	2.13	0.49
1:A:457:GLN:O	1:A:459:ALA:N	2.45	0.49
1:A:548:ARG:O	1:A:551:ALA:HB3	2.12	0.49
1:A:854:LEU:O	1:A:856:ALA:N	2.46	0.49
1:B:457:GLN:C	1:B:459:ALA:N	2.57	0.49
1:B:544:VAL:HG11	1:B:548:ARG:HH21	1.78	0.49
1:B:807:ASN:C	1:B:809:PHE:N	2.66	0.49
2:C:153:HIS:O	2:C:154:LYS:C	2.50	0.49
2:C:35:ASN:O	2:C:36:GLN:C	2.51	0.49
2:E:115:SER:O	2:E:119:LEU:HG	2.13	0.49
2:F:150:PHE:CD1	2:F:150:PHE:N	2.80	0.49
2:F:14:ALA:C	2:F:16:ASP:N	2.66	0.49
2:G:153:HIS:NE2	2:H:153:HIS:CD2	2.81	0.49
2:I:253:ILE:HD13	2:I:319:THR:HB	1.93	0.49
2:I:5:TYR:CE2	2:I:131:ASN:HA	2.47	0.49
2:L:139:TRP:HE1	2:L:143:ASN:HD22	1.61	0.49
2:M:5:TYR:HE2	2:M:131:ASN:HA	1.77	0.49
2:N:14:ALA:C	2:N:16:ASP:N	2.65	0.49
1:A:539:ARG:O	1:A:542:GLN:N	2.44	0.49
1:A:652:PHE:CD1	1:A:652:PHE:N	2.80	0.49
1:A:662:MET:O	1:A:665:LEU:CB	2.61	0.49
1:A:820:THR:O	1:A:820:THR:HG22	2.13	0.49
1:B:182:LEU:HD21	1:B:846:LEU:HD12	1.95	0.49
1:B:184:LYS:C	1:B:186:MET:H	2.15	0.49
1:B:288:MET:HA	1:B:288:MET:CE	2.42	0.49
1:B:487:GLY:O	1:B:488:VAL:HB	2.13	0.49
1:B:580:SER:O	1:B:581:VAL:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:854:LEU:CD2	1:B:855:LEU:N	2.76	0.49
2:E:110:ALA:HB1	2:E:111:PRO:HD2	1.95	0.49
2:E:21:GLY:O	2:E:22:THR:O	2.31	0.49
2:F:72:ASN:ND2	2:H:126:ARG:NH1	2.60	0.49
2:I:14:ALA:C	2:I:16:ASP:N	2.66	0.49
2:J:2:ASP:HB2	2:J:128:ASN:HD21	1.77	0.49
2:O:109:ILE:HB	2:O:380:ASP:HB3	1.94	0.49
3:W:748:LEU:O	3:W:748:LEU:HD23	2.13	0.49
1:A:192:ASN:O	1:A:193:SER:CB	2.49	0.49
1:B:139:GLU:O	1:B:141:GLU:N	2.46	0.49
1:B:428:GLN:O	1:B:432:VAL:HG23	2.13	0.49
1:B:501:HIS:O	1:B:503:ILE:HG13	2.12	0.49
1:B:676:VAL:O	1:B:680:ASP:HB2	2.13	0.49
1:B:845:ASN:HB3	1:B:848:PHE:HE1	1.77	0.49
2:D:35:ASN:O	2:D:36:GLN:C	2.51	0.49
2:F:101:VAL:HG23	2:F:102:ARG:N	2.27	0.49
2:F:46:PHE:CE2	2:F:119:LEU:HD21	2.48	0.49
2:G:42:ASN:HA	2:G:61:PHE:HB2	1.94	0.49
2:H:6:SER:O	2:H:8:SER:N	2.46	0.49
2:I:144:ARG:NH2	2:I:146:GLN:HE22	2.10	0.49
2:J:101:VAL:HG23	2:J:102:ARG:N	2.27	0.49
2:J:150:PHE:CD1	2:J:150:PHE:N	2.81	0.49
2:J:35:ASN:O	2:J:36:GLN:C	2.51	0.49
2:K:139:TRP:C	2:K:139:TRP:CD1	2.85	0.49
2:L:12:LYS:O	2:L:14:ALA:N	2.45	0.49
3:W:23:GLN:O	3:W:25:PRO:HD3	2.13	0.49
3:W:488:ARG:NH2	3:W:501:LEU:HD11	2.28	0.49
3:W:76:SER:O	3:W:748:LEU:HA	2.12	0.49
1:A:311:HIS:HE2	1:A:566:GLN:HE22	1.59	0.49
1:A:646:LEU:HD23	1:A:646:LEU:N	2.28	0.49
1:A:666:ARG:HG2	1:A:667:ASP:H	1.78	0.49
1:A:597:PRO:HB3	1:A:860:ALA:HB3	1.94	0.49
1:B:277:ARG:NH1	1:B:277:ARG:HB2	2.28	0.49
1:B:422:GLU:N	1:B:422:GLU:OE1	2.46	0.49
1:B:587:LEU:CG	1:B:587:LEU:O	2.60	0.49
2:C:106:ARG:HG2	2:C:107:ASN:H	1.77	0.49
2:G:12:LYS:O	2:G:14:ALA:N	2.46	0.49
1:B:473:HIS:CB	2:I:126:ARG:NH2	2.69	0.49
2:K:59:TRP:CD1	2:K:59:TRP:N	2.79	0.49
2:M:12:LYS:O	2:M:14:ALA:N	2.46	0.49
3:W:232:LEU:HD22	3:W:300:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:255:VAL:HG22	3:W:314:ARG:O	2.13	0.49
3:W:591:SER:HB2	3:W:596:THR:HG21	1.95	0.49
3:W:212:GLU:CB	3:W:696:LEU:HD12	2.39	0.49
1:A:122:LEU:HD11	1:A:201:ASP:CB	2.43	0.48
1:A:179:ASP:HA	1:A:677:ARG:NH2	2.27	0.48
1:A:271:PHE:CA	1:A:274:ILE:HD12	2.43	0.48
1:A:404:LEU:O	1:A:407:GLY:N	2.46	0.48
1:B:302:ASN:ND2	1:B:615:ASN:HB3	2.27	0.48
1:B:785:GLN:O	1:B:787:VAL:N	2.46	0.48
2:E:14:ALA:C	2:E:16:ASP:N	2.66	0.48
2:G:115:SER:O	2:G:119:LEU:HG	2.13	0.48
2:G:129:PHE:C	2:G:129:PHE:CD1	2.86	0.48
2:I:49:GLY:HA2	2:I:54:LEU:CD2	2.43	0.48
2:L:41:MET:O	2:L:42:ASN:C	2.51	0.48
2:O:69:THR:O	2:O:70:LEU:O	2.31	0.48
3:W:1047:LYS:O	3:W:1048:ASN:ND2	2.46	0.48
3:W:80:ASP:O	3:W:81:LYS:HG3	2.13	0.48
1:A:322:THR:O	1:A:323:THR:C	2.50	0.48
1:A:529:ILE:O	1:A:533:ILE:HG13	2.12	0.48
1:B:436:ILE:O	1:B:437:TYR:C	2.51	0.48
1:B:473:HIS:O	1:B:477:ASN:ND2	2.46	0.48
1:B:583:SER:O	1:B:587:LEU:HB3	2.12	0.48
1:B:789:LEU:O	1:B:790:ARG:C	2.51	0.48
2:K:30:LEU:O	2:K:31:ILE:C	2.52	0.48
2:K:6:SER:O	2:K:8:SER:N	2.46	0.48
2:L:109:ILE:HB	2:L:380:ASP:HB3	1.94	0.48
2:L:14:ALA:C	2:L:16:ASP:N	2.67	0.48
2:L:135:TYR:OH	2:L:340:GLU:OE1	2.30	0.48
2:M:38:ILE:HG22	2:M:42:ASN:ND2	2.27	0.48
2:M:6:SER:O	2:M:8:SER:N	2.45	0.48
2:N:53:ASN:ND2	2:N:354:ALA:HB3	2.28	0.48
2:O:48:THR:O	2:O:56:ILE:HA	2.12	0.48
3:W:396:SER:O	3:W:398:SER:N	2.46	0.48
3:W:477:VAL:HA	3:W:480:MET:HE3	1.94	0.48
1:A:434:THR:O	1:A:434:THR:CG2	2.61	0.48
1:B:477:ASN:HD21	2:I:39:ILE:HG21	1.77	0.48
1:B:486:ASP:O	1:B:488:VAL:N	2.46	0.48
1:B:522:PRO:O	1:B:525:TYR:HB2	2.14	0.48
1:B:765:PHE:CZ	1:B:767:THR:HG23	2.48	0.48
2:C:130:ASP:C	2:C:131:ASN:HD22	2.17	0.48
2:G:144:ARG:O	2:G:145:ARG:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:149:GLY:C	2:H:150:PHE:CD1	2.87	0.48
2:H:14:ALA:C	2:H:16:ASP:N	2.66	0.48
2:I:19:VAL:HG21	2:K:128:ASN:HB3	1.94	0.48
2:J:135:TYR:OH	2:J:340:GLU:OE1	2.30	0.48
2:M:123:LYS:HG3	2:M:124:PHE:CE1	2.49	0.48
2:M:131:ASN:O	2:N:16:ASP:HB3	2.13	0.48
2:O:144:ARG:C	2:O:145:ARG:HG2	2.33	0.48
3:W:1009:PHE:HE2	3:W:1042:ILE:HG13	1.78	0.48
3:W:498:ASN:HB2	3:W:1086:PHE:CE2	2.48	0.48
1:A:122:LEU:HD23	1:A:122:LEU:N	2.28	0.48
1:A:384:ALA:O	1:A:385:ALA:C	2.50	0.48
1:A:390:ARG:HE	1:A:574:GLU:HG2	1.78	0.48
1:A:704:ILE:O	1:A:823:THR:HB	2.14	0.48
1:B:228:MET:O	1:B:228:MET:HG3	2.12	0.48
1:B:231:ARG:CB	1:B:240:ASN:HB2	2.42	0.48
1:B:275:PRO:HD2	1:B:278:ILE:CD1	2.43	0.48
1:B:329:ALA:HB3	1:B:384:ALA:CB	2.43	0.48
1:B:422:GLU:O	1:B:425:VAL:HB	2.12	0.48
1:B:442:MET:O	1:B:443:GLN:C	2.50	0.48
2:E:133:SER:O	2:E:136:ILE:HG22	2.13	0.48
2:J:36:GLN:OE1	2:K:23:LEU:HD21	2.13	0.48
2:K:35:ASN:O	2:K:36:GLN:C	2.51	0.48
2:L:5:TYR:HE2	2:L:130:ASP:O	1.97	0.48
3:W:186:ASN:ND2	3:W:186:ASN:H	2.07	0.48
3:W:466:PRO:HD2	3:W:469:TYR:HD2	1.79	0.48
3:W:769:GLU:HG2	3:W:772:ILE:HD12	1.95	0.48
1:A:226:ALA:C	1:A:228:MET:H	2.15	0.48
1:A:305:GLN:OE1	1:A:564:ASN:ND2	2.44	0.48
1:A:484:VAL:CG1	1:A:485:ILE:H	2.25	0.48
1:A:486:ASP:OD2	1:A:490:ASN:HB2	2.13	0.48
1:A:545:ASP:O	1:A:546:LEU:C	2.51	0.48
1:A:545:ASP:OD1	1:A:548:ARG:NH1	2.46	0.48
1:A:170:TYR:CE1	1:A:682:PHE:HB2	2.49	0.48
1:B:108:LEU:C	1:B:110:ASP:N	2.67	0.48
1:B:176:GLU:O	1:B:178:PRO:CD	2.61	0.48
1:B:392:MET:CA	1:B:573:THR:HG23	2.43	0.48
1:B:521:MET:CB	1:B:522:PRO:CD	2.90	0.48
1:B:113:PRO:CD	1:B:609:ASN:HB3	2.43	0.48
2:D:125:LYS:O	2:D:127:ILE:N	2.46	0.48
2:E:6:SER:OG	2:E:128:ASN:HA	2.13	0.48
2:H:115:SER:O	2:H:119:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:22:THR:OG1	2:H:26:ASN:ND2	2.46	0.48
2:H:35:ASN:O	2:H:36:GLN:C	2.51	0.48
2:I:48:THR:O	2:I:56:ILE:HA	2.13	0.48
2:J:155:PRO:O	2:J:186:SER:HB3	2.14	0.48
2:O:14:ALA:O	2:O:18:ILE:CD1	2.61	0.48
2:O:42:ASN:HA	2:O:61:PHE:HB2	1.95	0.48
1:A:118:LYS:CG	1:A:119:GLN:N	2.73	0.48
1:A:404:LEU:CB	1:A:435:ILE:HD11	2.43	0.48
1:A:428:GLN:CB	1:A:456:PHE:HD1	2.22	0.48
1:A:460:GLU:C	1:A:462:GLN:H	2.16	0.48
1:A:516:GLN:CD	1:A:516:GLN:H	2.11	0.48
1:A:659:ASP:O	1:A:660:ASP:O	2.32	0.48
1:A:822:THR:O	1:A:823:THR:OG1	2.22	0.48
1:A:865:PRO:O	1:A:867:ASN:N	2.47	0.48
1:B:104:ILE:HD12	1:B:327:ILE:CD1	2.44	0.48
1:B:782:VAL:O	1:B:785:GLN:HB2	2.14	0.48
2:C:150:PHE:CD1	2:C:150:PHE:N	2.82	0.48
2:D:150:PHE:HB2	2:D:152:PHE:HE1	1.77	0.48
2:D:24:TYR:CE1	2:D:68:THR:HG22	2.48	0.48
2:D:31:ILE:O	2:D:34:PHE:HB3	2.13	0.48
2:E:35:ASN:O	2:E:36:GLN:C	2.52	0.48
2:F:53:ASN:ND2	2:F:354:ALA:HB3	2.28	0.48
2:G:54:LEU:HD12	2:G:55:PRO:HD2	1.96	0.48
2:M:128:ASN:HD22	2:N:19:VAL:HB	1.79	0.48
2:N:35:ASN:O	2:N:36:GLN:C	2.51	0.48
2:O:32:GLN:O	2:O:33:GLN:C	2.52	0.48
3:W:796:SER:C	3:W:798:ILE:H	2.16	0.48
3:W:825:ASN:HA	3:W:828:SER:CB	2.41	0.48
1:A:363:GLU:C	1:A:366:PHE:HE1	2.16	0.48
1:A:458:ILE:O	1:A:462:GLN:HG2	2.13	0.48
1:A:627:ALA:O	1:A:631:LEU:HG	2.13	0.48
1:A:629:ASN:C	1:A:631:LEU:N	2.61	0.48
1:B:190:ASN:O	1:B:190:ASN:CG	2.52	0.48
1:B:220:ALA:O	1:B:223:ARG:HB2	2.14	0.48
1:B:415:PRO:O	1:B:416:ASN:C	2.52	0.48
1:B:459:ALA:HB1	1:B:463:ILE:CD1	2.36	0.48
1:B:305:GLN:CG	1:B:564:ASN:HD21	2.26	0.48
1:B:723:ILE:O	1:B:724:ALA:CB	2.61	0.48
1:B:785:GLN:O	1:B:786:ILE:C	2.51	0.48
2:C:30:LEU:O	2:C:31:ILE:C	2.52	0.48
2:C:63:PHE:N	2:C:63:PHE:CD1	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:23:LEU:O	2:E:26:ASN:ND2	2.47	0.48
2:F:144:ARG:O	2:F:145:ARG:HG3	2.14	0.48
2:G:23:LEU:HD23	2:G:24:TYR:N	2.28	0.48
2:I:45:GLU:C	2:I:46:PHE:CD1	2.87	0.48
2:K:150:PHE:CD1	2:K:150:PHE:N	2.82	0.48
2:L:30:LEU:O	2:L:31:ILE:C	2.52	0.48
2:N:6:SER:O	2:N:8:SER:N	2.47	0.48
3:W:248:MET:O	3:W:252:VAL:HG13	2.14	0.48
3:W:626:ILE:O	3:W:627:ARG:NH1	2.43	0.48
1:A:145:ARG:HB3	1:A:147:TYR:CE1	2.49	0.48
1:A:589:GLY:C	1:A:591:ALA:N	2.66	0.48
1:B:233:GLN:HB2	1:B:238:VAL:HB	1.96	0.48
1:B:319:ASP:OD2	1:B:572:THR:N	2.46	0.48
1:B:452:PRO:O	1:B:453:GLN:OE1	2.32	0.48
1:B:594:ILE:HB	1:B:595:PRO:HD2	1.94	0.48
1:B:655:ALA:C	1:B:657:VAL:H	2.17	0.48
1:B:745:ALA:HA	1:B:748:THR:OG1	2.13	0.48
1:B:775:ILE:N	1:B:775:ILE:CD1	2.76	0.48
2:D:70:LEU:CG	2:D:71:LEU:N	2.76	0.48
2:I:128:ASN:O	2:J:22:THR:HB	2.14	0.48
2:M:22:THR:HG23	2:M:73:LEU:CD1	2.39	0.48
3:W:433:TYR:CE1	3:W:435:PRO:HD3	2.49	0.48
3:W:499:GLN:HE21	3:W:499:GLN:HB3	1.50	0.48
1:A:484:VAL:HG12	1:A:485:ILE:N	2.28	0.48
1:A:328:LEU:HG	1:A:603:TYR:HE1	1.79	0.48
1:A:769:SER:O	1:A:770:SER:C	2.51	0.48
1:A:817:TRP:CZ3	1:A:819:PRO:HA	2.49	0.48
1:A:239:VAL:HG21	1:A:845:ASN:O	2.13	0.48
1:B:214:ASP:O	1:B:216:GLU:N	2.47	0.48
1:B:517:GLN:N	1:B:518:PHE:CE1	2.79	0.48
1:B:536:LEU:CD2	1:B:536:LEU:N	2.77	0.48
1:B:712:LEU:HB3	1:B:819:PRO:HB2	1.96	0.48
1:B:811:LEU:HA	1:B:814:ASN:HD22	1.79	0.48
1:B:283:ASN:O	1:B:863:VAL:HG23	2.13	0.48
2:C:145:ARG:HB3	2:C:145:ARG:CZ	2.43	0.48
2:D:14:ALA:C	2:D:16:ASP:N	2.66	0.48
2:F:31:ILE:O	2:F:34:PHE:HB3	2.13	0.48
1:B:466:PHE:CD1	2:H:80:THR:HG22	2.48	0.48
2:I:37:MET:O	2:I:38:ILE:C	2.53	0.48
2:J:346:VAL:CG2	2:J:385:VAL:HG13	2.44	0.48
2:L:106:ARG:HG2	2:L:107:ASN:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:50:GLY:HA2	2:L:56:ILE:HD11	1.95	0.48
3:W:951:ILE:HG23	3:W:1071:TRP:HZ3	1.79	0.48
3:W:1082:ASN:O	3:W:1084:ASN:CG	2.52	0.48
3:W:464:ILE:HG22	3:W:464:ILE:O	2.14	0.48
3:W:519:THR:HG22	3:W:520:ASP:H	1.74	0.48
1:A:314:PHE:N	1:A:314:PHE:CD1	2.82	0.48
1:A:356:GLU:O	3:W:982:SER:HB2	2.14	0.48
1:A:365:GLN:C	1:A:366:PHE:CG	2.88	0.48
1:A:436:ILE:HD11	1:A:437:TYR:CE1	2.49	0.48
1:A:527:ARG:O	1:A:531:ARG:HG3	2.13	0.48
1:A:660:ASP:C	1:A:662:MET:N	2.66	0.48
1:A:694:ARG:HD2	1:A:828:GLN:HG3	1.96	0.48
1:B:126:PHE:HB3	1:B:149:LYS:O	2.14	0.48
1:B:236:ARG:O	1:B:237:ASN:CB	2.61	0.48
1:B:384:ALA:O	1:B:385:ALA:C	2.50	0.48
1:B:449:ASN:HD21	1:B:455:PRO:HG3	1.78	0.48
1:B:447:TYR:OH	1:B:458:ILE:HD11	2.13	0.48
1:B:478:ASN:C	1:B:480:PHE:H	2.17	0.48
1:B:533:ILE:O	1:B:536:LEU:HB2	2.14	0.48
1:B:540:LEU:C	1:B:540:LEU:HD23	2.34	0.48
1:B:639:LYS:O	1:B:640:ALA:C	2.52	0.48
1:B:89:GLU:C	1:B:91:LEU:H	2.16	0.48
2:F:38:ILE:HG22	2:F:42:ASN:ND2	2.27	0.48
2:I:35:ASN:O	2:I:36:GLN:C	2.52	0.48
2:I:346:VAL:CG2	2:I:385:VAL:HG13	2.44	0.48
2:I:41:MET:O	2:I:42:ASN:C	2.52	0.48
2:J:133:SER:O	2:J:136:ILE:HG22	2.13	0.48
2:J:19:VAL:O	2:J:21:GLY:N	2.47	0.48
2:K:115:SER:O	2:K:119:LEU:HG	2.14	0.48
2:L:139:TRP:HE1	2:L:143:ASN:ND2	2.11	0.48
2:M:14:ALA:C	2:M:16:ASP:N	2.66	0.48
2:M:30:LEU:O	2:M:31:ILE:C	2.52	0.48
2:M:35:ASN:O	2:M:36:GLN:C	2.51	0.48
2:O:35:ASN:O	2:O:36:GLN:C	2.52	0.48
2:O:346:VAL:CG2	2:O:385:VAL:HG13	2.44	0.48
2:O:63:PHE:CD2	2:O:84:THR:HG23	2.49	0.48
3:W:107:LEU:HB2	3:W:110:GLU:HG3	1.96	0.48
3:W:447:ILE:HG22	3:W:448:PRO:O	2.14	0.48
3:W:472:ALA:O	3:W:561:TYR:HD1	1.96	0.48
1:B:122:LEU:HD11	1:B:200:VAL:HG11	1.94	0.47
1:B:405:ILE:O	1:B:408:MET:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:131:ASN:ND2	2:C:131:ASN:N	2.62	0.47
2:D:66:LEU:O	2:D:67:GLY:O	2.31	0.47
2:E:131:ASN:HD22	2:E:131:ASN:N	2.11	0.47
2:I:48:THR:HG21	2:I:94:ASN:HB3	1.96	0.47
2:J:48:THR:O	2:J:56:ILE:HA	2.13	0.47
2:L:346:VAL:CG2	2:L:385:VAL:HG13	2.44	0.47
2:M:41:MET:O	2:M:42:ASN:C	2.52	0.47
2:N:152:PHE:N	2:N:152:PHE:CD1	2.82	0.47
2:N:42:ASN:HA	2:N:61:PHE:CB	2.44	0.47
2:N:99:GLU:OE2	2:N:112:GLN:HG2	2.13	0.47
2:O:12:LYS:O	2:O:14:ALA:N	2.46	0.47
3:W:772:ILE:HG23	3:W:1043:ASN:ND2	2.29	0.47
3:W:195:VAL:HG23	3:W:196:MET:N	2.29	0.47
3:W:497:SER:HB2	3:W:501:LEU:HD23	1.95	0.47
1:A:540:LEU:HA	1:A:543:LEU:HB2	1.96	0.47
1:B:822:THR:HG22	1:B:822:THR:O	2.14	0.47
2:C:5:TYR:HE2	2:C:131:ASN:HA	1.80	0.47
2:G:35:ASN:O	2:G:36:GLN:C	2.52	0.47
2:H:51:ILE:O	2:H:51:ILE:HG23	2.14	0.47
2:H:22:THR:HG23	2:H:73:LEU:CD1	2.43	0.47
2:M:115:SER:O	2:M:119:LEU:HG	2.14	0.47
3:W:387:ARG:HH11	3:W:387:ARG:CB	2.25	0.47
3:W:405:SER:HA	3:W:418:THR:HA	1.97	0.47
3:W:595:GLN:O	3:W:599:ALA:N	2.38	0.47
3:W:906:ASN:HD21	3:W:907:VAL:HG23	1.79	0.47
1:A:306:ASP:HB3	1:A:310:LEU:HD11	1.95	0.47
1:A:383:ILE:O	1:A:384:ALA:C	2.53	0.47
1:A:437:TYR:N	1:A:438:PRO:CD	2.73	0.47
1:A:503:ILE:HG12	1:A:547:THR:HG21	1.96	0.47
1:A:539:ARG:NH2	1:A:588:ILE:O	2.47	0.47
1:A:636:LYS:O	1:A:637:LYS:C	2.52	0.47
1:A:660:ASP:O	1:A:663:TYR:N	2.47	0.47
1:A:701:GLN:HB3	1:A:826:TYR:CD2	2.46	0.47
1:B:295:THR:O	1:B:297:ARG:HG2	2.14	0.47
1:B:296:ALA:C	1:B:297:ARG:HG2	2.35	0.47
1:B:493:LEU:HD11	1:B:567:HIS:HB2	1.95	0.47
1:B:638:MET:HE1	1:B:666:ARG:HH12	1.78	0.47
2:D:32:GLN:O	2:D:33:GLN:C	2.52	0.47
2:F:30:LEU:O	2:F:31:ILE:C	2.53	0.47
2:F:35:ASN:O	2:F:36:GLN:C	2.53	0.47
2:H:133:SER:O	2:H:136:ILE:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:33:GLN:HA	2:J:23:LEU:HD12	1.95	0.47
1:B:511:MET:HE3	2:J:70:LEU:HG	1.94	0.47
2:M:11:LEU:O	2:M:15:ARG:N	2.41	0.47
3:W:441:VAL:O	3:W:571:SER:HA	2.14	0.47
3:W:535:ARG:HH11	3:W:565:GLN:NE2	2.12	0.47
1:A:710:MET:HE1	1:A:824:LYS:HE2	1.97	0.47
1:A:714:ARG:HG2	1:A:720:TYR:HD2	1.79	0.47
1:A:827:LYS:O	1:A:828:GLN:O	2.32	0.47
1:B:355:LEU:HG	1:B:356:GLU:H	1.76	0.47
1:B:460:GLU:HG3	1:B:473:HIS:CD2	2.49	0.47
1:B:513:LEU:HA	1:B:516:GLN:HE22	1.71	0.47
2:D:48:THR:O	2:D:56:ILE:HA	2.14	0.47
2:E:30:LEU:O	2:E:31:ILE:C	2.51	0.47
2:G:346:VAL:CG2	2:G:385:VAL:HG13	2.45	0.47
2:H:151:THR:C	2:H:152:PHE:CD1	2.88	0.47
2:M:37:MET:O	2:M:38:ILE:C	2.53	0.47
2:N:32:GLN:O	2:N:33:GLN:C	2.53	0.47
2:O:153:HIS:O	2:O:154:LYS:C	2.52	0.47
3:W:382:ASP:O	3:W:387:ARG:HD2	2.14	0.47
3:W:385:LEU:HD13	3:W:939:VAL:HG22	1.96	0.47
1:A:148:TRP:CH2	1:A:246:HIS:HB2	2.49	0.47
1:A:311:HIS:N	1:A:311:HIS:ND1	2.63	0.47
1:A:742:GLY:CA	1:B:285:ILE:HD11	2.44	0.47
1:B:513:LEU:O	1:B:516:GLN:OE1	2.32	0.47
1:B:666:ARG:HG2	1:B:667:ASP:H	1.79	0.47
1:B:735:LEU:HD21	1:B:759:LEU:CB	2.45	0.47
1:B:95:ILE:O	1:B:97:THR:N	2.46	0.47
2:C:115:SER:O	2:C:119:LEU:HG	2.15	0.47
2:E:32:GLN:O	2:E:33:GLN:C	2.52	0.47
2:F:133:SER:O	2:F:136:ILE:HG22	2.14	0.47
1:B:481:ARG:HG2	2:I:65:LEU:CD1	2.44	0.47
2:J:129:PHE:O	2:J:131:ASN:ND2	2.47	0.47
2:K:125:LYS:O	2:K:127:ILE:N	2.45	0.47
2:N:23:LEU:HD23	2:N:24:TYR:N	2.29	0.47
2:O:115:SER:O	2:O:119:LEU:HG	2.14	0.47
1:A:338:GLU:O	1:A:338:GLU:HG3	2.14	0.47
1:A:527:ARG:HH11	1:A:531:ARG:HH21	1.63	0.47
1:A:596:SER:HB3	1:A:599:THR:OG1	2.15	0.47
1:A:723:ILE:O	1:A:824:LYS:HD2	2.14	0.47
1:B:593:VAL:HG12	1:B:594:ILE:N	2.30	0.47
2:E:346:VAL:CG2	2:E:385:VAL:HG13	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:78:VAL:O	2:F:81:ALA:HB3	2.14	0.47
2:G:153:HIS:O	2:G:154:LYS:C	2.53	0.47
2:I:144:ARG:O	2:I:145:ARG:HB2	2.15	0.47
2:K:100:MET:HG3	2:K:388:VAL:HG11	1.95	0.47
2:M:53:ASN:O	2:M:353:TYR:HD2	1.97	0.47
2:N:152:PHE:HD2	2:N:337:ASP:HB3	1.78	0.47
3:W:1058:TYR:HD2	3:W:1063:MET:HG2	1.79	0.47
1:A:248:ILE:O	1:A:251:ALA:HB3	2.14	0.47
1:A:454:THR:HB	1:A:457:GLN:CB	2.44	0.47
1:A:772:ILE:HA	1:A:775:ILE:CD1	2.45	0.47
1:B:308:LEU:HA	1:B:308:LEU:HD23	1.73	0.47
1:B:583:SER:O	1:B:584:LEU:C	2.53	0.47
2:F:142:GLN:HE21	2:F:143:ASN:N	2.12	0.47
2:F:72:ASN:ND2	2:H:126:ARG:HH11	2.12	0.47
2:H:23:LEU:N	2:H:26:ASN:HD22	2.12	0.47
2:I:124:PHE:C	2:I:126:ARG:N	2.68	0.47
2:I:139:TRP:HE1	2:I:143:ASN:HD22	1.62	0.47
2:J:63:PHE:CD2	2:J:84:THR:HG23	2.50	0.47
2:K:32:GLN:O	2:K:33:GLN:C	2.53	0.47
2:M:27:VAL:HG21	2:M:31:ILE:HD11	1.97	0.47
2:N:115:SER:O	2:N:119:LEU:HG	2.15	0.47
2:N:11:LEU:O	2:N:15:ARG:N	2.39	0.47
2:N:124:PHE:O	2:N:127:ILE:HG13	2.15	0.47
3:W:1068:LYS:HA	3:W:1068:LYS:HE3	1.96	0.47
3:W:24:ILE:HG21	3:W:46:LEU:CD1	2.44	0.47
3:W:449:LEU:HD22	3:W:573:VAL:HG11	1.95	0.47
3:W:633:ASN:O	3:W:633:ASN:OD1	2.33	0.47
1:A:133:ILE:O	1:A:134:TYR:HD2	1.97	0.47
1:A:205:ALA:O	1:A:206:SER:C	2.52	0.47
1:A:450:GLY:O	1:A:451:ASP:CB	2.62	0.47
1:A:494:ASN:CG	1:A:495:ASP:N	2.67	0.47
1:A:508:GLU:HG2	1:A:512:GLN:HE21	1.75	0.47
1:A:516:GLN:C	1:A:518:PHE:H	2.18	0.47
1:A:699:ILE:HA	1:A:763:LEU:O	2.14	0.47
1:B:122:LEU:O	1:B:253:ASN:OD1	2.32	0.47
1:B:211:ILE:C	1:B:213:GLN:N	2.67	0.47
1:B:548:ARG:O	1:B:551:ALA:HB3	2.15	0.47
1:B:721:VAL:CG1	1:B:722:ASN:N	2.77	0.47
1:B:725:ARG:H	1:B:725:ARG:CD	2.22	0.47
1:B:852:SER:O	1:B:854:LEU:N	2.46	0.47
2:I:102:ARG:HG2	2:I:102:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:128:ASN:ND2	2:M:19:VAL:HG21	2.30	0.47
2:L:32:GLN:O	2:L:33:GLN:C	2.52	0.47
2:L:37:MET:O	2:L:38:ILE:C	2.53	0.47
3:W:1013:ASP:O	3:W:1016:LYS:HG2	2.15	0.47
3:W:687:ILE:HG22	3:W:899:PHE:O	2.15	0.47
1:A:428:GLN:CD	1:A:456:PHE:N	2.67	0.47
1:A:510:LEU:HD12	1:A:513:LEU:HD12	1.96	0.47
1:A:510:LEU:CD2	1:A:540:LEU:HD13	2.29	0.47
1:A:578:LEU:HA	1:A:581:VAL:CG2	2.44	0.47
1:A:594:ILE:HG12	1:A:595:PRO:HD2	1.95	0.47
1:A:647:LYS:C	1:A:649:LEU:N	2.68	0.47
1:A:763:LEU:HD23	1:A:764:PRO:CD	2.44	0.47
1:B:360:ILE:O	1:B:361:GLN:HB2	2.15	0.47
1:B:458:ILE:HD12	1:B:459:ALA:CA	2.45	0.47
1:B:480:PHE:CE2	1:B:493:LEU:CB	2.96	0.47
1:B:549:LEU:HA	1:B:549:LEU:HD12	1.64	0.47
2:D:115:SER:O	2:D:119:LEU:HG	2.15	0.47
2:D:346:VAL:CG2	2:D:385:VAL:HG13	2.44	0.47
2:F:46:PHE:HE2	2:F:119:LEU:HD21	1.80	0.47
2:G:30:LEU:O	2:G:31:ILE:C	2.52	0.47
2:I:115:SER:O	2:I:119:LEU:HG	2.14	0.47
2:K:103:GLU:HG3	2:K:359:PRO:HD2	1.95	0.47
2:L:100:MET:HG3	2:L:388:VAL:HG11	1.95	0.47
2:N:346:VAL:CG2	2:N:385:VAL:HG13	2.44	0.47
2:O:104:SER:O	2:O:108:GLY:HA3	2.15	0.47
2:O:73:LEU:HD22	2:O:77:TYR:CD2	2.50	0.47
1:B:73:LEU:HB2	3:W:509:PHE:O	2.15	0.47
3:W:41:PHE:HD1	3:W:62:TYR:CD2	2.33	0.47
1:A:217:THR:O	1:A:218:GLU:HB2	2.13	0.47
1:A:332:VAL:O	1:A:333:VAL:C	2.53	0.47
1:A:277:ARG:CD	1:A:559:ALA:HB2	2.43	0.47
1:A:663:TYR:O	1:A:666:ARG:N	2.47	0.47
1:A:803:ASN:ND2	1:A:806:SER:H	2.13	0.47
1:B:653:ASP:O	1:B:653:ASP:CG	2.52	0.47
1:B:845:ASN:HB3	1:B:848:PHE:CE1	2.49	0.47
1:B:854:LEU:O	1:B:856:ALA:N	2.47	0.47
2:C:106:ARG:H	2:C:106:ARG:CD	2.10	0.47
2:E:5:TYR:HE2	2:E:130:ASP:O	1.98	0.47
2:F:53:ASN:HD22	2:F:354:ALA:CB	2.26	0.47
2:I:23:LEU:HD22	2:I:25:SER:OG	2.14	0.47
2:J:27:VAL:HG21	2:J:31:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:27:VAL:O	2:K:31:ILE:HG12	2.15	0.47
2:M:32:GLN:O	2:M:33:GLN:C	2.52	0.47
2:O:135:TYR:CZ	2:O:342:MET:HE3	2.50	0.47
3:W:134:ILE:CG2	3:W:136:THR:HG22	2.45	0.47
1:A:122:LEU:CD1	1:A:201:ASP:HB2	2.45	0.47
1:A:356:GLU:HB3	1:A:357:ALA:H	1.30	0.47
1:B:112:LYS:N	1:B:113:PRO:CD	2.78	0.47
1:B:354:GLN:HA	1:B:354:GLN:OE1	2.15	0.47
1:B:503:ILE:O	1:B:504:ASN:C	2.54	0.47
1:B:519:PRO:O	1:B:520:THR:OG1	2.32	0.47
1:B:383:ILE:HD11	1:B:550:LEU:HD23	1.97	0.47
1:B:645:PHE:HD2	1:B:646:LEU:CD2	2.25	0.47
1:B:752:LEU:C	1:B:754:ASN:N	2.63	0.47
1:B:87:GLN:C	1:B:89:GLU:N	2.68	0.47
2:C:150:PHE:HA	2:D:397:LYS:NZ	2.30	0.47
1:A:461:GLN:CA	2:F:32:GLN:NE2	2.75	0.47
2:G:32:GLN:O	2:G:33:GLN:C	2.53	0.47
2:H:11:LEU:O	2:H:15:ARG:N	2.39	0.47
2:H:346:VAL:CG2	2:H:385:VAL:HG13	2.44	0.47
2:K:109:ILE:HG13	2:K:110:ALA:N	2.29	0.47
2:N:37:MET:O	2:N:38:ILE:C	2.53	0.47
2:O:65:LEU:O	2:O:66:LEU:HD23	2.15	0.47
3:W:215:MET:CE	3:W:215:MET:HA	2.45	0.47
1:A:169:LEU:HA	1:A:169:LEU:HD12	1.62	0.46
1:A:180:TYR:CD1	1:A:181:LEU:N	2.83	0.46
1:A:286:LEU:H	1:A:286:LEU:CD2	2.10	0.46
1:B:409:TRP:O	1:B:412:THR:HB	2.16	0.46
1:B:479:GLN:O	1:B:480:PHE:HB3	2.16	0.46
2:C:129:PHE:CE1	2:C:130:ASP:HB2	2.50	0.46
2:D:128:ASN:HD22	2:E:19:VAL:HG21	1.80	0.46
2:E:41:MET:O	2:E:42:ASN:C	2.52	0.46
2:F:106:ARG:NH1	2:F:106:ARG:HB2	2.30	0.46
2:F:27:VAL:O	2:F:30:LEU:N	2.47	0.46
2:I:36:GLN:HE22	2:I:126:ARG:HD3	1.80	0.46
2:I:42:ASN:OD1	2:I:62:ASP:N	2.48	0.46
2:L:27:VAL:CG2	2:L:31:ILE:HD11	2.45	0.46
2:L:57:ARG:HB3	2:L:59:TRP:CZ2	2.49	0.46
2:N:124:PHE:O	2:N:126:ARG:N	2.49	0.46
2:N:30:LEU:O	2:N:31:ILE:C	2.54	0.46
3:W:300:LEU:N	3:W:300:LEU:HD12	2.30	0.46
3:W:402:ASN:N	3:W:420:LYS:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:400:ALA:HB2	3:W:470:PHE:CE2	2.50	0.46
3:W:283:GLN:HG2	3:W:649:GLN:HG3	1.97	0.46
3:W:924:ASP:C	3:W:944:ILE:HD13	2.35	0.46
3:W:827:VAL:HG13	3:W:940:TYR:CZ	2.50	0.46
1:A:419:PHE:CD1	1:A:419:PHE:N	2.82	0.46
1:A:746:GLN:O	1:A:750:MET:HG3	2.14	0.46
1:A:760:VAL:HG12	1:A:761:GLY:N	2.30	0.46
2:D:150:PHE:N	2:D:150:PHE:CD1	2.83	0.46
2:E:54:LEU:HD12	2:E:55:PRO:CD	2.42	0.46
2:I:128:ASN:HB3	2:J:19:VAL:CG2	2.44	0.46
2:I:144:ARG:O	2:I:145:ARG:CB	2.64	0.46
2:M:14:ALA:O	2:M:18:ILE:HD12	2.16	0.46
3:W:449:LEU:HD21	3:W:461:ILE:HD12	1.97	0.46
1:A:250:TYR:HB2	1:A:840:HIS:CD2	2.50	0.46
1:A:253:ASN:O	1:A:256:PHE:HB2	2.14	0.46
1:A:386:MET:HE3	1:A:414:VAL:HG13	1.96	0.46
1:A:499:ASN:CA	1:A:505:GLN:NE2	2.77	0.46
1:A:854:LEU:CD2	1:A:855:LEU:N	2.78	0.46
1:A:856:ALA:O	1:A:858:VAL:N	2.41	0.46
1:B:282:VAL:O	1:B:284:TYR:N	2.48	0.46
1:B:369:GLY:C	1:B:371:ASN:N	2.69	0.46
1:B:420:ILE:O	1:B:422:GLU:N	2.48	0.46
1:B:75:VAL:HG12	1:B:75:VAL:O	2.16	0.46
1:B:820:THR:O	1:B:820:THR:HG22	2.15	0.46
2:C:110:ALA:HB1	2:C:111:PRO:HD2	1.97	0.46
2:C:62:ASP:H	2:C:63:PHE:HD1	1.62	0.46
2:E:73:LEU:HD22	2:E:77:TYR:CD2	2.50	0.46
2:F:100:MET:HG3	2:F:388:VAL:HG11	1.97	0.46
2:I:32:GLN:O	2:I:33:GLN:C	2.54	0.46
2:L:153:HIS:O	2:L:154:LYS:C	2.54	0.46
2:N:66:LEU:O	2:N:67:GLY:C	2.53	0.46
2:N:76:ASN:HB2	2:O:76:ASN:HB2	1.97	0.46
3:W:109:TYR:HA	3:W:118:LEU:HD21	1.98	0.46
1:A:363:GLU:HA	1:A:366:PHE:HE1	1.80	0.46
1:A:428:GLN:HG3	1:A:456:PHE:HA	1.97	0.46
1:A:722:ASN:HB3	1:A:824:LYS:HA	1.96	0.46
1:B:500:GLY:HA3	1:B:871:PHE:HZ	1.80	0.46
1:B:818:VAL:HA	1:B:819:PRO:HD3	1.75	0.46
2:C:19:VAL:HG23	2:E:128:ASN:HB3	1.98	0.46
2:D:38:ILE:HG22	2:D:42:ASN:ND2	2.30	0.46
2:F:115:SER:O	2:F:119:LEU:HG	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:150:PHE:N	2:H:150:PHE:CD1	2.84	0.46
2:H:27:VAL:HG21	2:H:31:ILE:HD11	1.96	0.46
2:I:1:MET:C	2:I:3:VAL:N	2.67	0.46
2:J:32:GLN:O	2:J:33:GLN:C	2.54	0.46
2:K:63:PHE:N	2:K:63:PHE:CD1	2.82	0.46
2:L:153:HIS:NE2	2:M:153:HIS:CD2	2.84	0.46
2:M:128:ASN:HB3	2:N:19:VAL:HG23	1.97	0.46
3:W:1080:TYR:C	3:W:1082:ASN:H	2.19	0.46
3:W:129:LEU:HB2	3:W:201:TYR:OH	2.15	0.46
3:W:295:MET:O	3:W:300:LEU:HB2	2.15	0.46
1:A:145:ARG:HB3	1:A:147:TYR:HE1	1.79	0.46
1:A:151:LYS:O	1:A:152:LYS:CB	2.63	0.46
1:A:405:ILE:HG21	1:A:536:LEU:CG	2.43	0.46
1:A:775:ILE:C	1:A:777:LYS:H	2.19	0.46
1:A:548:ARG:HB2	1:A:877:MET:HE2	1.98	0.46
1:B:298:TYR:C	1:B:298:TYR:CD1	2.88	0.46
1:B:739:MET:C	1:B:741:THR:H	2.19	0.46
2:D:14:ALA:O	2:D:18:ILE:HD12	2.16	0.46
2:J:148:THR:OG1	2:J:332:GLU:HG2	2.15	0.46
2:J:153:HIS:O	2:J:154:LYS:C	2.53	0.46
2:K:54:LEU:HD12	2:K:55:PRO:CD	2.41	0.46
2:N:150:PHE:N	2:N:150:PHE:CD1	2.84	0.46
2:O:141:LEU:CD1	2:O:148:THR:HG21	2.46	0.46
2:O:1:MET:O	2:O:2:ASP:C	2.53	0.46
2:O:60:ASN:C	2:O:61:PHE:CD1	2.89	0.46
3:W:801:GLU:O	3:W:804:ALA:HB3	2.15	0.46
3:W:922:GLU:OE1	3:W:926:SER:N	2.49	0.46
1:A:197:GLY:O	1:A:198:LYS:O	2.34	0.46
1:A:122:LEU:CG	1:A:201:ASP:HB2	2.46	0.46
1:A:454:THR:HG22	1:A:457:GLN:H	1.80	0.46
1:A:639:LYS:HE3	1:A:659:ASP:OD1	2.15	0.46
1:A:772:ILE:O	1:A:773:SER:C	2.54	0.46
1:B:366:PHE:O	1:B:368:THR:N	2.48	0.46
1:B:490:ASN:O	1:B:492:VAL:HG23	2.15	0.46
1:B:605:ASN:ND2	1:B:855:LEU:HD12	2.30	0.46
2:I:61:PHE:N	2:I:61:PHE:CD1	2.83	0.46
2:O:139:TRP:NE1	2:O:143:ASN:ND2	2.63	0.46
3:W:180:TYR:CE1	3:W:200:PRO:HD3	2.51	0.46
1:A:299:ILE:O	1:A:301:PRO:HD3	2.15	0.46
1:A:314:PHE:CZ	1:A:664:ARG:HG2	2.51	0.46
1:A:329:ALA:HB3	1:A:384:ALA:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:PHE:O	1:A:602:HIS:C	2.54	0.46
1:A:620:ASP:O	1:A:624:ILE:HG13	2.15	0.46
1:B:413:VAL:CG1	1:B:414:VAL:H	2.26	0.46
1:B:608:VAL:O	1:B:609:ASN:C	2.54	0.46
1:B:857:PHE:CD1	1:B:857:PHE:N	2.72	0.46
2:D:123:LYS:HG3	2:D:124:PHE:CE1	2.50	0.46
2:D:61:PHE:N	2:D:61:PHE:CD1	2.84	0.46
2:F:22:THR:CG2	2:F:73:LEU:HD12	2.45	0.46
2:F:346:VAL:CG2	2:F:385:VAL:HG13	2.44	0.46
2:K:129:PHE:C	2:K:129:PHE:CD1	2.89	0.46
2:L:49:GLY:HA2	2:L:54:LEU:HD23	1.98	0.46
3:W:101:ASP:O	3:W:103:THR:N	2.48	0.46
3:W:426:ASP:O	3:W:430:ASN:HB2	2.15	0.46
3:W:760:ASN:ND2	3:W:760:ASN:C	2.67	0.46
3:W:865:VAL:HG22	3:W:865:VAL:O	2.16	0.46
1:A:404:LEU:HB3	1:A:435:ILE:HD11	1.98	0.46
1:A:506:LEU:HD23	1:A:544:VAL:CA	2.29	0.46
1:A:660:ASP:HB3	1:B:539:ARG:NH1	2.20	0.46
1:A:706:ALA:C	1:A:708:ARG:H	2.19	0.46
1:A:708:ARG:HD2	1:A:708:ARG:HA	1.80	0.46
1:B:373:GLN:O	1:B:376:ASN:N	2.49	0.46
1:B:478:ASN:O	1:B:480:PHE:N	2.45	0.46
1:B:601:PHE:HB3	1:B:855:LEU:HD13	1.98	0.46
1:B:770:SER:O	1:B:773:SER:HB2	2.15	0.46
1:B:854:LEU:O	1:B:855:LEU:C	2.54	0.46
2:C:346:VAL:CG2	2:C:385:VAL:HG13	2.44	0.46
2:C:41:MET:O	2:C:42:ASN:C	2.53	0.46
2:F:22:THR:HG23	2:F:73:LEU:HD12	1.98	0.46
2:G:41:MET:O	2:G:42:ASN:C	2.54	0.46
2:M:346:VAL:CG2	2:M:385:VAL:HG13	2.45	0.46
2:L:153:HIS:CD2	2:N:153:HIS:NE2	2.83	0.46
2:N:61:PHE:N	2:N:61:PHE:CD1	2.84	0.46
3:W:112:ASN:OD1	3:W:202:TYR:HB2	2.16	0.46
3:W:465:LEU:HB3	3:W:469:TYR:CD2	2.50	0.46
3:W:535:ARG:HH11	3:W:565:GLN:HE22	1.63	0.46
1:A:779:ASP:OD2	1:A:822:THR:O	2.34	0.46
1:A:846:LEU:HA	1:A:846:LEU:HD23	1.65	0.46
1:A:867:ASN:CG	1:A:867:ASN:O	2.54	0.46
1:B:118:LYS:CG	1:B:119:GLN:N	2.73	0.46
1:B:239:VAL:CG2	1:B:845:ASN:O	2.63	0.46
1:B:314:PHE:HZ	1:B:664:ARG:HG2	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:GLN:HG3	1:B:349:MET:CE	2.46	0.46
1:B:510:LEU:HD13	1:B:540:LEU:HB2	1.98	0.46
1:B:383:ILE:HD11	1:B:550:LEU:HD22	1.97	0.46
1:B:727:LEU:HG	1:B:727:LEU:O	2.15	0.46
1:B:783:PHE:O	1:B:784:ALA:C	2.54	0.46
1:B:848:PHE:O	1:B:849:THR:OG1	2.28	0.46
1:A:461:GLN:CB	2:F:32:GLN:NE2	2.79	0.46
2:I:155:PRO:O	2:I:186:SER:HB3	2.16	0.46
2:I:382:LEU:HD22	2:I:386:PHE:CE2	2.51	0.46
2:J:142:GLN:HE21	2:J:143:ASN:N	2.13	0.46
2:J:27:VAL:CG2	2:J:31:ILE:HD11	2.45	0.46
2:L:104:SER:HB3	2:L:108:GLY:CA	2.46	0.46
2:O:37:MET:O	2:O:38:ILE:C	2.54	0.46
2:O:22:THR:CG2	2:O:73:LEU:HD12	2.46	0.46
3:W:160:LEU:O	3:W:163:TYR:HB3	2.16	0.46
3:W:310:TRP:CZ2	3:W:319:PHE:HD1	2.34	0.46
3:W:438:ILE:HD11	3:W:563:GLN:CB	2.45	0.46
1:A:245:LEU:O	1:A:246:HIS:HB2	2.16	0.46
1:A:428:GLN:OE1	1:A:456:PHE:CB	2.38	0.46
1:A:509:ALA:O	1:A:513:LEU:CG	2.55	0.46
1:A:821:SER:OG	1:A:822:THR:N	2.46	0.46
1:B:340:VAL:O	1:B:341:SER:C	2.54	0.46
1:B:613:ASN:O	1:B:617:ARG:HG2	2.16	0.46
1:B:94:THR:O	1:B:94:THR:HG22	2.16	0.46
2:D:30:LEU:O	2:D:31:ILE:C	2.53	0.46
2:F:239:ASN:ND2	2:F:246:THR:HG22	2.29	0.46
2:H:106:ARG:O	2:H:107:ASN:CB	2.62	0.46
2:H:239:ASN:ND2	2:H:246:THR:HG22	2.30	0.46
2:I:135:TYR:CE1	2:I:342:MET:HE3	2.51	0.46
2:K:346:VAL:CG2	2:K:385:VAL:HG13	2.44	0.46
3:W:105:ASN:HD22	3:W:111:ASN:HA	1.76	0.46
3:W:290:GLN:HB2	3:W:290:GLN:HE21	1.54	0.46
3:W:467:TYR:C	3:W:467:TYR:CD1	2.89	0.46
3:W:598:ALA:O	3:W:602:ILE:HG13	2.16	0.46
1:A:549:LEU:HA	1:A:549:LEU:HD12	1.65	0.45
1:B:137:ASN:CG	1:B:137:ASN:O	2.55	0.45
1:B:170:TYR:CZ	1:B:682:PHE:HB2	2.52	0.45
1:B:637:LYS:HA	1:B:641:ILE:HD11	1.97	0.45
1:B:675:GLU:O	1:B:677:ARG:N	2.49	0.45
2:G:5:TYR:HE2	2:G:131:ASN:HA	1.80	0.45
2:H:62:ASP:H	2:H:63:PHE:HD1	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:382:LEU:HD22	2:J:386:PHE:CE2	2.52	0.45
2:J:37:MET:O	2:J:38:ILE:C	2.54	0.45
2:K:382:LEU:HD22	2:K:386:PHE:CE2	2.51	0.45
2:N:1:MET:O	2:N:2:ASP:C	2.55	0.45
2:N:1:MET:C	2:N:3:VAL:N	2.69	0.45
3:W:396:SER:OG	3:W:474:HIS:NE2	2.49	0.45
1:A:416:ASN:C	1:A:418:MET:N	2.70	0.45
1:B:282:VAL:HG13	1:B:283:ASN:N	2.31	0.45
1:B:583:SER:OG	1:B:584:LEU:N	2.48	0.45
1:B:772:ILE:HG22	1:B:809:PHE:CE2	2.51	0.45
2:C:135:TYR:CZ	2:C:342:MET:HE3	2.52	0.45
2:F:17:LYS:HE2	2:H:130:ASP:OD2	2.16	0.45
2:G:109:ILE:O	2:G:109:ILE:HD12	2.17	0.45
2:H:21:GLY:O	2:H:22:THR:O	2.34	0.45
2:I:136:ILE:HG23	2:I:137:GLU:N	2.31	0.45
2:I:1:MET:O	2:I:2:ASP:C	2.54	0.45
2:I:30:LEU:O	2:I:31:ILE:C	2.52	0.45
2:I:36:GLN:HB2	2:J:23:LEU:HD11	1.97	0.45
2:I:89:VAL:C	2:I:91:PHE:H	2.19	0.45
1:B:508:GLU:OE2	2:J:70:LEU:CD2	2.65	0.45
2:L:115:SER:O	2:L:119:LEU:HG	2.15	0.45
2:L:73:LEU:HD22	2:L:77:TYR:HD2	1.77	0.45
2:M:382:LEU:HD22	2:M:386:PHE:CE2	2.52	0.45
3:W:186:ASN:O	3:W:189:TYR:N	2.48	0.45
3:W:302:ASP:O	3:W:306:MET:HG3	2.17	0.45
3:W:422:MET:HA	3:W:425:MET:HG3	1.99	0.45
3:W:690:ARG:O	3:W:723:ARG:NH1	2.49	0.45
3:W:872:ILE:HG13	3:W:1072:ASN:O	2.17	0.45
1:A:526:LYS:HG3	1:A:527:ARG:N	2.31	0.45
1:A:353:LEU:HD22	1:A:531:ARG:HB3	1.98	0.45
1:A:608:VAL:O	1:A:609:ASN:C	2.55	0.45
1:A:688:ASN:O	1:A:691:GLN:N	2.49	0.45
1:A:706:ALA:O	1:A:708:ARG:N	2.45	0.45
1:B:542:GLN:OE1	1:B:542:GLN:N	2.49	0.45
1:B:594:ILE:HD12	1:B:594:ILE:O	2.17	0.45
1:B:633:LEU:O	1:B:635:GLN:N	2.48	0.45
1:B:872:ASP:CG	1:B:874:MET:H	2.20	0.45
2:C:124:PHE:O	2:C:127:ILE:HG13	2.16	0.45
2:C:59:TRP:N	2:C:59:TRP:CD1	2.83	0.45
2:E:190:VAL:HG21	2:E:210:HIS:HB2	1.99	0.45
2:F:32:GLN:O	2:F:33:GLN:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:382:LEU:HD22	2:H:386:PHE:CE2	2.51	0.45
1:B:498:ARG:CZ	2:J:25:SER:HB3	2.47	0.45
2:J:78:VAL:O	2:J:81:ALA:N	2.40	0.45
2:K:24:TYR:O	2:K:27:VAL:HG22	2.16	0.45
2:L:239:ASN:ND2	2:L:246:THR:HG22	2.29	0.45
2:L:22:THR:CG2	2:L:73:LEU:HD12	2.24	0.45
2:M:53:ASN:HD22	2:M:354:ALA:HB3	1.81	0.45
2:N:24:TYR:CE1	2:N:31:ILE:HG13	2.51	0.45
3:W:125:TYR:HE1	3:W:201:TYR:HE1	1.63	0.45
3:W:64:ASP:OD2	3:W:65:VAL:N	2.48	0.45
3:W:819:LEU:C	3:W:820:LEU:HD23	2.37	0.45
1:A:266:ASN:C	1:A:292:LEU:HD12	2.36	0.45
1:A:466:PHE:O	1:A:467:GLN:C	2.54	0.45
1:A:518:PHE:CB	1:A:519:PRO:CD	2.94	0.45
1:A:688:ASN:O	1:A:690:ASP:N	2.50	0.45
1:B:119:GLN:CG	1:B:181:LEU:HD11	2.46	0.45
1:B:159:ASP:O	1:B:162:VAL:HB	2.16	0.45
1:B:420:ILE:O	1:B:421:ARG:C	2.54	0.45
1:B:589:GLY:C	1:B:591:ALA:H	2.20	0.45
2:C:37:MET:O	2:C:38:ILE:C	2.55	0.45
2:D:1:MET:C	2:D:3:VAL:N	2.70	0.45
2:D:37:MET:O	2:D:38:ILE:C	2.55	0.45
2:J:1:MET:C	2:J:3:VAL:N	2.68	0.45
2:L:89:VAL:C	2:L:91:PHE:H	2.20	0.45
2:M:144:ARG:O	2:M:145:ARG:HB2	2.17	0.45
3:W:180:TYR:CD1	3:W:200:PRO:HD3	2.51	0.45
3:W:479:LYS:HD3	3:W:479:LYS:HA	1.85	0.45
3:W:705:THR:O	3:W:709:GLN:HB2	2.16	0.45
1:A:857:PHE:CD1	1:A:857:PHE:N	2.83	0.45
1:B:205:ALA:O	1:B:206:SER:C	2.55	0.45
1:B:434:THR:O	1:B:435:ILE:CG1	2.65	0.45
1:B:854:LEU:HD22	1:B:855:LEU:H	1.82	0.45
2:C:382:LEU:HD22	2:C:386:PHE:CE2	2.51	0.45
2:D:190:VAL:HG21	2:D:210:HIS:HB2	1.99	0.45
2:D:382:LEU:HD22	2:D:386:PHE:CE2	2.52	0.45
2:I:225:LEU:HD13	2:I:277:PHE:HD2	1.82	0.45
2:M:130:ASP:HA	2:N:17:LYS:HG2	1.98	0.45
2:N:110:ALA:HB1	2:N:111:PRO:HD2	1.99	0.45
3:W:161:LYS:HB3	3:W:165:ARG:NH1	2.28	0.45
3:W:247:PRO:O	3:W:251:LEU:HG	2.17	0.45
3:W:944:ILE:HG23	3:W:945:GLU:N	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:HIS:O	1:A:247:PRO:C	2.54	0.45
1:A:367:LEU:CD2	3:W:932:ARG:HB2	2.46	0.45
1:A:482:GLN:OE1	1:A:493:LEU:CD2	2.64	0.45
1:A:804:SER:HB2	1:A:810:TYR:CA	2.47	0.45
1:A:712:LEU:CG	1:A:819:PRO:HB2	2.40	0.45
1:A:822:THR:O	1:A:823:THR:CB	2.64	0.45
1:B:646:LEU:N	1:B:646:LEU:HD23	2.32	0.45
1:B:852:SER:O	1:B:853:ASP:HB3	2.16	0.45
2:C:128:ASN:O	2:D:22:THR:HB	2.17	0.45
2:C:190:VAL:HG21	2:C:210:HIS:HB2	1.99	0.45
2:D:24:TYR:O	2:D:26:ASN:N	2.50	0.45
2:D:78:VAL:O	2:D:81:ALA:HB3	2.17	0.45
2:E:312:GLN:HB3	2:E:313:PRO:HA	1.99	0.45
2:H:107:ASN:ND2	2:H:109:ILE:HG23	2.32	0.45
2:H:190:VAL:HG21	2:H:210:HIS:HB2	1.99	0.45
2:H:32:GLN:O	2:H:33:GLN:C	2.54	0.45
2:L:190:VAL:HG21	2:L:210:HIS:HB2	1.99	0.45
2:M:155:PRO:HA	2:M:337:ASP:HB2	1.99	0.45
3:W:410:PHE:CE2	3:W:415:ILE:HD11	2.52	0.45
3:W:477:VAL:HA	3:W:480:MET:HE2	1.99	0.45
3:W:501:LEU:HD12	3:W:501:LEU:O	2.17	0.45
3:W:4:TYR:CD1	3:W:733:LEU:HD22	2.33	0.45
3:W:874:ILE:CG2	3:W:875:ASN:N	2.80	0.45
1:A:155:LEU:HA	1:A:156:PRO:HD3	1.55	0.45
1:A:546:LEU:HD13	1:A:584:LEU:HD23	1.97	0.45
1:A:319:ASP:OD2	1:A:571:LEU:N	2.49	0.45
1:B:419:PHE:O	1:B:420:ILE:C	2.54	0.45
1:B:554:TYR:O	1:B:558:MET:HB2	2.17	0.45
1:B:577:GLN:O	1:B:579:THR:N	2.50	0.45
1:B:601:PHE:N	1:B:601:PHE:CD1	2.80	0.45
1:B:742:GLY:O	1:B:744:TYR:HE2	1.98	0.45
1:B:772:ILE:O	1:B:773:SER:C	2.54	0.45
1:B:85:GLU:O	1:B:86:ILE:C	2.54	0.45
2:D:54:LEU:HD12	2:D:55:PRO:CD	2.46	0.45
2:E:11:LEU:O	2:E:15:ARG:N	2.41	0.45
2:E:382:LEU:HD22	2:E:386:PHE:CE2	2.51	0.45
2:F:190:VAL:HG21	2:F:210:HIS:HB2	1.99	0.45
2:G:150:PHE:HB2	2:G:152:PHE:CZ	2.51	0.45
2:H:105:GLN:O	2:H:107:ASN:N	2.50	0.45
2:H:312:GLN:HB3	2:H:313:PRO:HA	1.99	0.45
2:J:60:ASN:C	2:J:61:PHE:CD1	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:382:LEU:HD22	2:L:386:PHE:CE2	2.52	0.45
2:M:110:ALA:HB1	2:M:111:PRO:HD2	1.99	0.45
2:N:23:LEU:HD22	2:N:25:SER:OG	2.17	0.45
3:W:448:PRO:HB2	3:W:464:ILE:HB	1.99	0.45
1:A:252:PHE:CD2	1:A:684:LEU:CD2	3.00	0.45
1:A:339:LEU:O	1:A:340:VAL:C	2.55	0.45
1:A:452:PRO:O	1:A:453:GLN:OE1	2.35	0.45
1:A:454:THR:O	1:A:457:GLN:HB3	2.17	0.45
1:A:503:ILE:O	1:A:505:GLN:N	2.50	0.45
1:A:506:LEU:CD2	1:A:544:VAL:CA	2.94	0.45
1:A:580:SER:O	1:A:581:VAL:C	2.55	0.45
1:B:400:ASN:O	1:B:404:LEU:CD1	2.65	0.45
1:B:601:PHE:O	1:B:602:HIS:C	2.53	0.45
2:D:225:LEU:HD13	2:D:277:PHE:HD2	1.82	0.45
2:E:154:LYS:N	2:E:327:GLU:O	2.42	0.45
2:E:37:MET:O	2:E:38:ILE:C	2.54	0.45
2:F:312:GLN:HB3	2:F:313:PRO:HA	1.99	0.45
2:G:382:LEU:HD22	2:G:386:PHE:CE2	2.51	0.45
2:H:48:THR:O	2:H:56:ILE:HA	2.17	0.45
2:I:145:ARG:O	2:I:146:GLN:CG	2.65	0.45
2:I:42:ASN:OD1	2:I:61:PHE:HB3	2.16	0.45
2:J:225:LEU:HD13	2:J:277:PHE:HD2	1.82	0.45
2:J:41:MET:O	2:J:42:ASN:C	2.54	0.45
2:M:225:LEU:HD13	2:M:277:PHE:HD2	1.82	0.45
2:O:217:VAL:HG22	2:O:286:ASP:HB3	1.99	0.45
3:W:538:ILE:HD12	3:W:565:GLN:NE2	2.31	0.45
3:W:695:LEU:HD21	3:W:732:ILE:CD1	2.47	0.45
3:W:840:ASN:OD1	3:W:846:SER:HA	2.16	0.45
1:A:186:MET:HG3	1:A:200:VAL:HG13	1.98	0.45
1:A:583:SER:OG	1:A:584:LEU:N	2.50	0.45
1:A:762:ALA:C	1:A:763:LEU:HG	2.37	0.45
1:A:783:PHE:N	1:A:783:PHE:CD1	2.72	0.45
1:B:119:GLN:NE2	1:B:181:LEU:HD11	2.32	0.45
1:B:277:ARG:HH11	1:B:277:ARG:HB3	1.80	0.45
1:B:496:ASN:HB3	1:B:499:ASN:H	1.82	0.45
1:B:573:THR:CG2	1:B:574:GLU:N	2.45	0.45
1:B:771:VAL:HG21	1:B:809:PHE:O	2.17	0.45
1:B:786:ILE:HG22	1:B:792:VAL:HG12	1.98	0.45
2:C:127:ILE:O	2:C:127:ILE:HG22	2.15	0.45
2:C:136:ILE:HG23	2:C:137:GLU:N	2.32	0.45
2:E:225:LEU:HD13	2:E:277:PHE:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:225:LEU:HD13	2:F:277:PHE:HD2	1.82	0.45
2:F:382:LEU:HD22	2:F:386:PHE:CE2	2.52	0.45
2:H:30:LEU:O	2:H:31:ILE:C	2.53	0.45
2:I:273:TYR:C	2:I:274:GLN:HE21	2.20	0.45
2:I:217:VAL:HG22	2:I:286:ASP:HB3	1.99	0.45
2:J:70:LEU:HD22	2:J:72:ASN:O	2.16	0.45
2:J:89:VAL:C	2:J:91:PHE:H	2.21	0.45
2:M:312:GLN:HB3	2:M:313:PRO:HA	1.99	0.45
2:N:89:VAL:C	2:N:91:PHE:H	2.21	0.45
2:O:131:ASN:HD22	2:O:131:ASN:N	2.14	0.45
2:O:190:VAL:HG21	2:O:210:HIS:HB2	1.99	0.45
2:O:225:LEU:HD13	2:O:277:PHE:HD2	1.82	0.45
2:O:273:TYR:C	2:O:274:GLN:HE21	2.21	0.45
3:W:301:VAL:O	3:W:304:PRO:HD2	2.17	0.45
1:A:224:PHE:O	1:A:225:ILE:C	2.55	0.45
1:A:269:ILE:HG21	1:A:298:TYR:CE2	2.51	0.45
1:A:428:GLN:HG2	1:A:429:LEU:H	1.79	0.45
1:A:866:ILE:HG22	1:A:866:ILE:O	2.17	0.45
1:B:467:GLN:HE21	1:B:511:MET:HG2	1.82	0.45
1:B:596:SER:O	1:B:597:PRO:C	2.55	0.45
1:B:772:ILE:CG2	1:B:809:PHE:HE2	2.29	0.45
1:B:846:LEU:HD12	1:B:847:THR:N	2.32	0.45
2:C:217:VAL:HG22	2:C:286:ASP:HB3	1.99	0.45
2:C:32:GLN:O	2:C:33:GLN:C	2.54	0.45
2:G:190:VAL:HG21	2:G:210:HIS:HB2	1.99	0.45
2:H:126:ARG:C	2:H:127:ILE:HG13	2.37	0.45
2:J:217:VAL:HG22	2:J:286:ASP:HB3	1.99	0.45
2:J:312:GLN:HB3	2:J:313:PRO:HA	1.99	0.45
2:K:190:VAL:HG21	2:K:210:HIS:HB2	1.99	0.45
2:M:42:ASN:HA	2:M:61:PHE:CB	2.46	0.45
2:N:135:TYR:CZ	2:N:342:MET:HE3	2.53	0.45
2:N:382:LEU:HD22	2:N:386:PHE:CE2	2.52	0.45
1:A:118:LYS:CG	1:A:119:GLN:H	2.29	0.44
1:A:117:LYS:HB2	1:A:179:ASP:CG	2.37	0.44
1:A:420:ILE:HD11	1:A:423:SER:HB2	1.99	0.44
1:A:587:LEU:O	1:A:587:LEU:HD22	2.17	0.44
1:A:680:ASP:HA	1:A:683:ASN:HD22	1.81	0.44
1:B:428:GLN:CB	1:B:456:PHE:CD1	2.90	0.44
1:B:763:LEU:HD22	1:B:764:PRO:HD3	1.99	0.44
2:C:1:MET:C	2:C:3:VAL:N	2.70	0.44
2:D:136:ILE:HG23	2:D:137:GLU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:217:VAL:HG22	2:D:286:ASP:HB3	1.99	0.44
2:E:44:ASN:HB3	2:E:46:PHE:HE1	1.81	0.44
2:G:273:TYR:C	2:G:274:GLN:HE21	2.20	0.44
2:G:312:GLN:HB3	2:G:313:PRO:HA	1.99	0.44
2:G:78:VAL:O	2:G:81:ALA:HB3	2.18	0.44
2:I:190:VAL:HG21	2:I:210:HIS:HB2	1.99	0.44
2:J:153:HIS:NE2	2:K:153:HIS:CD2	2.84	0.44
2:K:225:LEU:HD13	2:K:277:PHE:HD2	1.82	0.44
2:K:37:MET:O	2:K:38:ILE:C	2.55	0.44
2:L:225:LEU:HD13	2:L:277:PHE:HD2	1.82	0.44
2:L:312:GLN:HB3	2:L:313:PRO:HA	1.99	0.44
2:L:60:ASN:C	2:L:61:PHE:CD1	2.91	0.44
3:W:105:ASN:HB2	3:W:111:ASN:OD1	2.18	0.44
3:W:580:VAL:HG12	3:W:581:ILE:N	2.32	0.44
1:A:101:LYS:C	1:A:103:SER:H	2.20	0.44
1:A:270:ILE:HD11	1:A:292:LEU:CD1	2.23	0.44
1:A:286:LEU:O	1:A:287:ASN:CB	2.65	0.44
1:A:296:ALA:C	1:A:297:ARG:HG2	2.38	0.44
1:A:348:LYS:O	1:A:351:GLN:HB2	2.17	0.44
1:B:226:ALA:O	1:B:228:MET:N	2.50	0.44
1:B:248:ILE:O	1:B:251:ALA:HB3	2.17	0.44
1:B:420:ILE:O	1:B:420:ILE:HG23	2.18	0.44
1:B:463:ILE:HD12	1:B:472:LEU:CD1	2.47	0.44
1:B:374:ALA:O	1:B:580:SER:HB2	2.17	0.44
1:B:148:TRP:HE1	1:B:833:PHE:HD1	1.64	0.44
2:C:22:THR:HG23	2:C:73:LEU:CD1	2.46	0.44
2:C:54:LEU:HD12	2:C:55:PRO:CD	2.44	0.44
2:F:273:TYR:C	2:F:274:GLN:HE21	2.21	0.44
2:F:78:VAL:O	2:F:81:ALA:N	2.43	0.44
2:I:140:ASN:O	2:I:143:ASN:N	2.50	0.44
2:J:1:MET:O	2:J:2:ASP:C	2.54	0.44
2:M:239:ASN:ND2	2:M:246:THR:HG22	2.30	0.44
2:N:225:LEU:HD13	2:N:277:PHE:HD2	1.82	0.44
2:O:1:MET:C	2:O:3:VAL:N	2.68	0.44
2:O:382:LEU:HD22	2:O:386:PHE:CE2	2.51	0.44
3:W:437:ILE:O	3:W:439:PRO:HD3	2.17	0.44
1:A:229:ARG:O	1:A:242:PRO:HG3	2.18	0.44
1:A:556:THR:O	1:A:558:MET:N	2.51	0.44
1:A:660:ASP:OD1	1:A:661:GLN:N	2.50	0.44
1:A:674:VAL:HB	1:A:679:LEU:HB2	1.99	0.44
1:B:183:LEU:HD12	1:B:844:SER:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:THR:HG22	1:B:371:ASN:ND2	2.26	0.44
1:B:382:LEU:HA	1:B:382:LEU:HD12	1.62	0.44
1:B:447:TYR:C	1:B:448:ARG:HG2	2.38	0.44
1:B:674:VAL:O	1:B:675:GLU:C	2.54	0.44
1:B:757:VAL:HG12	1:B:758:ALA:N	2.32	0.44
2:C:27:VAL:O	2:C:30:LEU:HB3	2.17	0.44
2:C:69:THR:OG1	2:C:70:LEU:N	2.49	0.44
2:C:89:VAL:C	2:C:91:PHE:H	2.21	0.44
2:F:153:HIS:CD2	2:H:153:HIS:NE2	2.86	0.44
2:K:111:PRO:O	2:K:112:GLN:HG2	2.17	0.44
2:K:239:ASN:ND2	2:K:246:THR:HG22	2.29	0.44
2:K:78:VAL:O	2:K:81:ALA:N	2.40	0.44
2:L:136:ILE:HG23	2:L:137:GLU:N	2.32	0.44
1:A:597:PRO:HB3	1:A:860:ALA:HB1	1.99	0.44
1:A:804:SER:CB	1:A:810:TYR:HA	2.48	0.44
1:B:158:GLY:O	1:B:159:ASP:C	2.56	0.44
1:B:250:TYR:HB2	1:B:840:HIS:CD2	2.53	0.44
1:B:630:ARG:O	1:B:631:LEU:CG	2.62	0.44
1:B:751:LEU:O	1:B:754:ASN:HA	2.16	0.44
1:B:790:ARG:CG	1:B:791:LYS:N	2.71	0.44
2:C:145:ARG:HH11	2:C:145:ARG:CB	2.30	0.44
2:C:152:PHE:O	2:C:328:SER:HA	2.17	0.44
2:C:63:PHE:CD2	2:C:84:THR:HG23	2.52	0.44
2:E:1:MET:C	2:E:3:VAL:N	2.68	0.44
2:E:66:LEU:HB3	2:E:77:TYR:OH	2.16	0.44
2:E:78:VAL:O	2:E:81:ALA:HB3	2.17	0.44
2:F:48:THR:HG22	2:F:115:SER:OG	2.18	0.44
2:J:225:LEU:HD13	2:J:277:PHE:CD2	2.53	0.44
2:J:89:VAL:C	2:J:91:PHE:N	2.71	0.44
2:K:27:VAL:CG2	2:K:31:ILE:HD11	2.48	0.44
2:L:34:PHE:O	2:L:37:MET:HB3	2.17	0.44
2:N:190:VAL:HG21	2:N:210:HIS:HB2	1.99	0.44
2:O:89:VAL:C	2:O:91:PHE:H	2.21	0.44
3:W:223:TYR:CZ	3:W:227:LYS:HD2	2.53	0.44
3:W:473:GLN:NE2	3:W:593:GLU:HB3	2.29	0.44
1:B:361:GLN:NE2	3:W:624:LYS:HZ1	2.12	0.44
1:A:130:GLN:NE2	1:A:146:TRP:CZ2	2.85	0.44
1:A:513:LEU:CA	1:A:516:GLN:NE2	2.65	0.44
1:A:557:LEU:O	1:A:558:MET:C	2.55	0.44
1:A:870:ALA:C	1:A:872:ASP:H	2.20	0.44
1:B:277:ARG:CB	1:B:277:ARG:HH11	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:HIS:O	1:B:447:TYR:CB	2.49	0.44
1:B:498:ARG:HH11	1:B:502:VAL:HG11	1.83	0.44
1:B:707:TYR:N	1:B:707:TYR:CD1	2.85	0.44
2:G:239:ASN:ND2	2:G:246:THR:HG22	2.29	0.44
2:F:82:ARG:CZ	2:H:144:ARG:HD2	2.47	0.44
2:H:37:MET:O	2:H:38:ILE:C	2.55	0.44
2:I:101:VAL:HG11	2:I:355:ILE:HG13	1.99	0.44
2:J:273:TYR:C	2:J:274:GLN:HE21	2.20	0.44
2:K:136:ILE:HG23	2:K:137:GLU:N	2.32	0.44
2:K:1:MET:O	2:K:2:ASP:C	2.54	0.44
2:K:1:MET:C	2:K:3:VAL:N	2.68	0.44
2:L:273:TYR:C	2:L:274:GLN:HE21	2.21	0.44
2:D:75:ALA:HB3	2:L:76:ASN:HA	2.00	0.44
2:M:136:ILE:HG23	2:M:137:GLU:N	2.33	0.44
2:M:150:PHE:O	2:M:330:VAL:HG13	2.17	0.44
2:N:38:ILE:HG22	2:N:42:ASN:ND2	2.29	0.44
2:N:78:VAL:O	2:N:81:ALA:HB3	2.17	0.44
3:W:232:LEU:CD2	3:W:300:LEU:HD12	2.46	0.44
3:W:241:ALA:HB2	3:W:332:VAL:HG21	2.00	0.44
3:W:448:PRO:HD2	3:W:464:ILE:O	2.17	0.44
3:W:840:ASN:HA	3:W:845:ILE:HG21	1.97	0.44
1:A:488:VAL:O	1:A:490:ASN:N	2.51	0.44
1:A:516:GLN:OE1	1:A:517:GLN:N	2.50	0.44
1:A:727:LEU:O	1:A:727:LEU:CD1	2.65	0.44
1:A:771:VAL:HG13	1:A:772:ILE:N	2.22	0.44
1:A:701:GLN:CG	1:A:826:TYR:CD2	3.00	0.44
1:B:393:SER:HA	1:B:423:SER:CB	2.47	0.44
1:B:449:ASN:ND2	1:B:455:PRO:HG3	2.33	0.44
1:B:680:ASP:HA	1:B:683:ASN:HD22	1.82	0.44
1:B:727:LEU:HD23	1:B:826:TYR:CE1	2.53	0.44
2:E:225:LEU:HD13	2:E:277:PHE:CD2	2.53	0.44
2:E:273:TYR:C	2:E:274:GLN:HE21	2.21	0.44
2:F:11:LEU:O	2:F:15:ARG:N	2.40	0.44
2:F:249:PHE:CE2	2:F:251:PRO:HG3	2.53	0.44
2:F:37:MET:O	2:F:38:ILE:C	2.56	0.44
2:F:41:MET:O	2:F:42:ASN:C	2.56	0.44
2:G:104:SER:O	2:G:108:GLY:CA	2.66	0.44
2:G:33:GLN:HB2	2:H:26:ASN:OD1	2.16	0.44
2:H:67:GLY:O	2:H:69:THR:N	2.51	0.44
2:I:24:TYR:N	2:I:71:LEU:O	2.51	0.44
2:K:273:TYR:C	2:K:274:GLN:HE21	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:225:LEU:HD13	2:M:277:PHE:CD2	2.53	0.44
2:M:273:TYR:C	2:M:274:GLN:HE21	2.20	0.44
2:N:63:PHE:N	2:N:63:PHE:CD1	2.85	0.44
2:O:125:LYS:C	2:O:127:ILE:H	2.21	0.44
2:O:136:ILE:HG23	2:O:137:GLU:N	2.32	0.44
3:W:948:TYR:OH	3:W:1071:TRP:HA	2.18	0.44
3:W:123:GLU:CD	3:W:123:GLU:N	2.71	0.44
3:W:148:TRP:CE3	3:W:149:LEU:HD23	2.52	0.44
3:W:424:VAL:O	3:W:428:MET:HG3	2.17	0.44
1:A:312:ASP:O	1:A:313:ASN:CB	2.63	0.44
1:A:795:LEU:HA	1:A:795:LEU:HD12	1.74	0.44
1:B:428:GLN:HA	1:B:431:ILE:CD1	2.42	0.44
1:B:519:PRO:O	1:B:520:THR:CB	2.66	0.44
1:B:738:LEU:HD12	1:B:738:LEU:HA	1.82	0.44
2:C:3:VAL:O	2:C:4:LEU:C	2.56	0.44
2:D:249:PHE:CE2	2:D:251:PRO:HG3	2.53	0.44
2:D:73:LEU:N	2:D:73:LEU:HD23	2.33	0.44
2:G:23:LEU:C	2:G:23:LEU:HD23	2.38	0.44
2:H:142:GLN:NE2	2:H:143:ASN:N	2.65	0.44
2:H:249:PHE:CE2	2:H:251:PRO:HG3	2.53	0.44
2:H:217:VAL:HG22	2:H:286:ASP:HB3	2.00	0.44
2:I:225:LEU:HD13	2:I:277:PHE:CD2	2.53	0.44
2:I:46:PHE:HE2	2:I:119:LEU:HD21	1.83	0.44
2:J:78:VAL:O	2:J:81:ALA:HB3	2.17	0.44
2:K:110:ALA:HB1	2:K:111:PRO:HD2	2.00	0.44
2:K:14:ALA:O	2:K:16:ASP:N	2.51	0.44
2:K:312:GLN:HB3	2:K:313:PRO:HA	1.99	0.44
2:M:151:THR:C	2:M:152:PHE:CD1	2.91	0.44
2:M:249:PHE:CE2	2:M:251:PRO:HG3	2.53	0.44
2:N:217:VAL:HG22	2:N:286:ASP:HB3	2.00	0.44
2:O:153:HIS:CD2	2:O:154:LYS:N	2.86	0.44
2:O:169:SER:HA	2:O:176:LEU:HD23	2.00	0.44
2:O:225:LEU:HD13	2:O:277:PHE:CD2	2.53	0.44
3:W:770:ASP:O	3:W:771:PHE:HB2	2.18	0.44
1:A:625:ILE:H	1:A:625:ILE:HG13	1.62	0.44
1:B:108:LEU:CD2	1:B:108:LEU:N	2.79	0.44
1:B:155:LEU:HA	1:B:156:PRO:HD3	1.81	0.44
1:B:282:VAL:HG13	1:B:283:ASN:H	1.83	0.44
1:B:305:GLN:OE1	1:B:305:GLN:HA	2.18	0.44
1:B:404:LEU:O	1:B:405:ILE:C	2.55	0.44
1:B:487:GLY:O	1:B:488:VAL:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:GLU:O	1:B:512:GLN:NE2	2.48	0.44
2:C:249:PHE:CE2	2:C:251:PRO:HG3	2.53	0.44
2:D:66:LEU:HD23	2:D:66:LEU:HA	1.72	0.44
2:E:217:VAL:HG22	2:E:286:ASP:HB3	2.00	0.44
2:F:169:SER:HA	2:F:176:LEU:HD23	2.00	0.44
2:G:169:SER:HA	2:G:176:LEU:HD23	2.00	0.44
2:I:122:LEU:C	2:I:124:PHE:H	2.21	0.44
2:J:103:GLU:OE1	2:J:358:GLY:HA3	2.18	0.44
2:K:14:ALA:C	2:K:18:ILE:HD12	2.39	0.44
2:K:227:PRO:HD3	2:K:277:PHE:CG	2.53	0.44
2:L:225:LEU:HD13	2:L:277:PHE:CD2	2.53	0.44
2:M:217:VAL:HG22	2:M:286:ASP:HB3	1.99	0.44
2:O:312:GLN:HB3	2:O:313:PRO:HA	1.99	0.44
3:W:758:THR:HG22	3:W:766:PHE:C	2.37	0.44
3:W:897:GLN:N	3:W:897:GLN:OE1	2.49	0.44
1:A:245:LEU:O	1:A:246:HIS:CB	2.66	0.44
1:A:181:LEU:H	1:A:260:GLN:HE21	1.65	0.44
1:A:618:ILE:HD13	1:A:645:PHE:HZ	1.83	0.44
1:A:160:TYR:HE1	1:A:633:LEU:HA	1.83	0.44
1:A:799:LEU:HD22	1:A:800:TYR:H	1.82	0.44
1:B:101:LYS:HB2	1:B:102:GLU:H	1.68	0.44
1:B:111:ILE:HG22	1:B:113:PRO:CD	2.48	0.44
1:B:122:LEU:HD12	1:B:124:ARG:HH22	1.82	0.44
1:B:207:ILE:O	1:B:210:ALA:HB3	2.18	0.44
1:B:353:LEU:HD23	1:B:353:LEU:O	2.18	0.44
1:B:473:HIS:HB3	2:I:126:ARG:NH1	2.26	0.44
1:B:496:ASN:HD22	1:B:498:ARG:HB2	1.83	0.44
1:B:543:LEU:O	1:B:546:LEU:HB2	2.18	0.44
1:B:675:GLU:O	1:B:678:ARG:N	2.51	0.44
1:B:790:ARG:CG	1:B:791:LYS:H	2.18	0.44
1:B:870:ALA:O	1:B:871:PHE:C	2.55	0.44
2:C:273:TYR:C	2:C:274:GLN:HE21	2.21	0.44
2:D:169:SER:HA	2:D:176:LEU:HD23	2.00	0.44
2:D:5:TYR:CE2	2:D:131:ASN:HA	2.52	0.44
2:E:125:LYS:C	2:E:127:ILE:H	2.21	0.44
2:E:249:PHE:CE2	2:E:251:PRO:HG3	2.53	0.44
2:G:100:MET:HG3	2:G:388:VAL:HG11	1.99	0.44
2:G:150:PHE:N	2:G:150:PHE:CD1	2.86	0.44
2:G:37:MET:O	2:G:38:ILE:C	2.55	0.44
2:H:78:VAL:O	2:H:81:ALA:HB3	2.17	0.44
2:I:63:PHE:CD1	2:I:63:PHE:N	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:49:GLY:HA2	2:K:54:LEU:HD23	1.99	0.44
2:K:89:VAL:C	2:K:91:PHE:N	2.71	0.44
2:L:63:PHE:CD2	2:L:84:THR:HG23	2.53	0.44
2:M:190:VAL:HG21	2:M:210:HIS:HB2	1.99	0.44
2:N:169:SER:HA	2:N:176:LEU:HD23	2.00	0.44
2:N:21:GLY:O	2:N:22:THR:C	2.56	0.44
2:O:106:ARG:HG2	2:O:107:ASN:H	1.83	0.44
2:O:78:VAL:O	2:O:81:ALA:HB3	2.18	0.44
3:W:832:ALA:O	3:W:836:LYS:HG3	2.17	0.44
3:W:894:ILE:O	3:W:894:ILE:HG13	2.17	0.44
1:A:119:GLN:NE2	1:A:178:PRO:HG2	2.33	0.43
1:A:428:GLN:HE22	1:A:455:PRO:HB2	1.74	0.43
1:B:293:PRO:O	1:B:295:THR:N	2.50	0.43
1:B:321:ILE:O	1:B:322:THR:C	2.57	0.43
1:B:510:LEU:O	1:B:513:LEU:N	2.51	0.43
1:B:529:ILE:O	1:B:533:ILE:HG13	2.18	0.43
1:B:506:LEU:CD2	1:B:544:VAL:HA	2.39	0.43
2:C:225:LEU:HD13	2:C:277:PHE:HD2	1.82	0.43
2:D:273:TYR:C	2:D:274:GLN:HE21	2.21	0.43
2:D:312:GLN:HB3	2:D:313:PRO:HA	1.99	0.43
2:E:89:VAL:C	2:E:91:PHE:H	2.22	0.43
2:G:225:LEU:HD13	2:G:277:PHE:CD2	2.53	0.43
2:H:225:LEU:HD13	2:H:277:PHE:CD2	2.53	0.43
2:H:225:LEU:HD13	2:H:277:PHE:HD2	1.82	0.43
2:H:41:MET:O	2:H:42:ASN:C	2.56	0.43
2:I:89:VAL:C	2:I:91:PHE:N	2.70	0.43
2:J:125:LYS:O	2:J:127:ILE:N	2.42	0.43
2:L:217:VAL:HG22	2:L:286:ASP:HB3	2.00	0.43
2:L:3:VAL:O	2:L:4:LEU:C	2.56	0.43
2:M:89:VAL:C	2:M:91:PHE:H	2.21	0.43
2:N:151:THR:C	2:N:152:PHE:CD1	2.91	0.43
2:N:155:PRO:O	2:N:186:SER:HB3	2.17	0.43
2:N:2:ASP:HB2	2:N:128:ASN:HD21	1.83	0.43
2:N:62:ASP:H	2:N:63:PHE:HD1	1.66	0.43
2:O:227:PRO:HD3	2:O:277:PHE:CG	2.53	0.43
2:O:3:VAL:O	2:O:4:LEU:C	2.56	0.43
3:W:1006:LEU:HG	3:W:1086:PHE:CE1	2.49	0.43
3:W:527:SER:O	3:W:530:ASN:N	2.48	0.43
3:W:824:ASN:O	3:W:827:VAL:N	2.46	0.43
3:W:981:TYR:CZ	3:W:985:LYS:HD2	2.53	0.43
1:A:141:GLU:O	1:A:142:LEU:CB	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ALA:O	1:A:188:VAL:CG2	2.66	0.43
1:A:333:VAL:HB	1:A:380:LYS:HG2	2.00	0.43
1:A:416:ASN:C	1:A:418:MET:H	2.21	0.43
1:A:810:TYR:C	1:A:812:VAL:N	2.71	0.43
1:A:722:ASN:ND2	1:A:823:THR:O	2.51	0.43
1:A:854:LEU:O	1:A:855:LEU:C	2.56	0.43
1:B:138:GLY:O	1:B:804:SER:HB3	2.18	0.43
1:B:190:ASN:O	1:B:192:ASN:O	2.35	0.43
1:B:341:SER:O	1:B:342:THR:C	2.57	0.43
1:B:498:ARG:CD	2:I:32:GLN:NE2	2.82	0.43
1:B:503:ILE:HG12	1:B:547:THR:HB	2.00	0.43
1:B:491:GLN:CG	1:B:564:ASN:HB3	2.48	0.43
1:B:374:ALA:CB	1:B:580:SER:HB3	2.44	0.43
1:B:635:GLN:C	1:B:636:LYS:O	2.50	0.43
2:C:153:HIS:NE2	2:D:153:HIS:NE2	2.66	0.43
2:C:227:PRO:HD3	2:C:277:PHE:CG	2.53	0.43
2:C:239:ASN:ND2	2:C:246:THR:HG22	2.29	0.43
2:C:312:GLN:HB3	2:C:313:PRO:HA	1.99	0.43
2:D:99:GLU:CD	2:D:116:LEU:CD2	2.86	0.43
2:E:1:MET:O	2:E:2:ASP:C	2.56	0.43
2:G:61:PHE:N	2:G:61:PHE:CD1	2.86	0.43
2:I:36:GLN:CB	2:J:23:LEU:HD11	2.48	0.43
2:K:217:VAL:HG22	2:K:286:ASP:HB3	2.00	0.43
2:L:14:ALA:O	2:L:18:ILE:HD12	2.18	0.43
2:L:35:ASN:O	2:L:37:MET:N	2.51	0.43
2:M:169:SER:HA	2:M:176:LEU:HD23	2.00	0.43
2:M:22:THR:OG1	2:M:26:ASN:ND2	2.45	0.43
2:O:249:PHE:CE2	2:O:251:PRO:HG3	2.53	0.43
3:W:377:GLU:N	3:W:378:PRO:CD	2.81	0.43
3:W:595:GLN:O	3:W:599:ALA:HB3	2.18	0.43
3:W:786:ARG:HD3	3:W:869:SER:HB2	1.99	0.43
3:W:825:ASN:O	3:W:829:ARG:HG2	2.18	0.43
3:W:951:ILE:HG13	3:W:985:LYS:HG2	1.99	0.43
1:A:143:ARG:HG3	1:A:144:ASN:N	2.34	0.43
1:A:215:GLU:CD	1:A:215:GLU:H	2.21	0.43
1:A:181:LEU:N	1:A:260:GLN:HE21	2.16	0.43
1:A:396:PHE:HD2	1:A:578:LEU:HD11	1.84	0.43
1:A:501:HIS:CA	1:A:503:ILE:HG13	2.48	0.43
1:A:591:ALA:O	1:A:877:MET:SD	2.76	0.43
1:A:772:ILE:O	1:A:774:LEU:N	2.51	0.43
1:A:751:LEU:HD21	1:A:783:PHE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:SER:CB	1:A:807:ASN:OD1	2.60	0.43
1:B:309:ASN:HA	1:B:311:HIS:CE1	2.54	0.43
1:B:791:LYS:HB3	1:B:792:VAL:H	1.59	0.43
2:D:63:PHE:N	2:D:63:PHE:CD1	2.86	0.43
2:E:78:VAL:O	2:E:81:ALA:N	2.41	0.43
2:F:217:VAL:HG22	2:F:286:ASP:HB3	1.99	0.43
2:G:225:LEU:HD13	2:G:277:PHE:HD2	1.82	0.43
2:G:53:ASN:ND2	2:G:354:ALA:HB3	2.33	0.43
2:H:227:PRO:HD3	2:H:277:PHE:CG	2.53	0.43
2:I:169:SER:HA	2:I:176:LEU:HD23	2.00	0.43
2:J:3:VAL:O	2:J:4:LEU:C	2.56	0.43
2:K:3:VAL:O	2:K:4:LEU:C	2.56	0.43
2:K:5:TYR:HE2	2:K:131:ASN:HA	1.79	0.43
2:N:136:ILE:HG23	2:N:137:GLU:N	2.33	0.43
2:M:128:ASN:HB3	2:N:19:VAL:CG2	2.48	0.43
2:N:227:PRO:HD3	2:N:277:PHE:CG	2.53	0.43
3:W:165:ARG:HH11	3:W:165:ARG:HG3	1.84	0.43
3:W:586:TYR:HE2	3:W:588:ALA:HB3	1.81	0.43
3:W:81:LYS:O	3:W:82:TYR:HB2	2.19	0.43
3:W:854:ILE:O	3:W:858:LEU:HG	2.17	0.43
3:W:954:HIS:HB2	3:W:957:GLU:HG3	1.99	0.43
1:A:383:ILE:O	1:A:386:MET:N	2.52	0.43
1:A:750:MET:CE	1:A:757:VAL:HG21	2.48	0.43
1:A:781:THR:HG22	1:A:782:VAL:N	2.34	0.43
1:B:312:ASP:CG	1:B:312:ASP:O	2.56	0.43
1:B:510:LEU:HA	1:B:513:LEU:HD12	1.99	0.43
1:B:510:LEU:HD22	1:B:540:LEU:CD1	2.30	0.43
1:B:542:GLN:O	1:B:543:LEU:C	2.57	0.43
1:B:595:PRO:HB2	1:B:600:LEU:HD11	2.00	0.43
2:C:1:MET:O	2:C:2:ASP:C	2.56	0.43
2:E:142:GLN:HE21	2:E:143:ASN:N	2.16	0.43
2:E:227:PRO:HD3	2:E:277:PHE:CG	2.53	0.43
2:F:227:PRO:HD3	2:F:277:PHE:CG	2.53	0.43
2:G:249:PHE:CE2	2:G:251:PRO:HG3	2.53	0.43
2:G:6:SER:C	2:G:8:SER:N	2.72	0.43
2:H:169:SER:HA	2:H:176:LEU:HD23	2.00	0.43
2:I:146:GLN:O	2:I:148:THR:HG23	2.19	0.43
2:I:227:PRO:HD3	2:I:277:PHE:CG	2.53	0.43
2:I:312:GLN:HB3	2:I:313:PRO:HA	1.99	0.43
2:K:225:LEU:HD13	2:K:277:PHE:CD2	2.53	0.43
2:L:42:ASN:CA	2:L:61:PHE:HB2	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:89:VAL:C	2:L:91:PHE:N	2.71	0.43
2:M:24:TYR:N	2:M:71:LEU:O	2.49	0.43
2:N:153:HIS:O	2:N:154:LYS:C	2.57	0.43
2:N:225:LEU:HD13	2:N:277:PHE:CD2	2.53	0.43
2:N:101:VAL:HG11	2:N:355:ILE:HG13	2.01	0.43
3:W:650:ASP:O	3:W:654:ASP:OD1	2.36	0.43
1:A:243:SER:O	1:A:839:MET:HG2	2.19	0.43
1:A:415:PRO:O	1:A:417:ASP:N	2.43	0.43
1:A:408:MET:HG2	1:A:471:TRP:CH2	2.53	0.43
1:A:546:LEU:HD23	1:A:546:LEU:HA	1.86	0.43
1:A:548:ARG:HH11	1:A:877:MET:H	1.67	0.43
1:A:583:SER:O	1:A:584:LEU:C	2.56	0.43
1:A:714:ARG:HG2	1:A:720:TYR:CD2	2.54	0.43
1:A:717:MET:HE3	1:A:829:VAL:HG13	2.01	0.43
1:A:799:LEU:HD23	1:A:799:LEU:HA	1.68	0.43
1:B:309:ASN:HA	1:B:311:HIS:NE2	2.33	0.43
1:B:451:ASP:H	1:B:452:PRO:CD	2.20	0.43
1:B:540:LEU:HD23	1:B:541:GLY:CA	2.48	0.43
1:B:703:VAL:CG1	1:B:704:ILE:N	2.81	0.43
1:B:706:ALA:C	1:B:708:ARG:N	2.72	0.43
1:B:772:ILE:O	1:B:775:ILE:N	2.51	0.43
2:C:78:VAL:O	2:C:81:ALA:HB3	2.17	0.43
2:E:125:LYS:O	2:E:127:ILE:N	2.51	0.43
2:E:136:ILE:HG23	2:E:137:GLU:N	2.34	0.43
2:E:24:TYR:HE1	2:E:31:ILE:HG13	1.83	0.43
2:E:60:ASN:C	2:E:61:PHE:CD1	2.91	0.43
2:F:225:LEU:HD13	2:F:277:PHE:CD2	2.53	0.43
2:F:3:VAL:O	2:F:4:LEU:C	2.56	0.43
2:G:217:VAL:HG22	2:G:286:ASP:HB3	1.99	0.43
2:G:38:ILE:H	2:G:38:ILE:HG13	1.59	0.43
2:H:1:MET:O	2:H:2:ASP:C	2.57	0.43
2:I:34:PHE:O	2:I:37:MET:HB3	2.18	0.43
2:J:169:SER:HA	2:J:176:LEU:HD23	2.00	0.43
2:K:89:VAL:C	2:K:91:PHE:H	2.21	0.43
2:L:169:SER:HA	2:L:176:LEU:HD23	2.00	0.43
2:L:249:PHE:CE2	2:L:251:PRO:HG3	2.53	0.43
2:M:123:LYS:HG3	2:M:124:PHE:CD1	2.53	0.43
2:M:155:PRO:HA	2:M:337:ASP:CB	2.49	0.43
2:M:63:PHE:HD2	2:M:84:THR:HG23	1.81	0.43
2:N:145:ARG:HE	2:N:145:ARG:HA	1.83	0.43
2:N:24:TYR:HE1	2:N:31:ILE:HG13	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:312:GLN:HB3	2:N:313:PRO:HA	1.99	0.43
2:N:63:PHE:CD2	2:N:84:THR:HG23	2.54	0.43
3:W:296:ARG:HH22	3:W:308:GLN:NE2	2.05	0.43
3:W:427:ASP:OD1	3:W:432:ARG:NH2	2.52	0.43
3:W:686:LYS:HD3	3:W:901:PRO:HG2	2.01	0.43
1:A:298:TYR:CD1	1:A:298:TYR:C	2.91	0.43
1:A:353:LEU:C	1:A:354:GLN:HG2	2.37	0.43
1:A:501:HIS:HA	1:A:503:ILE:HG13	2.01	0.43
1:A:521:MET:CB	1:A:522:PRO:HD3	2.26	0.43
1:A:563:MET:O	1:A:564:ASN:C	2.56	0.43
1:A:675:GLU:HB3	1:A:678:ARG:HG2	2.01	0.43
1:B:224:PHE:CD1	2:O:71:LEU:HD13	2.54	0.43
1:B:231:ARG:HA	1:B:231:ARG:HD2	1.77	0.43
1:B:383:ILE:O	1:B:386:MET:N	2.51	0.43
1:B:772:ILE:CG2	1:B:773:SER:H	2.29	0.43
2:E:152:PHE:O	2:E:328:SER:HA	2.19	0.43
2:F:163:SER:HB3	2:F:181:TRP:CZ2	2.54	0.43
2:G:151:THR:C	2:G:152:PHE:CD1	2.92	0.43
2:G:89:VAL:C	2:G:91:PHE:H	2.22	0.43
2:O:62:ASP:H	2:O:63:PHE:HD1	1.66	0.43
3:W:1077:ARG:O	3:W:1078:SER:C	2.57	0.43
3:W:133:ALA:HB1	3:W:701:ARG:HG3	1.99	0.43
3:W:386:LEU:HB3	3:W:554:VAL:HG22	2.00	0.43
1:A:387:LEU:HD23	1:A:554:TYR:CE1	2.54	0.43
1:A:428:GLN:O	1:A:432:VAL:HG23	2.19	0.43
1:A:693:GLU:O	1:A:695:ALA:O	2.37	0.43
1:B:434:THR:C	1:B:435:ILE:HG13	2.37	0.43
1:B:508:GLU:OE1	2:J:71:LEU:HB3	2.18	0.43
1:B:620:ASP:O	1:B:624:ILE:HG13	2.19	0.43
1:B:666:ARG:HG2	1:B:667:ASP:N	2.32	0.43
1:B:743:ASP:CG	1:B:744:TYR:N	2.72	0.43
1:B:770:SER:O	1:B:771:VAL:C	2.57	0.43
2:C:78:VAL:O	2:C:81:ALA:N	2.40	0.43
2:D:11:LEU:O	2:D:15:ARG:N	2.40	0.43
2:D:89:VAL:C	2:D:91:PHE:H	2.22	0.43
2:E:169:SER:HA	2:E:176:LEU:HD23	2.00	0.43
2:H:273:TYR:C	2:H:274:GLN:HE21	2.21	0.43
2:H:35:ASN:O	2:H:37:MET:N	2.52	0.43
2:G:145:ARG:HE	2:I:142:GLN:NE2	2.17	0.43
2:J:136:ILE:HG23	2:J:137:GLU:N	2.33	0.43
2:J:14:ALA:O	2:J:16:ASP:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:78:VAL:O	2:L:81:ALA:HB3	2.18	0.43
2:N:154:LYS:N	2:N:155:PRO:CD	2.82	0.43
3:W:447:ILE:CG2	3:W:464:ILE:H	2.31	0.43
1:A:370:ILE:O	1:A:374:ALA:HB2	2.19	0.43
1:A:393:SER:C	1:A:394:LEU:HG	2.38	0.43
1:A:571:LEU:HD22	1:A:571:LEU:HA	1.74	0.43
1:A:709:ASP:O	1:A:710:MET:HB3	2.18	0.43
1:A:785:GLN:O	1:A:786:ILE:C	2.57	0.43
1:B:433:ASN:C	1:B:435:ILE:H	2.22	0.43
1:B:658:PRO:HB2	1:B:661:GLN:CG	2.39	0.43
1:B:776:ALA:O	1:B:778:LEU:N	2.52	0.43
1:B:871:PHE:CD1	1:B:872:ASP:N	2.87	0.43
2:C:53:ASN:HD22	2:C:354:ALA:HB3	1.83	0.43
2:I:11:LEU:O	2:I:15:ARG:N	2.38	0.43
2:I:4:LEU:O	2:I:5:TYR:C	2.57	0.43
2:J:190:VAL:HG21	2:J:210:HIS:HB2	1.99	0.43
2:M:74:ASP:O	2:M:75:ALA:C	2.57	0.43
2:N:125:LYS:C	2:N:127:ILE:H	2.22	0.43
2:N:249:PHE:CE2	2:N:251:PRO:HG3	2.53	0.43
2:N:3:VAL:O	2:N:4:LEU:C	2.56	0.43
3:W:173:VAL:O	3:W:177:ILE:HG12	2.19	0.43
3:W:169:LEU:HG	3:W:223:TYR:CE1	2.54	0.43
3:W:811:TYR:CZ	3:W:815:LEU:HD11	2.54	0.43
3:W:500:LEU:HD12	3:W:917:ARG:O	2.18	0.43
3:W:951:ILE:CG1	3:W:985:LYS:HA	2.47	0.43
1:A:396:PHE:HB3	1:A:578:LEU:HG	2.00	0.43
1:A:420:ILE:HD12	1:A:422:GLU:CG	2.49	0.43
1:A:481:ARG:HH12	1:A:497:ILE:CD1	2.32	0.43
1:A:510:LEU:HD13	1:A:540:LEU:HB2	2.01	0.43
1:A:393:SER:HB2	1:A:573:THR:CG2	2.48	0.43
1:A:815:TYR:HD1	1:A:815:TYR:H	1.62	0.43
1:B:409:TRP:CZ3	1:B:413:VAL:HG23	2.54	0.43
1:B:625:ILE:H	1:B:625:ILE:HG13	1.60	0.43
1:B:218:GLU:OE1	1:B:836:ARG:NH2	2.51	0.43
1:B:870:ALA:O	1:B:872:ASP:N	2.52	0.43
2:C:14:ALA:O	2:C:16:ASP:N	2.52	0.43
2:C:35:ASN:O	2:C:37:MET:N	2.52	0.43
2:C:89:VAL:C	2:C:91:PHE:N	2.72	0.43
2:D:89:VAL:C	2:D:91:PHE:N	2.72	0.43
2:E:70:LEU:HB3	2:E:72:ASN:O	2.19	0.43
2:G:3:VAL:O	2:G:4:LEU:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:135:TYR:CE1	2:H:342:MET:HE3	2.54	0.43
2:H:89:VAL:C	2:H:91:PHE:N	2.73	0.43
2:I:27:VAL:O	2:I:30:LEU:HB3	2.19	0.43
2:J:66:LEU:HD23	2:J:66:LEU:HA	1.81	0.43
2:I:16:ASP:HB3	2:K:131:ASN:O	2.18	0.43
2:K:163:SER:HB3	2:K:181:TRP:CZ2	2.54	0.43
2:M:1:MET:C	2:M:3:VAL:N	2.71	0.43
2:N:50:GLY:O	2:N:51:ILE:CG2	2.61	0.43
2:O:89:VAL:C	2:O:91:PHE:N	2.71	0.43
3:W:138:LEU:HA	3:W:141:ASN:HD22	1.84	0.43
3:W:181:GLY:O	3:W:183:PRO:HD3	2.19	0.43
3:W:754:GLU:O	3:W:758:THR:OG1	2.35	0.43
1:A:319:ASP:OD2	1:A:572:THR:N	2.52	0.43
1:A:396:PHE:HB3	1:A:578:LEU:CG	2.47	0.43
1:A:496:ASN:O	1:A:498:ARG:N	2.51	0.43
1:A:339:LEU:HD13	1:A:588:ILE:HG12	2.00	0.43
1:A:598:GLN:HG3	1:A:598:GLN:H	1.61	0.43
1:B:134:TYR:N	1:B:134:TYR:CD1	2.86	0.43
1:B:126:PHE:CB	1:B:149:LYS:O	2.67	0.43
1:A:656:ARG:HB3	1:B:347:GLN:NE2	2.34	0.43
1:B:477:ASN:ND2	2:I:39:ILE:CG2	2.81	0.43
1:B:810:TYR:C	1:B:812:VAL:HG12	2.38	0.43
1:B:89:GLU:O	1:B:91:LEU:N	2.52	0.43
2:D:225:LEU:HD13	2:D:277:PHE:CD2	2.53	0.43
2:E:49:GLY:HA2	2:E:54:LEU:HD23	2.01	0.43
2:F:89:VAL:C	2:F:91:PHE:H	2.22	0.43
2:I:149:GLY:C	2:I:150:PHE:CD1	2.92	0.43
2:J:34:PHE:O	2:J:37:MET:HB3	2.18	0.43
2:J:35:ASN:O	2:J:37:MET:N	2.52	0.43
2:K:27:VAL:O	2:K:30:LEU:N	2.52	0.43
2:M:34:PHE:O	2:M:37:MET:HB3	2.19	0.43
2:M:56:ILE:O	2:M:56:ILE:HG22	2.19	0.43
2:O:163:SER:HB3	2:O:181:TRP:CZ2	2.54	0.43
3:W:428:MET:SD	3:W:811:TYR:CD1	3.11	0.43
3:W:496:GLN:O	3:W:920:GLN:HG2	2.18	0.43
3:W:729:ARG:HD2	3:W:770:ASP:OD2	2.19	0.43
3:W:500:LEU:HD22	3:W:899:PHE:HE1	1.83	0.43
1:A:355:LEU:HA	1:A:355:LEU:HD23	1.79	0.42
1:B:249:ASP:O	1:B:250:TYR:C	2.58	0.42
1:B:251:ALA:HA	2:N:69:THR:CG2	2.42	0.42
1:B:305:GLN:HG3	1:B:489:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:698:LYS:C	1:B:699:ILE:CD1	2.87	0.42
1:B:795:LEU:O	1:B:797:PRO:HD3	2.18	0.42
1:B:548:ARG:CD	1:B:877:MET:H	2.31	0.42
1:B:99:GLU:HB3	1:B:100:PRO:CD	2.35	0.42
2:C:34:PHE:O	2:C:37:MET:HB3	2.19	0.42
2:C:38:ILE:HG13	2:C:38:ILE:H	1.58	0.42
2:D:150:PHE:HB2	2:D:152:PHE:CZ	2.53	0.42
2:D:227:PRO:HD3	2:D:277:PHE:CG	2.53	0.42
2:E:154:LYS:HG2	2:E:186:SER:OG	2.19	0.42
2:F:148:THR:HB	2:F:149:GLY:H	1.64	0.42
2:F:89:VAL:C	2:F:91:PHE:N	2.72	0.42
2:H:89:VAL:C	2:H:91:PHE:H	2.22	0.42
2:I:163:SER:HB3	2:I:181:TRP:CZ2	2.54	0.42
2:I:249:PHE:CE2	2:I:251:PRO:HG3	2.53	0.42
2:J:249:PHE:CE2	2:J:251:PRO:HG3	2.53	0.42
2:J:227:PRO:HD3	2:J:277:PHE:CG	2.53	0.42
2:K:125:LYS:C	2:K:127:ILE:H	2.22	0.42
2:L:38:ILE:H	2:L:38:ILE:HG13	1.55	0.42
2:N:27:VAL:O	2:N:28:SER:C	2.58	0.42
2:N:35:ASN:O	2:N:37:MET:N	2.52	0.42
2:O:23:LEU:CD2	2:O:24:TYR:N	2.82	0.42
3:W:324:LYS:HG2	3:W:328:TRP:NE1	2.33	0.42
3:W:109:TYR:OH	3:W:337:GLN:HB2	2.19	0.42
3:W:426:ASP:HB3	3:W:432:ARG:HH21	1.84	0.42
3:W:521:VAL:HG11	3:W:607:LEU:CD2	2.49	0.42
3:W:745:THR:OG1	3:W:748:LEU:HB3	2.19	0.42
3:W:863:LYS:HA	3:W:864:PRO:HD3	1.70	0.42
3:W:900:MET:N	3:W:901:PRO:HD3	2.34	0.42
1:A:124:ARG:C	1:A:125:ILE:HD12	2.37	0.42
1:A:273:TYR:O	1:A:273:TYR:HD2	2.01	0.42
1:A:587:LEU:HD22	1:A:587:LEU:C	2.39	0.42
1:A:613:ASN:O	1:A:617:ARG:HG2	2.19	0.42
1:A:633:LEU:C	1:A:635:GLN:N	2.72	0.42
1:B:308:LEU:HB3	1:B:310:LEU:CD2	2.49	0.42
1:B:346:ILE:HA	1:B:349:MET:HB2	2.01	0.42
1:B:393:SER:H	1:B:573:THR:CG2	2.31	0.42
1:B:413:VAL:O	1:B:414:VAL:C	2.58	0.42
1:B:491:GLN:NE2	1:B:566:GLN:CG	2.79	0.42
1:B:701:GLN:N	1:B:701:GLN:CD	2.72	0.42
2:C:163:SER:HB3	2:C:181:TRP:CZ2	2.54	0.42
2:C:169:SER:HA	2:C:176:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:225:LEU:HD13	2:C:277:PHE:CD2	2.53	0.42
2:C:4:LEU:O	2:C:5:TYR:C	2.58	0.42
2:D:14:ALA:O	2:D:16:ASP:N	2.52	0.42
2:D:3:VAL:O	2:D:4:LEU:C	2.57	0.42
2:E:150:PHE:HB2	2:E:152:PHE:HE1	1.81	0.42
2:E:6:SER:C	2:E:8:SER:N	2.73	0.42
2:G:227:PRO:HD3	2:G:277:PHE:CG	2.54	0.42
2:I:14:ALA:C	2:I:18:ILE:HD12	2.39	0.42
1:B:498:ARG:CD	2:I:32:GLN:HE21	2.32	0.42
2:I:51:ILE:O	2:I:54:LEU:HB3	2.19	0.42
2:I:61:PHE:O	2:I:62:ASP:HB3	2.19	0.42
2:J:54:LEU:HD12	2:J:55:PRO:HD2	2.00	0.42
2:K:169:SER:HA	2:K:176:LEU:HD23	2.00	0.42
2:K:249:PHE:CE2	2:K:251:PRO:HG3	2.53	0.42
2:L:227:PRO:HD3	2:L:277:PHE:CG	2.53	0.42
2:M:227:PRO:HD3	2:M:277:PHE:CG	2.53	0.42
2:M:89:VAL:C	2:M:91:PHE:N	2.72	0.42
2:O:113:SER:O	2:O:117:ARG:HG3	2.18	0.42
3:W:441:VAL:HB	3:W:447:ILE:CD1	2.33	0.42
1:A:265:LEU:HB3	1:A:296:ALA:HB1	2.00	0.42
1:A:370:ILE:O	1:A:374:ALA:CB	2.68	0.42
1:A:391:THR:O	1:A:573:THR:HA	2.19	0.42
1:A:510:LEU:HA	1:A:513:LEU:HD12	2.01	0.42
1:A:775:ILE:C	1:A:777:LYS:N	2.71	0.42
1:A:864:GLU:CD	1:A:865:PRO:HD2	2.40	0.42
1:A:548:ARG:NH1	1:A:877:MET:CA	2.78	0.42
1:B:380:LYS:O	1:B:381:THR:C	2.58	0.42
1:B:636:LYS:O	1:B:637:LYS:CB	2.66	0.42
2:C:111:PRO:HB3	2:C:116:LEU:HD23	2.01	0.42
2:C:26:ASN:N	2:C:26:ASN:OD1	2.52	0.42
2:D:27:VAL:CG2	2:D:31:ILE:HD11	2.49	0.42
2:D:35:ASN:O	2:D:37:MET:N	2.53	0.42
2:E:63:PHE:N	2:E:63:PHE:CD1	2.87	0.42
2:F:69:THR:O	2:F:70:LEU:C	2.56	0.42
2:H:38:ILE:HG13	2:H:38:ILE:H	1.57	0.42
2:I:36:GLN:NE2	2:I:126:ARG:HD3	2.34	0.42
2:I:17:LYS:HG2	2:K:130:ASP:HA	2.01	0.42
2:L:106:ARG:H	2:L:106:ARG:CD	2.20	0.42
2:L:140:ASN:O	2:L:143:ASN:N	2.50	0.42
2:N:116:LEU:O	2:N:119:LEU:N	2.48	0.42
2:N:273:TYR:C	2:N:274:GLN:HE21	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:1034:HIS:O	3:W:1037:ALA:HB3	2.20	0.42
3:W:409:LYS:HA	3:W:413:LYS:O	2.19	0.42
1:A:321:ILE:O	1:A:322:THR:C	2.58	0.42
1:A:383:ILE:HD11	1:A:550:LEU:CD2	2.49	0.42
1:A:548:ARG:HH11	1:A:877:MET:N	2.17	0.42
1:A:666:ARG:HA	1:A:669:LEU:HD12	2.00	0.42
1:A:714:ARG:CG	1:A:720:TYR:HD2	2.32	0.42
1:B:192:ASN:O	1:B:193:SER:HB3	2.19	0.42
1:B:300:ARG:HA	1:B:301:PRO:HD3	1.76	0.42
1:B:443:GLN:C	1:B:445:MET:H	2.21	0.42
1:B:482:GLN:CA	1:B:493:LEU:HD22	2.49	0.42
1:A:660:ASP:CA	1:B:539:ARG:NH1	2.83	0.42
1:B:557:LEU:O	1:B:558:MET:C	2.58	0.42
1:B:789:LEU:O	1:B:790:ARG:O	2.37	0.42
1:B:239:VAL:CG2	1:B:844:SER:O	2.61	0.42
1:B:853:ASP:O	1:B:854:LEU:CB	2.67	0.42
1:B:879:GLU:O	1:B:880:LEU:OXT	2.37	0.42
2:C:46:PHE:CE2	2:C:119:LEU:HD21	2.54	0.42
2:C:227:PRO:O	2:C:228:ASP:HB2	2.20	0.42
2:E:227:PRO:O	2:E:228:ASP:HB2	2.19	0.42
2:E:4:LEU:O	2:E:5:TYR:C	2.57	0.42
2:F:123:LYS:HG3	2:F:124:PHE:CD1	2.53	0.42
2:F:136:ILE:HG23	2:F:137:GLU:N	2.34	0.42
2:F:168:ARG:HD2	2:F:175:ASN:O	2.20	0.42
2:J:131:ASN:ND2	2:J:131:ASN:N	2.67	0.42
2:J:163:SER:HB3	2:J:181:TRP:CZ2	2.54	0.42
2:K:139:TRP:HE1	2:K:143:ASN:HD22	1.66	0.42
2:L:163:SER:HB3	2:L:181:TRP:CZ2	2.54	0.42
2:L:24:TYR:O	2:L:26:ASN:N	2.52	0.42
2:L:62:ASP:H	2:L:63:PHE:HD1	1.66	0.42
2:N:163:SER:HB3	2:N:181:TRP:CZ2	2.54	0.42
2:N:168:ARG:HD2	2:N:175:ASN:O	2.20	0.42
3:W:880:ASP:OD2	3:W:1069:LYS:HE3	2.19	0.42
3:W:319:PHE:N	3:W:320:PRO:HD2	2.34	0.42
3:W:61:GLU:O	3:W:61:GLU:HG2	2.19	0.42
3:W:777:THR:HG23	3:W:882:LYS:HD2	2.00	0.42
1:A:400:ASN:O	1:A:403:SER:HB2	2.20	0.42
1:A:319:ASP:OD2	1:A:570:THR:HG22	2.19	0.42
1:A:570:THR:CG2	1:A:571:LEU:N	2.74	0.42
1:B:146:TRP:O	1:B:833:PHE:HB3	2.20	0.42
1:B:113:PRO:CG	1:B:609:ASN:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:128:ASN:O	2:C:129:PHE:HB2	2.20	0.42
2:E:24:TYR:CE1	2:E:31:ILE:HG13	2.54	0.42
2:F:153:HIS:NE2	2:G:153:HIS:NE2	2.67	0.42
2:G:136:ILE:HG23	2:G:137:GLU:N	2.33	0.42
2:G:163:SER:HB3	2:G:181:TRP:CZ2	2.54	0.42
2:G:89:VAL:C	2:G:91:PHE:N	2.73	0.42
2:I:168:ARG:HD2	2:I:175:ASN:O	2.20	0.42
2:K:23:LEU:H	2:K:26:ASN:ND2	2.17	0.42
2:L:227:PRO:O	2:L:228:ASP:HB2	2.20	0.42
2:L:66:LEU:HB3	2:L:67:GLY:H	1.66	0.42
2:M:145:ARG:CB	2:M:145:ARG:HH11	2.32	0.42
2:M:14:ALA:O	2:M:16:ASP:N	2.52	0.42
2:M:78:VAL:O	2:M:81:ALA:HB3	2.19	0.42
2:N:21:GLY:O	2:N:22:THR:O	2.36	0.42
2:N:34:PHE:O	2:N:37:MET:HB3	2.20	0.42
2:O:227:PRO:O	2:O:228:ASP:HB2	2.20	0.42
3:W:108:ASP:HA	3:W:111:ASN:HD22	1.83	0.42
3:W:358:GLU:HG3	3:W:359:MET:N	2.33	0.42
3:W:64:ASP:OD2	3:W:65:VAL:HG23	2.20	0.42
1:A:200:VAL:CG2	1:A:241:TYR:HD2	2.32	0.42
1:A:259:HIS:O	1:A:260:GLN:C	2.56	0.42
1:A:271:PHE:HA	1:A:274:ILE:CD1	2.47	0.42
1:A:351:GLN:O	1:A:353:LEU:N	2.53	0.42
1:A:443:GLN:HE22	1:A:522:PRO:HG3	1.84	0.42
1:A:546:LEU:HD21	1:A:588:ILE:HD12	1.99	0.42
1:A:593:VAL:HG12	1:A:594:ILE:N	2.35	0.42
1:A:594:ILE:HG23	1:A:595:PRO:HD2	2.01	0.42
1:A:876:ILE:O	1:A:877:MET:CB	2.68	0.42
1:B:195:ASP:O	1:B:196:ALA:C	2.58	0.42
1:B:199:VAL:HG13	1:B:242:PRO:O	2.20	0.42
1:B:465:ASN:O	1:B:466:PHE:C	2.58	0.42
1:B:555:GLU:OE2	1:B:871:PHE:CE2	2.69	0.42
2:C:9:LYS:HE3	2:C:13:ASP:OD1	2.19	0.42
2:E:163:SER:HB3	2:E:181:TRP:CZ2	2.54	0.42
2:E:59:TRP:N	2:E:59:TRP:CD1	2.87	0.42
2:G:168:ARG:HD2	2:G:175:ASN:O	2.20	0.42
2:I:78:VAL:O	2:I:81:ALA:HB3	2.20	0.42
2:J:227:PRO:O	2:J:228:ASP:HB2	2.20	0.42
2:J:74:ASP:O	2:J:75:ALA:C	2.57	0.42
2:J:6:SER:C	2:J:8:SER:N	2.73	0.42
2:M:3:VAL:O	2:M:4:LEU:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:101:VAL:HG12	2:N:350:ARG:HG2	2.01	0.42
2:O:6:SER:C	2:O:8:SER:N	2.73	0.42
3:W:999:ILE:HD11	3:W:1009:PHE:HD1	1.81	0.42
1:A:125:ILE:H	1:A:125:ILE:HD12	1.77	0.42
1:A:211:ILE:C	1:A:213:GLN:H	2.23	0.42
1:A:409:TRP:CH2	1:A:547:THR:OG1	2.71	0.42
1:A:709:ASP:OD2	1:A:820:THR:HG21	2.20	0.42
1:A:775:ILE:HG13	1:A:775:ILE:H	1.35	0.42
1:A:839:MET:CG	1:A:840:HIS:N	2.83	0.42
1:A:853:ASP:O	1:A:854:LEU:HB2	2.18	0.42
1:B:390:ARG:HG3	1:B:391:THR:N	2.34	0.42
1:B:409:TRP:CZ3	1:B:413:VAL:CG2	3.02	0.42
1:B:496:ASN:HD22	1:B:498:ARG:CB	2.32	0.42
1:A:571:LEU:CD2	1:B:531:ARG:CZ	2.97	0.42
1:B:243:SER:HB3	1:B:842:LEU:HD12	2.01	0.42
2:E:168:ARG:HD2	2:E:175:ASN:O	2.20	0.42
2:F:227:PRO:O	2:F:228:ASP:HB2	2.20	0.42
2:G:9:LYS:HE3	2:G:13:ASP:OD1	2.19	0.42
2:H:136:ILE:HG23	2:H:137:GLU:N	2.34	0.42
2:K:78:VAL:O	2:K:81:ALA:HB3	2.19	0.42
2:L:168:ARG:HD2	2:L:175:ASN:O	2.20	0.42
2:N:227:PRO:O	2:N:228:ASP:HB2	2.19	0.42
3:W:114:MET:HB2	3:W:117:GLU:CG	2.50	0.42
3:W:3:LYS:O	3:W:7:ILE:HG13	2.18	0.42
3:W:72:LEU:HG	3:W:861:LEU:HG	2.00	0.42
3:W:840:ASN:HA	3:W:845:ILE:HG22	1.99	0.42
1:A:440:PHE:O	1:A:441:GLY:C	2.58	0.42
1:A:517:GLN:HG3	1:A:517:GLN:O	2.20	0.42
1:A:707:TYR:N	1:A:707:TYR:CD1	2.88	0.42
1:A:850:VAL:C	1:A:851:TYR:CD1	2.93	0.42
1:B:482:GLN:O	1:B:483:VAL:CG2	2.68	0.42
1:B:546:LEU:HD23	1:B:546:LEU:HA	1.81	0.42
2:C:155:PRO:HA	2:C:337:ASP:HB2	2.02	0.42
2:E:9:LYS:HE3	2:E:13:ASP:OD1	2.20	0.42
2:F:145:ARG:C	2:F:146:GLN:HG2	2.40	0.42
2:G:253:ILE:HG13	2:H:234:PHE:CE1	2.55	0.42
2:L:125:LYS:C	2:L:127:ILE:H	2.22	0.42
2:L:42:ASN:HB3	2:L:62:ASP:N	2.35	0.42
2:L:61:PHE:N	2:L:61:PHE:CD1	2.88	0.42
2:M:163:SER:HB3	2:M:181:TRP:CZ2	2.55	0.42
2:M:355:ILE:HA	2:M:356:PRO:HD3	1.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:124:PHE:O	2:O:127:ILE:HG13	2.19	0.42
2:O:23:LEU:HG	2:O:24:TYR:H	1.85	0.42
3:W:200:PRO:O	3:W:201:TYR:C	2.58	0.42
3:W:824:ASN:ND2	3:W:964:SER:HB2	2.35	0.42
1:A:141:GLU:O	1:A:142:LEU:HD12	2.20	0.42
1:A:216:GLU:N	1:A:216:GLU:OE1	2.50	0.42
1:A:487:GLY:O	1:A:488:VAL:CB	2.68	0.42
1:B:183:LEU:O	1:B:184:LYS:C	2.57	0.42
1:B:253:ASN:O	1:B:256:PHE:HB2	2.20	0.42
1:B:310:LEU:H	1:B:310:LEU:HG	1.44	0.42
1:B:454:THR:CG2	1:B:476:ASN:ND2	2.61	0.42
1:B:570:THR:HG22	1:B:571:LEU:N	2.34	0.42
1:B:646:LEU:H	1:B:646:LEU:HG	1.51	0.42
1:B:856:ALA:C	1:B:858:VAL:N	2.72	0.42
2:D:163:SER:HB3	2:D:181:TRP:CZ2	2.54	0.42
2:E:129:PHE:CE1	2:E:130:ASP:HB3	2.54	0.42
2:E:3:VAL:O	2:E:4:LEU:C	2.57	0.42
2:E:61:PHE:CD1	2:E:61:PHE:N	2.87	0.42
2:I:104:SER:HB3	2:I:108:GLY:HA2	2.02	0.42
2:J:73:LEU:HD22	2:J:77:TYR:CD2	2.54	0.42
2:K:9:LYS:HE3	2:K:13:ASP:OD1	2.20	0.42
2:I:397:LYS:NZ	2:K:150:PHE:HA	2.34	0.42
2:K:227:PRO:O	2:K:228:ASP:HB2	2.20	0.42
2:J:253:ILE:HG13	2:K:234:PHE:CE1	2.55	0.42
2:M:14:ALA:C	2:M:18:ILE:HD12	2.40	0.42
2:M:7:LEU:HG	2:M:7:LEU:H	1.53	0.42
2:N:14:ALA:O	2:N:16:ASP:N	2.53	0.42
2:N:4:LEU:O	2:N:5:TYR:C	2.58	0.42
2:O:153:HIS:C	2:O:155:PRO:N	2.71	0.42
3:W:214:LEU:C	3:W:214:LEU:HD12	2.40	0.42
3:W:516:VAL:HG21	3:W:675:ILE:HG21	2.01	0.42
3:W:827:VAL:O	3:W:831:ILE:HG13	2.20	0.42
3:W:922:GLU:HG3	3:W:991:SER:OG	2.20	0.42
1:A:201:ASP:O	1:A:204:THR:N	2.52	0.42
1:A:492:VAL:CG1	1:A:493:LEU:N	2.82	0.42
1:A:695:ALA:O	1:A:696:SER:HB3	2.20	0.42
1:A:134:TYR:CE1	1:A:803:ASN:CG	2.93	0.42
1:A:810:TYR:O	1:A:813:ALA:N	2.53	0.42
1:B:287:ASN:HD22	1:B:287:ASN:HA	1.60	0.42
1:B:544:VAL:HG12	1:B:548:ARG:HE	1.83	0.42
1:B:746:GLN:HE22	2:D:64:GLY:HA2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:TRP:NE1	1:B:833:PHE:HD1	2.18	0.42
2:C:168:ARG:HD2	2:C:175:ASN:O	2.20	0.42
2:D:51:ILE:O	2:D:52:GLY:C	2.58	0.42
2:E:14:ALA:O	2:E:16:ASP:N	2.52	0.42
2:G:23:LEU:HD23	2:G:25:SER:H	1.85	0.42
2:H:163:SER:HB3	2:H:181:TRP:CZ2	2.54	0.42
2:H:152:PHE:O	2:H:328:SER:HA	2.19	0.42
2:H:3:VAL:O	2:H:4:LEU:C	2.58	0.42
2:I:35:ASN:O	2:I:37:MET:N	2.52	0.42
2:I:74:ASP:O	2:I:75:ALA:C	2.57	0.42
2:K:35:ASN:O	2:K:37:MET:N	2.53	0.42
2:K:4:LEU:O	2:K:5:TYR:C	2.58	0.42
2:K:51:ILE:O	2:K:51:ILE:HG23	2.20	0.42
2:K:61:PHE:CD1	2:K:61:PHE:N	2.88	0.42
2:M:227:PRO:O	2:M:228:ASP:HB2	2.20	0.42
2:N:59:TRP:CD1	2:N:59:TRP:N	2.88	0.42
2:O:1:MET:HG3	2:O:2:ASP:N	2.34	0.42
2:O:239:ASN:ND2	2:O:246:THR:HG22	2.29	0.42
3:W:169:LEU:HG	3:W:223:TYR:HE1	1.85	0.42
3:W:516:VAL:N	3:W:671:SER:O	2.52	0.42
1:A:129:ARG:HG2	1:A:130:GLN:H	1.84	0.41
1:A:162:VAL:O	1:A:165:TYR:HB3	2.20	0.41
1:A:174:LEU:HA	1:A:177:MET:HB2	2.01	0.41
1:A:842:LEU:HD23	1:A:842:LEU:HA	1.76	0.41
1:A:853:ASP:OD1	1:A:854:LEU:N	2.53	0.41
1:B:224:PHE:CE1	2:O:71:LEU:N	2.87	0.41
1:B:501:HIS:O	1:B:503:ILE:N	2.53	0.41
1:B:526:LYS:O	1:B:530:GLN:HG2	2.20	0.41
2:C:235:PRO:HA	2:C:249:PHE:O	2.20	0.41
2:E:106:ARG:HB3	2:E:107:ASN:H	1.54	0.41
2:E:239:ASN:ND2	2:E:246:THR:HG22	2.30	0.41
2:E:89:VAL:C	2:E:91:PHE:N	2.73	0.41
2:H:227:PRO:O	2:H:228:ASP:HB2	2.20	0.41
2:I:27:VAL:O	2:I:31:ILE:HG12	2.19	0.41
2:L:124:PHE:O	2:L:126:ARG:N	2.53	0.41
2:L:235:PRO:HA	2:L:249:PHE:O	2.20	0.41
2:N:89:VAL:C	2:N:91:PHE:N	2.71	0.41
2:O:125:LYS:O	2:O:127:ILE:N	2.51	0.41
2:N:76:ASN:HA	2:O:75:ALA:HB3	2.01	0.41
3:W:441:VAL:HG11	3:W:465:LEU:HD22	2.02	0.41
3:W:542:LEU:HD11	3:W:561:TYR:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:962:LEU:HD22	3:W:967:ILE:HG12	2.02	0.41
1:A:124:ARG:HD2	1:A:203:GLU:OE1	2.20	0.41
1:A:275:PRO:C	1:A:277:ARG:H	2.23	0.41
1:A:275:PRO:CG	1:A:278:ILE:HD11	2.50	0.41
1:A:404:LEU:HD22	1:A:435:ILE:HD11	2.02	0.41
1:A:493:LEU:HD11	1:A:566:GLN:O	2.20	0.41
1:A:656:ARG:O	1:A:657:VAL:HG23	2.20	0.41
1:A:314:PHE:HZ	1:A:664:ARG:HG2	1.84	0.41
1:A:848:PHE:C	1:A:849:THR:OG1	2.58	0.41
1:B:371:ASN:O	1:B:372:SER:C	2.58	0.41
1:B:383:ILE:O	1:B:384:ALA:C	2.57	0.41
1:B:406:SER:O	1:B:409:TRP:N	2.51	0.41
1:B:466:PHE:CE1	2:H:80:THR:HG22	2.55	0.41
2:C:142:GLN:OE1	2:N:145:ARG:NH1	2.48	0.41
2:D:116:LEU:O	2:D:119:LEU:N	2.50	0.41
2:D:133:SER:O	2:D:134:GLU:C	2.59	0.41
2:D:1:MET:O	2:D:2:ASP:C	2.56	0.41
2:D:4:LEU:O	2:D:5:TYR:C	2.58	0.41
2:D:70:LEU:CD1	2:D:71:LEU:N	2.82	0.41
2:C:234:PHE:CE1	2:E:253:ILE:HG13	2.55	0.41
2:E:74:ASP:O	2:E:75:ALA:C	2.58	0.41
2:F:27:VAL:O	2:F:31:ILE:HG12	2.20	0.41
2:G:125:LYS:C	2:G:127:ILE:H	2.24	0.41
2:H:168:ARG:HD2	2:H:175:ASN:O	2.20	0.41
2:F:234:PHE:CE1	2:H:253:ILE:HG13	2.55	0.41
2:K:168:ARG:HD2	2:K:175:ASN:O	2.20	0.41
2:M:155:PRO:O	2:M:186:SER:HB3	2.20	0.41
2:O:38:ILE:HG22	2:O:42:ASN:ND2	2.33	0.41
3:W:729:ARG:HH11	3:W:770:ASP:CG	2.22	0.41
1:A:170:TYR:CZ	1:A:682:PHE:HB2	2.55	0.41
1:A:236:ARG:HB2	1:A:238:VAL:CG2	2.47	0.41
1:A:382:LEU:O	1:A:385:ALA:HB3	2.20	0.41
1:A:647:LYS:HG2	1:A:654:VAL:HG21	1.99	0.41
1:B:456:PHE:O	1:B:457:GLN:O	2.38	0.41
1:B:646:LEU:O	1:B:649:LEU:HB2	2.20	0.41
1:B:721:VAL:CG1	1:B:722:ASN:H	2.30	0.41
2:D:168:ARG:HD2	2:D:175:ASN:O	2.20	0.41
2:E:128:ASN:O	2:E:129:PHE:CB	2.68	0.41
2:E:35:ASN:O	2:E:37:MET:N	2.53	0.41
2:G:144:ARG:O	2:G:145:ARG:CB	2.67	0.41
2:G:235:PRO:HA	2:G:249:PHE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:14:ALA:O	2:I:16:ASP:N	2.53	0.41
2:J:239:ASN:ND2	2:J:246:THR:HG22	2.29	0.41
2:K:34:PHE:O	2:K:37:MET:HB3	2.20	0.41
2:L:151:THR:C	2:L:152:PHE:CD1	2.94	0.41
2:L:48:THR:O	2:L:56:ILE:HA	2.20	0.41
2:L:6:SER:C	2:L:8:SER:N	2.73	0.41
2:M:153:HIS:NE2	2:N:153:HIS:CD2	2.88	0.41
2:M:6:SER:C	2:M:8:SER:N	2.73	0.41
2:M:253:ILE:HG13	2:N:234:PHE:CE1	2.55	0.41
2:N:239:ASN:ND2	2:N:246:THR:HG22	2.29	0.41
2:N:148:THR:OG1	2:N:332:GLU:HG2	2.20	0.41
2:O:4:LEU:O	2:O:5:TYR:C	2.58	0.41
3:W:449:LEU:HD21	3:W:461:ILE:HD13	2.02	0.41
3:W:718:ILE:HG23	3:W:771:PHE:CE1	2.55	0.41
3:W:992:TYR:CE2	3:W:996:LEU:HD11	2.56	0.41
1:A:414:VAL:C	1:A:416:ASN:H	2.22	0.41
1:A:163:ARG:NE	1:A:631:LEU:O	2.54	0.41
1:A:807:ASN:C	1:A:809:PHE:N	2.73	0.41
1:B:275:PRO:HB2	1:B:278:ILE:HD13	2.03	0.41
1:B:322:THR:HG22	1:B:390:ARG:HD3	2.02	0.41
1:B:449:ASN:ND2	1:B:455:PRO:HB3	2.36	0.41
1:B:743:ASP:OD2	1:B:745:ALA:CA	2.68	0.41
1:B:776:ALA:O	1:B:777:LYS:C	2.58	0.41
2:C:253:ILE:HG13	2:D:234:PHE:CE1	2.55	0.41
2:D:14:ALA:C	2:D:18:ILE:HD12	2.41	0.41
2:D:34:PHE:O	2:D:37:MET:HB3	2.20	0.41
2:C:153:HIS:CD2	2:E:153:HIS:CE1	3.08	0.41
2:F:6:SER:C	2:F:8:SER:N	2.73	0.41
2:G:35:ASN:O	2:G:37:MET:N	2.54	0.41
2:J:149:GLY:C	2:J:150:PHE:CD1	2.94	0.41
2:M:35:ASN:O	2:M:37:MET:N	2.53	0.41
2:M:66:LEU:O	2:M:67:GLY:C	2.58	0.41
2:N:78:VAL:O	2:N:81:ALA:N	2.39	0.41
2:O:61:PHE:N	2:O:61:PHE:CD1	2.87	0.41
2:O:74:ASP:O	2:O:75:ALA:C	2.58	0.41
3:W:34:LEU:O	3:W:37:ARG:HB2	2.20	0.41
3:W:438:ILE:HD11	3:W:563:GLN:CG	2.50	0.41
3:W:619:HIS:ND1	3:W:619:HIS:N	2.65	0.41
1:A:542:GLN:OE1	1:A:542:GLN:N	2.53	0.41
1:B:191:LYS:HD3	1:B:191:LYS:HA	1.90	0.41
1:B:735:LEU:CG	1:B:760:VAL:O	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:807:ASN:C	1:B:809:PHE:H	2.23	0.41
1:B:812:VAL:C	1:B:814:ASN:H	2.23	0.41
2:D:227:PRO:O	2:D:228:ASP:HB2	2.20	0.41
2:D:253:ILE:HG13	2:E:234:PHE:CE1	2.55	0.41
2:D:74:ASP:O	2:D:75:ALA:C	2.59	0.41
2:D:6:SER:C	2:D:8:SER:N	2.73	0.41
2:G:11:LEU:HA	2:G:14:ALA:HB3	2.02	0.41
2:G:34:PHE:O	2:G:37:MET:HB3	2.20	0.41
2:H:9:LYS:HE3	2:H:13:ASP:OD1	2.20	0.41
2:H:34:PHE:O	2:H:37:MET:HB3	2.20	0.41
2:L:9:LYS:HE3	2:L:13:ASP:OD1	2.21	0.41
2:N:74:ASP:O	2:N:75:ALA:C	2.58	0.41
2:O:53:ASN:HD22	2:O:354:ALA:HB3	1.86	0.41
3:W:191:TYR:CZ	3:W:204:VAL:HG11	2.56	0.41
3:W:292:LEU:HD13	3:W:308:GLN:NE2	2.35	0.41
3:W:467:TYR:O	3:W:471:ILE:HD13	2.20	0.41
3:W:908:GLN:O	3:W:912:GLN:HG3	2.21	0.41
1:A:855:LEU:O	1:A:856:ALA:C	2.56	0.41
1:B:190:ASN:HB2	1:B:199:VAL:CG2	2.50	0.41
1:B:270:ILE:HG23	1:B:854:LEU:HD21	2.03	0.41
1:B:493:LEU:CD1	1:B:567:HIS:HB2	2.50	0.41
1:B:712:LEU:HG	1:B:721:VAL:O	2.19	0.41
1:B:786:ILE:O	1:B:787:VAL:C	2.59	0.41
2:D:239:ASN:ND2	2:D:246:THR:HG22	2.29	0.41
2:I:239:ASN:ND2	2:I:246:THR:HG22	2.30	0.41
2:I:235:PRO:HA	2:I:249:PHE:O	2.21	0.41
2:I:253:ILE:HG13	2:J:234:PHE:CE1	2.55	0.41
2:I:3:VAL:O	2:I:4:LEU:C	2.57	0.41
2:J:59:TRP:N	2:J:59:TRP:CD1	2.86	0.41
2:I:234:PHE:CE1	2:K:253:ILE:HG13	2.55	0.41
2:O:14:ALA:O	2:O:16:ASP:N	2.52	0.41
3:W:574:GLN:HG2	3:W:581:ILE:CG2	2.50	0.41
3:W:772:ILE:HD11	3:W:1047:LYS:HB2	2.02	0.41
3:W:934:ILE:HG23	3:W:965:LEU:CD1	2.49	0.41
1:A:178:PRO:CD	1:A:256:PHE:HE2	2.32	0.41
1:A:345:GLN:HG3	1:A:349:MET:CE	2.51	0.41
1:A:396:PHE:CD2	1:A:578:LEU:HD11	2.56	0.41
1:A:405:ILE:O	1:A:408:MET:HB2	2.21	0.41
1:A:304:LEU:H	1:A:615:ASN:ND2	2.19	0.41
1:A:679:LEU:O	1:A:681:ILE:N	2.54	0.41
1:B:136:ALA:O	1:B:137:ASN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:PHE:CE2	1:B:689:MET:CA	2.99	0.41
1:B:178:PRO:CD	1:B:256:PHE:CE2	3.04	0.41
1:B:515:ARG:O	1:B:515:ARG:HG3	2.21	0.41
1:B:521:MET:SD	1:B:521:MET:N	2.94	0.41
1:B:552:TYR:O	1:B:553:ASN:C	2.58	0.41
2:C:61:PHE:CD1	2:C:61:PHE:N	2.89	0.41
2:C:6:SER:C	2:C:8:SER:N	2.74	0.41
2:D:124:PHE:CD1	2:D:124:PHE:N	2.89	0.41
2:F:253:ILE:HG13	2:G:234:PHE:CE1	2.55	0.41
2:G:227:PRO:O	2:G:228:ASP:HB2	2.20	0.41
2:J:11:LEU:HA	2:J:14:ALA:HB3	2.03	0.41
2:J:14:ALA:O	2:J:18:ILE:HD12	2.21	0.41
2:K:110:ALA:HB1	2:K:111:PRO:CD	2.50	0.41
2:L:21:GLY:O	2:L:22:THR:O	2.38	0.41
2:M:235:PRO:HA	2:M:249:PHE:O	2.21	0.41
2:O:35:ASN:O	2:O:37:MET:N	2.53	0.41
3:W:205:THR:HG23	3:W:206:TRP:N	2.36	0.41
3:W:229:LEU:HD21	3:W:244:VAL:HG21	2.01	0.41
3:W:255:VAL:HG23	3:W:310:TRP:CH2	2.56	0.41
3:W:54:SER:O	3:W:55:LEU:HD23	2.20	0.41
1:A:120:THR:HB	1:A:121:LYS:H	1.66	0.41
1:A:503:ILE:H	1:A:503:ILE:HG13	1.72	0.41
1:A:310:LEU:HD11	1:A:614:TYR:OH	2.21	0.41
1:A:701:GLN:CB	1:A:826:TYR:HD2	2.33	0.41
1:B:252:PHE:O	1:B:253:ASN:C	2.59	0.41
1:B:286:LEU:O	1:B:287:ASN:ND2	2.54	0.41
1:B:721:VAL:HG12	1:B:799:LEU:HD21	1.98	0.41
2:C:145:ARG:CB	2:C:145:ARG:NH1	2.79	0.41
2:C:100:MET:HG3	2:C:388:VAL:HG11	2.01	0.41
2:D:9:LYS:HE3	2:D:13:ASP:OD1	2.21	0.41
2:G:14:ALA:O	2:G:16:ASP:N	2.54	0.41
2:H:235:PRO:HA	2:H:249:PHE:O	2.21	0.41
2:H:6:SER:C	2:H:8:SER:N	2.74	0.41
2:J:136:ILE:HD12	2:J:139:TRP:HB3	2.03	0.41
2:I:153:HIS:CD2	2:K:153:HIS:CE1	3.08	0.41
2:L:23:LEU:HD22	2:L:72:ASN:OD1	2.21	0.41
2:L:253:ILE:HG13	2:M:234:PHE:CE1	2.55	0.41
2:L:150:PHE:O	2:L:330:VAL:HG13	2.20	0.41
2:L:35:ASN:OD1	2:L:65:LEU:HD22	2.21	0.41
2:M:124:PHE:CD1	2:M:124:PHE:N	2.89	0.41
2:M:168:ARG:HD2	2:M:175:ASN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:7:LEU:H	2:N:7:LEU:HG	1.54	0.41
2:O:168:ARG:HD2	2:O:175:ASN:O	2.20	0.41
3:W:887:VAL:HG12	3:W:1054:LEU:HG	2.02	0.41
3:W:200:PRO:O	3:W:203:LEU:N	2.54	0.41
3:W:690:ARG:HH11	3:W:690:ARG:CB	2.34	0.41
3:W:802:ILE:O	3:W:808:PHE:HB2	2.21	0.41
1:A:368:THR:HG23	1:A:579:THR:O	2.21	0.41
1:A:472:LEU:N	1:A:472:LEU:HD23	2.36	0.41
1:A:374:ALA:HB1	1:A:580:SER:HA	2.02	0.41
1:A:782:VAL:CG2	1:A:798:ILE:HD11	2.51	0.41
1:A:862:THR:HG22	1:A:863:VAL:N	2.36	0.41
1:B:349:MET:HB2	1:B:349:MET:HE2	1.88	0.41
1:B:489:LEU:C	1:B:489:LEU:HD23	2.41	0.41
2:D:235:PRO:HA	2:D:249:PHE:O	2.21	0.41
2:F:135:TYR:CZ	2:F:342:MET:HE3	2.56	0.41
2:F:9:LYS:HE3	2:F:13:ASP:OD1	2.21	0.41
2:I:106:ARG:HG2	2:I:107:ASN:H	1.84	0.41
2:I:72:ASN:CG	2:K:126:ARG:NH1	2.74	0.41
2:J:9:LYS:HE3	2:J:13:ASP:OD1	2.21	0.41
2:J:27:VAL:O	2:J:28:SER:C	2.57	0.41
2:L:1:MET:O	2:L:2:ASP:C	2.59	0.41
2:L:4:LEU:O	2:L:5:TYR:C	2.59	0.41
2:O:147:ARG:O	2:O:148:THR:CB	2.66	0.41
2:O:152:PHE:CD1	2:O:152:PHE:N	2.89	0.41
2:O:34:PHE:O	2:O:35:ASN:C	2.59	0.41
3:W:884:PHE:CG	3:W:1058:TYR:CD1	3.09	0.41
3:W:871:LYS:HD3	3:W:1074:THR:HG21	2.01	0.41
3:W:1078:SER:HA	3:W:1079:PRO:HD3	1.76	0.41
3:W:169:LEU:HD21	3:W:227:LYS:HG3	2.03	0.41
3:W:499:GLN:NE2	3:W:689:PHE:HE1	2.19	0.41
3:W:675:ILE:C	3:W:675:ILE:HD12	2.41	0.41
3:W:503:TYR:HB2	3:W:687:ILE:HD13	2.02	0.41
3:W:133:ALA:CB	3:W:701:ARG:HG3	2.50	0.41
3:W:810:ASN:O	3:W:814:ARG:HB2	2.20	0.41
1:A:202:SER:O	1:A:205:ALA:HB3	2.21	0.41
1:A:283:ASN:HD21	1:A:869:VAL:H	1.69	0.41
1:A:382:LEU:HD12	1:A:382:LEU:HA	1.60	0.41
1:A:552:TYR:O	1:A:553:ASN:C	2.59	0.41
1:A:601:PHE:CD1	1:A:601:PHE:N	2.80	0.41
1:A:622:VAL:O	1:A:623:ALA:C	2.59	0.41
1:A:756:PRO:C	1:A:757:VAL:CG2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ASN:O	1:A:858:VAL:HA	2.20	0.41
1:B:159:ASP:OD2	1:B:761:GLY:CA	2.69	0.41
1:B:492:VAL:O	1:B:493:LEU:O	2.38	0.41
1:B:763:LEU:HD23	1:B:763:LEU:HA	1.80	0.41
1:B:771:VAL:O	1:B:775:ILE:HD13	2.21	0.41
1:B:791:LYS:O	1:B:792:VAL:CG1	2.66	0.41
2:C:33:GLN:O	2:C:36:GLN:HB3	2.21	0.41
2:D:128:ASN:HD22	2:E:19:VAL:CG2	2.34	0.41
2:D:31:ILE:O	2:D:32:GLN:C	2.59	0.41
2:E:23:LEU:HD22	2:E:25:SER:OG	2.21	0.41
2:F:24:TYR:C	2:F:26:ASN:H	2.24	0.41
2:H:91:PHE:O	2:H:95:VAL:HG23	2.21	0.41
2:I:9:LYS:HE3	2:I:13:ASP:OD1	2.20	0.41
2:I:227:PRO:O	2:I:228:ASP:HB2	2.20	0.41
2:I:397:LYS:HZ1	2:K:150:PHE:HA	1.86	0.41
2:J:168:ARG:HD2	2:J:175:ASN:O	2.20	0.41
2:L:14:ALA:O	2:L:16:ASP:N	2.54	0.41
2:N:124:PHE:C	2:N:126:ARG:H	2.24	0.41
2:L:26:ASN:OD1	2:N:33:GLN:HB2	2.21	0.41
2:O:23:LEU:CG	2:O:24:TYR:N	2.83	0.41
2:O:5:TYR:CE2	2:O:131:ASN:HA	2.55	0.41
3:W:802:ILE:HG13	3:W:808:PHE:HD2	1.85	0.41
1:A:609:ASN:O	1:A:610:PHE:C	2.59	0.41
1:A:726:ASN:HD22	1:A:726:ASN:HA	1.60	0.41
1:A:763:LEU:HA	1:A:764:PRO:HD3	1.68	0.41
1:A:771:VAL:HG12	1:A:809:PHE:CB	2.51	0.41
1:B:207:ILE:HG13	1:B:207:ILE:H	1.62	0.41
1:B:229:ARG:HD2	1:B:230:GLN:NE2	2.31	0.41
1:B:288:MET:HE1	1:B:288:MET:HA	2.02	0.41
1:B:379:PHE:O	1:B:380:LYS:C	2.59	0.41
1:B:411:LEU:HA	1:B:411:LEU:HD23	1.83	0.41
1:B:451:ASP:N	1:B:452:PRO:CD	2.82	0.41
1:B:415:PRO:HB3	1:B:480:PHE:HB2	2.01	0.41
1:B:672:LEU:O	1:B:673:PRO:O	2.38	0.41
2:C:5:TYR:HE2	2:C:130:ASP:O	2.04	0.41
2:C:204:ASN:HB3	2:C:296:ARG:HB3	2.03	0.41
2:C:67:GLY:C	2:C:69:THR:N	2.72	0.41
2:D:204:ASN:HB3	2:D:296:ARG:HB3	2.03	0.41
2:D:34:PHE:O	2:D:35:ASN:C	2.59	0.41
2:F:74:ASP:O	2:F:75:ALA:C	2.59	0.41
2:H:123:LYS:HG3	2:H:124:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:14:ALA:O	2:H:16:ASP:N	2.54	0.41
2:J:27:VAL:O	2:J:31:ILE:HG12	2.20	0.41
2:I:16:ASP:HB3	2:K:131:ASN:C	2.42	0.41
2:K:235:PRO:HA	2:K:249:PHE:O	2.21	0.41
2:L:42:ASN:CB	2:L:62:ASP:HA	2.51	0.41
2:N:235:PRO:HA	2:N:249:PHE:O	2.21	0.41
2:N:34:PHE:O	2:N:35:ASN:C	2.59	0.41
3:W:929:ALA:N	3:W:984:ASP:OD2	2.53	0.41
1:A:370:ILE:HD11	3:W:933:LEU:HA	2.01	0.41
1:A:594:ILE:HA	1:A:595:PRO:HD3	1.86	0.40
1:B:401:TYR:N	1:B:401:TYR:CD1	2.74	0.40
1:B:743:ASP:OD1	1:B:744:TYR:N	2.53	0.40
1:B:747:ILE:H	1:B:747:ILE:HG22	1.51	0.40
1:B:854:LEU:HD22	1:B:855:LEU:N	2.36	0.40
1:B:869:VAL:HG13	1:B:873:ASN:CA	2.51	0.40
2:D:144:ARG:O	2:D:145:ARG:CB	2.65	0.40
2:D:38:ILE:HG13	2:D:38:ILE:H	1.57	0.40
2:E:235:PRO:HA	2:E:249:PHE:O	2.21	0.40
2:H:34:PHE:O	2:H:35:ASN:C	2.60	0.40
2:I:116:LEU:O	2:I:119:LEU:N	2.50	0.40
2:I:11:LEU:HA	2:I:14:ALA:HB3	2.02	0.40
2:J:110:ALA:CB	2:J:111:PRO:CD	2.96	0.40
2:J:133:SER:O	2:J:134:GLU:C	2.59	0.40
2:J:355:ILE:HA	2:J:356:PRO:HD3	1.96	0.40
2:I:144:ARG:HD2	2:J:82:ARG:CZ	2.51	0.40
2:K:38:ILE:H	2:K:38:ILE:HG13	1.58	0.40
2:J:126:ARG:NH1	2:K:72:ASN:ND2	2.69	0.40
2:L:131:ASN:HD22	2:L:131:ASN:N	2.19	0.40
2:L:234:PHE:CE1	2:N:253:ILE:HG13	2.55	0.40
3:W:444:ASP:C	3:W:446:PRO:HD3	2.41	0.40
3:W:490:TYR:HA	3:W:628:VAL:HG22	2.02	0.40
3:W:524:TRP:CD1	3:W:607:LEU:HD22	2.55	0.40
3:W:798:ILE:HB	3:W:845:ILE:HG12	2.03	0.40
3:W:873:THR:HA	3:W:1073:ILE:CG2	2.50	0.40
3:W:917:ARG:HD2	3:W:919:TYR:CZ	2.56	0.40
1:A:200:VAL:O	1:A:201:ASP:HB3	2.21	0.40
1:A:249:ASP:O	1:A:250:TYR:C	2.60	0.40
1:A:264:PRO:O	1:A:265:LEU:HB2	2.22	0.40
1:A:283:ASN:ND2	1:A:869:VAL:H	2.18	0.40
1:A:594:ILE:HG23	1:A:595:PRO:N	2.36	0.40
1:A:714:ARG:O	1:A:715:ASP:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:GLN:HB2	1:A:786:ILE:H	1.60	0.40
1:A:793:ASP:OD1	1:A:793:ASP:N	2.54	0.40
1:B:224:PHE:HE1	2:O:70:LEU:C	2.24	0.40
1:B:543:LEU:O	1:B:544:VAL:C	2.58	0.40
1:B:558:MET:O	1:B:559:ALA:C	2.60	0.40
1:B:150:LEU:CD1	1:B:696:SER:HA	2.50	0.40
1:B:847:THR:HG22	1:B:847:THR:O	2.20	0.40
2:D:214:LEU:N	2:D:214:LEU:HD23	2.36	0.40
2:E:65:LEU:C	2:E:66:LEU:HG	2.42	0.40
2:E:91:PHE:O	2:E:95:VAL:HG23	2.22	0.40
2:F:65:LEU:HB3	2:F:66:LEU:H	1.69	0.40
2:G:104:SER:O	2:G:108:GLY:HA2	2.21	0.40
2:H:152:PHE:HB3	2:H:337:ASP:CB	2.51	0.40
2:H:65:LEU:O	2:H:66:LEU:HD23	2.22	0.40
2:I:204:ASN:HB3	2:I:296:ARG:HB3	2.03	0.40
2:L:153:HIS:CE1	2:M:153:HIS:CD2	3.09	0.40
3:W:193:TYR:O	3:W:197:LYS:HB2	2.21	0.40
3:W:62:TYR:O	3:W:66:ILE:HG12	2.22	0.40
3:W:75:LEU:N	3:W:75:LEU:HD12	2.37	0.40
1:A:338:GLU:O	1:A:339:LEU:HG	2.22	0.40
1:A:362:SER:HA	1:A:365:GLN:HE21	1.87	0.40
1:A:451:ASP:O	1:A:452:PRO:O	2.39	0.40
1:A:506:LEU:HD21	1:A:544:VAL:N	2.36	0.40
1:A:542:GLN:HA	1:A:545:ASP:OD2	2.20	0.40
1:A:707:TYR:H	1:A:707:TYR:HD1	1.69	0.40
1:A:715:ASP:O	1:A:718:TYR:O	2.39	0.40
1:B:497:ILE:HG23	2:I:68:THR:CG2	2.52	0.40
1:B:622:VAL:O	1:B:623:ALA:C	2.59	0.40
1:B:743:ASP:OD2	1:B:745:ALA:N	2.54	0.40
2:C:214:LEU:HD23	2:C:214:LEU:N	2.37	0.40
2:E:136:ILE:HD12	2:E:139:TRP:HB3	2.04	0.40
2:F:155:PRO:O	2:F:186:SER:HB3	2.21	0.40
2:F:14:ALA:O	2:F:16:ASP:N	2.54	0.40
2:F:204:ASN:HB3	2:F:296:ARG:HB3	2.03	0.40
2:G:4:LEU:O	2:G:5:TYR:C	2.59	0.40
2:H:23:LEU:H	2:H:26:ASN:HD21	1.67	0.40
2:I:145:ARG:NH1	2:I:145:ARG:CB	2.65	0.40
2:J:124:PHE:O	2:J:126:ARG:N	2.54	0.40
2:K:48:THR:O	2:K:56:ILE:HA	2.20	0.40
2:K:88:PHE:O	2:K:91:PHE:HB3	2.22	0.40
2:M:131:ASN:ND2	2:M:131:ASN:N	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:11:LEU:HA	2:M:14:ALA:HB3	2.04	0.40
2:M:204:ASN:HB3	2:M:296:ARG:HB3	2.04	0.40
2:O:204:ASN:HB3	2:O:296:ARG:HB3	2.03	0.40
2:O:9:LYS:HE3	2:O:13:ASP:OD1	2.21	0.40
3:W:539:ILE:HG23	3:W:562:LYS:CG	2.42	0.40
3:W:687:ILE:O	3:W:687:ILE:CG2	2.69	0.40
1:A:154:THR:O	1:A:155:LEU:C	2.59	0.40
1:A:304:LEU:N	1:A:615:ASN:ND2	2.67	0.40
1:A:536:LEU:HD22	1:A:536:LEU:N	2.36	0.40
1:A:657:VAL:HA	1:A:658:PRO:HD3	1.64	0.40
1:A:163:ARG:NH2	1:A:736:GLU:OE1	2.52	0.40
1:A:854:LEU:HD22	1:A:855:LEU:H	1.86	0.40
1:B:190:ASN:HB3	1:B:197:GLY:O	2.21	0.40
1:B:239:VAL:HG21	1:B:845:ASN:O	2.21	0.40
1:B:244:ILE:O	1:B:244:ILE:HG23	2.22	0.40
1:B:639:LYS:O	1:B:641:ILE:N	2.55	0.40
1:B:804:SER:O	1:B:805:ASP:HB2	2.22	0.40
1:B:870:ALA:C	1:B:872:ASP:H	2.21	0.40
2:D:11:LEU:HA	2:D:14:ALA:HB3	2.03	0.40
2:D:124:PHE:O	2:D:126:ARG:N	2.54	0.40
2:F:11:LEU:HB2	2:F:395:LEU:HD21	2.04	0.40
2:H:108:GLY:C	2:H:110:ALA:N	2.75	0.40
2:I:31:ILE:O	2:I:32:GLN:C	2.59	0.40
2:K:11:LEU:HA	2:K:14:ALA:HB3	2.03	0.40
2:K:133:SER:O	2:K:134:GLU:C	2.60	0.40
2:L:59:TRP:CD1	2:L:59:TRP:N	2.88	0.40
2:M:31:ILE:O	2:M:32:GLN:C	2.60	0.40
2:N:91:PHE:O	2:N:95:VAL:HG23	2.21	0.40
2:O:100:MET:HG3	2:O:388:VAL:CG1	2.51	0.40
2:O:144:ARG:O	2:O:145:ARG:CG	2.69	0.40
2:O:34:PHE:O	2:O:37:MET:HB3	2.21	0.40
3:W:288:LEU:O	3:W:288:LEU:HD12	2.20	0.40
3:W:844:PRO:O	3:W:848:GLU:HB2	2.20	0.40
3:W:865:VAL:HG13	3:W:866:THR:HG23	2.02	0.40
1:A:131:LEU:HA	1:A:132:PRO:HD3	1.90	0.40
1:A:303:LEU:HA	1:A:615:ASN:HD21	1.82	0.40
1:A:359:THR:HG22	1:A:359:THR:O	2.22	0.40
1:A:421:ARG:C	1:A:423:SER:H	2.25	0.40
1:A:510:LEU:HA	1:A:513:LEU:CD1	2.51	0.40
1:A:536:LEU:CD2	1:A:536:LEU:N	2.85	0.40
1:A:815:TYR:CD1	1:A:815:TYR:N	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:GLN:O	1:B:374:ALA:C	2.59	0.40
1:B:477:ASN:C	1:B:479:GLN:N	2.75	0.40
1:B:556:THR:HG22	1:B:557:LEU:N	2.36	0.40
1:B:746:GLN:O	1:B:750:MET:HG3	2.21	0.40
1:B:87:GLN:C	1:B:89:GLU:H	2.25	0.40
2:C:14:ALA:O	2:C:18:ILE:HD12	2.21	0.40
2:D:128:ASN:O	2:D:129:PHE:HB3	2.21	0.40
2:D:378:ARG:O	2:D:382:LEU:HB2	2.22	0.40
2:E:100:MET:HG3	2:E:388:VAL:HG11	2.04	0.40
2:F:235:PRO:HA	2:F:249:PHE:O	2.21	0.40
2:G:131:ASN:N	2:G:131:ASN:HD22	2.20	0.40
2:G:34:PHE:O	2:G:35:ASN:C	2.60	0.40
2:K:116:LEU:O	2:K:119:LEU:N	2.50	0.40
2:K:204:ASN:HB3	2:K:296:ARG:HB3	2.04	0.40
2:L:355:ILE:HA	2:L:356:PRO:HD3	1.96	0.40
2:L:74:ASP:O	2:L:75:ALA:C	2.59	0.40
2:M:4:LEU:O	2:M:5:TYR:C	2.58	0.40
2:O:101:VAL:HG23	2:O:102:ARG:N	2.36	0.40
3:W:255:VAL:HG11	3:W:316:ILE:HB	2.02	0.40
3:W:463:PHE:O	3:W:464:ILE:HG12	2.21	0.40
3:W:982:SER:O	3:W:985:LYS:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	779/880 (88%)	431 (55%)	199 (26%)	149 (19%)	0	2
1	B	808/880 (92%)	458 (57%)	204 (25%)	146 (18%)	0	2
2	C	395/397 (100%)	318 (80%)	54 (14%)	23 (6%)	1	20
2	D	395/397 (100%)	315 (80%)	50 (13%)	30 (8%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	395/397 (100%)	323 (82%)	49 (12%)	23 (6%)	1	20
2	F	395/397 (100%)	324 (82%)	47 (12%)	24 (6%)	1	18
2	G	395/397 (100%)	323 (82%)	49 (12%)	23 (6%)	1	20
2	H	395/397 (100%)	323 (82%)	50 (13%)	22 (6%)	2	20
2	I	395/397 (100%)	320 (81%)	51 (13%)	24 (6%)	1	18
2	J	395/397 (100%)	320 (81%)	53 (13%)	22 (6%)	2	20
2	K	395/397 (100%)	318 (80%)	52 (13%)	25 (6%)	1	18
2	L	395/397 (100%)	322 (82%)	47 (12%)	26 (7%)	1	17
2	M	395/397 (100%)	322 (82%)	52 (13%)	21 (5%)	2	21
2	N	395/397 (100%)	317 (80%)	50 (13%)	28 (7%)	1	16
2	O	395/397 (100%)	317 (80%)	47 (12%)	31 (8%)	1	14
3	W	933/1089 (86%)	807 (86%)	93 (10%)	33 (4%)	3	28
All	All	7655/8010 (96%)	5858 (76%)	1147 (15%)	650 (8%)	1	12

All (650) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	LYS
1	A	130	GLN
1	A	193	SER
1	A	198	LYS
1	A	220	ALA
1	A	234	ALA
1	A	246	HIS
1	A	252	PHE
1	A	260	GLN
1	A	275	PRO
1	A	283	ASN
1	A	287	ASN
1	A	306	ASP
1	A	315	GLU
1	A	338	GLU
1	A	340	VAL
1	A	356	GLU
1	A	358	LEU
1	A	370	ILE
1	A	413	VAL
1	A	443	GLN

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Mol	Chain	Res	Type
1	A	446	HIS
1	A	451	ASP
1	A	452	PRO
1	A	453	GLN
1	A	484	VAL
1	A	485	ILE
1	A	488	VAL
1	A	489	LEU
1	A	501	HIS
1	A	523	VAL
1	A	558	MET
1	A	564	ASN
1	A	570	THR
1	A	573	THR
1	A	585	CYS
1	A	650	HIS
1	A	651	ILE
1	A	660	ASP
1	A	661	GLN
1	A	689	MET
1	A	701	GLN
1	A	715	ASP
1	A	743	ASP
1	A	745	ALA
1	A	770	SER
1	A	771	VAL
1	A	772	ILE
1	A	781	THR
1	A	782	VAL
1	A	785	GLN
1	A	786	ILE
1	A	808	ASP
1	A	811	LEU
1	A	814	ASN
1	A	828	GLN
1	A	854	LEU
1	A	855	LEU
1	A	856	ALA
1	A	857	PHE
1	B	191	LYS
1	B	194	ARG
1	B	195	ASP

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Mol	Chain	Res	Type
1	B	196	ALA
1	B	200	VAL
1	B	215	GLU
1	B	218	GLU
1	B	226	ALA
1	B	227	GLU
1	B	252	PHE
1	B	306	ASP
1	B	355	LEU
1	B	361	GLN
1	B	369	GLY
1	B	400	ASN
1	B	417	ASP
1	B	446	HIS
1	B	447	TYR
1	B	451	ASP
1	B	457	GLN
1	B	458	ILE
1	B	479	GLN
1	B	481	ARG
1	B	503	ILE
1	B	504	ASN
1	B	574	GLU
1	B	585	CYS
1	B	634	TYR
1	B	640	ALA
1	B	651	ILE
1	B	655	ALA
1	B	673	PRO
1	B	699	ILE
1	B	702	GLY
1	B	724	ALA
1	B	764	PRO
1	B	765	PHE
1	B	777	LYS
1	B	782	VAL
1	B	785	GLN
1	B	786	ILE
1	B	790	ARG
1	B	792	VAL
1	B	805	ASP
1	B	806	SER

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Mol	Chain	Res	Type
1	B	855	LEU
1	B	856	ALA
1	B	875	ARG
2	C	22	THR
2	C	70	LEU
2	C	134	GLU
2	D	25	SER
2	D	70	LEU
2	D	126	ARG
2	D	128	ASN
2	D	134	GLU
2	D	148	THR
2	E	22	THR
2	E	25	SER
2	E	106	ARG
2	E	134	GLU
2	F	22	THR
2	F	62	ASP
2	F	70	LEU
2	F	105	GLN
2	F	134	GLU
2	F	145	ARG
2	F	148	THR
2	G	20	GLU
2	G	22	THR
2	G	134	GLU
2	G	148	THR
2	H	22	THR
2	H	107	ASN
2	H	134	GLU
2	I	25	SER
2	I	62	ASP
2	I	134	GLU
2	I	148	THR
2	J	20	GLU
2	J	70	LEU
2	J	106	ARG
2	J	134	GLU
2	K	22	THR
2	K	70	LEU
2	K	126	ARG
2	K	128	ASN

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Mol	Chain	Res	Type
2	K	134	GLU
2	K	148	THR
2	L	22	THR
2	L	62	ASP
2	L	126	ARG
2	L	134	GLU
2	L	145	ARG
2	L	148	THR
2	M	22	THR
2	M	25	SER
2	M	128	ASN
2	M	134	GLU
2	N	22	THR
2	N	25	SER
2	N	70	LEU
2	N	128	ASN
2	N	134	GLU
2	N	148	THR
2	O	65	LEU
2	O	68	THR
2	O	70	LEU
2	O	134	GLU
2	O	145	ARG
2	O	148	THR
3	W	54	SER
3	W	397	MET
3	W	401	SER
3	W	864	PRO
3	W	1082	ASN
3	W	1083	ALA
3	W	1084	ASN
1	A	143	ARG
1	A	202	SER
1	A	215	GLU
1	A	219	GLY
1	A	226	ALA
1	A	227	GLU
1	A	253	ASN
1	A	264	PRO
1	A	307	ARG
1	A	336	LEU
1	A	352	ASP

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Mol	Chain	Res	Type
1	A	369	GLY
1	A	415	PRO
1	A	438	PRO
1	A	441	GLY
1	A	458	ILE
1	A	465	ASN
1	A	503	ILE
1	A	559	ALA
1	A	571	LEU
1	A	590	ASN
1	A	608	VAL
1	A	630	ARG
1	A	654	VAL
1	A	680	ASP
1	A	739	MET
1	A	804	SER
1	A	815	TYR
1	A	823	THR
1	A	847	THR
1	A	866	ILE
1	B	73	LEU
1	B	141	GLU
1	B	142	LEU
1	B	212	PHE
1	B	230	GLN
1	B	253	ASN
1	B	261	LEU
1	B	264	PRO
1	B	265	LEU
1	B	278	ILE
1	B	282	VAL
1	B	283	ASN
1	B	307	ARG
1	B	313	ASN
1	B	338	GLU
1	B	388	SER
1	B	436	ILE
1	B	438	PRO
1	B	443	GLN
1	B	452	PRO
1	B	465	ASN
1	B	478	ASN

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Mol	Chain	Res	Type
1	B	487	GLY
1	B	488	VAL
1	B	489	LEU
1	B	493	LEU
1	B	496	ASN
1	B	500	GLY
1	B	520	THR
1	B	524	ASP
1	B	608	VAL
1	B	631	LEU
1	B	637	LYS
1	B	638	MET
1	B	654	VAL
1	B	674	VAL
1	B	676	VAL
1	B	787	VAL
1	B	854	LEU
2	C	7	LEU
2	C	20	GLU
2	C	25	SER
2	C	62	ASP
2	C	106	ARG
2	C	130	ASP
2	C	148	THR
2	D	7	LEU
2	D	20	GLU
2	D	42	ASN
2	D	65	LEU
2	D	67	GLY
2	D	69	THR
2	D	72	ASN
2	D	90	ASP
2	D	106	ARG
2	D	147	ARG
2	E	7	LEU
2	E	62	ASP
2	E	90	ASP
2	E	126	ARG
2	E	128	ASN
2	E	130	ASP
2	E	148	THR
2	F	7	LEU

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Mol	Chain	Res	Type
2	F	25	SER
2	F	128	ASN
2	G	7	LEU
2	G	25	SER
2	G	125	LYS
2	G	126	ARG
2	H	7	LEU
2	H	25	SER
2	H	42	ASN
2	H	51	ILE
2	H	62	ASP
2	H	68	THR
2	H	109	ILE
2	H	128	ASN
2	I	7	LEU
2	I	90	ASP
2	I	125	LYS
2	I	147	ARG
2	J	7	LEU
2	J	51	ILE
2	J	62	ASP
2	J	90	ASP
2	J	126	ARG
2	J	128	ASN
2	J	130	ASP
2	K	7	LEU
2	K	20	GLU
2	K	62	ASP
2	K	106	ARG
2	K	125	LYS
2	L	7	LEU
2	L	25	SER
2	L	69	THR
2	L	72	ASN
2	L	106	ARG
2	L	128	ASN
2	L	147	ARG
2	M	7	LEU
2	M	42	ASN
2	M	90	ASP
2	N	7	LEU
2	N	42	ASN

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Mol	Chain	Res	Type
2	N	62	ASP
2	N	65	LEU
2	N	90	ASP
2	N	145	ARG
2	O	7	LEU
2	O	22	THR
2	O	25	SER
2	O	62	ASP
2	O	90	ASP
2	O	105	GLN
3	W	102	LEU
3	W	201	TYR
3	W	521	VAL
3	W	825	ASN
3	W	862	GLN
3	W	865	VAL
3	W	1002	GLY
1	A	137	ASN
1	A	142	LEU
1	A	218	GLU
1	A	254	GLU
1	A	265	LEU
1	A	276	GLU
1	A	496	ASN
1	A	497	ILE
1	A	521	MET
1	A	525	TYR
1	A	579	THR
1	A	597	PRO
1	A	648	ARG
1	A	658	PRO
1	A	676	VAL
1	A	687	MET
1	A	696	SER
1	A	773	SER
1	A	816	ASP
1	A	849	THR
1	B	237	ASN
1	B	254	GLU
1	B	273	TYR
1	B	359	THR
1	B	387	LEU

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Mol	Chain	Res	Type
1	B	421	ARG
1	B	549	LEU
1	B	579	THR
1	B	581	VAL
1	B	590	ASN
1	B	635	GLN
1	B	656	ARG
1	B	670	ARG
1	B	675	GLU
1	B	794	THR
1	B	849	THR
2	C	13	ASP
2	C	42	ASN
2	C	69	THR
2	C	90	ASP
2	C	126	ARG
2	D	13	ASP
2	D	32	GLN
2	D	62	ASP
2	D	68	THR
2	D	125	LYS
2	E	13	ASP
2	E	32	GLN
2	E	70	LEU
2	F	13	ASP
2	F	32	GLN
2	F	90	ASP
2	F	126	ARG
2	F	130	ASP
2	G	13	ASP
2	G	32	GLN
2	G	42	ASN
2	G	90	ASP
2	G	128	ASN
2	H	13	ASP
2	H	32	GLN
2	H	90	ASP
2	I	13	ASP
2	I	32	GLN
2	I	126	ARG
2	I	128	ASN
2	I	146	GLN

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Mol	Chain	Res	Type
2	J	13	ASP
2	J	42	ASN
2	K	13	ASP
2	K	25	SER
2	K	32	GLN
2	K	90	ASP
2	K	111	PRO
2	L	13	ASP
2	L	20	GLU
2	L	41	MET
2	L	90	ASP
2	L	125	LYS
2	M	13	ASP
2	M	106	ARG
2	N	13	ASP
2	N	67	GLY
2	N	106	ARG
2	N	125	LYS
2	N	155	PRO
2	O	20	GLU
2	O	24	TYR
2	O	32	GLN
2	O	42	ASN
2	O	73	LEU
2	O	106	ARG
2	O	126	ARG
2	O	155	PRO
3	W	81	LYS
3	W	582	LYS
3	W	870	SER
1	A	131	LEU
1	A	144	ASN
1	A	155	LEU
1	A	187	ALA
1	A	195	ASP
1	A	206	SER
1	A	212	PHE
1	A	299	ILE
1	A	333	VAL
1	A	372	SER
1	A	387	LEU
1	A	457	GLN

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Mol	Chain	Res	Type
1	A	518	PHE
1	A	524	ASP
1	A	549	LEU
1	A	552	TYR
1	A	557	LEU
1	A	581	VAL
1	A	700	ALA
1	A	730	PHE
1	A	853	ASP
1	A	877	MET
1	B	85	GLU
1	B	101	LYS
1	B	185	ASP
1	B	193	SER
1	B	206	SER
1	B	294	SER
1	B	302	ASN
1	B	372	SER
1	B	442	MET
1	B	466	PHE
1	B	483	VAL
1	B	552	TYR
1	B	564	ASN
1	B	597	PRO
1	B	639	LYS
1	B	680	ASP
1	B	731	GLN
2	C	32	GLN
2	C	38	ILE
2	C	89	VAL
2	D	38	ILE
2	D	41	MET
2	D	89	VAL
2	D	123	LYS
2	D	145	ARG
2	E	38	ILE
2	F	20	GLU
2	F	38	ILE
2	F	42	ASN
2	G	38	ILE
2	G	130	ASP
2	G	145	ARG

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Mol	Chain	Res	Type
2	H	36	GLN
2	H	38	ILE
2	H	89	VAL
2	H	106	ARG
2	I	36	GLN
2	I	38	ILE
2	I	42	ASN
2	I	89	VAL
2	I	145	ARG
2	J	32	GLN
2	J	36	GLN
2	J	38	ILE
2	J	89	VAL
2	K	9	LYS
2	K	36	GLN
2	K	38	ILE
2	K	89	VAL
2	L	32	GLN
2	L	36	GLN
2	L	38	ILE
2	M	20	GLU
2	M	32	GLN
2	M	38	ILE
2	M	55	PRO
2	M	89	VAL
2	M	126	ARG
2	N	20	GLU
2	N	32	GLN
2	N	36	GLN
2	N	38	ILE
2	N	89	VAL
2	N	126	ARG
2	O	13	ASP
2	O	38	ILE
2	O	89	VAL
2	O	128	ASN
3	W	256	ASP
3	W	463	PHE
3	W	464	ILE
3	W	596	THR
3	W	760	ASN
3	W	790	SER

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Mol	Chain	Res	Type
3	W	795	LYS
1	A	152	LYS
1	A	196	ALA
1	A	351	GLN
1	B	86	ILE
1	B	103	SER
1	B	207	ILE
1	B	277	ARG
1	B	399	THR
1	B	416	ASN
1	B	437	TYR
1	B	827	LYS
2	C	36	GLN
2	C	145	ARG
2	D	9	LYS
2	D	36	GLN
2	E	36	GLN
2	E	55	PRO
2	E	89	VAL
2	F	9	LYS
2	F	36	GLN
2	F	89	VAL
2	G	36	GLN
2	G	89	VAL
2	G	123	LYS
2	G	155	PRO
2	H	9	LYS
2	H	130	ASP
2	I	9	LYS
2	I	41	MET
2	J	125	LYS
2	K	42	ASN
2	K	130	ASP
2	L	9	LYS
2	L	65	LEU
2	L	89	VAL
2	M	36	GLN
2	M	41	MET
2	M	145	ARG
2	N	9	LYS
2	N	69	THR
2	O	9	LYS

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Mol	Chain	Res	Type
2	O	36	GLN
2	O	41	MET
3	W	192	GLU
3	W	586	TYR
1	A	207	ILE
1	A	422	GLU
1	A	622	VAL
1	A	733	ILE
1	A	819	PRO
1	B	521	MET
1	B	557	LEU
1	B	622	VAL
1	B	677	ARG
1	B	781	THR
1	B	857	PHE
2	C	3	VAL
2	E	9	LYS
2	E	20	GLU
2	E	42	ASN
2	F	55	PRO
2	G	3	VAL
2	G	9	LYS
2	I	123	LYS
2	J	3	VAL
2	J	9	LYS
2	J	69	THR
2	K	3	VAL
2	K	147	ARG
2	L	3	VAL
2	N	3	VAL
2	O	3	VAL
3	W	1078	SER
1	A	247	PRO
1	A	334	PRO
1	B	519	PRO
1	B	723	ILE
1	B	865	PRO
2	D	3	VAL
2	E	3	VAL
2	F	3	VAL
2	H	3	VAL
2	I	3	VAL

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Mol	Chain	Res	Type
2	M	3	VAL
3	W	200	PRO
3	W	246	SER
3	W	301	VAL
3	W	901	PRO
1	A	502	VAL
1	A	606	VAL
1	B	415	PRO
2	E	78	VAL
2	I	78	VAL
2	I	101	VAL
2	L	78	VAL
2	N	78	VAL
3	W	798	ILE
1	A	405	ILE
1	A	699	ILE
1	B	128	PRO
1	B	370	ILE
1	B	405	ILE
1	B	413	VAL
2	C	78	VAL
2	F	78	VAL
2	H	78	VAL
2	J	78	VAL
2	K	78	VAL
2	M	78	VAL
2	M	101	VAL
2	N	101	VAL
2	O	51	ILE
2	O	78	VAL
2	O	101	VAL
3	W	446	PRO
1	A	500	GLY
1	B	435	ILE
1	B	606	VAL
2	C	67	GLY
2	D	78	VAL
2	G	78	VAL
1	A	787	VAL
1	B	246	HIS
1	B	544	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	715/809 (88%)	603 (84%)	112 (16%)	2	15
1	B	744/809 (92%)	635 (85%)	109 (15%)	3	16
2	C	350/350 (100%)	325 (93%)	25 (7%)	14	41
2	D	350/350 (100%)	322 (92%)	28 (8%)	12	37
2	E	350/350 (100%)	325 (93%)	25 (7%)	14	41
2	F	350/350 (100%)	327 (93%)	23 (7%)	16	43
2	G	350/350 (100%)	327 (93%)	23 (7%)	16	43
2	H	350/350 (100%)	329 (94%)	21 (6%)	19	46
2	I	350/350 (100%)	327 (93%)	23 (7%)	16	43
2	J	350/350 (100%)	327 (93%)	23 (7%)	16	43
2	K	350/350 (100%)	327 (93%)	23 (7%)	16	43
2	L	350/350 (100%)	321 (92%)	29 (8%)	11	36
2	M	350/350 (100%)	325 (93%)	25 (7%)	14	41
2	N	350/350 (100%)	324 (93%)	26 (7%)	13	40
2	O	350/350 (100%)	329 (94%)	21 (6%)	19	46
3	W	885/990 (89%)	828 (94%)	57 (6%)	17	44
All	All	6894/7158 (96%)	6301 (91%)	593 (9%)	10	35

All (593) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	PRO
1	A	122	LEU
1	A	125	ILE
1	A	126	PHE
1	A	142	LEU
1	A	147	TYR
1	A	154	THR
1	A	157	ASP

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Mol	Chain	Res	Type
1	A	169	LEU
1	A	180	TYR
1	A	193	SER
1	A	204	THR
1	A	215	GLU
1	A	216	GLU
1	A	229	ARG
1	A	230	GLN
1	A	239	VAL
1	A	247	PRO
1	A	259	HIS
1	A	271	PHE
1	A	273	TYR
1	A	278	ILE
1	A	280	ASN
1	A	286	LEU
1	A	288	MET
1	A	295	THR
1	A	298	TYR
1	A	303	LEU
1	A	305	GLN
1	A	310	LEU
1	A	311	HIS
1	A	316	SER
1	A	318	TRP
1	A	342	THR
1	A	347	GLN
1	A	348	LYS
1	A	354	GLN
1	A	366	PHE
1	A	371	ASN
1	A	382	LEU
1	A	389	GLN
1	A	391	THR
1	A	392	MET
1	A	395	ASP
1	A	401	TYR
1	A	414	VAL
1	A	419	PHE
1	A	423	SER
1	A	424	LEU
1	A	428	GLN

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Mol	Chain	Res	Type
1	A	436	ILE
1	A	443	GLN
1	A	445	MET
1	A	447	TYR
1	A	449	ASN
1	A	471	TRP
1	A	473	HIS
1	A	480	PHE
1	A	495	ASP
1	A	505	GLN
1	A	515	ARG
1	A	516	GLN
1	A	520	THR
1	A	521	MET
1	A	525	TYR
1	A	534	LEU
1	A	540	LEU
1	A	563	MET
1	A	564	ASN
1	A	565	MET
1	A	571	LEU
1	A	587	LEU
1	A	594	ILE
1	A	600	LEU
1	A	601	PHE
1	A	616	GLU
1	A	634	TYR
1	A	638	MET
1	A	641	ILE
1	A	646	LEU
1	A	676	VAL
1	A	680	ASP
1	A	701	GLN
1	A	704	ILE
1	A	707	TYR
1	A	717	MET
1	A	718	TYR
1	A	720	TYR
1	A	723	ILE
1	A	726	ASN
1	A	730	PHE
1	A	743	ASP

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Mol	Chain	Res	Type
1	A	744	TYR
1	A	747	ILE
1	A	753	ASN
1	A	759	LEU
1	A	765	PHE
1	A	771	VAL
1	A	775	ILE
1	A	782	VAL
1	A	793	ASP
1	A	798	ILE
1	A	799	LEU
1	A	802	ILE
1	A	816	ASP
1	A	829	VAL
1	A	837	ASN
1	A	839	MET
1	A	848	PHE
1	A	849	THR
1	A	861	ASP
1	A	872	ASP
1	B	74	GLU
1	B	126	PHE
1	B	134	TYR
1	B	135	ARG
1	B	153	ASP
1	B	157	ASP
1	B	169	LEU
1	B	180	TYR
1	B	182	LEU
1	B	190	ASN
1	B	194	ARG
1	B	201	ASP
1	B	204	THR
1	B	215	GLU
1	B	217	THR
1	B	239	VAL
1	B	271	PHE
1	B	286	LEU
1	B	287	ASN
1	B	298	TYR
1	B	310	LEU
1	B	311	HIS

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Mol	Chain	Res	Type
1	B	312	ASP
1	B	314	PHE
1	B	316	SER
1	B	318	TRP
1	B	336	LEU
1	B	347	GLN
1	B	348	LYS
1	B	352	ASP
1	B	353	LEU
1	B	358	LEU
1	B	382	LEU
1	B	389	GLN
1	B	392	MET
1	B	396	PHE
1	B	397	VAL
1	B	401	TYR
1	B	424	LEU
1	B	428	GLN
1	B	436	ILE
1	B	451	ASP
1	B	453	GLN
1	B	457	GLN
1	B	471	TRP
1	B	476	ASN
1	B	494	ASN
1	B	495	ASP
1	B	497	ILE
1	B	498	ARG
1	B	499	ASN
1	B	505	GLN
1	B	518	PHE
1	B	521	MET
1	B	525	TYR
1	B	534	LEU
1	B	540	LEU
1	B	542	GLN
1	B	560	CYS
1	B	562	THR
1	B	590	ASN
1	B	600	LEU
1	B	601	PHE
1	B	616	GLU

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Mol	Chain	Res	Type
1	B	634	TYR
1	B	638	MET
1	B	641	ILE
1	B	646	LEU
1	B	652	PHE
1	B	660	ASP
1	B	674	VAL
1	B	676	VAL
1	B	680	ASP
1	B	697	ASP
1	B	707	TYR
1	B	709	ASP
1	B	710	MET
1	B	725	ARG
1	B	727	LEU
1	B	728	ASP
1	B	730	PHE
1	B	734	ASN
1	B	744	TYR
1	B	747	ILE
1	B	759	LEU
1	B	765	PHE
1	B	771	VAL
1	B	774	LEU
1	B	782	VAL
1	B	783	PHE
1	B	786	ILE
1	B	789	LEU
1	B	790	ARG
1	B	791	LYS
1	B	798	ILE
1	B	799	LEU
1	B	808	ASP
1	B	810	TYR
1	B	812	VAL
1	B	818	VAL
1	B	823	THR
1	B	832	GLN
1	B	836	ARG
1	B	839	MET
1	B	841	MET
1	B	857	PHE

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Mol	Chain	Res	Type
1	B	871	PHE
1	B	872	ASP
1	B	876	ILE
2	C	1	MET
2	C	2	ASP
2	C	13	ASP
2	C	22	THR
2	C	26	ASN
2	C	59	TRP
2	C	68	THR
2	C	106	ARG
2	C	128	ASN
2	C	129	PHE
2	C	142	GLN
2	C	147	ARG
2	C	150	PHE
2	C	152	PHE
2	C	170	GLN
2	C	214	LEU
2	C	225	LEU
2	C	255	ARG
2	C	274	GLN
2	C	284	ASN
2	C	370	LEU
2	C	374	TYR
2	C	378	ARG
2	C	382	LEU
2	C	385	VAL
2	D	1	MET
2	D	2	ASP
2	D	13	ASP
2	D	19	VAL
2	D	68	THR
2	D	70	LEU
2	D	73	LEU
2	D	103	GLU
2	D	106	ARG
2	D	109	ILE
2	D	117	ARG
2	D	129	PHE
2	D	142	GLN
2	D	143	ASN

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Mol	Chain	Res	Type
2	D	147	ARG
2	D	150	PHE
2	D	152	PHE
2	D	170	GLN
2	D	214	LEU
2	D	225	LEU
2	D	255	ARG
2	D	274	GLN
2	D	284	ASN
2	D	370	LEU
2	D	374	TYR
2	D	378	ARG
2	D	382	LEU
2	D	385	VAL
2	E	1	MET
2	E	2	ASP
2	E	13	ASP
2	E	26	ASN
2	E	59	TRP
2	E	69	THR
2	E	103	GLU
2	E	109	ILE
2	E	128	ASN
2	E	129	PHE
2	E	142	GLN
2	E	148	THR
2	E	150	PHE
2	E	152	PHE
2	E	170	GLN
2	E	214	LEU
2	E	225	LEU
2	E	255	ARG
2	E	274	GLN
2	E	284	ASN
2	E	370	LEU
2	E	374	TYR
2	E	378	ARG
2	E	382	LEU
2	E	385	VAL
2	F	2	ASP
2	F	13	ASP
2	F	60	ASN

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Mol	Chain	Res	Type
2	F	61	PHE
2	F	105	GLN
2	F	109	ILE
2	F	128	ASN
2	F	129	PHE
2	F	142	GLN
2	F	148	THR
2	F	150	PHE
2	F	152	PHE
2	F	170	GLN
2	F	214	LEU
2	F	225	LEU
2	F	255	ARG
2	F	274	GLN
2	F	284	ASN
2	F	370	LEU
2	F	374	TYR
2	F	378	ARG
2	F	382	LEU
2	F	385	VAL
2	G	2	ASP
2	G	13	ASP
2	G	26	ASN
2	G	63	PHE
2	G	106	ARG
2	G	109	ILE
2	G	117	ARG
2	G	129	PHE
2	G	142	GLN
2	G	143	ASN
2	G	145	ARG
2	G	152	PHE
2	G	170	GLN
2	G	214	LEU
2	G	225	LEU
2	G	255	ARG
2	G	274	GLN
2	G	284	ASN
2	G	370	LEU
2	G	374	TYR
2	G	378	ARG
2	G	382	LEU

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Mol	Chain	Res	Type
2	G	385	VAL
2	H	1	MET
2	H	2	ASP
2	H	13	ASP
2	H	103	GLU
2	H	106	ARG
2	H	128	ASN
2	H	129	PHE
2	H	142	GLN
2	H	150	PHE
2	H	152	PHE
2	H	170	GLN
2	H	214	LEU
2	H	225	LEU
2	H	255	ARG
2	H	274	GLN
2	H	284	ASN
2	H	370	LEU
2	H	374	TYR
2	H	378	ARG
2	H	382	LEU
2	H	385	VAL
2	I	1	MET
2	I	2	ASP
2	I	13	ASP
2	I	48	THR
2	I	61	PHE
2	I	106	ARG
2	I	109	ILE
2	I	117	ARG
2	I	129	PHE
2	I	142	GLN
2	I	150	PHE
2	I	152	PHE
2	I	170	GLN
2	I	214	LEU
2	I	225	LEU
2	I	255	ARG
2	I	274	GLN
2	I	284	ASN
2	I	370	LEU
2	I	374	TYR

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Mol	Chain	Res	Type
2	I	378	ARG
2	I	382	LEU
2	I	385	VAL
2	J	1	MET
2	J	2	ASP
2	J	13	ASP
2	J	19	VAL
2	J	59	TRP
2	J	106	ARG
2	J	109	ILE
2	J	128	ASN
2	J	129	PHE
2	J	142	GLN
2	J	150	PHE
2	J	152	PHE
2	J	170	GLN
2	J	214	LEU
2	J	225	LEU
2	J	255	ARG
2	J	274	GLN
2	J	284	ASN
2	J	370	LEU
2	J	374	TYR
2	J	378	ARG
2	J	382	LEU
2	J	385	VAL
2	K	1	MET
2	K	2	ASP
2	K	13	ASP
2	K	59	TRP
2	K	62	ASP
2	K	106	ARG
2	K	109	ILE
2	K	129	PHE
2	K	142	GLN
2	K	143	ASN
2	K	150	PHE
2	K	152	PHE
2	K	170	GLN
2	K	214	LEU
2	K	225	LEU
2	K	255	ARG

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Mol	Chain	Res	Type
2	K	274	GLN
2	K	284	ASN
2	K	370	LEU
2	K	374	TYR
2	K	378	ARG
2	K	382	LEU
2	K	385	VAL
2	L	1	MET
2	L	2	ASP
2	L	13	ASP
2	L	19	VAL
2	L	22	THR
2	L	25	SER
2	L	59	TRP
2	L	62	ASP
2	L	72	ASN
2	L	103	GLU
2	L	106	ARG
2	L	109	ILE
2	L	125	LYS
2	L	129	PHE
2	L	142	GLN
2	L	143	ASN
2	L	150	PHE
2	L	152	PHE
2	L	170	GLN
2	L	214	LEU
2	L	225	LEU
2	L	255	ARG
2	L	274	GLN
2	L	284	ASN
2	L	370	LEU
2	L	374	TYR
2	L	378	ARG
2	L	382	LEU
2	L	385	VAL
2	M	1	MET
2	M	2	ASP
2	M	13	ASP
2	M	22	THR
2	M	59	TRP
2	M	71	LEU

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Mol	Chain	Res	Type
2	M	103	GLU
2	M	106	ARG
2	M	117	ARG
2	M	125	LYS
2	M	129	PHE
2	M	142	GLN
2	M	150	PHE
2	M	152	PHE
2	M	170	GLN
2	M	214	LEU
2	M	225	LEU
2	M	255	ARG
2	M	274	GLN
2	M	284	ASN
2	M	370	LEU
2	M	374	TYR
2	M	378	ARG
2	M	382	LEU
2	M	385	VAL
2	N	1	MET
2	N	2	ASP
2	N	13	ASP
2	N	58	ASN
2	N	60	ASN
2	N	66	LEU
2	N	73	LEU
2	N	103	GLU
2	N	106	ARG
2	N	109	ILE
2	N	129	PHE
2	N	142	GLN
2	N	145	ARG
2	N	150	PHE
2	N	152	PHE
2	N	170	GLN
2	N	214	LEU
2	N	225	LEU
2	N	255	ARG
2	N	274	GLN
2	N	284	ASN
2	N	370	LEU
2	N	374	TYR

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Mol	Chain	Res	Type
2	N	378	ARG
2	N	382	LEU
2	N	385	VAL
2	O	2	ASP
2	O	13	ASP
2	O	23	LEU
2	O	25	SER
2	O	106	ARG
2	O	107	ASN
2	O	109	ILE
2	O	129	PHE
2	O	142	GLN
2	O	150	PHE
2	O	170	GLN
2	O	214	LEU
2	O	225	LEU
2	O	255	ARG
2	O	274	GLN
2	O	284	ASN
2	O	370	LEU
2	O	374	TYR
2	O	378	ARG
2	O	382	LEU
2	O	385	VAL
3	W	48	ASN
3	W	70	THR
3	W	79	TYR
3	W	121	THR
3	W	130	MET
3	W	143	ASN
3	W	150	GLU
3	W	155	ASP
3	W	166	ARG
3	W	178	ASN
3	W	186	ASN
3	W	195	VAL
3	W	198	ASP
3	W	246	SER
3	W	283	GLN
3	W	290	GLN
3	W	305	LYS
3	W	311	LEU

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Mol	Chain	Res	Type
3	W	320	PRO
3	W	341	ASP
3	W	394	LEU
3	W	404	GLU
3	W	408	LEU
3	W	426	ASP
3	W	430	ASN
3	W	439	PRO
3	W	451	ARG
3	W	499	GLN
3	W	503	TYR
3	W	518	TYR
3	W	619	HIS
3	W	623	THR
3	W	628	VAL
3	W	629	ASP
3	W	663	ASN
3	W	690	ARG
3	W	709	GLN
3	W	717	TYR
3	W	721	ARG
3	W	723	ARG
3	W	734	THR
3	W	750	LEU
3	W	758	THR
3	W	782	VAL
3	W	808	PHE
3	W	820	LEU
3	W	835	GLU
3	W	886	THR
3	W	892	LEU
3	W	906	ASN
3	W	932	ARG
3	W	939	VAL
3	W	1003	CYS
3	W	1050	SER
3	W	1068	LYS
3	W	1078	SER
3	W	1084	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (253) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	137	ASN
1	A	168	ASN
1	A	230	GLN
1	A	246	HIS
1	A	260	GLN
1	A	309	ASN
1	A	365	GLN
1	A	428	GLN
1	A	443	GLN
1	A	453	GLN
1	A	462	GLN
1	A	473	HIS
1	A	490	ASN
1	A	496	ASN
1	A	553	ASN
1	A	605	ASN
1	A	609	ASN
1	A	613	ASN
1	A	615	ASN
1	A	661	GLN
1	A	683	ASN
1	A	701	GLN
1	A	722	ASN
1	A	726	ASN
1	A	803	ASN
1	A	807	ASN
1	A	840	HIS
1	A	873	ASN
1	B	119	GLN
1	B	168	ASN
1	B	190	ASN
1	B	230	GLN
1	B	237	ASN
1	B	240	ASN
1	B	246	HIS
1	B	287	ASN
1	B	302	ASN
1	B	305	GLN
1	B	311	HIS
1	B	347	GLN
1	B	361	GLN
1	B	371	ASN

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Mol	Chain	Res	Type
1	B	449	ASN
1	B	465	ASN
1	B	473	HIS
1	B	476	ASN
1	B	477	ASN
1	B	491	GLN
1	B	517	GLN
1	B	553	ASN
1	B	564	ASN
1	B	590	ASN
1	B	602	HIS
1	B	605	ASN
1	B	609	ASN
1	B	611	HIS
1	B	615	ASN
1	B	629	ASN
1	B	635	GLN
1	B	683	ASN
1	B	746	GLN
1	B	807	ASN
1	B	814	ASN
1	B	831	GLN
1	B	840	HIS
1	B	878	ASN
2	C	26	ASN
2	C	35	ASN
2	C	53	ASN
2	C	72	ASN
2	C	128	ASN
2	C	131	ASN
2	C	143	ASN
2	C	146	GLN
2	C	167	ASN
2	C	239	ASN
2	C	274	GLN
2	C	284	ASN
2	C	345	ASN
2	D	26	ASN
2	D	128	ASN
2	D	131	ASN
2	D	142	GLN
2	D	146	GLN

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Mol	Chain	Res	Type
2	D	167	ASN
2	D	239	ASN
2	D	274	GLN
2	D	284	ASN
2	D	345	ASN
2	E	26	ASN
2	E	53	ASN
2	E	94	ASN
2	E	131	ASN
2	E	142	GLN
2	E	167	ASN
2	E	239	ASN
2	E	274	GLN
2	E	284	ASN
2	E	345	ASN
2	F	32	GLN
2	F	53	ASN
2	F	72	ASN
2	F	94	ASN
2	F	128	ASN
2	F	131	ASN
2	F	142	GLN
2	F	167	ASN
2	F	239	ASN
2	F	274	GLN
2	F	284	ASN
2	F	345	ASN
2	G	26	ASN
2	G	35	ASN
2	G	53	ASN
2	G	128	ASN
2	G	131	ASN
2	G	142	GLN
2	G	167	ASN
2	G	239	ASN
2	G	274	GLN
2	G	284	ASN
2	G	345	ASN
2	H	26	ASN
2	H	53	ASN
2	H	83	ASN
2	H	94	ASN

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Mol	Chain	Res	Type
2	H	107	ASN
2	H	128	ASN
2	H	131	ASN
2	H	142	GLN
2	H	167	ASN
2	H	239	ASN
2	H	274	GLN
2	H	284	ASN
2	H	345	ASN
2	I	32	GLN
2	I	53	ASN
2	I	76	ASN
2	I	94	ASN
2	I	128	ASN
2	I	131	ASN
2	I	143	ASN
2	I	146	GLN
2	I	167	ASN
2	I	239	ASN
2	I	274	GLN
2	I	284	ASN
2	I	345	ASN
2	J	26	ASN
2	J	53	ASN
2	J	94	ASN
2	J	128	ASN
2	J	131	ASN
2	J	142	GLN
2	J	146	GLN
2	J	167	ASN
2	J	239	ASN
2	J	274	GLN
2	J	284	ASN
2	J	345	ASN
2	K	26	ASN
2	K	53	ASN
2	K	72	ASN
2	K	94	ASN
2	K	131	ASN
2	K	143	ASN
2	K	167	ASN
2	K	239	ASN

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Mol	Chain	Res	Type
2	K	274	GLN
2	K	284	ASN
2	K	345	ASN
2	L	53	ASN
2	L	72	ASN
2	L	131	ASN
2	L	140	ASN
2	L	143	ASN
2	L	146	GLN
2	L	167	ASN
2	L	239	ASN
2	L	274	GLN
2	L	284	ASN
2	L	345	ASN
2	M	36	GLN
2	M	53	ASN
2	M	128	ASN
2	M	131	ASN
2	M	142	GLN
2	M	143	ASN
2	M	167	ASN
2	M	239	ASN
2	M	274	GLN
2	M	284	ASN
2	M	345	ASN
2	N	26	ASN
2	N	32	GLN
2	N	53	ASN
2	N	94	ASN
2	N	128	ASN
2	N	131	ASN
2	N	140	ASN
2	N	142	GLN
2	N	146	GLN
2	N	167	ASN
2	N	239	ASN
2	N	274	GLN
2	N	284	ASN
2	N	345	ASN
2	O	35	ASN
2	O	53	ASN
2	O	131	ASN

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Mol	Chain	Res	Type
2	O	140	ASN
2	O	142	GLN
2	O	143	ASN
2	O	153	HIS
2	O	167	ASN
2	O	239	ASN
2	O	274	GLN
2	O	284	ASN
2	O	345	ASN
3	W	31	ASN
3	W	36	ASN
3	W	42	HIS
3	W	48	ASN
3	W	68	ASN
3	W	143	ASN
3	W	185	HIS
3	W	186	ASN
3	W	283	GLN
3	W	290	GLN
3	W	308	GLN
3	W	423	HIS
3	W	473	GLN
3	W	499	GLN
3	W	565	GLN
3	W	585	GLN
3	W	604	ASN
3	W	653	ASN
3	W	703	GLN
3	W	706	GLN
3	W	760	ASN
3	W	794	GLN
3	W	810	ASN
3	W	818	GLN
3	W	824	ASN
3	W	853	GLN
3	W	862	GLN
3	W	906	ASN
3	W	956	ASN
3	W	1005	GLN
3	W	1010	ASN
3	W	1043	ASN
3	W	1048	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.