



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:59 PM GMT

PDB ID : 1I6V  
Title : THERMUS AQUATICUS CORE RNA POLYMERASE-RIFAMPICIN COMPLEX  
Authors : Campbell, E.A.; Korzheva, N.; Mustaev, A.; Murakami, K.; Goldfarb, A.; Darst, S.A.  
Deposited on : 2001-03-05  
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865



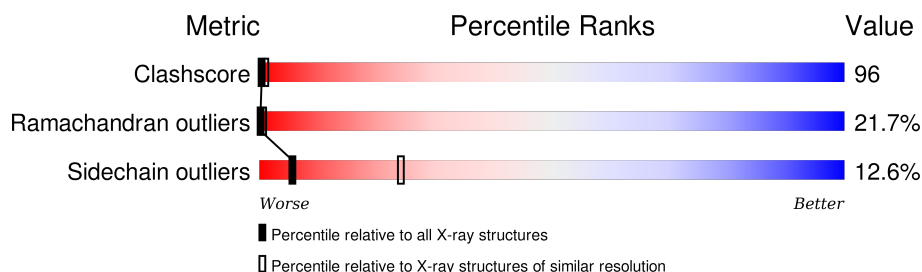
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	314	
1	B	314	
2	C	1118	
3	D	1264	
4	E	99	



## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21292 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1741	1109	299	330	3			
1	B	230	Total	C	N	O	S	0	0	0
			1761	1122	299	337	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	VAL	GLY	CONFLICT	UNP Q9KWU8
A	232	SER	LEU	CONFLICT	UNP Q9KWU8
B	112	VAL	GLY	CONFLICT	UNP Q9KWU8
B	232	SER	LEU	CONFLICT	UNP Q9KWU8

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1113	Total	C	N	O	S	12	0	0
			8508	5386	1514	1585	23			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	LYS	GLU	CONFLICT	UNP Q9KWU7
C	?	-	GLU	DELETION	UNP Q9KWU7
C	1111	VAL	ILE	CONFLICT	UNP Q9KWU7

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1174	Total	C	N	O	S	17	0	0
			8502	5329	1550	1596	27			



There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	70	ALA	GLY	CONFLICT	UNP Q9KWU6
D	77	ALA	GLY	CONFLICT	UNP Q9KWU6
D	91	ALA	GLY	CONFLICT	UNP Q9KWU6
D	113	ALA	GLY	CONFLICT	UNP Q9KWU6
D	139	ALA	GLY	CONFLICT	UNP Q9KWU6
D	144	ALA	GLY	CONFLICT	UNP Q9KWU6
D	863	THR	VAL	CONFLICT	UNP Q9KWU6
D	866	THR	VAL	CONFLICT	UNP Q9KWU6
D	1009	ASN	LYS	CONFLICT	UNP Q9KWU6

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	98	Total	C	N	O	S	0	0	0
			719	453	132	130	4			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

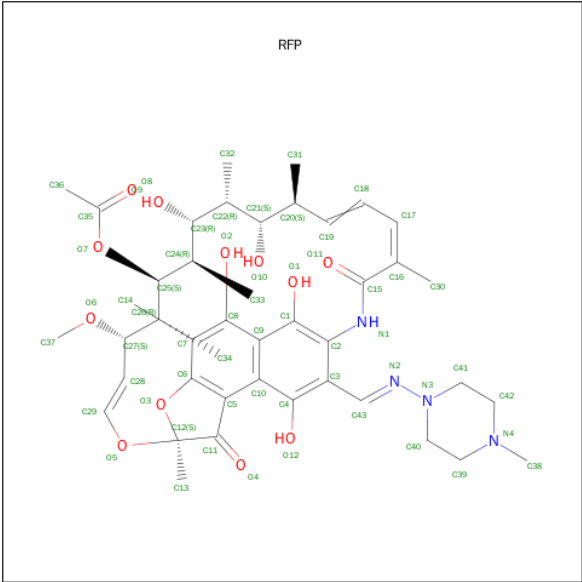
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Zn	0	0
			1	1		

- Molecule 7 is RIFAMPICIN (three-letter code: RFP) (formula: C<sub>43</sub>H<sub>58</sub>N<sub>4</sub>O<sub>12</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			59	43	4	12		

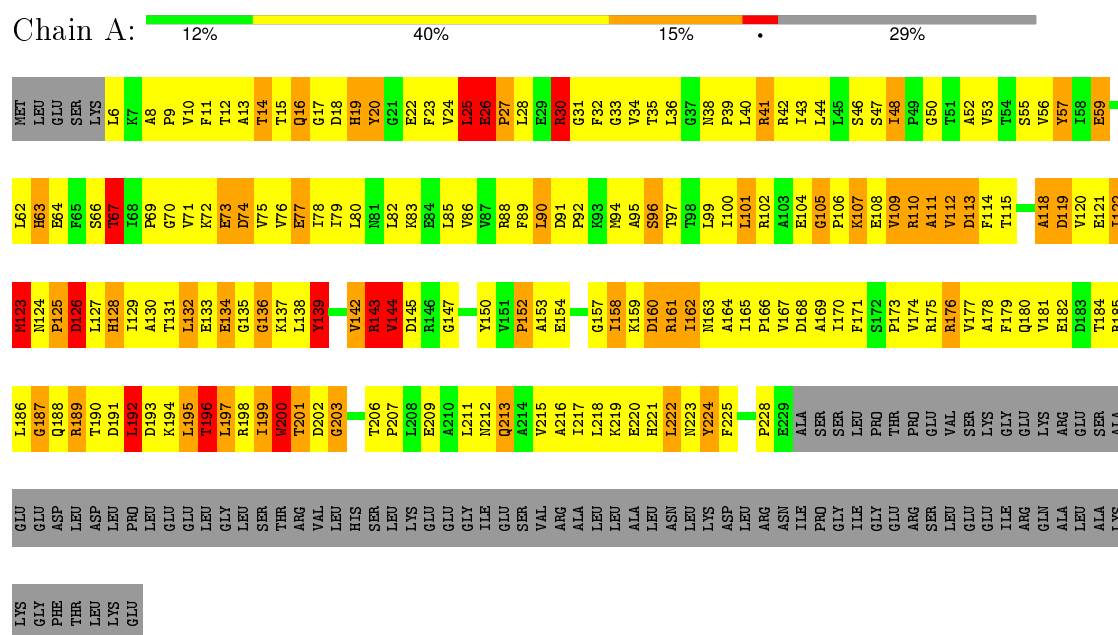


### 3 Residue-property plots

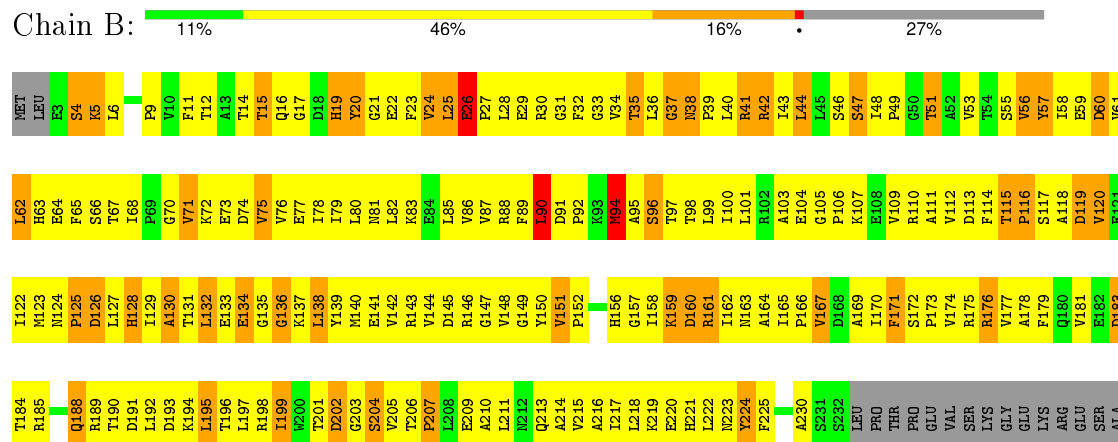
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

#### • Molecule 1: DNA-DIRECTED RNA POLYMERASE




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GLU	LYS
GLY	GLY
ASP	PHE
LEU	THR
ASP	LEU
LEU	LYS
PRO	LEU
LEU	GLU
GLU	GLU
LEU	LEU
GLY	GLY
LEU	LEU
SER	SER
THR	THR
VAL	VAL
GLU	GLU
GLY	GLY
GLY	ILE
ILE	GLU
GLU	SER
SER	LEU
LEU	GLU
GLY	ILE
GLY	GLY
ARG	ARG
SER	SER
LEU	LEU
GLU	GLU
ILE	ILE
ARG	ARG
GLN	ALA
ALA	LEU
LEU	ALA
LEU	LYS

• Molecule 2: DNA-DIRECTED RNA POLYMERASE

Chain C:  14% 60% 24%

MET	G62	T122	M184	G246	Y309	A370	H431	E491	D553	B616	D680	I742	R805
R2	G63	E123	K185	D246	L310	K371	R432	D491	D554	D617	G681	V743	L806
I3	L64	D124	M187	P248	F311	L372	T433	R493	A555	G618	N682	R744	R807
R4	V65	G125	K187	P248	F311	N373	T434	Y494	N556	R619	N683	I745	
R5	L66	S126	K190	K250	T314	N374	Y435	T495	R557	V621	F684	G746	D810
R6	D67	S127	K191	K251	T315	N375	R436	I496	A558	V622	E685	A747	P811
G7	F68	I128	F191	D251	A315	R376	R437	A497	L559	H623	D686	V748	G812
R8	L69	I129	F192	K252	G316	F377	I438	Q498	M560	P624	A687	V749	G813
R9	E70	G131	L193	K253	P317	L378	Q439	A499	G561	L625	N688	K750	E814
R10	Y71		L194	L254	G318	A380	P440	N500	M564	R626	V689	D753	L815
R11	Y72		L195	A255	P319	E379	A441	T501	Q565	R627	G690	I754	K816
Y12	I73		L196	A256	G320	A381	T442	P502	T566	Y628	E691	P754	P817
I13	G74		L197	L257	E321	L382	T443	L503	Q567	A629	E692	L755	G818
P14	D75		R198	F288	V322	R383	P444	R507	A568	R630	E693	V756	V819
L15	P76		V199	G259	D323	E384	E445	R508	A569	S631	L694	G757	R820
P16	P77		G206	L260	D324	F385	G446	L508	F578	N632	L695	L758	E821
P17	F78		G207	L261	R331	Q392	A447	A509	P570	Q633	G696	T759	V822
Y18	S79		Y202	L262	R332	F394	N448	T510	L571	G634	R697	S760	V823
L19	Q80		D203	D263	H327	R388	I449	D511	L572	T635	D698	F761	R824
E20	D81		Q204	P264	L328	L391	G450	R512	A573	A636	F699	K762	V825
I21	L88		E205	K265	T335	L451	L451	R513	A574	P637	Y700	G763	F826
K28	L89		S212	R266	R330	Q393	I452	V514	Q575	R643	T701	E764	A828
A29	Q91		A213	Y275	R331	Q393	T453	A515	A576	Q1639	S702	L773	V835
L30	Q92		P152	K276	R332	F394	S454	R516	P577	R640	G702	L774	G836
Q31	A92		A153	L269	R333	K395	L455	R517	Q578	P641	H704	R775	D837
A32	P93		D216	G270	R334	S402	A456	R518	L579	R642	I705	S776	K838
D33	L94		L217	E278	N340	S403	A463	A525	R586	V643	E706	E770	K839
V34	Y95		L218	L281	A341	L404	L464	P526	F587	R644	T707	E771	A840
P35	A96		Q219	G282	Q343	R405	G465	E527	L588	V645	L715	G772	Q834
R97	R97		G220	V283	F344	H406	F466	E528	R589	V646	K716	G773	V835
P36	L98		L221	G284	R345	K407	I467	V529	L592	A656	L717	K781	R843
E37	Q99		L222	L285	V346	R408	R468	E530	L593	D657	G718	A782	G844
K38	L100		D223	L286	G347	R409	T469	P531	L595	G688	F719	R783	N845
R39	I101		E224	S286	L348	L410	P470	N532	F596	P659	E720	V784	K846
V42	H02		A225	G287	A349	S411	Y471	D533	Y597	A660	R721	K785	G847
G43	K103		V226	R288	R350	A412	R472	V534	A597	S661	I722	K786	V848
I44	D104		L227	T289	L351	G413	R473	S535	E598	E662	R723	D787	V849
Q45	T105		A228	L290	A352	L414	V474	P536	E599	B663	R724	T788	A850
A46	G106		M229	V291	R353	P415	K475	K537	D600	G684	D725	S789	K851
A47	L107		R168	R292	V354	G416	N476	Q538	G601	P665	I726	V791	L852
F48	I108		P231		V355	G417	V477	V539	E602	L666	P727	K791	G853
R49	K109		E232	D295	R356	L418	V478	P540	V603	A667	H728	V792	P854
E50	E110		E233	F298	E357	T419	V479	S541	V604	L668	R729	P793	V855
T51	D111		A234	K299	R358	R420	T480	L542	K605	G669	S730	P794	K856
F52	E112		A235	K299	M359	E421	E481	N543	V606	Q670	E731	G795	D857
P53	V113		V236	D300	V360	R422	E482	T544	D607	N671	A732	E796	N858
I54	F114		R237	E301	M361	A423	V483	N545	G608	V672	A733	E797	P859
E55	L115		L238	V302	G362	G424	V484	L546	T609	L673	H734	G798	H860
ARG	E116		P239	F303	S363	F425	Y485	P547	R610	V674	R735	V799	P861
GLN	G57		T240	L304	P364	D426	V486	P548	L611	A675	D736	V800	L862
B58	L118		L241	P305		V427	T487	P549	A612	L676	L737	V801	D863
R59	P119		R242	T306	L367	R428	A488	E551	V613	P677	D738	G802	G864
A60	L120		R243	L307	T368	R429	S489	R551	R614	P678	E739	R803	T865
M61	M121		P244	R308	P369	V430	E490	H552	V615	F679	L804		P866







[illegible]

Chain E:  19% 62% 18%

M63	M64	M65	M66	M67	M68	M69	M70	M71	M72	M73	M74	M75	M76	M77	M78	M79	M80	M81	M82	M83	M84	M85	M86	M87	M88	M89	M90	M91	M92	M93	M94	M95	M96	M97	M98	M99	M100	M101	M102	M103	M104	M105	M106	M107	M108	M109	M110	M111	M112	M113	M114	M115	M116	M117	M118	M119	M120	M121	M122	M123	M124	M125	M126	M127	M128	M129	M130	M131	M132	M133	M134	M135	M136	M137	M138	M139	M140	M141	M142	M143	M144	M145	M146	M147	M148	M149	M150	M151	M152	M153	M154	M155	M156	M157	M158	M159	M160	M161	M162	M163	M164	M165	M166	M167	M168	M169	M170	M171	M172	M173	M174	M175	M176	M177	M178	M179	M180	M181	M182	M183	M184	M185	M186	M187	M188	M189	M190	M191	M192	M193	M194	M195	M196	M197	M198	M199	M200	M201	M202	M203	M204	M205	M206	M207	M208	M209	M210	M211	M212	M213	M214	M215	M216	M217	M218	M219	M220	M221	M222	M223	M224	M225	M226	M227	M228	M229	M230	M231	M232	M233	M234	M235	M236	M237	M238	M239	M240	M241	M242	M243	M244	M245	M246	M247	M248	M249	M250	M251	M252	M253	M254	M255	M256	M257	M258	M259	M260	M261	M262	M263	M264	M265	M266	M267	M268	M269	M270	M271	M272	M273	M274	M275	M276	M277	M278	M279	M280	M281	M282	M283	M284	M285	M286	M287	M288	M289	M290	M291	M292	M293	M294	M295	M296	M297	M298	M299	M300	M301	M302	M303	M304	M305	M306	M307	M308	M309	M310	M311	M312	M313	M314	M315	M316	M317	M318	M319	M320	M321	M322	M323	M324	M325	M326	M327	M328	M329	M330	M331	M332	M333	M334	M335	M336	M337	M338	M339	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353	M354	M355	M356	M357	M358	M359	M360	M361	M362	M363	M364	M365	M366	M367	M368	M369	M370	M371	M372	M373	M374	M375	M376	M377	M378	M379	M380	M381	M382	M383	M384	M385	M386	M387	M388	M389	M390	M391	M392	M393	M394	M395	M396	M397	M398	M399	M400	M401	M402	M403	M404	M405	M406	M407	M408	M409	M410	M411	M412	M413	M414	M415	M416	M417	M418	M419	M420	M421	M422	M423	M424	M425	M426	M427	M428	M429	M430	M431	M432	M433	M434	M435	M436	M437	M438	M439	M440	M441	M442	M443	M444	M445	M446	M447	M448	M449	M450	M451	M452	M453	M454	M455	M456	M457	M458	M459	M460	M461	M462	M463	M464	M465	M466	M467	M468	M469	M470	M471	M472	M473	M474	M475	M476	M477	M478	M479	M480	M481	M482	M483	M484	M485	M486	M487	M488	M489	M490	M491	M492	M493	M494	M495	M496	M497	M498	M499	M500	M501	M502	M503	M504	M505	M506	M507	M508	M509	M510	M511	M512	M513	M514	M515	M516	M517	M518	M519	M520	M521	M522	M523	M524	M525	M526	M527	M528	M529	M530	M531	M532	M533	M534	M535	M536	M537	M538	M539	M540	M541	M542	M543	M544	M545	M546	M547	M548	M549	M550	M551	M552	M553	M554	M555	M556	M557	M558	M559	M560	M561	M562	M563	M564	M565	M566	M567	M568	M569	M570	M571	M572	M573	M574	M575	M576	M577	M578	M579	M580	M581	M582	M583	M584	M585	M586	M587	M588	M589	M590	M591	M592	M593	M594	M595	M596	M597	M598	M599	M600	M601	M602	M603	M604	M605	M606	M607	M608	M609	M610	M611	M612	M613	M614	M615	M616	M617	M618	M619	M620	M621	M622	M623	M624	M625	M626	M627	M628	M629	M630	M631	M632	M633	M634	M635	M636	M637	M638	M639	M640	M641	M642	M643	M644	M645	M646	M647	M648	M649	M650	M651	M652	M653	M654	M655	M656	M657	M658	M659	M660	M661	M662	M663	M664	M665	M666	M667	M668	M669	M670	M671	M672	M673	M674	M675	M676	M677	M678	M679	M680	M681	M682	M683	M684	M685	M686	M687	M688	M689	M690	M691	M692	M693	M694	M695	M696	M697	M698	M699	M700	M701	M702	M703	M704	M705	M706	M707	M708	M709	M710	M711	M712	M713	M714	M715	M716	M717	M718	M719	M720	M721	M722	M723	M724	M725	M726	M727	M728	M729	M730	M731	M732	M733	M734	M735	M736	M737	M738	M739	M740	M741	M742	M743	M744	M745	M746	M747	M748	M749	M750	M751	M752	M753	M754	M755	M756	M757	M758	M759	M760	M761	M762	M763	M764	M765	M766	M767	M768	M769	M770	M771	M772	M773	M774	M775	M776	M777	M778	M779	M780	M781	M782	M783	M784	M785	M786	M787	M788	M789	M790	M791	M792	M793	M794	M795	M796	M797	M798	M799	M800	M801	M802	M803	M804	M805	M806	M807	M808	M809	M810	M811	M812	M813	M814	M815	M816	M817	M818	M819	M820	M821	M822	M823	M824	M825	M826	M827	M828	M829	M830	M831	M832	M833	M834	M835	M836	M837	M838	M839	M840	M841	M842	M843	M844	M845	M846	M847	M848	M849	M850	M851	M852	M853	M854	M855	M856	M857	M858	M859	M860	M861	M862	M863	M864	M865	M866	M867	M868	M869	M870	M871	M872	M873	M874	M875	M876	M877	M878	M879	M880	M881	M882	M883	M884	M885	M886	M887	M888	M889	M890	M891	M892	M893	M894	M895	M896	M897	M898	M899	M900	M901	M902	M903	M904	M905	M906	M907	M908	M909	M910	M911	M912	M913	M914	M915	M916	M917	M918	M919	M920	M921	M922	M923	M924	M925	M926	M927	M928	M929	M930	M931	M932	M933	M934	M935	M936	M937	M938	M939	M940	M941	M942	M943	M944	M945	M946	M947	M948	M949	M950	M951	M952	M953	M954	M955	M956	M957	M958	M959	M960	M961	M962	M963	M964	M965	M966	M967	M968	M969	M970	M971	M972	M973	M974	M975	M976	M977	M978	M979	M980	M981	M982	M983	M984	M985	M986	M987	M988	M989	M990	M991	M992	M993	M994	M995	M996	M997	M998	M999	M1000	M1001	M1002	M1003	M1004	M1005	M1006	M1007	M1008	M1009	M1010	M1011	M1012	M1013	M1014	M1015	M1016	M1017	M1018	M1019	M1020	M1021	M1022	M1023	M1024	M1025	M1026	M1027	M1028	M1029	M1030	M1031	M1032	M1033	M1034	M1035	M1036	M1037	M1038	M1039	M1040	M1041	M1042	M1043	M1044	M1045	M1046	M1047	M1048	M1049	M1050	M1051	M1052	M1053	M1054	M1055	M1056	M1057	M1058	M1059	M1060	M1061	M1062	M1063	M1064	M1065	M1066	M1067	M1068	M1069	M1070	M1071	M1072	M1073	M1074	M1075	M1076	M1077	M1078	M1079	M1080	M1081	M1082	M1083	M1084	M1085	M1086	M1087	M1088	M1089	M1090	M1091	M1092	M1093	M1094	M1095	M1096	M1097	M1098	M1099	M1100	M1101	M1102	M1103	M1104	M1105	M1106	M1107	M1108	M1109	M1110	M1111	M1112	M1113	M1114	M1115	M1116	M1117	M1118	M1119	M1120	M1121	M1122	M1123	M1124	M1125	M1126	M1127	M1128	M1129	M1130	M1131	M1132	M1133	M1134	M1135	M1136	M1137	M1138	M1139	M1140	M1141	M1142	M1143	M1144	M1145	M1146	M1147	M1148	M1149	M1150	M1151	M1152	M1153	M1154	M1155	M1156	M1157	M1158	M1159	M1160	M1161	M1162	M1163	M1164	M1165	M1166	M1167	M1168	M1169	M1170	M1171	M1172	M1173	M1174	M1175	M1176	M1177	M1178	M1179	M1180	M1181	M1182	M1183	M1184	M1185	M1186	M1187	M1188	M1189	M1190	M1191	M1192	M1193	M1194	M1195	M1196	M1197	M1198	M1199	M1200	M1201	M1202	M1203	M1204	M1205	M1206	M1207	M1208	M1209	M1210	M1211	M1212	M1213	M1214	M1215	M1216	M1217	M1218	M1219	M1220	M1221	M1222	M1223	M1224	M1225	M1226	M1227	M1228	M1229	M1230	M1231	M1232	M1233	M1234	M1235	M1236	M1237	M1238	M1239	M1240	M1241	M1242	M1243	M1244	M1245	M1246	M1247	M1248	M1249	M1250	M1251	M1252	M1253	M1254	M1255	M1256	M1257	M1258	M1259	M1260	M1261	M1262	M1263	M1264	M1265	M1266	M1267	M1268	M1269	M1270	M1271	M1272	M1273	M1274	M1275	M1276	M1277	M1278	M1279	M1280	M1281	M1282	M1283	M1284	M1285	M1286	M1287	M1288	M1289	M1290	M1291	M1292	M1293	M1294	M1295	M1296	M1297	M1298	M1299	M1300	M1301	M1302	M1303	M1304	M1305	M1306	M1307	M1308	M1309	M1310	M1311	M1312	M1313	M1314	M1315	M1316	M1317	M1318	M1319	M1320	M1321	M1322	M1323	M1324	M1325	M1326	M1327	M1328	M1329	M1330	M1331	M1332	M1333	M1334	M1335	M1336	M1337	M1338	M1339	M1340	M1341	M1342	M1343	M1344	M1345	M1346	M1347	M1348	M1349	M1350	M1351	M1352	M1353	M1354	M1355	M1356	M1357	M1358	M1359	M1360	M1361	M1362	M1363	M1364	M1365	M1366	M1367	M1368	M1369	M1370	M1371	M1372	M1373	M1374	M1375	M1376	M1377	M1378	M1379	M1380	M1381	M1382	M1383	M1384	M1385	M1386	M1387	M1388	M1389	M1390	M1391	M1392	M1393	M1394	M1395	M1396	M1397	M1398	M1399	M1400	M1401	M1402	M1403	M1404	M1405	M1406	M1407	M1408	M1409	M1410	M1411	M1412	M1413	M1414	M1415	M1416	M1417	M1418	M1419	M1420	M1421	M1422	M1423	M1424	M1425	M1426	M1427	M1428	M1429	M1430	M1431	M1432	M1433	M1434	M1435	M1436	M1437	M1438	M1439	M1440	M1441	M1442	M1443	M1444	M1445	M1446	M1447	M1448	M1449	M1450	M1451	M1452	M1453	M1454	M1455	M1456	M1457	M1458	M1459	M1460	M1461	M1462	M1463	M1464	M1465	M1466	M1467	M1468	M1469	M1470	M1471	M1472	M1473	M1474	M1475	M1476	M1477	M1478	M1479	M1480	M1481	M1482	M1483	M1484	M1485	M1486	M1487	M1488	M1489	M1490	M1491	M1492	M1493	M1494	M1495	M1496	M1497	M1498	M1499	M1500	M1501	M1502	M1503	M1504	M1505	M1506	M1507	M1508	M1509	M1510	M1511	M1512	M1513	M1514	M1515	M1516	M1517	M1518	M1519	M1520	M1521	M1522	M1523	M1524	M1525	M1526	M1527	M1528	M1529	M1530	M1531	M1532	M1533	M1534	M1535	M1536	M1537	M1538	M1539	M1540	M1541	M1542	M1543	M1544	M1545	M1546</
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## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	199.45Å 199.45Å 289.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.30)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.276 , 0.359	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21292	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.43	0/1775	0.77	1/2417 (0.0%)
1	B	0.42	1/1795 (0.1%)	0.77	1/2447 (0.0%)
2	C	0.41	0/8672	0.80	7/11752 (0.1%)
3	D	0.44	1/8439 (0.0%)	0.84	19/11447 (0.2%)
4	E	0.37	0/730	0.71	0/991
All	All	0.42	2/21411 (0.0%)	0.81	28/29054 (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
2	C	0	1
3	D	0	3
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1270	ALA	C-N	-12.09	1.06	1.34
1	B	94	MET	SD-CE	5.75	2.10	1.77

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1270	ALA	O-C-N	-19.05	92.23	122.70
3	D	1270	ALA	C-N-CA	13.67	155.87	121.70
3	D	1270	ALA	CA-C-N	12.08	143.77	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	580	MET	N-CA-C	6.98	129.85	111.00
3	D	1166	LEU	CA-CB-CG	6.22	129.61	115.30
3	D	508	ARG	N-CA-C	-6.00	94.79	111.00
1	A	25	LEU	N-CA-C	-5.91	95.05	111.00
3	D	954	ALA	N-CA-C	-5.87	95.16	111.00
2	C	836	GLY	N-CA-C	-5.82	98.55	113.10
3	D	137	PRO	N-CA-CB	5.80	110.26	103.30
3	D	775	GLY	N-CA-C	5.78	127.55	113.10
3	D	512	MET	N-CA-C	-5.73	95.53	111.00
3	D	834	THR	N-CA-C	-5.61	95.86	111.00
2	C	571	LEU	CA-CB-CG	5.57	128.10	115.30
1	B	26	GLU	N-CA-C	5.46	125.75	111.00
3	D	98	PRO	N-CA-CB	5.40	109.78	103.30
2	C	467	ILE	N-CA-C	5.38	125.54	111.00
3	D	29	PRO	N-CA-CB	5.33	109.69	103.30
3	D	1069	GLU	N-CA-C	-5.26	96.79	111.00
3	D	1042	ARG	N-CA-C	-5.24	96.86	111.00
2	C	329	GLY	N-CA-C	-5.23	100.02	113.10
3	D	826	PRO	N-CA-CB	5.23	109.57	103.30
3	D	146	PRO	N-CA-CB	5.17	109.50	103.30
3	D	109	PRO	N-CA-CB	5.16	109.50	103.30
2	C	379	GLU	N-CA-C	-5.14	97.13	111.00
3	D	1388	ARG	N-CA-C	5.12	124.82	111.00
2	C	655	LEU	CA-CB-CG	5.07	126.95	115.30
3	D	1018	ASN	C-N-CD	5.04	139.00	128.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	TYR	Sidechain
2	C	1013	TYR	Sidechain
3	D	1165	TYR	Sidechain
3	D	1268	PRO	Mainchain
3	D	1270	ALA	Mainchain

## 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	1741	0	1747	348	0
1	B	1761	0	1754	316	0
2	C	8508	0	8421	1817	0
3	D	8502	0	8002	1671	0
4	E	719	0	685	138	0
5	D	1	0	0	0	0
6	D	1	0	0	0	0
7	C	59	0	56	6	0
All	All	21292	0	20665	4041	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 96.

All (4041) 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:94:MET:SD	1:B:94:MET:CE	2.10	1.39
2:C:690:ILE:HB	2:C:852:ILE:HG22	1.19	1.18
3:D:1280:VAL:HG12	3:D:1281:VAL:HG23	1.25	1.16
2:C:491:GLU:HA	2:C:531:PHE:HA	1.29	1.15
3:D:772:PRO:HG3	3:D:778:LEU:HB2	1.28	1.14
2:C:861:LEU:HG	2:C:862:PRO:HD2	1.23	1.14
3:D:1280:VAL:HG13	3:D:1315:ASP:HA	1.25	1.13
2:C:613:VAL:HG21	2:C:619:ARG:HG2	1.31	1.13
3:D:129:PHE:HA	3:D:454:ALA:HB1	1.24	1.12
2:C:208:VAL:HG11	2:C:218:VAL:HG11	1.27	1.12
1:A:96:SER:HB3	1:A:145:ASP:HA	1.16	1.11
3:D:890:VAL:HG12	3:D:891:GLY:H	1.12	1.10
3:D:1101:VAL:HG21	3:D:1424:VAL:HG22	1.33	1.10
3:D:1015:TYR:HB3	3:D:1019:PRO:HD3	1.33	1.10
3:D:483:HIS:H	3:D:484:PRO:HD2	1.00	1.09
2:C:17:PRO:HD2	2:C:20:GLU:HB2	1.32	1.09
2:C:261:LEU:HG	2:C:263:ASP:HB3	1.33	1.09
2:C:262:ALA:HB1	2:C:266:ARG:HD3	1.15	1.08
2:C:129:ILE:HG21	2:C:387:SER:HB2	1.36	1.08
1:A:26:GLU:HB3	1:A:27:PRO:CD	1.81	1.08
3:D:691:LEU:HD12	3:D:691:LEU:H	1.18	1.08
2:C:12:VAL:HG12	2:C:13:ILE:H	1.17	1.07
2:C:115:LEU:HD12	2:C:116:GLY:H	1.12	1.06
3:D:876:SER:H	3:D:879:ARG:HG3	1.20	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:399:ASN:C	2:C:399:ASN:HD22	1.59	1.06
3:D:772:PRO:CG	3:D:778:LEU:HB2	1.86	1.06
2:C:376:ARG:H	2:C:377:PRO:HD2	1.20	1.05
1:A:30:ARG:HD2	1:A:191:ASP:HB3	1.37	1.05
3:D:1019:PRO:HB2	3:D:1022:VAL:HG23	1.37	1.05
2:C:873:PRO:O	2:C:877:PRO:HD2	1.56	1.05
3:D:1154:GLU:HB3	3:D:1159:ARG:HG2	1.38	1.05
2:C:333:ILE:HD11	2:C:468:ARG:HE	1.20	1.05
2:C:474:VAL:HG22	2:C:530:GLU:HA	1.37	1.04
2:C:1008:ARG:HD3	2:C:1029:GLY:H	1.19	1.04
3:D:1273:VAL:HG23	3:D:1324:PRO:HG3	1.37	1.04
3:D:886:VAL:HG11	3:D:900:ILE:HD11	1.36	1.03
2:C:253:ALA:HA	2:C:256:TYR:HB2	1.36	1.03
3:D:811:GLU:HA	3:D:814:ALA:HB3	1.34	1.03
2:C:456:ALA:HB3	2:C:459:ALA:HB2	1.34	1.02
3:D:879:ARG:NH2	3:D:904:VAL:HA	1.75	1.02
2:C:710:ILE:HD11	2:C:790:LEU:HD22	1.05	1.02
1:B:195:LEU:HD11	1:B:197:LEU:HD13	1.42	1.02
2:C:140:ILE:HG22	2:C:333:ILE:HG12	1.40	1.01
1:B:26:GLU:HG3	1:B:194:LYS:HD2	1.38	1.01
1:A:26:GLU:HB3	1:A:27:PRO:HD3	1.43	1.01
1:B:97:THR:CG2	1:B:120:VAL:HG21	1.91	1.00
3:D:521:PRO:HG2	3:D:522:PRO:HD3	1.41	1.00
1:A:158:ILE:HD11	1:A:161:ARG:HE	1.23	1.00
2:C:525:ALA:HB1	2:C:526:PRO:HD2	1.44	1.00
1:A:131:THR:HG23	2:C:644:ARG:HH21	1.24	1.00
2:C:1045:ALA:HB1	2:C:1048:THR:HB	1.40	0.99
1:B:97:THR:HG21	1:B:120:VAL:HG21	1.42	0.99
3:D:772:PRO:HD2	3:D:776:GLU:O	1.62	0.99
2:C:72:ARG:HD3	2:C:112:GLU:OE1	1.62	0.99
3:D:1236:LEU:HB2	3:D:1256:LEU:HB2	1.45	0.99
2:C:755:LEU:HD12	2:C:790:LEU:HD23	1.41	0.99
3:D:1353:GLN:HE21	3:D:1368:ILE:HD11	1.24	0.98
3:D:1141:GLU:HA	3:D:1171:VAL:HG11	1.42	0.98
3:D:1092:GLY:HA2	3:D:1096:ARG:HE	1.29	0.98
3:D:860:LEU:HA	3:D:877:PRO:HG2	1.43	0.98
1:A:143:ARG:HE	1:A:159:LYS:HE2	1.24	0.98
2:C:110:GLU:HG2	2:C:369:PRO:HG2	1.44	0.98
3:D:483:HIS:H	3:D:484:PRO:CD	1.75	0.98
3:D:699:VAL:HB	3:D:716:PHE:O	1.63	0.97
3:D:721:VAL:HG12	3:D:722:GLU:H	1.28	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1055:ILE:H	2:C:1055:ILE:HD12	1.26	0.97
2:C:384:GLU:O	2:C:388:ARG:HB2	1.65	0.97
3:D:89:ARG:C	3:D:520:LEU:HD21	1.85	0.97
1:A:96:SER:CB	1:A:145:ASP:HA	1.95	0.97
2:C:567:GLN:HB2	2:C:997:LEU:HD22	1.44	0.96
2:C:946:ARG:HE	3:D:861:GLN:HE22	1.10	0.96
3:D:836:VAL:O	3:D:865:THR:HG23	1.65	0.96
1:B:106:PRO:HA	1:B:133:GLU:HA	1.46	0.96
2:C:159:ILE:HD11	2:C:310:LEU:HB2	1.48	0.96
2:C:195:LEU:HD13	2:C:227:LEU:HD13	1.48	0.96
2:C:497:ALA:HA	2:C:502:PRO:HG3	1.47	0.96
2:C:165:LEU:HD22	2:C:334:ARG:HD3	1.48	0.95
2:C:710:ILE:HG13	2:C:790:LEU:HD13	1.46	0.95
3:D:1310:ARG:HA	3:D:1323:GLN:O	1.66	0.94
3:D:483:HIS:HA	3:D:489:ARG:HG3	1.49	0.94
2:C:438:ILE:HD13	2:C:470:PRO:HD3	1.49	0.94
2:C:1001:VAL:HG11	3:D:724:GLN:HB3	1.49	0.94
3:D:1251:ASP:H	3:D:1269:LYS:HZ2	0.99	0.93
2:C:1038:TRP:NE1	3:D:1099:VAL:HG11	1.82	0.93
3:D:639:LEU:H	3:D:729:HIS:CD2	1.83	0.93
1:B:106:PRO:HB3	1:B:133:GLU:HG3	1.51	0.93
3:D:1336:LEU:HB2	3:D:1344:VAL:HG21	1.49	0.93
3:D:899:LEU:O	3:D:900:ILE:HG13	1.66	0.93
1:B:26:GLU:HB3	1:B:27:PRO:HD3	1.48	0.93
3:D:857:LEU:HD12	3:D:858:LEU:H	1.34	0.93
3:D:1118:ILE:HD13	3:D:1190:SER:HB3	1.51	0.93
2:C:585:GLU:HG2	2:C:665:PHE:HE2	1.33	0.92
2:C:710:ILE:HD11	2:C:790:LEU:CD2	1.97	0.92
2:C:115:LEU:HD12	2:C:116:GLY:N	1.83	0.92
2:C:690:ILE:CB	2:C:852:ILE:HG22	1.99	0.92
3:D:1236:LEU:HD11	3:D:1356:TYR:HE2	1.31	0.92
1:A:30:ARG:H	1:A:30:ARG:HD3	1.35	0.92
2:C:946:ARG:HE	3:D:861:GLN:NE2	1.67	0.92
1:B:25:LEU:HD11	1:B:28:LEU:HD11	1.51	0.92
2:C:613:VAL:HG13	2:C:620:LEU:H	1.33	0.92
3:D:806:PHE:H	3:D:827:ILE:HA	1.35	0.92
2:C:198:ARG:HG2	2:C:228:ALA:HA	1.52	0.92
2:C:585:GLU:HG2	2:C:665:PHE:CE2	2.05	0.91
3:D:699:VAL:H	3:D:756:GLN:NE2	1.68	0.91
1:A:38:ASN:ND2	2:C:980:GLY:HA2	1.84	0.91
3:D:900:ILE:HG22	3:D:902:MET:H	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:HB3	1:A:41:ARG:NH1	1.85	0.91
3:D:1382:THR:HG21	3:D:1418:LYS:HE3	1.52	0.91
1:A:197:LEU:HD23	1:A:197:LEU:H	1.35	0.91
3:D:1147:ARG:NH1	3:D:1190:SER:HB2	1.86	0.91
2:C:852:ILE:N	2:C:852:ILE:HD13	1.84	0.90
3:D:860:LEU:C	3:D:862:ASP:H	1.69	0.90
2:C:605:LYS:HG2	2:C:607:ASP:H	1.33	0.90
3:D:615:ARG:HA	3:D:618:LEU:HD12	1.52	0.90
2:C:749:VAL:HG11	2:C:792:VAL:HG21	1.53	0.90
3:D:728:LEU:HD22	3:D:745:MET:HE1	1.52	0.90
2:C:31:GLN:OE1	2:C:39:ARG:HB3	1.71	0.90
2:C:203:ASP:O	2:C:206:THR:HG22	1.72	0.90
3:D:483:HIS:N	3:D:484:PRO:HD2	1.86	0.90
2:C:564:MET:SD	2:C:840:ALA:HB1	2.12	0.90
3:D:552:ASN:HA	3:D:555:LYS:HB3	1.53	0.90
3:D:1278:ASP:HA	3:D:1318:TYR:HA	1.54	0.90
3:D:643:GLY:HA3	3:D:727:GLN:H	1.37	0.90
2:C:256:TYR:HA	2:C:260:LEU:HD13	1.54	0.89
4:E:31:LEU:HD12	4:E:35:PHE:HA	1.54	0.89
3:D:901:GLN:HB2	3:D:905:PRO:HG3	1.52	0.89
1:A:88:ARG:HD3	1:A:121:GLU:OE2	1.72	0.89
3:D:1321:ALA:O	3:D:1323:GLN:N	2.05	0.89
1:A:160:ASP:O	1:A:162:ILE:HG22	1.72	0.89
1:A:15:THR:HG22	1:B:230:ALA:HB1	1.53	0.89
3:D:1253:THR:HA	3:D:1258:ARG:HD2	1.53	0.89
2:C:99:GLN:HB3	2:C:109:LYS:HG2	1.54	0.89
3:D:1008:PHE:HE1	3:D:1035:ILE:HG13	1.37	0.89
3:D:1231:GLU:HB3	3:D:1232:PRO:HD3	1.53	0.89
2:C:246:ASP:HB3	2:C:247:PRO:HD2	1.54	0.89
2:C:1103:ASP:HB2	2:C:1108:PRO:HB2	1.55	0.89
2:C:1095:LEU:HD12	3:D:603:LEU:HD23	1.55	0.89
1:B:78:ILE:HG13	1:B:130:ALA:HB2	1.52	0.89
2:C:260:LEU:O	2:C:261:LEU:HD23	1.73	0.89
2:C:159:ILE:HD13	2:C:306:THR:HG23	1.55	0.89
3:D:631:ILE:HD13	3:D:745:MET:HE2	1.55	0.88
3:D:1024:ALA:HA	3:D:1028:ALA:HB3	1.51	0.88
1:A:72:LYS:HA	2:C:607:ASP:HB3	1.55	0.88
2:C:110:GLU:CG	2:C:369:PRO:HG2	2.03	0.88
2:C:701:THR:HG22	2:C:832:LYS:HA	1.56	0.88
2:C:1017:THR:O	2:C:1018:GLN:HB2	1.71	0.88
2:C:257:LEU:HD23	2:C:261:LEU:HD21	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:699:VAL:H	3:D:756:GLN:HE22	1.19	0.88
2:C:726:ILE:HD12	2:C:726:ILE:H	1.37	0.88
2:C:631:SER:HB2	2:C:635:THR:H	1.36	0.88
2:C:605:LYS:HA	2:C:612:ALA:HB3	1.53	0.88
2:C:32:ALA:HA	2:C:71:TYR:HE1	1.38	0.87
2:C:493:ARG:HH12	3:D:1069:GLU:HA	1.36	0.87
3:D:1015:TYR:CB	3:D:1019:PRO:HD3	2.05	0.87
2:C:889:HIS:CE1	3:D:951:ILE:H	1.92	0.87
2:C:588:VAL:HG12	2:C:588:VAL:O	1.74	0.87
3:D:1043:GLY:HA2	3:D:1057:VAL:HG23	1.54	0.87
2:C:290:LEU:HD11	2:C:298:PHE:HB3	1.56	0.87
3:D:704:ARG:HH12	3:D:743:ASP:CG	1.78	0.87
2:C:551:GLU:HA	2:C:906:PHE:HE2	1.39	0.87
4:E:78:ASN:OD1	4:E:79:LEU:HG	1.73	0.87
2:C:762:LYS:HD2	2:C:786:LYS:HD2	1.56	0.87
3:D:783:ARG:O	3:D:784:ASP:HB2	1.71	0.87
2:C:1040:LEU:HD12	2:C:1045:ALA:HB3	1.57	0.87
2:C:674:VAL:HB	2:C:869:VAL:HG13	1.56	0.87
1:A:79:ILE:HD11	1:A:165:ILE:HD12	1.57	0.87
3:D:1466:VAL:O	3:D:1469:GLY:N	2.08	0.86
1:B:211:LEU:O	1:B:215:VAL:HG23	1.74	0.86
2:C:892:LEU:H	2:C:892:LEU:CD2	1.88	0.86
2:C:15:LEU:HD11	2:C:461:VAL:HG21	1.57	0.86
2:C:396:ASP:OD1	2:C:402:SER:HB3	1.75	0.86
3:D:129:PHE:HA	3:D:454:ALA:CB	2.05	0.86
3:D:1019:PRO:C	3:D:1021:TYR:H	1.77	0.86
2:C:1008:ARG:HD3	2:C:1029:GLY:N	1.91	0.86
1:A:79:ILE:HD11	1:A:165:ILE:CD1	2.05	0.86
2:C:115:LEU:CD1	2:C:116:GLY:H	1.89	0.86
3:D:1194:CYS:HB3	3:D:1373:ARG:NH2	1.90	0.86
1:A:59:GLU:HG2	1:A:137:LYS:HE3	1.56	0.86
3:D:890:VAL:HG12	3:D:891:GLY:N	1.90	0.86
2:C:1052:MET:O	2:C:1053:LEU:HD13	1.74	0.86
2:C:569:VAL:HG13	2:C:569:VAL:O	1.73	0.86
2:C:9:ILE:HG22	2:C:10:ARG:N	1.89	0.85
3:D:1043:GLY:HA3	3:D:1057:VAL:H	1.41	0.85
1:A:131:THR:HG23	2:C:644:ARG:NH2	1.91	0.85
3:D:876:SER:N	3:D:879:ARG:HG3	1.91	0.85
3:D:890:VAL:HG11	3:D:922:LEU:HD13	1.59	0.85
1:A:88:ARG:HB3	1:A:121:GLU:HB2	1.56	0.85
1:B:214:ALA:HA	1:B:217:ILE:HD12	1.55	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:959:PRO:HG2	2:C:960:GLU:H	1.41	0.85
3:D:1261:GLU:CD	3:D:1268:PRO:HB3	1.97	0.85
3:D:1132:LEU:HD13	3:D:1184:ARG:HH12	1.41	0.85
2:C:323:ASP:C	2:C:325:ILE:H	1.79	0.85
2:C:642:ARG:HG2	2:C:643:VAL:HG23	1.56	0.85
3:D:113:ALA:HB2	3:D:495:ARG:HH22	1.38	0.85
3:D:855:HIS:H	3:D:855:HIS:CD2	1.93	0.85
2:C:443:THR:HG21	2:C:454:SER:HB2	1.56	0.84
3:D:1047:LYS:HA	3:D:1053:PHE:CE1	2.12	0.84
3:D:1280:VAL:HG12	3:D:1281:VAL:CG2	2.08	0.84
2:C:613:VAL:CG2	2:C:619:ARG:HG2	2.06	0.84
2:C:162:ILE:HG13	2:C:171:TRP:CZ3	2.11	0.84
3:D:772:PRO:HG3	3:D:778:LEU:CB	2.07	0.84
2:C:12:VAL:HG12	2:C:13:ILE:N	1.90	0.84
3:D:1147:ARG:HH12	3:D:1190:SER:HB2	1.42	0.84
3:D:502:PHE:HE1	3:D:1452:ILE:HG13	1.41	0.84
1:A:143:ARG:HE	1:A:159:LYS:CE	1.90	0.84
2:C:852:ILE:H	2:C:852:ILE:HD13	1.37	0.84
2:C:882:LEU:N	2:C:882:LEU:HD23	1.91	0.84
1:B:98:THR:HG22	1:B:99:LEU:N	1.92	0.84
2:C:440:PRO:HB3	2:C:541:SER:HB3	1.58	0.84
2:C:843:HIS:CD2	2:C:884:GLN:HA	2.13	0.84
2:C:89:THR:O	2:C:91:GLN:HG3	1.78	0.84
2:C:1008:ARG:CZ	2:C:1020:PRO:HB3	2.07	0.83
2:C:324:ASP:O	2:C:326:ASP:N	2.10	0.83
2:C:278:GLU:HG3	2:C:284:GLY:H	1.43	0.83
2:C:13:ILE:HG22	2:C:15:LEU:H	1.43	0.83
1:B:86:VAL:HG23	1:B:124:ASN:ND2	1.92	0.83
3:D:879:ARG:NE	3:D:904:VAL:HG22	1.94	0.83
2:C:333:ILE:HD11	2:C:468:ARG:NE	1.92	0.83
2:C:352:ALA:HA	2:C:355:VAL:HG12	1.59	0.83
2:C:198:ARG:CG	2:C:228:ALA:HA	2.08	0.83
2:C:1107:ASN:N	2:C:1108:PRO:HD3	1.93	0.83
3:D:879:ARG:CD	3:D:904:VAL:HG22	2.07	0.83
3:D:1450:ALA:HA	3:D:1455:LYS:HG3	1.61	0.83
2:C:672:VAL:HG22	2:C:868:ASP:OD2	1.77	0.83
2:C:58:ASP:CB	2:C:61:LYS:HG3	2.09	0.83
3:D:1015:TYR:HB3	3:D:1018:ASN:HB2	1.61	0.83
3:D:908:LYS:HG3	3:D:1027:GLY:CA	2.07	0.83
4:E:38:THR:HG22	4:E:40:LEU:H	1.43	0.83
1:A:131:THR:O	1:A:131:THR:HG22	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:465:LEU:HD23	3:D:509:PRO:HB3	1.59	0.83
3:D:1011:PHE:HA	3:D:1014:ASN:O	1.76	0.83
3:D:860:LEU:C	3:D:862:ASP:N	2.32	0.83
2:C:1051:GLU:HG2	2:C:1056:LYS:HE2	1.58	0.83
3:D:590:PRO:HB3	3:D:599:PRO:HA	1.60	0.83
4:E:9:LEU:HA	4:E:12:MET:HE2	1.59	0.83
3:D:511:TRP:O	3:D:512:MET:HG3	1.79	0.83
1:A:143:ARG:NE	1:A:159:LYS:HE2	1.94	0.82
3:D:1282:ARG:CG	3:D:1293:PHE:HB2	2.10	0.82
2:C:875:GLY:HA2	2:C:879:ARG:HG3	1.61	0.82
3:D:1003:VAL:O	3:D:1007:VAL:HG12	1.79	0.82
3:D:1107:VAL:HG21	3:D:1215:VAL:HG11	1.61	0.82
3:D:900:ILE:HG22	3:D:902:MET:N	1.94	0.82
3:D:1154:GLU:HA	3:D:1159:ARG:HA	1.61	0.82
2:C:924:LEU:N	2:C:924:LEU:HD23	1.94	0.82
3:D:792:ILE:HG21	3:D:881:LEU:HD23	1.60	0.82
2:C:1012:PRO:HB3	2:C:1023:GLY:HA3	1.58	0.82
1:B:25:LEU:HD11	1:B:28:LEU:HD21	1.59	0.82
3:D:1213:ARG:HG3	3:D:1214:PRO:N	1.95	0.82
3:D:521:PRO:CG	3:D:522:PRO:HD3	2.09	0.82
1:B:103:ALA:HB3	1:B:137:LYS:O	1.80	0.82
4:E:48:MET:HG2	4:E:49:ARG:H	1.45	0.82
2:C:110:GLU:H	2:C:369:PRO:HG3	1.44	0.82
3:D:1251:ASP:H	3:D:1269:LYS:NZ	1.76	0.82
3:D:1376:LEU:HD11	3:D:1421:LEU:HD12	1.62	0.82
3:D:1250:THR:HG23	3:D:1269:LYS:HD3	1.61	0.82
2:C:564:MET:SD	2:C:846:LYS:HB3	2.20	0.82
2:C:695:LEU:HD21	2:C:833:LEU:HB3	1.60	0.82
3:D:1403:LEU:HD21	3:D:1415:VAL:H	1.44	0.82
2:C:15:LEU:HD21	2:C:461:VAL:CG2	2.09	0.81
3:D:890:VAL:HG11	3:D:922:LEU:CD1	2.08	0.81
3:D:731:LEU:HD11	3:D:931:LEU:HD12	1.61	0.81
3:D:1277:ILE:HD12	3:D:1294:VAL:HG12	1.61	0.81
2:C:32:ALA:HA	2:C:71:TYR:CE1	2.14	0.81
2:C:604:VAL:HG11	2:C:619:ARG:NH2	1.94	0.81
2:C:1030:GLN:O	3:D:622:ARG:HA	1.79	0.81
1:B:151:VAL:HG23	1:B:169:ALA:HB3	1.62	0.81
2:C:1005:MET:O	2:C:1005:MET:HG3	1.80	0.81
3:D:1096:ARG:HH11	3:D:1096:ARG:HG3	1.42	0.81
2:C:836:GLY:HA3	2:C:1001:VAL:CG2	2.10	0.81
2:C:260:LEU:HD23	2:C:261:LEU:N	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1119:SER:HB3	3:D:1185:GLU:HB3	1.62	0.81
3:D:582:ILE:O	3:D:584:ASN:N	2.14	0.81
2:C:892:LEU:H	2:C:892:LEU:HD22	1.46	0.81
2:C:376:ARG:N	2:C:377:PRO:HD2	1.95	0.81
3:D:1037:GLN:HG3	3:D:1042:ARG:HG2	1.63	0.81
3:D:1403:LEU:O	3:D:1407:LEU:HB2	1.81	0.81
2:C:467:ILE:CG2	2:C:484:VAL:HG21	2.11	0.81
2:C:589:ARG:HH21	2:C:654:LEU:HD12	1.45	0.81
1:A:10:VAL:HB	1:A:26:GLU:CG	2.11	0.81
1:A:180:GLN:HE21	2:C:934:PHE:HB3	1.45	0.81
1:B:109:VAL:O	1:B:129:ILE:HB	1.80	0.81
3:D:1459:LEU:HB3	3:D:1465:ASN:HD22	1.46	0.81
3:D:1258:ARG:CZ	3:D:1262:LEU:HD11	2.11	0.80
2:C:1053:LEU:HD12	3:D:621:LYS:HD2	1.63	0.80
3:D:882:PHE:HA	3:D:885:ILE:HD12	1.63	0.80
2:C:136:ILE:HG21	2:C:336:VAL:HG13	1.60	0.80
3:D:969:ARG:HG3	3:D:970:LYS:N	1.95	0.80
2:C:969:LEU:HD11	3:D:952:ASP:H	1.42	0.80
2:C:671:ASN:HA	2:C:993:PHE:HA	1.62	0.80
2:C:216:ASP:O	2:C:218:VAL:HG23	1.80	0.80
1:A:158:ILE:HG23	1:A:159:LYS:H	1.45	0.80
1:B:26:GLU:HB3	1:B:27:PRO:CD	2.11	0.80
1:B:41:ARG:HD3	1:B:42:ARG:N	1.96	0.80
2:C:889:HIS:HE1	3:D:951:ILE:H	1.26	0.80
3:D:968:ASP:O	3:D:970:LYS:N	2.14	0.80
3:D:795:VAL:HG13	3:D:864:VAL:CG2	2.10	0.80
2:C:613:VAL:HG12	2:C:614:ARG:N	1.96	0.80
2:C:580:MET:HB2	2:C:584:GLU:OE1	1.81	0.80
2:C:572:ILE:O	2:C:573:ARG:HB2	1.81	0.80
2:C:261:LEU:CG	2:C:263:ASP:HB3	2.12	0.80
2:C:108:ILE:HD13	2:C:368:THR:HG22	1.64	0.80
2:C:654:LEU:O	2:C:655:LEU:HB3	1.81	0.80
3:D:881:LEU:O	3:D:885:ILE:HG13	1.82	0.80
2:C:84:ARG:HA	2:C:131:GLY:HA2	1.64	0.80
3:D:1062:ARG:HG3	3:D:1062:ARG:HH11	1.45	0.80
3:D:1351:GLU:OE1	3:D:1354:LYS:HD2	1.82	0.80
2:C:1005:MET:HB2	3:D:629:SER:HB2	1.63	0.80
1:A:24:VAL:HG12	1:A:25:LEU:O	1.82	0.80
3:D:1086:LEU:HD13	3:D:1238:MET:HB2	1.63	0.80
3:D:1067:VAL:HG12	3:D:1069:GLU:HB2	1.64	0.80
3:D:890:VAL:CG1	3:D:922:LEU:HD13	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:9:ILE:HG22	2:C:10:ARG:H	1.47	0.80
3:D:772:PRO:HD3	3:D:778:LEU:H	1.47	0.79
2:C:460:ARG:NH1	2:C:464:LEU:HD21	1.97	0.79
2:C:631:SER:HB2	2:C:635:THR:N	1.96	0.79
2:C:149:THR:OG1	2:C:323:ASP:HA	1.82	0.79
3:D:886:VAL:CG1	3:D:900:ILE:HD11	2.12	0.79
2:C:147:TYR:O	2:C:322:VAL:HG13	1.83	0.79
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.63	0.79
3:D:876:SER:H	3:D:879:ARG:CG	1.95	0.79
3:D:1378:TYR:HE2	3:D:1431:THR:HB	1.45	0.79
2:C:290:LEU:HD12	2:C:291:VAL:H	1.45	0.79
2:C:921:ALA:H	2:C:924:LEU:HD21	1.47	0.79
2:C:440:PRO:HG3	2:C:454:SER:H	1.46	0.79
2:C:149:THR:HB	2:C:158:TYR:HE1	1.46	0.79
3:D:1459:LEU:CD1	3:D:1470:ARG:HH11	1.96	0.79
2:C:140:ILE:CG2	2:C:333:ILE:HG12	2.12	0.79
2:C:474:VAL:HG13	2:C:529:VAL:O	1.83	0.79
3:D:113:ALA:HB2	3:D:495:ARG:NH2	1.98	0.79
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.64	0.79
2:C:478:VAL:O	2:C:479:VAL:HG13	1.81	0.79
2:C:613:VAL:HG11	2:C:619:ARG:CG	2.12	0.79
1:A:163:ASN:O	1:A:165:ILE:HG23	1.82	0.79
3:D:721:VAL:HG12	3:D:722:GLU:N	1.98	0.79
2:C:452:ILE:HG21	7:C:1640:RFP:O11	1.82	0.79
2:C:807:ARG:O	2:C:810:ASP:HB2	1.83	0.79
2:C:839:LEU:HD12	2:C:994:ILE:CG2	2.12	0.79
3:D:1483:PHE:CZ	4:E:18:ARG:HG3	2.17	0.79
2:C:531:PHE:O	2:C:532:MET:HB2	1.82	0.79
2:C:577:PRO:HG2	2:C:580:MET:HB3	1.65	0.78
2:C:163:ILE:HG22	2:C:164:PRO:HD2	1.65	0.78
3:D:1207:TYR:HA	3:D:1213:ARG:O	1.82	0.78
3:D:728:LEU:HD22	3:D:745:MET:CE	2.13	0.78
2:C:873:PRO:HG2	2:C:874:LEU:H	1.46	0.78
2:C:862:PRO:HA	2:C:975:TYR:HE1	1.48	0.78
2:C:690:ILE:HB	2:C:852:ILE:CG2	2.08	0.78
2:C:399:ASN:C	2:C:399:ASN:ND2	2.36	0.78
1:A:222:LEU:HD12	1:B:215:VAL:HG13	1.63	0.78
3:D:1160:LEU:HD22	3:D:1164:ARG:NH1	1.98	0.78
2:C:952:LEU:HD23	2:C:966:LEU:HD11	1.65	0.78
3:D:1196:THR:HB	3:D:1199:GLY:O	1.84	0.78
2:C:225:ALA:O	2:C:229:MET:HG2	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LEU:O	1:B:174:VAL:HG21	1.83	0.78
3:D:1019:PRO:HB2	3:D:1022:VAL:CG2	2.14	0.78
2:C:401:LEU:HD21	2:C:543:ASN:HB3	1.64	0.78
2:C:666:LEU:HD11	2:C:668:LEU:HD21	1.66	0.78
3:D:765:SER:O	3:D:769:LEU:HB2	1.83	0.78
3:D:947:ILE:HG13	3:D:947:ILE:O	1.83	0.78
3:D:948:THR:O	3:D:1020:LEU:HB2	1.84	0.78
1:B:169:ALA:HB1	1:B:171:PHE:CZ	2.19	0.78
2:C:533:ASP:HB3	2:C:538:GLN:NE2	1.99	0.78
2:C:602:GLU:H	2:C:647:GLN:HA	1.49	0.78
2:C:460:ARG:HH11	2:C:464:LEU:HD21	1.48	0.78
2:C:597:ALA:HA	2:C:614:ARG:HH11	1.48	0.78
1:A:20:TYR:O	1:A:207:PRO:HG2	1.82	0.78
1:B:195:LEU:CD1	1:B:197:LEU:HD13	2.14	0.78
3:D:1280:VAL:CG1	3:D:1281:VAL:HG23	2.11	0.78
3:D:1484:THR:O	3:D:1486:VAL:HG23	1.83	0.78
3:D:905:PRO:O	3:D:906:GLN:HB2	1.84	0.77
1:A:23:PHE:CD2	1:A:211:LEU:HD22	2.19	0.77
3:D:1459:LEU:HD13	3:D:1470:ARG:HH11	1.47	0.77
1:B:47:SER:O	1:B:48:ILE:HG13	1.84	0.77
3:D:1007:VAL:HG21	3:D:1039:CYS:HB2	1.65	0.77
2:C:474:VAL:HG22	2:C:530:GLU:CA	2.14	0.77
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.19	0.77
3:D:544:TYR:O	3:D:548:ILE:HG12	1.85	0.77
3:D:1205:TYR:HD2	3:D:1215:VAL:HG21	1.49	0.77
3:D:648:MET:O	3:D:652:LEU:HD23	1.85	0.77
3:D:1290:LEU:HB2	3:D:1305:LEU:O	1.85	0.77
2:C:376:ARG:H	2:C:377:PRO:CD	1.96	0.77
2:C:551:GLU:HA	2:C:906:PHE:CE2	2.18	0.77
2:C:256:TYR:O	2:C:261:LEU:HD22	1.85	0.77
2:C:813:VAL:HG12	2:C:815:LEU:HD11	1.64	0.77
1:A:195:LEU:HD23	1:A:196:THR:H	1.49	0.77
3:D:1282:ARG:HG2	3:D:1293:PHE:HB2	1.64	0.77
2:C:460:ARG:HD2	2:C:464:LEU:HD22	1.67	0.77
2:C:475:LYS:O	2:C:477:GLY:N	2.18	0.77
2:C:966:LEU:HD11	2:C:986:PRO:HG3	1.66	0.77
2:C:944:LEU:HD21	2:C:963:LEU:HD22	1.66	0.77
2:C:333:ILE:CD1	2:C:468:ARG:HE	1.97	0.77
2:C:159:ILE:CG1	2:C:310:LEU:HD13	2.14	0.77
3:D:547:LEU:HD13	3:D:577:ALA:O	1.85	0.77
2:C:13:ILE:CG2	2:C:15:LEU:H	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:VAL:HG23	1:A:130:ALA:O	1.85	0.77
2:C:1054:THR:HB	2:C:1055:ILE:HD12	1.67	0.77
2:C:493:ARG:NH1	3:D:1069:GLU:HA	2.00	0.77
3:D:731:LEU:CD1	3:D:931:LEU:HD12	2.15	0.77
2:C:256:TYR:C	2:C:260:LEU:HB3	2.06	0.76
1:A:173:PRO:O	1:A:202:ASP:HA	1.85	0.76
2:C:257:LEU:HD22	2:C:264:PRO:HG3	1.67	0.76
2:C:274:ARG:HE	2:C:275:TYR:HE1	1.31	0.76
3:D:465:LEU:HD22	3:D:512:MET:SD	2.26	0.76
2:C:969:LEU:HD21	3:D:952:ASP:HB2	1.66	0.76
2:C:810:ASP:OD1	2:C:811:PRO:HD2	1.85	0.76
3:D:822:ALA:HA	3:D:832:ARG:HB3	1.65	0.76
3:D:855:HIS:HD2	3:D:855:HIS:H	1.30	0.76
2:C:163:ILE:HD12	2:C:163:ILE:H	1.47	0.76
2:C:890:LEU:HG	2:C:890:LEU:O	1.85	0.76
2:C:963:LEU:HD12	2:C:972:VAL:HG22	1.65	0.76
3:D:1043:GLY:CA	3:D:1057:VAL:HG23	2.15	0.76
2:C:437:ARG:HB3	3:D:1071:PHE:CE1	2.20	0.76
3:D:1376:LEU:CD1	3:D:1421:LEU:HD12	2.16	0.76
1:B:98:THR:CG2	1:B:99:LEU:N	2.48	0.76
3:D:1481:VAL:O	3:D:1482:ARG:HG3	1.85	0.76
2:C:139:GLN:CD	2:C:334:ARG:HH21	1.88	0.76
2:C:79:SER:OG	2:C:82:GLU:HB2	1.86	0.76
3:D:795:VAL:H	3:D:862:ASP:CB	1.99	0.76
3:D:1252:ILE:O	3:D:1258:ARG:HB2	1.85	0.76
3:D:767:HIS:CE1	4:E:6:ILE:HG13	2.20	0.76
2:C:398:THR:OG1	2:C:633:GLN:HG3	1.86	0.76
2:C:181:VAL:HG12	2:C:182:VAL:HG23	1.67	0.76
2:C:1016:ILE:HD12	3:D:536:ALA:HA	1.66	0.76
2:C:605:LYS:CA	2:C:612:ALA:HB3	2.16	0.76
3:D:1103:HIS:C	3:D:1105:ILE:H	1.89	0.76
3:D:1273:VAL:H	3:D:1324:PRO:HG3	1.51	0.76
3:D:1273:VAL:N	3:D:1324:PRO:HG3	2.01	0.76
3:D:1378:TYR:CD1	3:D:1422:MET:HG3	2.20	0.76
1:A:41:ARG:NE	2:C:860:HIS:NE2	2.34	0.76
2:C:348:LEU:HD12	2:C:378:LEU:HD11	1.67	0.76
1:A:215:VAL:O	1:A:219:LYS:HG3	1.85	0.76
3:D:691:LEU:H	3:D:691:LEU:CD1	1.98	0.76
3:D:1156:LEU:HD12	3:D:1177:ALA:HA	1.68	0.76
3:D:806:PHE:HA	3:D:827:ILE:O	1.86	0.76
2:C:387:SER:O	2:C:388:ARG:HG3	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:208:VAL:CG1	2:C:218:VAL:HG11	2.12	0.75
3:D:1443:THR:HG22	3:D:1447:LEU:HD22	1.67	0.75
3:D:1126:ASP:OD1	3:D:1128:VAL:HB	1.86	0.75
3:D:790:TYR:CE2	3:D:906:GLN:HB3	2.22	0.75
3:D:1235:GLN:O	3:D:1236:LEU:HD23	1.87	0.75
1:A:197:LEU:H	1:A:197:LEU:CD2	1.98	0.75
3:D:518:PRO:HB3	3:D:544:TYR:CE1	2.21	0.75
3:D:506:GLY:O	3:D:507:ASN:HB3	1.86	0.75
2:C:80:GLN:O	2:C:81:ASP:HB2	1.84	0.75
1:A:72:LYS:CA	2:C:607:ASP:HB3	2.17	0.75
2:C:1053:LEU:CD1	3:D:621:LYS:HD2	2.15	0.75
1:A:35:THR:HG21	1:B:43:ILE:HD11	1.67	0.75
1:B:199:ILE:HG23	1:B:201:THR:HG23	1.68	0.75
2:C:710:ILE:N	2:C:710:ILE:HD12	2.01	0.75
1:B:103:ALA:HB1	1:B:132:LEU:HD11	1.67	0.75
3:D:865:THR:HG22	3:D:866:THR:N	2.01	0.75
2:C:440:PRO:HD3	2:C:455:LEU:N	2.02	0.75
2:C:659:PRO:O	2:C:660:ALA:HB2	1.85	0.75
2:C:239:PHE:CE1	2:C:254:LEU:HD23	2.22	0.75
1:A:39:PRO:O	1:A:43:ILE:HG12	1.86	0.75
2:C:748:GLU:HA	2:C:799:ILE:HA	1.66	0.75
1:B:100:ILE:HG23	1:B:141:GLU:HG2	1.69	0.75
3:D:1481:VAL:CG1	4:E:21:VAL:HG21	2.17	0.75
3:D:1283:ILE:HG12	3:D:1292:VAL:HG22	1.69	0.75
3:D:626:SER:HA	3:D:652:LEU:HD11	1.68	0.75
3:D:881:LEU:HG	3:D:885:ILE:HD11	1.68	0.75
4:E:40:LEU:C	4:E:42:PRO:HD2	2.06	0.75
2:C:730:SER:HA	2:C:734:LEU:HD11	1.67	0.75
1:B:78:ILE:CG1	1:B:130:ALA:HB2	2.16	0.75
3:D:855:HIS:O	3:D:857:LEU:N	2.20	0.75
2:C:438:ILE:HD12	2:C:484:VAL:HG22	1.69	0.75
2:C:705:ILE:HD12	2:C:705:ILE:H	1.51	0.75
2:C:251:ASP:O	2:C:252:LYS:HB3	1.84	0.75
1:B:33:GLY:O	1:B:195:LEU:HD23	1.87	0.75
3:D:100:ALA:HB1	3:D:579:ASP:OD1	1.87	0.75
3:D:968:ASP:O	3:D:971:LEU:N	2.19	0.75
2:C:17:PRO:O	2:C:18:LEU:HB2	1.86	0.75
3:D:1047:LYS:HB3	3:D:1048:PRO:HD2	1.69	0.75
1:B:214:ALA:HA	1:B:217:ILE:CD1	2.17	0.75
3:D:1280:VAL:HG12	3:D:1281:VAL:N	2.02	0.74
3:D:1282:ARG:O	3:D:1283:ILE:HG13	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1069:GLU:HG3	3:D:1072:ILE:HD13	1.69	0.74
1:B:98:THR:HG23	1:B:142:VAL:O	1.87	0.74
3:D:1092:GLY:HA2	3:D:1096:ARG:NE	2.01	0.74
1:A:101:LEU:HD12	1:A:102:ARG:N	2.01	0.74
2:C:958:SER:O	2:C:962:GLN:HG3	1.85	0.74
3:D:1031:ASN:O	3:D:1035:ILE:HG12	1.88	0.74
3:D:1322:GLY:O	3:D:1323:GLN:HB2	1.86	0.74
2:C:168:ARG:NH2	2:C:266:ARG:HG2	2.03	0.74
3:D:827:ILE:O	3:D:828:VAL:HG23	1.87	0.74
2:C:106:GLY:O	2:C:107:LEU:HD23	1.86	0.74
2:C:571:LEU:HD22	2:C:670:GLN:HG3	1.70	0.74
3:D:1150:ALA:HB2	3:D:1189:ARG:HG2	1.67	0.74
2:C:260:LEU:HD23	2:C:261:LEU:HB3	1.68	0.74
3:D:1459:LEU:HB3	3:D:1465:ASN:ND2	2.01	0.74
1:B:178:ALA:HB3	1:B:198:ARG:HE	1.52	0.74
2:C:401:LEU:HD21	2:C:543:ASN:CB	2.16	0.74
3:D:752:SER:O	3:D:754:PHE:N	2.21	0.74
3:D:675:ARG:HA	3:D:678:GLU:HB2	1.69	0.74
2:C:861:LEU:CG	2:C:862:PRO:HD2	2.10	0.74
2:C:922:PHE:C	2:C:924:LEU:H	1.89	0.74
2:C:148:PHE:O	2:C:149:THR:HB	1.87	0.74
2:C:305:PRO:O	2:C:308:ARG:HB3	1.88	0.74
1:A:94:MET:CE	1:A:119:ASP:HB2	2.17	0.74
1:A:89:PHE:O	1:A:119:ASP:HB3	1.86	0.74
2:C:911:GLU:O	2:C:915:LYS:HG2	1.85	0.74
2:C:1030:GLN:HE22	3:D:628:ARG:HD3	1.52	0.74
2:C:328:LEU:O	2:C:467:ILE:HD13	1.87	0.74
2:C:290:LEU:HA	2:C:300:ASP:HA	1.68	0.74
1:B:25:LEU:HD11	1:B:28:LEU:CD1	2.16	0.74
3:D:1042:ARG:HG3	3:D:1042:ARG:O	1.87	0.74
3:D:1060:SER:O	3:D:1062:ARG:N	2.19	0.74
3:D:1364:HIS:CG	3:D:1365:ASP:H	2.06	0.74
2:C:256:TYR:O	2:C:260:LEU:HD22	1.87	0.74
3:D:795:VAL:HG23	3:D:904:VAL:HG11	1.68	0.74
2:C:710:ILE:CG1	2:C:790:LEU:HD13	2.18	0.74
2:C:34:VAL:HG11	2:C:39:ARG:HG2	1.69	0.74
3:D:1109:GLU:HG3	3:D:1110:ALA:N	2.02	0.74
3:D:639:LEU:N	3:D:729:HIS:CD2	2.56	0.74
2:C:355:VAL:HG23	2:C:372:LEU:HB3	1.69	0.73
2:C:262:ALA:HB1	2:C:266:ARG:CD	2.09	0.73
2:C:290:LEU:HD21	2:C:298:PHE:HD2	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:10:ILE:HG13	3:D:11:ALA:H	1.52	0.73
2:C:492:ASP:H	2:C:532:MET:H	1.36	0.73
3:D:1275:SER:H	3:D:1322:GLY:HA2	1.52	0.73
1:A:165:ILE:O	1:A:165:ILE:HG13	1.87	0.73
1:B:174:VAL:HG12	1:B:201:THR:HG21	1.69	0.73
2:C:755:LEU:HD12	2:C:790:LEU:CD2	2.18	0.73
3:D:519:VAL:HG12	3:D:520:LEU:H	1.50	0.73
3:D:1118:ILE:CD1	3:D:1190:SER:HB3	2.18	0.73
2:C:285:LEU:HD23	2:C:286:SER:H	1.53	0.73
2:C:613:VAL:HG11	2:C:619:ARG:HG2	1.70	0.73
2:C:291:VAL:HB	2:C:299:LYS:HG3	1.71	0.73
2:C:727:PRO:HG3	2:C:785:VAL:HG12	1.69	0.73
3:D:1045:MET:CE	3:D:1045:MET:HA	2.18	0.73
3:D:630:VAL:O	3:D:725:SER:HA	1.86	0.73
2:C:256:TYR:O	2:C:260:LEU:HB3	1.88	0.73
1:A:83:LYS:HE2	1:A:168:ASP:HB2	1.70	0.73
3:D:1281:VAL:HG12	3:D:1282:ARG:N	2.04	0.73
2:C:391:LEU:HD22	2:C:415:PRO:CD	2.17	0.73
3:D:1106:VAL:HG21	3:D:1474:ALA:HB2	1.71	0.73
2:C:285:LEU:HD11	2:C:302:VAL:HG21	1.70	0.73
1:A:184:THR:O	1:A:185:ARG:HD3	1.89	0.73
2:C:753:ASP:O	2:C:791:ARG:HA	1.89	0.73
3:D:1481:VAL:HG11	4:E:21:VAL:HG21	1.69	0.73
3:D:1338:ALA:O	3:D:1339:LYS:HB2	1.87	0.73
3:D:1314:LYS:O	3:D:1315:ASP:O	2.07	0.73
2:C:129:ILE:CG2	2:C:387:SER:HB2	2.17	0.73
2:C:629:ALA:O	2:C:630:ARG:HD3	1.88	0.73
3:D:1483:PHE:CE1	4:E:22:VAL:HG23	2.24	0.73
3:D:508:ARG:O	3:D:510:GLU:N	2.21	0.73
3:D:790:TYR:CD2	3:D:906:GLN:HB3	2.24	0.73
3:D:879:ARG:HD2	3:D:904:VAL:HG22	1.69	0.73
2:C:110:GLU:CB	2:C:369:PRO:HG2	2.19	0.73
2:C:553:ASP:OD2	2:C:843:HIS:ND1	2.20	0.73
2:C:66:LEU:HA	2:C:100:LEU:HA	1.70	0.73
2:C:552:HIS:CE1	3:D:1064:GLY:H	2.07	0.73
3:D:1145:TYR:C	3:D:1145:TYR:HD2	1.90	0.73
2:C:1094:ALA:HB1	3:D:603:LEU:HD21	1.71	0.73
3:D:578:VAL:C	3:D:580:ALA:H	1.91	0.73
2:C:363:SER:O	2:C:367:LEU:HG	1.89	0.72
2:C:267:TYR:N	2:C:267:TYR:CD2	2.56	0.72
3:D:1147:ARG:HB3	3:D:1188:VAL:CG2	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:795:GLY:O	2:C:797:GLY:N	2.21	0.72
3:D:580:ALA:O	3:D:584:ASN:HB2	1.89	0.72
2:C:676:ILE:O	2:C:677:MET:HB3	1.89	0.72
1:A:90:LEU:HB2	1:A:119:ASP:HB3	1.70	0.72
3:D:893:GLU:O	3:D:894:LYS:HB2	1.88	0.72
2:C:597:ALA:HB2	2:C:655:LEU:HD13	1.69	0.72
1:A:12:THR:HB	1:A:24:VAL:HB	1.71	0.72
3:D:879:ARG:CZ	3:D:904:VAL:HA	2.19	0.72
2:C:559:LEU:HD12	2:C:560:MET:N	2.04	0.72
2:C:277:ALA:HB1	2:C:281:LEU:HD12	1.70	0.72
2:C:775:ARG:O	2:C:780:GLU:N	2.22	0.72
2:C:801:VAL:CG2	2:C:828:ALA:HB2	2.18	0.72
1:A:142:VAL:HG22	1:A:142:VAL:O	1.89	0.72
2:C:421:GLU:HG3	2:C:423:ALA:H	1.54	0.72
3:D:1281:VAL:CG1	3:D:1282:ARG:H	2.01	0.72
3:D:865:THR:HG22	3:D:866:THR:H	1.53	0.72
2:C:399:ASN:ND2	2:C:401:LEU:N	2.38	0.72
1:A:143:ARG:O	1:A:144:VAL:HG13	1.89	0.72
3:D:1402:ALA:HB1	3:D:1415:VAL:HG11	1.72	0.72
2:C:897:LEU:HD23	2:C:899:GLN:OE1	1.89	0.72
2:C:946:ARG:NE	2:C:984:GLU:HB2	2.05	0.72
2:C:139:GLN:HE22	2:C:416:GLY:HA3	1.53	0.72
3:D:1033:GLN:HA	3:D:1036:ARG:HD3	1.72	0.72
3:D:1205:TYR:CD2	3:D:1215:VAL:HG21	2.25	0.72
1:A:41:ARG:HB3	1:A:41:ARG:HH11	1.54	0.72
1:B:55:SER:HA	1:B:166:PRO:HA	1.70	0.72
3:D:1034:GLN:O	3:D:1037:GLN:HB3	1.90	0.72
3:D:609:GLY:HA2	3:D:615:ARG:CZ	2.19	0.72
1:A:42:ARG:HH21	1:B:34:VAL:HB	1.55	0.72
1:A:90:LEU:HD12	1:A:119:ASP:HA	1.69	0.72
3:D:668:PRO:HG2	3:D:672:ALA:CB	2.19	0.72
2:C:877:PRO:HA	2:C:882:LEU:HD21	1.72	0.71
3:D:1094:LEU:HD22	3:D:1256:LEU:HD11	1.72	0.71
1:A:162:ILE:HG23	1:A:163:ASN:N	2.05	0.71
2:C:688:ILE:HG23	2:C:871:LEU:HD12	1.70	0.71
2:C:710:ILE:CD1	2:C:790:LEU:HD22	2.02	0.71
1:B:66:SER:OG	1:B:67:THR:N	2.19	0.71
2:C:469:THR:HG22	2:C:483:VAL:HA	1.72	0.71
3:D:1356:TYR:HB3	3:D:1361:VAL:HB	1.70	0.71
2:C:253:ALA:O	2:C:254:LEU:HB3	1.90	0.71
1:A:212:ASN:O	1:A:215:VAL:HG22	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:80:GLN:HE22	2:C:122:THR:HG23	1.55	0.71
3:D:756:GLN:O	3:D:760:ARG:HG2	1.90	0.71
3:D:1443:THR:CG2	3:D:1447:LEU:HD22	2.20	0.71
2:C:1012:PRO:CB	2:C:1023:GLY:HA3	2.21	0.71
2:C:775:ARG:HA	2:C:780:GLU:CB	2.20	0.71
2:C:921:ALA:N	2:C:924:LEU:HD21	2.05	0.71
2:C:940:GLU:HG2	2:C:973:VAL:HG21	1.73	0.71
2:C:262:ALA:CB	2:C:266:ARG:HD3	2.08	0.71
1:A:10:VAL:H	1:A:26:GLU:HB2	1.55	0.71
1:B:174:VAL:HA	1:B:201:THR:HG22	1.72	0.71
3:D:564:GLU:HG3	3:D:568:ARG:HE	1.55	0.71
2:C:399:ASN:HD21	2:C:401:LEU:HB3	1.56	0.71
2:C:570:PRO:HB3	2:C:659:PRO:O	1.90	0.71
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.72	0.71
2:C:523:ILE:O	2:C:525:ALA:N	2.23	0.71
2:C:525:ALA:CB	2:C:526:PRO:HD2	2.20	0.71
1:B:82:LEU:HD21	1:B:142:VAL:HG21	1.72	0.71
3:D:728:LEU:HD13	3:D:745:MET:HE3	1.73	0.71
2:C:166:PRO:HB3	2:C:417:GLY:H	1.56	0.71
3:D:705:ALA:HB3	3:D:706:PRO:CD	2.21	0.71
2:C:51:THR:OG1	2:C:348:LEU:HD23	1.91	0.71
3:D:1486:VAL:HG21	4:E:25:LYS:HZ1	1.55	0.71
3:D:899:LEU:N	3:D:899:LEU:HD13	2.06	0.71
3:D:691:LEU:HD12	3:D:691:LEU:N	1.98	0.71
2:C:910:THR:HG22	2:C:912:PRO:HD2	1.72	0.71
1:A:75:VAL:HA	1:A:78:ILE:HD12	1.71	0.71
3:D:699:VAL:CB	3:D:716:PHE:O	2.36	0.71
3:D:688:TRP:O	3:D:690:ALA:N	2.24	0.71
1:A:110:ARG:HB2	1:A:126:ASP:O	1.90	0.71
1:B:213:GLN:O	1:B:217:ILE:HG13	1.90	0.71
2:C:939:ARG:HD3	2:C:975:TYR:HE2	1.55	0.71
2:C:1066:ALA:O	2:C:1070:ILE:HD13	1.90	0.71
2:C:877:PRO:O	2:C:881:ASN:N	2.22	0.71
2:C:144:PRO:HA	2:C:162:ILE:CG2	2.21	0.71
3:D:586:ARG:O	3:D:588:GLY:N	2.23	0.71
3:D:486:ARG:HG3	3:D:487:ALA:H	1.55	0.71
2:C:467:ILE:HG21	2:C:484:VAL:HG21	1.71	0.70
2:C:630:ARG:HA	2:C:705:ILE:HD13	1.73	0.70
3:D:1311:LEU:HB2	3:D:1323:GLN:OE1	1.91	0.70
1:A:112:VAL:O	1:A:114:PHE:N	2.24	0.70
1:A:47:SER:O	1:A:48:ILE:HG13	1.88	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:460:ALA:O	3:D:463:GLU:HB3	1.90	0.70
2:C:564:MET:HG3	2:C:997:LEU:HD11	1.72	0.70
2:C:196:LEU:O	2:C:200:LEU:HG	1.91	0.70
1:B:26:GLU:CB	1:B:27:PRO:HD3	2.20	0.70
3:D:631:ILE:CD1	3:D:745:MET:HE2	2.21	0.70
3:D:571:LYS:C	3:D:573:MET:H	1.94	0.70
1:A:85:LEU:HA	1:A:124:ASN:HD21	1.55	0.70
1:A:106:PRO:O	1:A:107:LYS:HB3	1.91	0.70
3:D:645:PRO:HD2	3:D:648:MET:SD	2.30	0.70
3:D:899:LEU:HD11	3:D:921:ARG:HD2	1.73	0.70
1:A:30:ARG:HD2	1:A:191:ASP:CB	2.19	0.70
3:D:1457:ASP:CG	3:D:1459:LEU:HD23	2.11	0.70
3:D:1402:ALA:CB	3:D:1415:VAL:HG11	2.22	0.70
3:D:1281:VAL:HG12	3:D:1282:ARG:H	1.55	0.70
2:C:922:PHE:HA	2:C:925:TYR:HB3	1.73	0.70
2:C:943:VAL:HG21	2:C:973:VAL:HG13	1.73	0.70
2:C:613:VAL:HG22	2:C:620:LEU:C	2.12	0.70
2:C:801:VAL:HG21	2:C:828:ALA:HB2	1.74	0.70
3:D:1432:LYS:HG3	3:D:1433:SER:H	1.55	0.70
3:D:502:PHE:HE2	3:D:509:PRO:HG3	1.56	0.70
3:D:1273:VAL:CG2	3:D:1324:PRO:HG3	2.18	0.70
3:D:1145:TYR:C	3:D:1145:TYR:CD2	2.63	0.70
3:D:590:PRO:O	3:D:600:LEU:HD11	1.92	0.70
2:C:90:TYR:CE2	2:C:120:LEU:HB2	2.27	0.70
2:C:841:ASN:C	2:C:841:ASN:HD22	1.94	0.70
2:C:148:PHE:CZ	2:C:309:TYR:HD2	2.10	0.70
2:C:197:LEU:HD22	2:C:202:TYR:HD1	1.54	0.70
1:A:30:ARG:NH1	1:A:191:ASP:HB2	2.06	0.70
3:D:688:TRP:C	3:D:690:ALA:H	1.94	0.70
2:C:1099:VAL:HG22	3:D:10:ILE:HD12	1.73	0.70
2:C:874:LEU:HD13	3:D:787:LEU:HD22	1.73	0.70
3:D:1104:GLU:O	3:D:1104:GLU:HG2	1.91	0.70
3:D:1265:ALA:O	3:D:1266:ARG:HG3	1.91	0.70
2:C:142:ARG:HG2	2:C:147:TYR:CZ	2.26	0.70
3:D:890:VAL:CG1	3:D:891:GLY:H	1.97	0.70
3:D:890:VAL:HG13	3:D:926:LYS:HE2	1.74	0.70
2:C:565:GLN:HG3	2:C:995:MET:CE	2.21	0.70
3:D:1211:MET:CE	4:E:16:LYS:HD2	2.21	0.70
3:D:1431:THR:O	3:D:1432:LYS:HG2	1.92	0.70
1:B:25:LEU:HD11	1:B:28:LEU:CD2	2.22	0.70
1:A:66:SER:HB2	1:A:75:VAL:HG21	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:26:ARG:NE	4:E:67:GLU:OE2	2.25	0.70
2:C:291:VAL:HG11	2:C:299:LYS:HE2	1.74	0.70
2:C:674:VAL:HG22	2:C:675:ALA:N	2.07	0.70
3:D:1019:PRO:CB	3:D:1022:VAL:HG23	2.19	0.69
2:C:588:VAL:HG23	2:C:666:LEU:HB2	1.74	0.69
3:D:657:LEU:O	3:D:660:LYS:N	2.24	0.69
3:D:1403:LEU:HG	3:D:1415:VAL:HB	1.73	0.69
2:C:862:PRO:HA	2:C:975:TYR:CE1	2.27	0.69
2:C:950:LEU:O	3:D:1018:ASN:OD1	2.10	0.69
3:D:836:VAL:HG11	3:D:858:LEU:HG	1.72	0.69
2:C:177:GLU:HG2	2:C:181:VAL:H	1.55	0.69
1:B:199:ILE:HG23	1:B:201:THR:CG2	2.22	0.69
1:B:25:LEU:HD11	1:B:28:LEU:CG	2.23	0.69
2:C:498:GLN:H	2:C:502:PRO:HD3	1.56	0.69
3:D:587:ARG:HG2	3:D:588:GLY:N	2.07	0.69
2:C:391:LEU:HD22	2:C:415:PRO:HD2	1.74	0.69
2:C:536:PRO:HB3	3:D:1068:LEU:HD11	1.75	0.69
3:D:1107:VAL:HG21	3:D:1215:VAL:CG1	2.21	0.69
3:D:1202:GLN:O	3:D:1203:LYS:HB2	1.92	0.69
2:C:500:ASN:C	2:C:502:PRO:HD2	2.12	0.69
2:C:312:ALA:HB1	2:C:318:PRO:CG	2.22	0.69
2:C:666:LEU:HD11	2:C:668:LEU:CD2	2.22	0.69
1:A:206:THR:HB	1:A:209:GLU:HG3	1.75	0.69
3:D:1108:ARG:O	3:D:1109:GLU:HG2	1.92	0.69
3:D:701:LEU:HD12	3:D:715:ALA:HB2	1.75	0.69
2:C:142:ARG:HA	2:C:330:ASN:O	1.91	0.69
2:C:299:LYS:O	2:C:299:LYS:HG3	1.91	0.69
1:A:109:VAL:O	1:A:129:ILE:HB	1.93	0.69
2:C:352:ALA:O	2:C:355:VAL:HG12	1.92	0.69
3:D:1145:TYR:HD2	3:D:1146:GLY:N	1.91	0.69
3:D:552:ASN:HA	3:D:555:LYS:CB	2.22	0.69
3:D:1270:ALA:CB	3:D:1328:GLY:HA3	2.22	0.69
1:B:179:PHE:HB2	1:B:197:LEU:HD12	1.73	0.69
2:C:889:HIS:C	2:C:891:GLY:H	1.95	0.69
1:A:6:LEU:C	1:A:8:ALA:H	1.94	0.69
2:C:1052:MET:HG2	3:D:623:VAL:HG22	1.75	0.69
4:E:59:ASN:ND2	4:E:61:VAL:HG23	2.08	0.69
2:C:796:GLU:HG2	3:D:681:ARG:HH12	1.57	0.69
3:D:1144:LEU:O	3:D:1147:ARG:HG2	1.92	0.69
2:C:726:ILE:HD12	2:C:726:ILE:N	2.07	0.69
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:126:SER:HB3	2:C:135:VAL:HG13	1.73	0.69
3:D:42(U):UNK:O	3:D:43(U):UNK:O	2.10	0.69
2:C:1005:MET:HA	3:D:628:ARG:O	1.92	0.69
2:C:333:ILE:HG21	2:C:460:ARG:HH22	1.58	0.69
2:C:683:ASN:HB2	2:C:872:ASN:HB2	1.74	0.69
3:D:1251:ASP:C	3:D:1253:THR:H	1.95	0.69
2:C:323:ASP:C	2:C:325:ILE:N	2.47	0.69
1:B:59:GLU:O	1:B:60:ASP:HB2	1.93	0.69
3:D:1147:ARG:HB3	3:D:1188:VAL:HG22	1.74	0.69
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.74	0.69
2:C:42:VAL:N	2:C:46:ALA:HB2	2.08	0.69
2:C:469:THR:HB	2:C:482:GLU:O	1.93	0.69
3:D:1201:CYS:SG	3:D:1202:GLN:N	2.65	0.69
3:D:886:VAL:HG11	3:D:900:ILE:CD1	2.18	0.69
3:D:493:ARG:O	3:D:496:LEU:HB3	1.93	0.69
3:D:808:THR:N	3:D:809:PRO:HD3	2.08	0.69
4:E:50:THR:O	4:E:52:GLU:N	2.26	0.69
3:D:456:MET:HG2	3:D:457:GLY:N	2.08	0.69
1:A:72:LYS:HG3	2:C:607:ASP:OD1	1.92	0.68
2:C:613:VAL:HG21	2:C:619:ARG:CG	2.17	0.68
3:D:1104:GLU:HB2	3:D:1461:GLY:HA2	1.75	0.68
4:E:30:LEU:C	4:E:32:ARG:H	1.97	0.68
1:B:44:LEU:HG	1:B:199:ILE:HD11	1.74	0.68
3:D:115:LEU:C	3:D:117:ASP:H	1.93	0.68
3:D:1014:ASN:O	3:D:1015:TYR:CG	2.47	0.68
2:C:837:ASP:N	2:C:837:ASP:OD2	2.24	0.68
3:D:1105:ILE:HD11	3:D:1374:GLN:NE2	2.07	0.68
2:C:211:LEU:HD22	2:C:304:LEU:HD12	1.75	0.68
3:D:1160:LEU:HD22	3:D:1164:ARG:HH12	1.58	0.68
1:A:105:GLY:N	1:A:136:GLY:HA3	2.07	0.68
2:C:54:ILE:HD11	2:C:356:ARG:HB2	1.75	0.68
2:C:545:ASN:HB3	2:C:583:LEU:HD12	1.75	0.68
2:C:64:LEU:HD11	2:C:367:LEU:HD12	1.73	0.68
2:C:569:VAL:HG12	2:C:996:LYS:O	1.94	0.68
3:D:765:SER:HB2	3:D:769:LEU:HD12	1.76	0.68
2:C:1052:MET:C	2:C:1053:LEU:HD22	2.14	0.68
2:C:139:GLN:NE2	2:C:334:ARG:HH21	1.91	0.68
2:C:881:ASN:N	2:C:881:ASN:ND2	2.42	0.68
3:D:1062:ARG:HG3	3:D:1062:ARG:NH1	2.08	0.68
2:C:759:THR:HB	2:C:785:VAL:CG1	2.23	0.68
2:C:22:GLN:HE21	2:C:336:VAL:CG2	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:401:LEU:HD13	2:C:587:VAL:HG11	1.74	0.68
2:C:613:VAL:HG12	2:C:614:ARG:H	1.58	0.68
2:C:660:ALA:O	2:C:667:ALA:N	2.24	0.68
3:D:750:PRO:HG2	3:D:756:GLN:OE1	1.93	0.68
2:C:816:LYS:HD2	2:C:817:PRO:HD2	1.74	0.68
2:C:502:PRO:O	2:C:507:ARG:NH2	2.26	0.68
2:C:852:ILE:CD1	2:C:852:ILE:N	2.57	0.68
2:C:939:ARG:HD3	2:C:975:TYR:CE2	2.29	0.68
2:C:142:ARG:NE	2:C:324:ASP:HA	2.08	0.68
2:C:261:LEU:C	2:C:263:ASP:H	1.97	0.68
1:A:175:ARG:HB2	1:A:201:THR:HB	1.76	0.68
3:D:836:VAL:HG11	3:D:858:LEU:CG	2.22	0.68
3:D:859:ASP:O	3:D:860:LEU:HB3	1.94	0.68
2:C:193:LEU:HD13	2:C:193:LEU:O	1.94	0.68
2:C:313:LEU:HD13	2:C:319:GLY:O	1.94	0.68
2:C:1089:VAL:O	2:C:1093:GLN:HG3	1.94	0.68
2:C:770:GLU:O	2:C:774:LEU:HG	1.94	0.68
3:D:112:ILE:O	3:D:114:THR:N	2.26	0.68
2:C:924:LEU:O	2:C:928:LYS:HG3	1.94	0.68
2:C:54:ILE:HG12	2:C:355:VAL:HG13	1.76	0.68
2:C:836:GLY:HA3	2:C:1001:VAL:HG21	1.76	0.68
4:E:81:PRO:HG3	4:E:84:ARG:HD2	1.76	0.68
2:C:99:GLN:CB	2:C:109:LYS:HG2	2.22	0.68
1:B:147:GLY:HA3	1:B:171:PHE:CD1	2.29	0.68
2:C:1054:THR:O	2:C:1056:LYS:N	2.27	0.68
3:D:770:LEU:H	3:D:770:LEU:HD12	1.59	0.68
3:D:789:LEU:HD13	3:D:882:PHE:HE1	1.58	0.68
2:C:204:GLN:HG3	2:C:205:GLU:HG2	1.75	0.68
1:A:157:GLY:HA3	1:A:166:PRO:HB3	1.76	0.68
3:D:662:GLU:HB2	3:D:670:VAL:HG22	1.75	0.68
2:C:147:TYR:O	2:C:148:PHE:HB2	1.93	0.68
1:B:49:PRO:HB3	1:B:146:ARG:NH2	2.10	0.68
2:C:145:GLY:O	2:C:146:VAL:HG23	1.93	0.68
2:C:410:ILE:HG12	2:C:468:ARG:HH21	1.58	0.67
2:C:635:THR:O	2:C:636:ALA:HB3	1.94	0.67
3:D:721:VAL:CG1	3:D:722:GLU:H	2.06	0.67
2:C:754:ILE:CD1	2:C:791:ARG:HE	2.07	0.67
2:C:755:LEU:HD23	2:C:792:VAL:CG2	2.24	0.67
1:B:56:VAL:O	1:B:164:ALA:O	2.12	0.67
3:D:509:PRO:HA	3:D:511:TRP:NE1	2.09	0.67
3:D:1123:PHE:CE2	3:D:1184:ARG:HG2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1106:VAL:O	3:D:1108:ARG:HG3	1.94	0.67
3:D:709:HIS:HD2	3:D:711:LEU:HB2	1.59	0.67
4:E:29:GLN:N	4:E:32:ARG:HG2	2.10	0.67
2:C:285:LEU:HD11	2:C:302:VAL:CG2	2.24	0.67
2:C:729:LEU:HB2	2:C:787:ASP:OD2	1.93	0.67
3:D:631:ILE:HG21	3:D:745:MET:HE2	1.77	0.67
3:D:26:VAL:C	3:D:28:LYS:H	1.95	0.67
3:D:502:PHE:CE1	3:D:1452:ILE:HG13	2.28	0.67
3:D:126:VAL:H	3:D:456:MET:HE2	1.58	0.67
2:C:35:PRO:O	2:C:37:GLU:N	2.27	0.67
2:C:328:LEU:O	2:C:467:ILE:HG21	1.94	0.67
3:D:1033:GLN:O	3:D:1036:ARG:HG2	1.94	0.67
3:D:957:PRO:HB2	3:D:959:GLU:HG2	1.76	0.67
1:B:16:GLN:HB3	1:B:19:HIS:O	1.93	0.67
1:B:26:GLU:O	1:B:28:LEU:HG	1.95	0.67
3:D:1207:TYR:HA	3:D:1214:PRO:HA	1.76	0.67
3:D:578:VAL:O	3:D:582:ILE:HG13	1.94	0.67
3:D:1153:VAL:O	3:D:1153:VAL:HG12	1.95	0.67
2:C:903:SER:HB2	2:C:909:ALA:HB2	1.77	0.67
2:C:605:LYS:HD3	2:C:607:ASP:HA	1.76	0.67
3:D:1327:ARG:HB3	3:D:1327:ARG:NH1	2.10	0.67
3:D:639:LEU:H	3:D:729:HIS:HD2	1.38	0.67
2:C:257:LEU:O	2:C:259:GLY:N	2.28	0.67
2:C:285:LEU:CD2	2:C:286:SER:H	2.06	0.67
1:B:72:LYS:N	1:B:131:THR:O	2.27	0.67
3:D:551:ASN:O	3:D:555:LYS:HB2	1.93	0.67
2:C:674:VAL:CG2	2:C:675:ALA:N	2.57	0.67
2:C:892:LEU:HD23	2:C:893:ALA:H	1.60	0.67
1:B:202:ASP:C	1:B:204:SER:H	1.98	0.67
2:C:246:ASP:HB3	2:C:247:PRO:CD	2.25	0.67
2:C:423:ALA:HA	2:C:427:VAL:HG21	1.77	0.67
2:C:440:PRO:HD3	2:C:455:LEU:CA	2.24	0.67
2:C:579:VAL:HG21	2:C:887:GLU:HG3	1.75	0.67
2:C:159:ILE:O	2:C:173:ASP:HA	1.93	0.67
4:E:48:MET:HG2	4:E:49:ARG:N	2.10	0.67
3:D:612:GLY:O	3:D:614:PHE:N	2.27	0.67
2:C:1034:GLU:CD	3:D:1096:ARG:HH12	1.98	0.67
3:D:699:VAL:HG22	3:D:756:GLN:NE2	2.10	0.67
3:D:709:HIS:CD2	3:D:711:LEU:HB2	2.30	0.67
3:D:947:ILE:HD12	3:D:1020:LEU:HB3	1.77	0.67
2:C:164:PRO:HD3	2:C:267:TYR:CD2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:553:ARG:O	3:D:554:LEU:HD23	1.95	0.67
3:D:465:LEU:HD22	3:D:512:MET:CE	2.25	0.67
2:C:673:LEU:O	2:C:868:ASP:HB2	1.95	0.67
3:D:1125:MET:HB2	3:D:1132:LEU:HD23	1.75	0.67
4:E:82:GLU:O	4:E:85:LEU:HB3	1.95	0.67
3:D:906:GLN:OE1	3:D:906:GLN:N	2.28	0.67
2:C:640:ARG:HH11	2:C:640:ARG:HG3	1.60	0.67
3:D:1043:GLY:O	3:D:1056:PRO:HA	1.95	0.67
3:D:1103:HIS:HB2	3:D:1462:LEU:HD12	1.77	0.67
1:B:76:VAL:HB	3:D:872:ARG:HH22	1.58	0.67
3:D:891:GLY:N	3:D:926:LYS:HZ1	1.92	0.67
1:A:44:LEU:HD13	1:A:199:ILE:HG13	1.75	0.67
1:B:25:LEU:HD12	1:B:25:LEU:C	2.15	0.67
1:B:30:ARG:HA	1:B:193:ASP:OD1	1.95	0.67
1:A:180:GLN:HG3	2:C:934:PHE:CD2	2.30	0.67
3:D:557:LEU:HD11	3:D:563:PRO:HD2	1.77	0.67
3:D:795:VAL:HG13	3:D:864:VAL:HG22	1.77	0.67
2:C:605:LYS:HA	2:C:612:ALA:CB	2.24	0.67
3:D:1252:ILE:C	3:D:1254:GLN:H	1.96	0.67
4:E:29:GLN:CA	4:E:32:ARG:HG2	2.25	0.67
1:A:194:LYS:O	1:A:196:THR:HG22	1.94	0.67
1:A:197:LEU:HD23	1:A:197:LEU:N	2.08	0.67
3:D:100:ALA:CB	3:D:575:GLN:HG3	2.25	0.67
3:D:1136:LYS:O	3:D:1138:SER:N	2.28	0.67
2:C:882:LEU:CD2	2:C:882:LEU:N	2.59	0.66
3:D:760:ARG:HH12	4:E:59:ASN:HD21	1.42	0.66
3:D:705:ALA:CB	3:D:706:PRO:CD	2.73	0.66
3:D:777:PRO:HG2	3:D:912:LYS:HG3	1.76	0.66
3:D:947:ILE:HB	3:D:1020:LEU:HD22	1.76	0.66
4:E:25:LYS:HA	4:E:28:GLN:HB3	1.77	0.66
2:C:929:ARG:C	2:C:931:GLY:H	1.98	0.66
2:C:438:ILE:CD1	2:C:484:VAL:HG22	2.25	0.66
2:C:676:ILE:CG2	2:C:873:PRO:HB3	2.25	0.66
3:D:103:TRP:O	3:D:104:PHE:CB	2.43	0.66
3:D:510:GLU:O	3:D:512:MET:N	2.28	0.66
2:C:440:PRO:HG3	2:C:454:SER:N	2.10	0.66
2:C:876:VAL:HB	2:C:877:PRO:CD	2.25	0.66
3:D:764:LEU:HG	3:D:766:ALA:H	1.60	0.66
2:C:266:ARG:NE	2:C:268:ASP:HB3	2.10	0.66
2:C:323:ASP:O	2:C:325:ILE:N	2.24	0.66
1:A:62:LEU:HD13	2:C:745:ILE:HB	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:755:LEU:CD1	2:C:790:LEU:HD23	2.23	0.66
2:C:1018:GLN:HA	2:C:1018:GLN:OE1	1.95	0.66
3:D:1304:LYS:N	3:D:1304:LYS:HD3	2.10	0.66
3:D:849:ALA:O	3:D:853:VAL:HG23	1.95	0.66
2:C:148:PHE:O	2:C:149:THR:CB	2.42	0.66
1:A:195:LEU:HD23	1:A:196:THR:N	2.11	0.66
1:B:25:LEU:CD1	1:B:28:LEU:HD21	2.25	0.66
2:C:710:ILE:HG12	2:C:790:LEU:HB2	1.77	0.66
3:D:1141:GLU:HA	3:D:1171:VAL:CG1	2.22	0.66
3:D:91:ALA:O	3:D:517:VAL:HG13	1.96	0.66
3:D:108:VAL:N	3:D:511:TRP:HH2	1.94	0.66
3:D:1486:VAL:HG21	4:E:25:LYS:NZ	2.11	0.66
1:A:41:ARG:HG2	1:A:177:VAL:CG1	2.25	0.66
2:C:712:ALA:HB2	2:C:722:ILE:HD12	1.78	0.66
1:B:106:PRO:CA	1:B:133:GLU:HA	2.24	0.66
2:C:922:PHE:C	2:C:924:LEU:N	2.49	0.66
3:D:904:VAL:HG12	3:D:906:GLN:OE1	1.95	0.66
3:D:879:ARG:NH2	3:D:905:PRO:HD2	2.11	0.66
2:C:881:ASN:HD22	2:C:881:ASN:N	1.92	0.66
3:D:1236:LEU:HD11	3:D:1356:TYR:CE2	2.22	0.66
3:D:546:ARG:HH12	3:D:589:SER:HB2	1.59	0.66
3:D:1396:GLU:O	3:D:1400:VAL:HG23	1.95	0.66
2:C:862:PRO:HG3	2:C:925:TYR:OH	1.96	0.66
1:A:211:LEU:O	1:A:215:VAL:HG13	1.95	0.66
1:A:217:ILE:HG22	1:A:221:HIS:CD2	2.31	0.66
2:C:892:LEU:N	2:C:892:LEU:CD2	2.54	0.66
2:C:953:VAL:HG11	2:C:962:GLN:HB3	1.78	0.66
2:C:839:LEU:HD12	2:C:994:ILE:HG22	1.77	0.66
3:D:1142:SER:O	3:D:1365:ASP:HB2	1.95	0.66
3:D:91:ALA:HB3	3:D:518:PRO:HG2	1.76	0.66
3:D:772:PRO:HG3	3:D:778:LEU:CD2	2.26	0.66
3:D:908:LYS:HG3	3:D:1027:GLY:HA3	1.77	0.66
3:D:792:ILE:HG22	3:D:792:ILE:O	1.95	0.66
2:C:502:PRO:HB2	2:C:507:ARG:HH12	1.59	0.66
2:C:626:ARG:NE	2:C:637:PHE:HZ	1.94	0.65
4:E:40:LEU:HB3	4:E:44:GLU:O	1.96	0.65
2:C:163:ILE:HG23	2:C:265:LYS:NZ	2.11	0.65
3:D:772:PRO:HD3	3:D:778:LEU:N	2.11	0.65
2:C:336:VAL:HA	2:C:339:LEU:HD12	1.78	0.65
3:D:1112:CYS:SG	3:D:1113:GLY:N	2.69	0.65
3:D:1273:VAL:HG23	3:D:1324:PRO:CG	2.19	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ARG:HG3	1:B:30:ARG:O	1.95	0.65
2:C:958:SER:HB2	2:C:959:PRO:HD2	1.78	0.65
2:C:721:ARG:O	2:C:758:ARG:HB2	1.95	0.65
3:D:90:MET:N	3:D:520:LEU:HD21	2.10	0.65
3:D:91:ALA:HB3	3:D:518:PRO:HD2	1.78	0.65
2:C:943:VAL:O	2:C:946:ARG:N	2.28	0.65
2:C:613:VAL:CG1	2:C:620:LEU:H	2.05	0.65
2:C:648:ARG:HG2	2:C:648:ARG:HH11	1.61	0.65
3:D:1069:GLU:O	3:D:1072:ILE:N	2.28	0.65
3:D:681:ARG:O	3:D:682:ASP:HB2	1.97	0.65
2:C:1045:ALA:HB1	2:C:1048:THR:CB	2.23	0.65
1:B:150:TYR:CE1	1:B:170:ILE:HG22	2.31	0.65
2:C:410:ILE:HG12	2:C:468:ARG:NH2	2.11	0.65
2:C:576:ALA:H	2:C:662:GLU:HG2	1.62	0.65
2:C:1034:GLU:HB3	3:D:618:LEU:O	1.96	0.65
3:D:754:PHE:O	3:D:758:GLU:HG2	1.96	0.65
3:D:789:LEU:HD11	3:D:934:LEU:HD22	1.78	0.65
2:C:142:ARG:HH12	2:C:171:TRP:HH2	1.45	0.65
2:C:159:ILE:HG12	2:C:310:LEU:HD13	1.76	0.65
1:A:162:ILE:HG12	1:A:163:ASN:OD1	1.95	0.65
1:B:174:VAL:HG12	1:B:201:THR:CG2	2.26	0.65
1:B:58:ILE:HG23	1:B:140:MET:HG2	1.77	0.65
1:B:94:MET:HB2	1:B:94:MET:CE	2.27	0.65
3:D:860:LEU:HA	3:D:877:PRO:CG	2.21	0.65
2:C:1020:PRO:HD2	3:D:622:ARG:O	1.96	0.65
1:A:35:THR:HG22	1:B:218:LEU:HD13	1.77	0.65
2:C:796:GLU:HG2	3:D:681:ARG:HH22	1.62	0.65
2:C:857:ASP:O	2:C:858:MET:HB2	1.95	0.65
2:C:1008:ARG:HB2	2:C:1028:GLY:HA3	1.77	0.65
2:C:467:ILE:HG22	2:C:484:VAL:HG21	1.77	0.65
2:C:564:MET:CG	2:C:997:LEU:HD11	2.26	0.65
2:C:404:LEU:HD23	2:C:587:VAL:HG13	1.79	0.65
2:C:604:VAL:HG11	2:C:619:ARG:HH22	1.61	0.65
2:C:575:GLN:O	2:C:667:ALA:HB1	1.96	0.65
3:D:129:PHE:CA	3:D:454:ALA:HB1	2.15	0.65
1:A:213:GLN:O	1:A:216:ALA:HB3	1.97	0.65
2:C:953:VAL:CG2	2:C:966:LEU:HD13	2.27	0.65
2:C:813:VAL:CG1	2:C:815:LEU:HD11	2.26	0.65
3:D:916:TYR:C	3:D:916:TYR:CD2	2.71	0.65
3:D:1017:PHE:HA	3:D:1023:MET:SD	2.37	0.65
2:C:439:CYS:SG	2:C:440:PRO:HD2	2.37	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:631:SER:OG	2:C:635:THR:HG22	1.97	0.65
3:D:877:PRO:O	3:D:880:ILE:HB	1.95	0.65
2:C:1008:ARG:CD	2:C:1029:GLY:H	2.02	0.65
2:C:94:LEU:O	2:C:115:LEU:HB3	1.97	0.65
2:C:688:ILE:CG2	2:C:871:LEU:HD12	2.27	0.65
2:C:495:THR:HG22	2:C:496:ILE:H	1.61	0.65
2:C:813:VAL:HG12	2:C:815:LEU:CD1	2.27	0.65
2:C:910:THR:C	2:C:912:PRO:HD2	2.17	0.65
3:D:670:VAL:O	3:D:673:ALA:HB3	1.97	0.65
2:C:360:VAL:O	2:C:361:MET:C	2.35	0.65
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.79	0.65
2:C:1063:ARG:O	2:C:1066:ALA:HB3	1.97	0.64
2:C:184:MET:HB3	2:C:191:PHE:CZ	2.32	0.64
3:D:657:LEU:O	3:D:658:LEU:C	2.35	0.64
2:C:605:LYS:CG	2:C:607:ASP:H	2.10	0.64
2:C:163:ILE:HG21	2:C:169:GLY:HA3	1.79	0.64
1:A:23:PHE:HZ	1:A:207:PRO:HB2	1.63	0.64
3:D:1277:ILE:HG22	3:D:1279:GLY:H	1.62	0.64
2:C:573:ARG:HG3	2:C:573:ARG:HH11	1.62	0.64
3:D:1093:TYR:HE2	3:D:1097:LYS:NZ	1.96	0.64
3:D:1364:HIS:O	3:D:1365:ASP:HB3	1.97	0.64
3:D:1457:ASP:OD1	3:D:1459:LEU:HD23	1.96	0.64
3:D:978:TYR:C	3:D:980:MET:H	2.01	0.64
2:C:839:LEU:HD23	2:C:849:VAL:HG22	1.80	0.64
3:D:1348:LEU:O	3:D:1352:ILE:HG13	1.97	0.64
3:D:1118:ILE:HD12	3:D:1118:ILE:N	2.11	0.64
3:D:1136:LYS:HE3	3:D:1139:ASP:OD1	1.96	0.64
2:C:1019:GLN:HB3	2:C:1057:SER:OG	1.96	0.64
3:D:1093:TYR:HE2	3:D:1097:LYS:HZ2	1.45	0.64
3:D:641:GLN:HB3	3:D:719:VAL:HG21	1.79	0.64
3:D:578:VAL:HG12	3:D:582:ILE:HD11	1.79	0.64
2:C:1113:GLU:O	2:C:1115:LEU:HD23	1.98	0.64
3:D:1282:ARG:CB	3:D:1293:PHE:HB2	2.26	0.64
3:D:793:THR:HG22	3:D:879:ARG:HH22	1.61	0.64
2:C:34:VAL:CG1	2:C:38:LYS:HG3	2.27	0.64
2:C:331:ARG:O	2:C:467:ILE:HG12	1.96	0.64
3:D:764:LEU:HD23	3:D:767:HIS:NE2	2.12	0.64
2:C:151:ASP:H	2:C:157:ARG:HA	1.63	0.64
3:D:1381:VAL:HG12	3:D:1382:THR:H	1.62	0.64
2:C:589:ARG:NH2	2:C:654:LEU:HA	2.13	0.64
3:D:1037:GLN:HG3	3:D:1042:ARG:CG	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1323:GLN:N	3:D:1324:PRO:CD	2.61	0.64
3:D:996:TRP:HA	3:D:999:THR:HG22	1.78	0.64
2:C:304:LEU:N	2:C:305:PRO:CD	2.61	0.64
2:C:859:PRO:O	2:C:867:VAL:HG23	1.98	0.64
3:D:968:ASP:O	3:D:969:ARG:C	2.36	0.64
2:C:768:SER:HB2	2:C:769:PRO:HD2	1.79	0.64
2:C:12:VAL:HG21	2:C:479:VAL:HG11	1.79	0.64
3:D:1142:SER:O	3:D:1364:HIS:HD2	1.80	0.64
2:C:256:TYR:CA	2:C:260:LEU:HD13	2.28	0.64
3:D:886:VAL:HG21	3:D:914:LEU:HD11	1.79	0.64
3:D:1086:LEU:O	3:D:1089:ALA:HB3	1.98	0.64
2:C:946:ARG:HH11	2:C:946:ARG:HG2	1.63	0.64
4:E:59:ASN:HD22	4:E:62:THR:HG1	1.46	0.64
3:D:1378:TYR:CE2	3:D:1431:THR:HB	2.30	0.64
3:D:1433:SER:HB3	3:D:1464:GLU:OE2	1.98	0.64
3:D:626:SER:HB2	3:D:748:HIS:HA	1.80	0.64
4:E:59:ASN:HD21	4:E:61:VAL:HG23	1.63	0.64
3:D:1326:THR:O	3:D:1327:ARG:HB3	1.97	0.63
3:D:1484:THR:HG21	4:E:79:LEU:HB2	1.79	0.63
1:B:14:THR:CB	1:B:22:GLU:HB3	2.27	0.63
3:D:606:ILE:HD12	3:D:606:ILE:H	1.63	0.63
4:E:47:LYS:HD3	4:E:54:LEU:HD23	1.80	0.63
3:D:840:LYS:CB	3:D:846:PRO:HA	2.28	0.63
3:D:1280:VAL:HG12	3:D:1281:VAL:H	1.63	0.63
2:C:831:ARG:HH12	2:C:1002:GLU:HB2	1.63	0.63
1:B:23:PHE:HD1	1:B:211:LEU:HD22	1.63	0.63
1:B:76:VAL:HB	3:D:872:ARG:NH2	2.13	0.63
1:A:88:ARG:HB2	1:A:123:MET:SD	2.38	0.63
2:C:66:LEU:HD11	2:C:98:LEU:CB	2.27	0.63
3:D:1096:ARG:HG3	3:D:1096:ARG:NH1	2.10	0.63
3:D:723:GLY:O	3:D:724:GLN:HB2	1.98	0.63
3:D:496:LEU:HD12	3:D:500:ARG:HG2	1.81	0.63
2:C:1087:VAL:HG12	2:C:1091:GLU:OE2	1.97	0.63
3:D:965:GLU:O	3:D:968:ASP:HB2	1.97	0.63
3:D:969:ARG:HG3	3:D:970:LYS:H	1.60	0.63
1:A:115:THR:HG23	1:A:115:THR:O	1.98	0.63
3:D:1282:ARG:HB3	3:D:1293:PHE:HB2	1.80	0.63
3:D:1043:GLY:HA2	3:D:1057:VAL:CG2	2.28	0.63
3:D:769:LEU:HD22	3:D:779:ALA:HB2	1.80	0.63
3:D:788:GLY:O	3:D:792:ILE:HD13	1.97	0.63
2:C:303:PHE:H	2:C:305:PRO:HD2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:580:ALA:HB2	3:D:587:ARG:HH22	1.63	0.63
2:C:129:ILE:CD1	2:C:386:PHE:HB3	2.29	0.63
2:C:38:LYS:O	2:C:39:ARG:HB2	1.98	0.63
2:C:408:ARG:NH2	2:C:456:ALA:O	2.28	0.63
2:C:580:MET:HB2	2:C:584:GLU:CD	2.19	0.63
2:C:602:GLU:O	2:C:603:VAL:HG13	1.99	0.63
2:C:66:LEU:CA	2:C:100:LEU:HA	2.28	0.63
3:D:1103:HIS:C	3:D:1105:ILE:N	2.50	0.63
2:C:475:LYS:C	2:C:477:GLY:H	2.02	0.63
2:C:1089:VAL:HG13	2:C:1099:VAL:HB	1.80	0.63
3:D:976:GLN:C	3:D:978:TYR:H	2.02	0.63
3:D:880:ILE:O	3:D:883:ALA:HB3	1.98	0.63
2:C:401:LEU:O	2:C:404:LEU:HB3	1.99	0.63
2:C:588:VAL:CG1	2:C:588:VAL:O	2.46	0.63
2:C:874:LEU:O	2:C:876:VAL:HG23	1.98	0.63
3:D:643:GLY:HA2	3:D:721:VAL:HG21	1.80	0.63
2:C:202:TYR:CE1	2:C:304:LEU:HB3	2.32	0.63
3:D:89:ARG:O	3:D:520:LEU:HD11	1.97	0.63
1:A:131:THR:CG2	2:C:644:ARG:HE	2.12	0.63
3:D:1403:LEU:HD12	3:D:1417:TRP:HZ3	1.64	0.63
3:D:972:ARG:O	3:D:976:GLN:HB2	1.99	0.63
2:C:87:ASP:OD2	2:C:824:ARG:NH2	2.31	0.63
2:C:685:GLU:OE1	2:C:685:GLU:HA	1.99	0.63
1:B:174:VAL:HA	1:B:201:THR:CB	2.28	0.63
3:D:1139:ASP:O	3:D:1143:GLY:N	2.32	0.63
3:D:1304:LYS:H	3:D:1304:LYS:HD3	1.61	0.63
1:B:87:VAL:HG12	1:B:88:ARG:N	2.14	0.63
1:B:90:LEU:HB2	1:B:119:ASP:HA	1.80	0.63
2:C:492:ASP:O	2:C:532:MET:HA	1.98	0.63
2:C:26:TYR:O	2:C:30:LEU:N	2.29	0.63
1:A:46:SER:OG	2:C:856:GLU:HG2	1.98	0.63
3:D:1154:GLU:O	3:D:1155:ALA:HB2	1.98	0.63
3:D:679:ARG:O	3:D:681:ARG:N	2.32	0.63
3:D:519:VAL:HG12	3:D:520:LEU:N	2.13	0.63
4:E:14:ASP:CG	4:E:15:SER:N	2.51	0.63
3:D:456:MET:HG2	3:D:457:GLY:H	1.64	0.63
3:D:35(U):UNK:O	3:D:36(U):UNK:CB	2.47	0.63
3:D:908:LYS:HD3	3:D:909:ASN:HB2	1.81	0.63
3:D:1236:LEU:HD12	3:D:1256:LEU:HD13	1.81	0.63
3:D:1324:PRO:HG2	3:D:1325:LEU:N	2.14	0.63
2:C:202:TYR:HB3	2:C:207:LEU:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:257:LEU:CD2	2:C:264:PRO:HG3	2.29	0.63
2:C:268:ASP:O	2:C:270:GLY:N	2.31	0.63
2:C:816:LYS:HD2	2:C:817:PRO:CD	2.28	0.63
3:D:678:GLU:C	3:D:680:GLN:H	2.02	0.63
1:A:86:VAL:HG12	1:A:124:ASN:CG	2.18	0.63
2:C:110:GLU:HB2	2:C:369:PRO:HG2	1.80	0.62
1:A:217:ILE:HG22	1:A:221:HIS:NE2	2.14	0.62
2:C:787:ASP:O	2:C:787:ASP:OD1	2.17	0.62
1:B:98:THR:CG2	1:B:99:LEU:H	2.12	0.62
1:B:115:THR:O	1:B:117:SER:N	2.32	0.62
2:C:66:LEU:HD11	2:C:98:LEU:HB3	1.80	0.62
2:C:676:ILE:O	2:C:677:MET:CB	2.47	0.62
2:C:722:ILE:HA	2:C:758:ARG:CB	2.29	0.62
2:C:1107:ASN:N	2:C:1108:PRO:CD	2.62	0.62
3:D:502:PHE:CE2	3:D:509:PRO:HG3	2.33	0.62
2:C:1034:GLU:HA	2:C:1037:VAL:HG23	1.81	0.62
2:C:603:VAL:HG21	2:C:646:GLY:H	1.65	0.62
3:D:767:HIS:HE1	4:E:2:ALA:HB1	1.64	0.62
2:C:1012:PRO:HB3	2:C:1023:GLY:CA	2.29	0.62
3:D:1083:ASP:O	3:D:1086:LEU:HB2	1.99	0.62
3:D:770:LEU:CD1	3:D:770:LEU:H	2.11	0.62
2:C:208:VAL:HG12	2:C:209:ARG:HG3	1.80	0.62
2:C:324:ASP:C	2:C:326:ASP:H	2.02	0.62
3:D:554:LEU:O	3:D:558:LEU:HD12	1.99	0.62
2:C:1001:VAL:O	2:C:1004:LYS:N	2.27	0.62
2:C:100:LEU:HD11	2:C:369:PRO:HD3	1.81	0.62
1:A:28:LEU:HD12	1:A:195:LEU:HB2	1.81	0.62
3:D:688:TRP:HA	3:D:688:TRP:CE3	2.34	0.62
1:A:173:PRO:O	1:A:203:GLY:N	2.31	0.62
2:C:911:GLU:HA	2:C:914:ILE:HD12	1.81	0.62
3:D:1291:SER:HA	3:D:1303:TYR:O	1.99	0.62
2:C:946:ARG:NE	3:D:861:GLN:HE22	1.89	0.62
2:C:595:LEU:HD21	2:C:623:HIS:HB3	1.82	0.62
2:C:1038:TRP:CD1	3:D:1099:VAL:HG11	2.34	0.62
3:D:1462:LEU:HD23	3:D:1473:PRO:HG2	1.80	0.62
1:B:76:VAL:O	1:B:80:LEU:HG	1.98	0.62
3:D:558:LEU:CD2	3:D:567:ILE:HG13	2.30	0.62
3:D:1019:PRO:C	3:D:1021:TYR:N	2.48	0.62
3:D:795:VAL:HG12	3:D:796:ARG:N	2.15	0.62
3:D:793:THR:CG2	3:D:879:ARG:HH22	2.12	0.62
3:D:639:LEU:HD23	3:D:729:HIS:CD2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:VAL:HA	1:B:201:THR:CG2	2.29	0.62
1:B:53:VAL:HG11	1:B:82:LEU:HG	1.82	0.62
2:C:502:PRO:HB2	2:C:507:ARG:NH1	2.14	0.62
3:D:3(U):UNK:O	3:D:39(U):UNK:O	2.16	0.62
2:C:635:THR:HG22	2:C:636:ALA:N	2.14	0.62
2:C:565:GLN:HG3	2:C:995:MET:HE1	1.81	0.62
3:D:1075:HIS:O	3:D:1077:ALA:N	2.32	0.62
3:D:1266:ARG:O	3:D:1268:PRO:HD3	2.00	0.62
2:C:1052:MET:HE1	3:D:748:HIS:HB3	1.82	0.62
3:D:903:ASP:OD1	3:D:903:ASP:O	2.18	0.62
3:D:637:LEU:O	3:D:638:LYS:O	2.17	0.62
2:C:168:ARG:HH21	2:C:266:ARG:HG2	1.64	0.62
1:B:80:LEU:O	1:B:83:LYS:HB2	2.00	0.62
3:D:952:ASP:C	3:D:954:ALA:H	2.03	0.62
1:B:49:PRO:HD2	1:B:213:GLN:NE2	2.15	0.62
3:D:658:LEU:HA	3:D:661:MET:HE2	1.81	0.62
3:D:793:THR:CG2	3:D:879:ARG:HH12	2.13	0.62
3:D:863:THR:N	3:D:876:SER:OG	2.33	0.62
2:C:379:GLU:O	2:C:380:ALA:HB3	1.99	0.62
2:C:629:ALA:C	2:C:630:ARG:HD3	2.21	0.62
3:D:1059:SER:O	3:D:1061:PHE:N	2.33	0.62
3:D:1394:VAL:HG12	3:D:1395:LEU:N	2.15	0.62
3:D:1403:LEU:CD2	3:D:1415:VAL:H	2.11	0.62
3:D:1304:LYS:O	3:D:1304:LYS:HG2	2.00	0.62
2:C:1113:GLU:C	2:C:1115:LEU:H	2.02	0.62
2:C:22:GLN:O	2:C:24:GLU:N	2.32	0.61
2:C:22:GLN:HE21	2:C:336:VAL:HG21	1.64	0.61
2:C:559:LEU:HD12	2:C:559:LEU:C	2.21	0.61
3:D:1263:PHE:CE2	3:D:1352:ILE:HD13	2.35	0.61
3:D:757:ALA:HB2	4:E:61:VAL:CG1	2.30	0.61
1:A:224:TYR:CD1	1:B:9:PRO:HD2	2.35	0.61
1:A:110:ARG:HD3	1:A:113:ASP:OD2	2.00	0.61
3:D:10:ILE:HG21	3:D:1450:ALA:HB1	1.82	0.61
2:C:946:ARG:NE	3:D:861:GLN:NE2	2.43	0.61
2:C:438:ILE:HG23	2:C:470:PRO:HB3	1.81	0.61
2:C:613:VAL:CG1	2:C:614:ARG:N	2.64	0.61
3:D:1262:LEU:HD21	3:D:1351:GLU:HG3	1.81	0.61
3:D:1264:GLU:HG2	3:D:1266:ARG:NH2	2.15	0.61
2:C:159:ILE:HG21	2:C:306:THR:CG2	2.30	0.61
1:A:15:THR:OG1	1:A:16:GLN:N	2.32	0.61
1:A:35:THR:HG21	1:B:43:ILE:CD1	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:14:PRO:O	2:C:15:LEU:HB3	1.99	0.61
3:D:1103:HIS:O	3:D:1104:GLU:HB3	2.01	0.61
3:D:1270:ALA:HB3	3:D:1328:GLY:HA3	1.82	0.61
3:D:1333:HIS:CE1	3:D:1421:LEU:HB3	2.35	0.61
3:D:770:LEU:HD12	3:D:770:LEU:N	2.15	0.61
3:D:891:GLY:N	3:D:926:LYS:NZ	2.47	0.61
3:D:921:ARG:O	3:D:922:LEU:HD23	2.00	0.61
1:B:188:GLN:CG	3:D:688:TRP:HD1	2.13	0.61
3:D:518:PRO:CB	3:D:544:TYR:CE1	2.82	0.61
2:C:686:ASP:OD2	3:D:739:ASP:OD2	2.18	0.61
2:C:614:ARG:O	2:C:616:GLU:N	2.30	0.61
3:D:699:VAL:HG12	3:D:717:GLN:CG	2.30	0.61
3:D:638:LYS:HA	3:D:729:HIS:CG	2.35	0.61
1:A:142:VAL:O	1:A:143:ARG:O	2.18	0.61
1:A:86:VAL:HG21	1:A:203:GLY:C	2.20	0.61
3:D:1045:MET:HE2	3:D:1045:MET:HA	1.82	0.61
3:D:633:VAL:HG22	3:D:634:GLY:N	2.15	0.61
2:C:348:LEU:CD1	2:C:378:LEU:HD11	2.30	0.61
2:C:605:LYS:HA	2:C:612:ALA:H	1.65	0.61
2:C:588:VAL:CG2	2:C:666:LEU:HB2	2.29	0.61
3:D:1036:ARG:O	3:D:1040:GLY:O	2.18	0.61
3:D:1150:ALA:HB2	3:D:1189:ARG:CG	2.29	0.61
2:C:184:MET:HB3	2:C:191:PHE:CE1	2.36	0.61
2:C:729:LEU:O	2:C:731:GLU:N	2.33	0.61
1:A:169:ALA:O	1:A:170:ILE:HD13	2.01	0.61
1:A:31:GLY:H	1:A:193:ASP:CG	2.03	0.61
2:C:342:ASP:O	2:C:345:ARG:HB2	2.01	0.61
2:C:466:PHE:CE1	2:C:467:ILE:HD12	2.35	0.61
2:C:1005:MET:HB2	3:D:629:SER:CB	2.29	0.61
3:D:760:ARG:NH1	4:E:59:ASN:HD21	1.98	0.61
3:D:792:ILE:N	3:D:792:ILE:HD12	2.16	0.61
1:A:10:VAL:HB	1:A:26:GLU:HG3	1.82	0.61
1:B:125:PRO:HG2	1:B:126:ASP:H	1.65	0.61
2:C:9:ILE:CG2	2:C:10:ARG:N	2.61	0.61
2:C:491:GLU:O	2:C:509:ALA:HB1	2.01	0.61
3:D:607:LEU:O	3:D:608:SER:HB2	2.00	0.61
2:C:1101:THR:O	2:C:1110:ASP:N	2.33	0.61
3:D:1372:VAL:HG22	3:D:1375:MET:HE3	1.80	0.61
3:D:1278:ASP:HA	3:D:1317:ASP:O	2.01	0.61
3:D:1017:PHE:HA	3:D:1023:MET:HE1	1.81	0.61
3:D:509:PRO:HA	3:D:511:TRP:HE1	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:590:PRO:HA	3:D:600:LEU:HG	1.82	0.61
2:C:1067:TYR:O	2:C:1067:TYR:CG	2.54	0.61
3:D:985:ASP:O	3:D:988:ARG:HB3	2.00	0.61
3:D:1379:VAL:O	3:D:1393:GLN:HA	2.01	0.61
2:C:482:GLU:HA	2:C:486:MET:CE	2.31	0.61
2:C:552:HIS:CE1	3:D:1064:GLY:N	2.69	0.61
2:C:327:HIS:C	2:C:329:GLY:H	2.03	0.61
1:B:26:GLU:HG3	1:B:194:LYS:CD	2.22	0.61
1:A:180:GLN:HE21	2:C:934:PHE:CB	2.12	0.61
3:D:545:ARG:HG3	3:D:546:ARG:N	2.15	0.61
1:A:175:ARG:O	1:A:176:ARG:HB2	2.01	0.61
2:C:963:LEU:CD1	2:C:972:VAL:HG22	2.30	0.60
3:D:857:LEU:O	3:D:858:LEU:C	2.39	0.60
2:C:569:VAL:O	2:C:569:VAL:CG1	2.44	0.60
3:D:1356:TYR:HD1	3:D:1363:LEU:HD21	1.65	0.60
2:C:8:ARG:HH11	2:C:495:THR:HG23	1.65	0.60
3:D:1485:GLN:CB	4:E:22:VAL:HG22	2.31	0.60
3:D:916:TYR:HD2	3:D:917:GLN:N	1.99	0.60
1:B:175:ARG:O	1:B:176:ARG:HB2	2.01	0.60
3:D:1192:LEU:HD13	3:D:1345:GLU:OE1	2.01	0.60
2:C:491:GLU:HG3	2:C:510:THR:HB	1.81	0.60
2:C:589:ARG:NH1	2:C:596:TYR:HB3	2.16	0.60
2:C:598:GLU:OE2	2:C:614:ARG:NH2	2.33	0.60
3:D:1324:PRO:HG2	3:D:1325:LEU:H	1.67	0.60
3:D:638:LYS:C	3:D:639:LEU:O	2.38	0.60
3:D:747:VAL:O	3:D:747:VAL:HG22	2.01	0.60
2:C:475:LYS:CB	2:C:527:GLU:H	2.14	0.60
1:B:86:VAL:HG23	1:B:124:ASN:CG	2.22	0.60
1:B:143:ARG:HD2	1:B:159:LYS:CG	2.31	0.60
2:C:1055:ILE:H	2:C:1055:ILE:CD1	2.02	0.60
2:C:342:ASP:O	2:C:346:VAL:HG23	2.01	0.60
2:C:588:VAL:HG11	2:C:661:SER:HB3	1.81	0.60
3:D:948:THR:H	3:D:1020:LEU:HD13	1.66	0.60
1:B:42:ARG:HG3	1:B:42:ARG:HH11	1.65	0.60
2:C:729:LEU:HB3	2:C:734:LEU:HD21	1.83	0.60
2:C:165:LEU:HD13	2:C:342:ASP:OD2	2.01	0.60
3:D:1003:VAL:O	3:D:1006:ALA:HB3	2.02	0.60
3:D:1272:ALA:CB	3:D:1325:LEU:HA	2.31	0.60
3:D:1364:HIS:CD2	3:D:1365:ASP:H	2.19	0.60
4:E:29:GLN:HA	4:E:32:ARG:HG2	1.84	0.60
3:D:566:ILE:C	3:D:570:GLU:HG3	2.21	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:100:ALA:HB2	3:D:575:GLN:HG3	1.83	0.60
1:B:148:VAL:HG23	1:B:149:GLY:N	2.16	0.60
3:D:1346:ARG:HH12	3:D:1349:VAL:HG11	1.66	0.60
2:C:875:GLY:HA3	2:C:879:ARG:HD2	1.84	0.60
3:D:1236:LEU:CB	3:D:1256:LEU:HB2	2.27	0.60
3:D:609:GLY:HA2	3:D:615:ARG:NH2	2.15	0.60
3:D:10:ILE:HG13	3:D:11:ALA:N	2.17	0.60
2:C:317:VAL:H	2:C:318:PRO:HD2	1.66	0.60
1:B:51:THR:HG21	1:B:87:VAL:O	2.01	0.60
2:C:706:GLU:HG3	2:C:707:ARG:N	2.15	0.60
2:C:110:GLU:HB2	2:C:369:PRO:CG	2.32	0.60
2:C:391:LEU:HD22	2:C:415:PRO:HD3	1.82	0.60
2:C:636:ALA:HB2	2:C:705:ILE:HD11	1.82	0.60
3:D:932:ASP:O	3:D:933:ALA:C	2.40	0.60
1:A:30:ARG:HH11	1:A:191:ASP:HB2	1.66	0.60
2:C:519:GLY:C	2:C:521:PRO:HD3	2.22	0.60
3:D:465:LEU:HD22	3:D:512:MET:HE1	1.83	0.60
2:C:1033:GLY:O	2:C:1035:MET:N	2.35	0.60
2:C:440:PRO:CG	2:C:454:SER:H	2.15	0.60
2:C:460:ARG:HD2	2:C:464:LEU:CD2	2.30	0.60
3:D:1194:CYS:SG	3:D:1201:CYS:HB2	2.41	0.60
4:E:30:LEU:O	4:E:32:ARG:N	2.31	0.60
2:C:152:PRO:HD2	2:C:158:TYR:CE2	2.35	0.60
2:C:184:MET:HE1	2:C:303:PHE:CZ	2.37	0.60
1:A:16:GLN:HG3	1:A:20:TYR:HB2	1.83	0.60
2:C:730:SER:O	2:C:731:GLU:C	2.40	0.60
3:D:88:TYR:O	3:D:520:LEU:HD13	2.01	0.60
3:D:566:ILE:O	3:D:566:ILE:HG22	2.01	0.60
3:D:969:ARG:CG	3:D:970:LYS:N	2.62	0.60
2:C:572:ILE:O	2:C:573:ARG:CB	2.49	0.60
1:A:41:ARG:HH11	1:A:41:ARG:C	2.04	0.60
2:C:743:VAL:HG11	2:C:800:VAL:HG21	1.83	0.60
3:D:91:ALA:HB3	3:D:518:PRO:CG	2.31	0.60
4:E:14:ASP:CG	4:E:15:SER:H	2.05	0.60
3:D:901:GLN:CB	3:D:905:PRO:HG3	2.28	0.60
2:C:1054:THR:CB	2:C:1055:ILE:HD12	2.32	0.60
2:C:613:VAL:HG11	2:C:619:ARG:HA	1.83	0.60
2:C:253:ALA:CA	2:C:256:TYR:HB2	2.22	0.60
1:A:44:LEU:O	1:A:174:VAL:HG21	2.01	0.60
2:C:712:ALA:HB1	2:C:720:GLU:O	2.02	0.60
3:D:587:ARG:HG2	3:D:588:GLY:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:969:ARG:CG	3:D:970:LYS:H	2.14	0.60
2:C:815:LEU:N	2:C:815:LEU:HD12	2.16	0.60
3:D:1219:GLU:O	3:D:1221:VAL:N	2.33	0.60
3:D:637:LEU:CB	3:D:641:GLN:HG3	2.32	0.60
2:C:261:LEU:O	2:C:263:ASP:N	2.35	0.60
2:C:759:THR:HB	2:C:785:VAL:HG13	1.83	0.60
2:C:423:ALA:HA	2:C:427:VAL:CG2	2.32	0.60
2:C:77:PRO:HD3	2:C:92:ALA:HA	1.83	0.60
3:D:1192:LEU:HD13	3:D:1345:GLU:HB3	1.83	0.60
3:D:854:ALA:O	3:D:855:HIS:C	2.41	0.59
1:A:158:ILE:HD11	1:A:161:ARG:NE	2.06	0.59
2:C:721:ARG:C	2:C:758:ARG:HB2	2.22	0.59
3:D:1382:THR:HG21	3:D:1418:LYS:CE	2.29	0.59
2:C:8:ARG:NH1	2:C:495:THR:HG23	2.17	0.59
2:C:80:GLN:NE2	2:C:122:THR:HG23	2.17	0.59
2:C:1054:THR:CG2	2:C:1055:ILE:HD12	2.32	0.59
3:D:638:LYS:HA	3:D:729:HIS:CD2	2.37	0.59
3:D:1435:LEU:HD21	3:D:1468:LEU:HD21	1.85	0.59
3:D:1435:LEU:O	3:D:1438:ALA:HB3	2.02	0.59
2:C:1085:PHE:CE1	3:D:1468:LEU:HD13	2.36	0.59
3:D:1275:SER:H	3:D:1322:GLY:CA	2.14	0.59
2:C:149:THR:HG23	2:C:150:PRO:HD2	1.84	0.59
1:A:30:ARG:CD	1:A:191:ASP:HB3	2.23	0.59
1:B:37:GLY:HA3	1:B:195:LEU:HD21	1.82	0.59
3:D:21:TRP:O	3:D:23:TYR:N	2.35	0.59
1:A:57:TYR:CD2	1:A:57:TYR:C	2.74	0.59
3:D:860:LEU:O	3:D:862:ASP:N	2.34	0.59
2:C:89:THR:HG23	2:C:129:ILE:HA	1.84	0.59
2:C:31:GLN:O	2:C:33:ASP:N	2.36	0.59
3:D:767:HIS:CE1	4:E:2:ALA:HB1	2.38	0.59
1:A:100:ILE:HG22	1:A:101:LEU:N	2.17	0.59
2:C:850:ALA:HA	3:D:632:VAL:HG11	1.84	0.59
3:D:24(U):UNK:O	3:D:25(U):UNK:CB	2.50	0.59
3:D:1014:ASN:O	3:D:1015:TYR:CD2	2.54	0.59
2:C:369:PRO:O	2:C:370:ALA:HB3	2.02	0.59
2:C:539:VAL:HG12	2:C:539:VAL:O	2.02	0.59
4:E:68:LEU:CD1	4:E:73:LEU:HD12	2.32	0.59
1:A:162:ILE:HG23	1:A:163:ASN:H	1.67	0.59
3:D:612:GLY:C	3:D:614:PHE:H	2.05	0.59
2:C:981:GLU:HB3	2:C:982:PRO:HD2	1.85	0.59
3:D:466:LYS:O	3:D:468:LEU:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:861:LEU:HG	2:C:862:PRO:CD	2.16	0.59
2:C:679:PHE:O	2:C:681:GLY:N	2.35	0.59
3:D:1222:GLY:O	3:D:1225:ALA:HB3	2.02	0.59
3:D:1364:HIS:CG	3:D:1365:ASP:N	2.69	0.59
3:D:701:LEU:HD12	3:D:715:ALA:CB	2.33	0.59
2:C:9:ILE:N	2:C:9:ILE:HD12	2.18	0.59
3:D:964:LEU:O	3:D:966:GLU:N	2.33	0.59
3:D:1017:PHE:HA	3:D:1023:MET:CE	2.33	0.59
3:D:850:LEU:HA	3:D:853:VAL:HB	1.85	0.59
2:C:1034:GLU:HA	2:C:1037:VAL:CG2	2.33	0.59
2:C:480:THR:HG23	2:C:480:THR:O	2.03	0.59
2:C:564:MET:SD	2:C:840:ALA:CB	2.87	0.59
2:C:577:PRO:HA	2:C:671:ASN:HD22	1.67	0.59
3:D:1107:VAL:HG13	3:D:1202:GLN:HA	1.84	0.59
3:D:1109:GLU:HG3	3:D:1110:ALA:H	1.67	0.59
3:D:719:VAL:O	3:D:721:VAL:HG23	2.02	0.59
2:C:527:GLU:O	2:C:528:GLU:C	2.41	0.59
1:B:79:ILE:HG23	1:B:167:VAL:HG12	1.85	0.59
3:D:518:PRO:HB3	3:D:544:TYR:CZ	2.38	0.59
2:C:769:PRO:O	2:C:771:GLU:N	2.34	0.59
3:D:978:TYR:CG	3:D:988:ARG:HD2	2.37	0.59
2:C:950:LEU:HB3	3:D:1018:ASN:OD1	2.03	0.59
3:D:795:VAL:HG21	3:D:904:VAL:HG21	1.85	0.59
2:C:367:LEU:HD13	2:C:372:LEU:HD21	1.85	0.59
2:C:439:CYS:HB2	2:C:468:ARG:NH1	2.17	0.59
2:C:882:LEU:HD11	2:C:884:GLN:HE21	1.67	0.59
3:D:1431:THR:C	3:D:1432:LYS:HG2	2.23	0.59
1:B:223:ASN:O	1:B:225:PHE:N	2.36	0.59
1:B:42:ARG:HG3	1:B:42:ARG:NH1	2.18	0.59
2:C:11:GLU:OE1	2:C:473:ARG:HG3	2.03	0.59
1:B:214:ALA:HA	1:B:217:ILE:CG1	2.32	0.59
2:C:972:VAL:O	2:C:974:LEU:N	2.35	0.59
3:D:927:THR:HG22	3:D:931:LEU:HD23	1.84	0.59
1:B:199:ILE:O	1:B:199:ILE:HG22	2.03	0.59
3:D:590:PRO:CB	3:D:599:PRO:HA	2.33	0.59
3:D:961:GLN:O	3:D:962:ARG:C	2.40	0.59
3:D:916:TYR:C	3:D:918:ALA:H	2.05	0.59
3:D:7(U):UNK:O	3:D:35(U):UNK:N	2.36	0.59
2:C:1021:LEU:HG	3:D:622:ARG:HD2	1.84	0.59
2:C:368:THR:HB	2:C:369:PRO:HD2	1.85	0.59
2:C:461:VAL:O	2:C:462:ASP:CB	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:467:ILE:O	2:C:469:THR:HG23	2.03	0.59
2:C:568:ALA:O	2:C:569:VAL:HB	2.03	0.59
2:C:613:VAL:CG1	2:C:614:ARG:H	2.16	0.59
2:C:181:VAL:HG21	2:C:220:GLY:HA3	1.85	0.59
2:C:525:ALA:O	2:C:526:PRO:C	2.40	0.59
3:D:1147:ARG:CB	3:D:1188:VAL:HG21	2.32	0.59
1:A:101:LEU:C	1:A:101:LEU:HD12	2.22	0.59
2:C:1103:ASP:HB2	2:C:1108:PRO:CB	2.30	0.59
1:B:149:GLY:HA2	1:B:172:SER:OG	2.03	0.59
3:D:126:VAL:H	3:D:456:MET:CE	2.15	0.59
4:E:86:GLN:O	4:E:89:MET:HB2	2.03	0.59
2:C:440:PRO:HG3	2:C:454:SER:HB3	1.85	0.58
2:C:882:LEU:H	2:C:882:LEU:HD23	1.68	0.58
3:D:948:THR:N	3:D:1020:LEU:HD13	2.18	0.58
3:D:762:GLN:NE2	4:E:20:THR:HG21	2.18	0.58
2:C:162:ILE:CG2	2:C:163:ILE:N	2.66	0.58
1:A:185:ARG:HH21	1:A:194:LYS:HE3	1.68	0.58
1:A:221:HIS:HA	1:A:224:TYR:CD2	2.38	0.58
2:C:755:LEU:O	2:C:755:LEU:HD13	2.03	0.58
2:C:989:VAL:HG12	2:C:990:GLY:N	2.16	0.58
3:D:879:ARG:HG2	3:D:879:ARG:HH11	1.68	0.58
2:C:839:LEU:O	2:C:995:MET:O	2.21	0.58
3:D:1273:VAL:N	3:D:1324:PRO:CG	2.67	0.58
2:C:164:PRO:HG2	2:C:168:ARG:HG2	1.84	0.58
2:C:110:GLU:H	2:C:369:PRO:CG	2.16	0.58
2:C:483:VAL:O	2:C:486:MET:N	2.36	0.58
2:C:603:VAL:CG2	2:C:646:GLY:H	2.16	0.58
2:C:841:ASN:ND2	2:C:845:ASN:H	2.00	0.58
3:D:701:LEU:HD11	3:D:759:ALA:HB1	1.85	0.58
3:D:757:ALA:HB2	4:E:61:VAL:HG11	1.86	0.58
1:B:14:THR:OG1	1:B:22:GLU:HB3	2.03	0.58
1:B:101:LEU:HD13	1:B:114:PHE:HA	1.85	0.58
1:B:80:LEU:HD13	3:D:839:LEU:CB	2.33	0.58
3:D:1165:TYR:CZ	3:D:1214:PRO:HB3	2.38	0.58
2:C:348:LEU:C	2:C:350:ARG:H	2.06	0.58
2:C:636:ALA:CB	2:C:705:ILE:HD11	2.33	0.58
2:C:885:ILE:O	2:C:887:GLU:N	2.37	0.58
3:D:1200:VAL:HA	3:D:1373:ARG:HH12	1.69	0.58
1:A:224:TYR:CE1	1:B:9:PRO:HD2	2.39	0.58
2:C:11:GLU:OE2	2:C:473:ARG:NE	2.36	0.58
3:D:1125:MET:HG2	3:D:1126:ASP:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:850:ALA:HA	3:D:632:VAL:CG1	2.34	0.58
2:C:945:ALA:O	2:C:949:LYS:HG3	2.03	0.58
3:D:907:GLU:HB3	3:D:911:LEU:HD22	1.86	0.58
2:C:483:VAL:O	2:C:486:MET:HB2	2.03	0.58
2:C:565:GLN:HG3	2:C:995:MET:HE3	1.85	0.58
3:D:1353:GLN:HE21	3:D:1368:ILE:CD1	2.07	0.58
3:D:948:THR:H	3:D:1020:LEU:CD1	2.16	0.58
3:D:129:PHE:O	3:D:130:ASN:CB	2.50	0.58
2:C:501:THR:O	2:C:502:PRO:C	2.42	0.58
2:C:1098:ASP:OD1	2:C:1100:GLN:HG3	2.02	0.58
3:D:599:PRO:O	3:D:600:LEU:HD23	2.04	0.58
3:D:798:GLU:HG3	3:D:821:VAL:CB	2.32	0.58
2:C:987:ILE:HD11	3:D:946:GLY:C	2.23	0.58
3:D:699:VAL:HA	3:D:717:GLN:HA	1.84	0.58
3:D:1211:MET:HE2	4:E:16:LYS:HD2	1.84	0.58
2:C:419:THR:O	2:C:420:ARG:C	2.42	0.58
1:B:94:MET:HE1	1:B:119:ASP:HB2	1.86	0.58
2:C:1052:MET:HE3	2:C:1056:LYS:HZ1	1.69	0.58
2:C:613:VAL:CG1	2:C:619:ARG:HG2	2.33	0.58
3:D:1035:ILE:C	3:D:1037:GLN:H	2.05	0.58
2:C:198:ARG:NH1	2:C:231:PRO:HD3	2.19	0.58
1:A:131:THR:HG23	2:C:644:ARG:HE	1.68	0.58
3:D:551:ASN:HA	3:D:574:LEU:HD13	1.84	0.58
3:D:582:ILE:HG22	3:D:583:ASP:H	1.68	0.58
2:C:1100:GLN:O	3:D:8:VAL:O	2.22	0.58
2:C:312:ALA:HB1	2:C:318:PRO:HG3	1.85	0.58
3:D:959:GLU:O	3:D:963:TYR:CD1	2.56	0.58
1:A:143:ARG:HD3	1:A:145:ASP:OD1	2.04	0.58
1:A:158:ILE:HG13	1:A:161:ARG:HG2	1.86	0.58
3:D:898:GLU:C	3:D:899:LEU:HD13	2.24	0.58
1:B:36:LEU:O	1:B:39:PRO:HD2	2.03	0.58
3:D:642:CYS:SG	3:D:702:LEU:HD23	2.43	0.58
3:D:704:ARG:NH1	3:D:743:ASP:CG	2.53	0.58
1:A:90:LEU:HB2	1:A:119:ASP:CB	2.34	0.58
1:B:55:SER:OG	1:B:157:GLY:HA3	2.03	0.58
2:C:395:LYS:HG3	2:C:397:GLU:HG3	1.85	0.58
1:A:181:VAL:O	1:A:181:VAL:HG12	2.04	0.58
3:D:1281:VAL:HA	3:D:1314:LYS:HA	1.85	0.58
3:D:1014:ASN:C	3:D:1015:TYR:CG	2.76	0.58
2:C:1008:ARG:NH2	2:C:1020:PRO:HB3	2.18	0.58
2:C:386:PHE:O	2:C:392:SER:OG	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1008:PHE:CE1	3:D:1035:ILE:HG13	2.28	0.58
3:D:1194:CYS:HB3	3:D:1373:ARG:HH22	1.66	0.58
3:D:1486:VAL:O	4:E:79:LEU:HD12	2.04	0.58
1:A:198:ARG:HH12	2:C:932:GLU:HB3	1.68	0.58
3:D:1452:ILE:HG22	3:D:1453:ALA:N	2.19	0.58
2:C:684:PHE:CD2	2:C:685:GLU:HG2	2.39	0.58
2:C:487:THR:O	2:C:489:SER:N	2.37	0.58
3:D:1059:SER:O	3:D:1060:SER:C	2.38	0.58
3:D:1261:GLU:OE1	3:D:1268:PRO:HB3	2.02	0.58
2:C:758:ARG:HH11	2:C:758:ARG:HG3	1.68	0.58
2:C:1082:PRO:HG2	2:C:1085:PHE:CB	2.34	0.58
2:C:128:ILE:N	2:C:128:ILE:HD12	2.19	0.58
3:D:1234:THR:HG22	3:D:1234:THR:O	2.04	0.58
3:D:794:GLN:O	3:D:795:VAL:HB	2.03	0.57
2:C:349:ALA:C	2:C:350:ARG:HG3	2.23	0.57
2:C:579:VAL:CG2	2:C:887:GLU:HG3	2.34	0.57
2:C:635:THR:O	2:C:636:ALA:CB	2.51	0.57
3:D:1031:ASN:OD1	3:D:1033:GLN:HG2	2.04	0.57
3:D:1059:SER:C	3:D:1061:PHE:N	2.56	0.57
3:D:789:LEU:HD13	3:D:882:PHE:CE1	2.39	0.57
4:E:68:LEU:HD13	4:E:73:LEU:HD12	1.84	0.57
2:C:281:LEU:HD21	2:C:306:THR:OG1	2.04	0.57
1:A:124:ASN:O	1:A:125:PRO:O	2.22	0.57
2:C:926:PHE:CE1	2:C:929:ARG:HD2	2.39	0.57
2:C:946:ARG:O	2:C:950:LEU:HG	2.04	0.57
2:C:136:ILE:CG2	2:C:336:VAL:HG13	2.33	0.57
3:D:959:GLU:O	3:D:963:TYR:HD1	1.87	0.57
2:C:695:LEU:O	2:C:698:ASP:N	2.35	0.57
2:C:137:VAL:CG1	2:C:411:SER:HB2	2.34	0.57
2:C:26:TYR:CE2	2:C:30:LEU:HD22	2.39	0.57
2:C:399:ASN:ND2	2:C:401:LEU:H	2.01	0.57
2:C:551:GLU:HG3	2:C:906:PHE:CD2	2.39	0.57
3:D:1103:HIS:H	3:D:1222:GLY:HA3	1.70	0.57
3:D:1109:GLU:O	3:D:1217:ILE:HD11	2.03	0.57
2:C:742:ILE:HG23	2:C:756:VAL:HG22	1.86	0.57
3:D:969:ARG:HG3	3:D:970:LYS:HG3	1.85	0.57
3:D:1076:GLY:O	3:D:1079:LYS:HG2	2.04	0.57
1:A:106:PRO:O	1:A:107:LYS:CB	2.52	0.57
3:D:772:PRO:CD	3:D:778:LEU:HB2	2.34	0.57
1:A:178:ALA:O	1:A:179:PHE:HB3	2.04	0.57
2:C:64:LEU:CD1	2:C:367:LEU:HD12	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:466:PHE:CD1	2:C:467:ILE:HG13	2.39	0.57
3:D:1204:CYS:C	3:D:1206:GLY:H	2.08	0.57
2:C:157:ARG:HG3	2:C:313:LEU:HG	1.85	0.57
1:A:222:LEU:HD12	1:B:215:VAL:CG1	2.33	0.57
1:B:73:GLU:OE2	1:B:73:GLU:N	2.38	0.57
1:A:71:VAL:HG13	1:A:132:LEU:HB3	1.85	0.57
3:D:1280:VAL:HG13	3:D:1315:ASP:CA	2.18	0.57
3:D:1280:VAL:CG1	3:D:1281:VAL:N	2.68	0.57
2:C:34:VAL:HG11	2:C:38:LYS:HG3	1.86	0.57
3:D:1275:SER:N	3:D:1322:GLY:HA2	2.18	0.57
3:D:1353:GLN:HB3	3:D:1357:ARG:CD	2.34	0.57
3:D:639:LEU:HD23	3:D:729:HIS:HD2	1.68	0.57
4:E:38:THR:HG22	4:E:39:VAL:N	2.20	0.57
1:A:228:PRO:HA	1:B:11:PHE:O	2.05	0.57
3:D:1084:THR:C	3:D:1086:LEU:H	2.07	0.57
3:D:829:VAL:O	3:D:830:ALA:HB3	2.05	0.57
1:B:95:ALA:O	1:B:96:SER:HB3	2.05	0.57
2:C:1054:THR:C	2:C:1056:LYS:H	2.08	0.57
2:C:662:GLU:O	2:C:663:GLU:HB2	2.04	0.57
3:D:1430:SER:O	3:D:1431:THR:HB	2.05	0.57
3:D:758:GLU:O	3:D:762:GLN:HG3	2.04	0.57
2:C:142:ARG:CD	2:C:324:ASP:HA	2.34	0.57
1:B:19:HIS:HB3	1:B:201:THR:O	2.04	0.57
4:E:17:TYR:O	4:E:21:VAL:HG23	2.05	0.57
2:C:3:ILE:CG2	2:C:902:ILE:HD13	2.35	0.57
2:C:374:ASN:O	2:C:376:ARG:N	2.38	0.57
4:E:79:LEU:O	4:E:81:PRO:HD2	2.04	0.57
2:C:202:TYR:CD1	2:C:304:LEU:HD13	2.39	0.57
1:A:56:VAL:HB	1:A:142:VAL:HB	1.86	0.57
3:D:890:VAL:HG11	3:D:922:LEU:HD11	1.87	0.57
2:C:747:ALA:O	2:C:749:VAL:HG23	2.05	0.57
2:C:760:SER:O	2:C:785:VAL:HG22	2.05	0.57
3:D:558:LEU:HD21	3:D:567:ILE:HG13	1.86	0.57
3:D:1014:ASN:O	3:D:1015:TYR:CB	2.53	0.57
2:C:410:ILE:HG21	2:C:468:ARG:NH2	2.19	0.57
2:C:1052:MET:HE2	3:D:623:VAL:HG11	1.87	0.57
2:C:149:THR:HB	2:C:158:TYR:CE1	2.34	0.57
2:C:162:ILE:HG22	2:C:163:ILE:N	2.20	0.57
2:C:211:LEU:HD22	2:C:304:LEU:CD1	2.34	0.57
1:A:41:ARG:HG2	1:A:177:VAL:HB	1.85	0.57
1:A:225:PHE:CZ	1:B:25:LEU:HD23	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:LEU:CD1	1:B:28:LEU:HD11	2.29	0.57
3:D:1312:LEU:O	3:D:1313:VAL:CB	2.53	0.57
3:D:853:VAL:HG21	3:D:877:PRO:CB	2.35	0.57
2:C:51:THR:HG1	2:C:348:LEU:HD23	1.70	0.57
2:C:988:VAL:HG12	3:D:948:THR:OG1	2.04	0.57
2:C:260:LEU:HD12	2:C:292:ARG:CB	2.35	0.57
3:D:480:GLU:HA	3:D:493:ARG:NH1	2.19	0.57
3:D:1479:ASP:C	3:D:1481:VAL:H	2.07	0.57
3:D:1023:MET:SD	3:D:1023:MET:N	2.77	0.57
2:C:12:VAL:O	2:C:13:ILE:HD12	2.05	0.57
2:C:545:ASN:CB	2:C:583:LEU:HD12	2.35	0.57
2:C:659:PRO:O	2:C:660:ALA:CB	2.52	0.57
3:D:1250:THR:HG21	3:D:1270:ALA:HB2	1.86	0.57
3:D:626:SER:HA	3:D:652:LEU:CD1	2.35	0.57
4:E:3:GLU:HB3	4:E:4:PRO:CD	2.35	0.57
1:B:26:GLU:CB	1:B:27:PRO:CD	2.79	0.57
1:B:129:ILE:O	1:B:130:ALA:HB2	2.04	0.57
3:D:69:GLU:O	3:D:70:ALA:HB3	2.05	0.57
3:D:1277:ILE:HG22	3:D:1278:ASP:N	2.20	0.56
3:D:777:PRO:CG	3:D:912:LYS:HG3	2.34	0.56
2:C:1077:PRO:O	2:C:1079:PRO:HD3	2.05	0.56
2:C:468:ARG:O	2:C:469:THR:O	2.23	0.56
2:C:597:ALA:HA	2:C:614:ARG:NH1	2.19	0.56
1:A:72:LYS:N	2:C:607:ASP:HB3	2.20	0.56
2:C:843:HIS:HD2	2:C:884:GLN:HA	1.66	0.56
2:C:874:LEU:CD2	3:D:784:ASP:HA	2.35	0.56
3:D:1379:VAL:HG22	3:D:1394:VAL:O	2.04	0.56
3:D:934:LEU:O	3:D:935:LYS:C	2.44	0.56
2:C:728:HIS:CD2	2:C:783:ARG:HH11	2.22	0.56
1:A:101:LEU:HD21	1:A:109:VAL:HG11	1.85	0.56
2:C:892:LEU:HD23	2:C:892:LEU:N	2.19	0.56
3:D:663:GLU:C	3:D:665:ALA:H	2.09	0.56
1:B:150:TYR:CD1	1:B:170:ILE:HG22	2.40	0.56
2:C:100:LEU:HD21	2:C:368:THR:CA	2.36	0.56
2:C:1055:ILE:CG2	2:C:1066:ALA:HB2	2.34	0.56
2:C:129:ILE:HD12	2:C:386:PHE:HB3	1.85	0.56
2:C:568:ALA:O	2:C:569:VAL:CB	2.53	0.56
3:D:957:PRO:HG3	3:D:1007:VAL:HB	1.87	0.56
2:C:163:ILE:CG2	2:C:164:PRO:HD2	2.34	0.56
2:C:142:ARG:HE	2:C:324:ASP:HA	1.69	0.56
1:B:72:LYS:HB3	1:B:131:THR:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:VAL:HG12	1:B:167:VAL:HG21	1.86	0.56
3:D:702:LEU:HD12	3:D:745:MET:SD	2.45	0.56
3:D:461:ILE:HG22	3:D:465:LEU:CD1	2.35	0.56
3:D:580:ALA:HB2	3:D:587:ARG:NH2	2.21	0.56
2:C:317:VAL:N	2:C:318:PRO:HD2	2.20	0.56
2:C:640:ARG:NH1	2:C:640:ARG:HG3	2.20	0.56
2:C:873:PRO:HG2	2:C:874:LEU:N	2.18	0.56
2:C:159:ILE:HD11	2:C:310:LEU:CB	2.29	0.56
2:C:169:GLY:HA2	2:C:264:PRO:O	2.06	0.56
3:D:1154:GLU:CB	3:D:1159:ARG:HG2	2.25	0.56
3:D:811:GLU:CA	3:D:814:ALA:HB3	2.24	0.56
2:C:735:ARG:HA	2:C:737:LEU:O	2.04	0.56
3:D:88:TYR:C	3:D:520:LEU:HD13	2.25	0.56
3:D:88:TYR:O	3:D:89:ARG:CB	2.53	0.56
1:B:126:ASP:O	1:B:127:LEU:HB3	2.05	0.56
1:B:77:GLU:HA	1:B:77:GLU:OE1	2.05	0.56
1:B:100:ILE:HA	1:B:141:GLU:HA	1.86	0.56
3:D:1381:VAL:HG12	3:D:1382:THR:N	2.20	0.56
3:D:91:ALA:CB	3:D:518:PRO:HG2	2.36	0.56
2:C:726:ILE:CD1	2:C:726:ILE:H	2.14	0.56
3:D:1475:GLY:C	3:D:1477:GLY:N	2.59	0.56
2:C:989:VAL:CG1	2:C:990:GLY:N	2.68	0.56
1:A:52:ALA:HB3	1:A:171:PHE:CE1	2.39	0.56
2:C:940:GLU:HA	2:C:973:VAL:HG21	1.87	0.56
2:C:100:LEU:HD21	2:C:368:THR:HA	1.87	0.56
2:C:493:ARG:HH12	3:D:1069:GLU:CD	2.08	0.56
2:C:873:PRO:CG	2:C:874:LEU:H	2.18	0.56
3:D:1062:ARG:HD3	3:D:1062:ARG:C	2.25	0.56
3:D:1208:ASP:HA	3:D:1215:VAL:HG22	1.87	0.56
3:D:1376:LEU:HD11	3:D:1421:LEU:CD1	2.32	0.56
3:D:1463:LYS:O	3:D:1467:ILE:HG13	2.05	0.56
3:D:898:GLU:OE1	3:D:921:ARG:NH1	2.38	0.56
1:A:26:GLU:OE2	1:A:185:ARG:CZ	2.53	0.56
1:A:99:LEU:O	1:A:100:ILE:HD13	2.06	0.56
3:D:1483:PHE:HE2	4:E:18:ARG:NE	2.03	0.56
3:D:20(U):UNK:O	3:D:21(U):UNK:CB	2.53	0.56
2:C:944:LEU:C	2:C:946:ARG:H	2.07	0.56
2:C:1076:VAL:HG21	3:D:753:SER:HB3	1.88	0.56
2:C:443:THR:N	2:C:444:PRO:CD	2.69	0.56
2:C:456:ALA:HB3	2:C:459:ALA:CB	2.24	0.56
3:D:616:GLN:O	3:D:617:ASN:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ILE:HG22	1:A:199:ILE:O	2.05	0.56
3:D:87:ARG:CB	3:D:522:PRO:HG2	2.36	0.56
2:C:1087:VAL:O	2:C:1087:VAL:HG12	2.06	0.56
2:C:918:LEU:HD13	2:C:968:ASP:HA	1.87	0.56
2:C:681:GLY:HA2	3:D:939:PHE:CE2	2.40	0.56
3:D:1266:ARG:O	3:D:1268:PRO:CD	2.54	0.56
2:C:151:ASP:HB2	2:C:156:GLY:O	2.04	0.56
1:A:159:LYS:C	1:A:161:ARG:H	2.09	0.56
1:A:185:ARG:NH2	1:A:194:LYS:HE3	2.20	0.56
1:B:188:GLN:HG2	3:D:688:TRP:CD1	2.40	0.56
3:D:502:PHE:CD1	3:D:1452:ILE:HG23	2.40	0.56
3:D:1079:LYS:C	3:D:1081:GLY:H	2.07	0.56
2:C:314:THR:O	2:C:315:ALA:CB	2.53	0.56
1:B:94:MET:SD	1:B:97:THR:HG22	2.45	0.56
3:D:795:VAL:N	3:D:862:ASP:CB	2.67	0.56
2:C:100:LEU:CD1	2:C:108:ILE:HB	2.35	0.56
2:C:337:GLY:O	2:C:341:ALA:HB2	2.06	0.56
2:C:328:LEU:C	2:C:467:ILE:HD13	2.26	0.56
2:C:605:LYS:HG3	2:C:611:ILE:HA	1.88	0.56
3:D:1030:GLY:O	3:D:1031:ASN:HB3	2.06	0.56
3:D:1194:CYS:HB3	3:D:1373:ARG:HH21	1.70	0.56
4:E:10:PHE:CE2	4:E:16:LYS:HG3	2.41	0.56
2:C:260:LEU:CD2	2:C:261:LEU:HB3	2.34	0.56
2:C:325:ILE:C	2:C:327:HIS:H	2.07	0.56
1:A:157:GLY:CA	1:A:166:PRO:HB3	2.35	0.56
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.41	0.56
3:D:1381:VAL:HB	3:D:1390:LEU:O	2.06	0.56
3:D:554:LEU:HD11	3:D:571:LYS:HA	1.87	0.56
2:C:693:GLU:OE1	2:C:693:GLU:HA	2.06	0.56
2:C:1008:ARG:NE	2:C:1010:THR:O	2.39	0.56
2:C:31:GLN:HG2	2:C:39:ARG:HD2	1.86	0.56
2:C:440:PRO:HG2	2:C:453:THR:OG1	2.06	0.56
2:C:144:PRO:HA	2:C:162:ILE:HG21	1.87	0.56
1:A:198:ARG:O	1:A:199:ILE:C	2.44	0.56
1:A:41:ARG:HH21	2:C:860:HIS:CD2	2.24	0.56
1:B:78:ILE:HA	1:B:81:ASN:HD22	1.71	0.56
2:C:498:GLN:H	2:C:502:PRO:CD	2.18	0.56
3:D:897:GLN:HE21	3:D:897:GLN:HA	1.71	0.56
3:D:1280:VAL:CG1	3:D:1281:VAL:H	2.18	0.56
2:C:1008:ARG:HH12	2:C:1021:LEU:N	2.04	0.56
2:C:352:ALA:CA	2:C:355:VAL:HG12	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1353:GLN:HB3	3:D:1357:ARG:HD2	1.87	0.56
2:C:233:GLU:O	2:C:237:ARG:HG2	2.06	0.56
2:C:263:ASP:OD2	2:C:264:PRO:HD3	2.05	0.56
2:C:750:LYS:HE3	3:D:680:GLN:HE22	1.71	0.56
3:D:1450:ALA:CA	3:D:1455:LYS:HG3	2.33	0.56
2:C:395:LYS:CE	2:C:403:SER:HB2	2.35	0.56
3:D:978:TYR:C	3:D:980:MET:N	2.59	0.56
2:C:183:THR:HG21	2:C:190:LYS:HG3	1.88	0.56
3:D:1015:TYR:CB	3:D:1018:ASN:HB2	2.34	0.56
2:C:841:ASN:C	2:C:841:ASN:ND2	2.59	0.56
3:D:1031:ASN:HD21	3:D:1034:GLN:HB2	1.71	0.56
3:D:699:VAL:HG12	3:D:717:GLN:HG2	1.87	0.56
2:C:203:ASP:N	2:C:207:LEU:HB2	2.21	0.56
3:D:808:THR:N	3:D:809:PRO:CD	2.69	0.56
2:C:731:GLU:O	2:C:733:ALA:N	2.38	0.56
1:B:103:ALA:HB1	1:B:132:LEU:CD1	2.36	0.56
3:D:971:LEU:O	3:D:974:ILE:N	2.36	0.56
2:C:166:PRO:CB	2:C:417:GLY:H	2.19	0.56
3:D:904:VAL:HG12	3:D:906:GLN:CD	2.26	0.55
2:C:605:LYS:CD	2:C:607:ASP:HA	2.35	0.55
2:C:567:GLN:O	2:C:997:LEU:HA	2.06	0.55
3:D:936:TYR:O	3:D:940:THR:HG22	2.05	0.55
2:C:208:VAL:HG21	2:C:218:VAL:HG13	1.87	0.55
1:A:143:ARG:HG3	1:A:159:LYS:HG3	1.88	0.55
1:A:121:GLU:O	1:A:123:MET:N	2.31	0.55
3:D:603:LEU:HA	3:D:606:ILE:HD13	1.87	0.55
3:D:99:ALA:HB3	3:D:458:ALA:HB1	1.87	0.55
2:C:867:VAL:HG12	2:C:868:ASP:H	1.70	0.55
3:D:1483:PHE:HE1	4:E:22:VAL:HG23	1.72	0.55
3:D:659:LYS:C	3:D:659:LYS:HD3	2.27	0.55
2:C:343:GLN:HG2	2:C:385:PHE:CB	2.36	0.55
3:D:1437:ALA:HA	3:D:1440:PHE:HD1	1.71	0.55
1:B:94:MET:CB	1:B:94:MET:CE	2.84	0.55
2:C:21:ILE:O	2:C:25:SER:HB2	2.06	0.55
2:C:31:GLN:HG2	2:C:39:ARG:CD	2.35	0.55
2:C:355:VAL:HG13	2:C:356:ARG:N	2.21	0.55
2:C:580:MET:O	2:C:581:THR:HB	2.07	0.55
2:C:595:LEU:HG	2:C:655:LEU:CD2	2.37	0.55
2:C:665:PHE:O	2:C:666:LEU:C	2.44	0.55
2:C:845:ASN:ND2	2:C:884:GLN:OE1	2.36	0.55
3:D:1008:PHE:CD2	3:D:1008:PHE:O	2.59	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1109:GLU:CG	3:D:1110:ALA:N	2.68	0.55
3:D:1335:LEU:HD23	3:D:1344:VAL:HG22	1.88	0.55
1:A:131:THR:HG23	2:C:644:ARG:CZ	2.37	0.55
2:C:501:THR:N	2:C:502:PRO:HD2	2.20	0.55
2:C:360:VAL:HG12	2:C:361:MET:N	2.20	0.55
3:D:25(U):UNK:HA	3:D:40(U):UNK:O	2.06	0.55
3:D:857:LEU:CD1	3:D:858:LEU:H	2.14	0.55
3:D:865:THR:CG2	3:D:866:THR:N	2.69	0.55
2:C:549:PHE:HE1	2:C:579:VAL:HG11	1.71	0.55
2:C:603:VAL:HG21	2:C:645:VAL:HA	1.87	0.55
2:C:831:ARG:O	2:C:832:LYS:O	2.25	0.55
2:C:755:LEU:HB3	2:C:790:LEU:HD23	1.86	0.55
3:D:1141:GLU:CA	3:D:1171:VAL:HG11	2.27	0.55
3:D:1475:GLY:C	3:D:1477:GLY:H	2.08	0.55
3:D:1429:LEU:HD12	3:D:1429:LEU:O	2.07	0.55
3:D:865:THR:CG2	3:D:866:THR:H	2.18	0.55
3:D:907:GLU:CG	3:D:911:LEU:HD13	2.37	0.55
2:C:837:ASP:H	2:C:1001:VAL:HG23	1.71	0.55
2:C:30:LEU:O	2:C:32:ALA:N	2.40	0.55
2:C:163:ILE:HG23	2:C:265:LYS:HZ1	1.72	0.55
2:C:177:GLU:CG	2:C:181:VAL:H	2.19	0.55
2:C:304:LEU:HD23	2:C:305:PRO:CD	2.37	0.55
2:C:313:LEU:HD13	2:C:319:GLY:C	2.27	0.55
1:A:198:ARG:NH1	2:C:934:PHE:CE1	2.74	0.55
3:D:807:ALA:C	3:D:809:PRO:HD3	2.27	0.55
3:D:675:ARG:HA	3:D:678:GLU:CB	2.37	0.55
2:C:796:GLU:HA	3:D:681:ARG:HH22	1.72	0.55
3:D:100:ALA:HA	3:D:575:GLN:OE1	2.06	0.55
3:D:502:PHE:CD2	3:D:507:ASN:ND2	2.73	0.55
3:D:1402:ALA:C	3:D:1404:ASN:H	2.10	0.55
3:D:772:PRO:O	3:D:772:PRO:HG2	2.06	0.55
2:C:142:ARG:HG2	2:C:147:TYR:OH	2.07	0.55
1:A:16:GLN:HG3	1:A:20:TYR:CB	2.36	0.55
1:B:173:PRO:HG3	1:B:204:SER:OG	2.06	0.55
2:C:754:ILE:HD13	2:C:791:ARG:HE	1.71	0.55
3:D:681:ARG:O	3:D:682:ASP:CB	2.55	0.55
1:A:131:THR:O	1:A:131:THR:CG2	2.52	0.55
3:D:728:LEU:HD13	3:D:745:MET:CE	2.36	0.55
1:A:122:ILE:HG22	1:A:122:ILE:O	2.06	0.55
2:C:1009:SER:HB2	3:D:651:GLU:O	2.07	0.55
2:C:852:ILE:O	2:C:852:ILE:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1283:ILE:HD12	3:D:1312:LEU:HA	1.89	0.55
3:D:793:THR:HG21	3:D:907:GLU:OE1	2.06	0.55
3:D:864:VAL:H	3:D:876:SER:HG	1.51	0.55
2:C:15:LEU:HD21	2:C:461:VAL:HG21	1.86	0.55
3:D:1069:GLU:HG3	3:D:1072:ILE:CD1	2.35	0.55
3:D:1324:PRO:CG	3:D:1325:LEU:H	2.20	0.55
3:D:648:MET:CE	3:D:747:VAL:HG11	2.36	0.55
2:C:803:ARG:HB3	2:C:825:VAL:HG22	1.88	0.55
3:D:1459:LEU:CD1	3:D:1470:ARG:NH1	2.69	0.55
3:D:1083:ASP:O	3:D:1086:LEU:N	2.37	0.55
3:D:1471:LEU:O	3:D:1471:LEU:HG	2.06	0.55
2:C:1073:GLY:HA2	3:D:659:LYS:HE3	1.88	0.55
2:C:1020:PRO:O	2:C:1021:LEU:HG	2.06	0.55
2:C:881:ASN:ND2	3:D:1034:GLN:CD	2.60	0.55
2:C:44:ILE:HD12	2:C:44:ILE:H	1.71	0.55
2:C:479:VAL:O	2:C:480:THR:O	2.25	0.55
3:D:616:GLN:O	3:D:617:ASN:CB	2.54	0.55
2:C:327:HIS:O	2:C:329:GLY:N	2.36	0.55
2:C:816:LYS:HG3	2:C:819:VAL:HG23	1.89	0.55
2:C:688:ILE:HG22	2:C:869:VAL:HG23	1.89	0.55
2:C:1012:PRO:CG	2:C:1023:GLY:HA3	2.37	0.55
3:D:965:GLU:O	3:D:968:ASP:N	2.40	0.55
1:B:12:THR:HB	1:B:24:VAL:HB	1.88	0.55
3:D:30(U):UNK:O	3:D:31(U):UNK:CB	2.55	0.55
3:D:1281:VAL:HG13	3:D:1314:LYS:CB	2.36	0.55
2:C:924:LEU:N	2:C:924:LEU:CD2	2.66	0.55
2:C:601:GLY:O	2:C:602:GLU:CB	2.54	0.55
2:C:613:VAL:HG11	2:C:619:ARG:HG3	1.87	0.55
2:C:831:ARG:HG2	2:C:1002:GLU:OE2	2.06	0.55
2:C:839:LEU:O	2:C:840:ALA:O	2.25	0.55
2:C:676:ILE:HG21	2:C:873:PRO:HB3	1.87	0.55
2:C:1005:MET:HG2	3:D:724:GLN:HG3	1.88	0.55
1:A:56:VAL:O	1:A:165:ILE:HG12	2.07	0.55
1:A:95:ALA:O	1:A:96:SER:HB3	2.06	0.55
3:D:1402:ALA:O	3:D:1406:ARG:HB2	2.06	0.55
1:B:143:ARG:HG2	1:B:144:VAL:N	2.21	0.55
1:B:104:GLU:O	1:B:136:GLY:HA3	2.06	0.55
2:C:552:HIS:CE1	3:D:1064:GLY:HA2	2.42	0.55
3:D:1436:SER:HB3	3:D:1464:GLU:HG2	1.88	0.55
2:C:291:VAL:O	2:C:299:LYS:N	2.38	0.55
1:B:78:ILE:HG13	1:B:129:ILE:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1148:VAL:HG23	3:D:1165:TYR:CD2	2.42	0.55
2:C:672:VAL:HG22	2:C:673:LEU:H	1.71	0.55
2:C:700:TYR:HB2	2:C:833:LEU:HD22	1.89	0.55
3:D:1407:LEU:C	3:D:1409:ALA:H	2.10	0.55
3:D:970:LYS:HA	3:D:973:GLN:HB2	1.87	0.55
3:D:669:ASN:O	3:D:672:ALA:HB3	2.06	0.55
1:B:62:LEU:HD23	1:B:163:ASN:OD1	2.07	0.55
3:D:666:PHE:O	3:D:667:ALA:HB3	2.06	0.55
2:C:440:PRO:HG3	2:C:454:SER:CB	2.36	0.54
2:C:472:ARG:HH11	2:C:472:ARG:HG2	1.73	0.54
3:D:1324:PRO:CG	3:D:1325:LEU:N	2.70	0.54
3:D:1142:SER:O	3:D:1364:HIS:CD2	2.59	0.54
3:D:762:GLN:O	3:D:768:ASN:HB2	2.07	0.54
2:C:163:ILE:HD12	2:C:163:ILE:N	2.20	0.54
2:C:203:ASP:O	2:C:204:GLN:O	2.25	0.54
2:C:257:LEU:O	2:C:258:PHE:C	2.46	0.54
2:C:200:LEU:HD22	2:C:290:LEU:HD13	1.88	0.54
1:B:100:ILE:HA	1:B:140:MET:O	2.06	0.54
3:D:26:VAL:C	3:D:28:LYS:N	2.60	0.54
3:D:1434:TRP:CD1	3:D:1447:LEU:HD12	2.43	0.54
2:C:889:HIS:C	2:C:891:GLY:N	2.60	0.54
2:C:495:THR:HG22	2:C:496:ILE:N	2.21	0.54
2:C:5:ARG:HH22	2:C:10:ARG:NH1	2.05	0.54
3:D:660:LYS:O	3:D:664:LYS:HB2	2.06	0.54
1:B:151:VAL:HG23	1:B:169:ALA:CB	2.32	0.54
2:C:780:GLU:O	2:C:781:LYS:C	2.46	0.54
4:E:27:ALA:HB1	4:E:60:ALA:HB1	1.89	0.54
1:A:72:LYS:HA	2:C:607:ASP:CB	2.32	0.54
2:C:17:PRO:HD2	2:C:20:GLU:CB	2.23	0.54
2:C:410:ILE:HB	2:C:453:THR:HG23	1.89	0.54
4:E:38:THR:HG22	4:E:40:LEU:N	2.18	0.54
2:C:202:TYR:HE1	2:C:304:LEU:HB3	1.73	0.54
2:C:291:VAL:HB	2:C:299:LYS:CG	2.37	0.54
3:D:564:GLU:CG	3:D:568:ARG:HE	2.20	0.54
3:D:104:PHE:O	3:D:511:TRP:HZ3	1.90	0.54
2:C:1111:VAL:HG12	2:C:1111:VAL:O	2.07	0.54
3:D:905:PRO:O	3:D:906:GLN:CB	2.54	0.54
2:C:101:ILE:HG22	2:C:102:HIS:H	1.72	0.54
2:C:439:CYS:HB2	2:C:468:ARG:HH11	1.72	0.54
3:D:1105:ILE:HG23	3:D:1200:VAL:CB	2.37	0.54
2:C:1052:MET:HG2	3:D:623:VAL:CG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:629:SER:HB3	3:D:726:ILE:HD12	1.88	0.54
3:D:699:VAL:CA	3:D:716:PHE:O	2.55	0.54
1:A:26:GLU:CB	1:A:27:PRO:CD	2.72	0.54
1:B:173:PRO:O	1:B:201:THR:HB	2.07	0.54
3:D:542:ASP:O	3:D:543:LEU:C	2.45	0.54
3:D:91:ALA:HB3	3:D:518:PRO:CD	2.36	0.54
3:D:1444:THR:O	3:D:1448:THR:N	2.35	0.54
3:D:461:ILE:HG22	3:D:465:LEU:HD13	1.89	0.54
3:D:952:ASP:O	3:D:954:ALA:N	2.41	0.54
1:B:147:GLY:HA3	1:B:171:PHE:CG	2.43	0.54
1:B:170:ILE:HD12	1:B:170:ILE:O	2.07	0.54
2:C:492:ASP:HA	2:C:509:ALA:CB	2.37	0.54
2:C:470:PRO:HG3	2:C:472:ARG:NH2	2.23	0.54
3:D:1236:LEU:CD1	3:D:1259:VAL:HG21	2.37	0.54
2:C:1038:TRP:HE1	3:D:1463:LYS:HE3	1.73	0.54
4:E:42:PRO:HG2	4:E:44:GLU:HG2	1.89	0.54
3:D:688:TRP:C	3:D:690:ALA:N	2.60	0.54
1:B:73:GLU:OE1	1:B:128:HIS:CE1	2.60	0.54
3:D:1118:ILE:HD11	3:D:1193:THR:HG22	1.90	0.54
3:D:573:MET:HA	3:D:576:GLU:HB2	1.88	0.54
3:D:965:GLU:HA	3:D:968:ASP:HB2	1.89	0.54
3:D:897:GLN:NE2	3:D:897:GLN:HA	2.22	0.54
3:D:772:PRO:CB	3:D:778:LEU:HB2	2.36	0.54
3:D:911:LEU:O	3:D:915:VAL:HG23	2.08	0.54
2:C:1052:MET:HG3	2:C:1056:LYS:HE3	1.89	0.54
2:C:328:LEU:CB	2:C:484:VAL:HG11	2.38	0.54
2:C:574:ALA:C	2:C:575:GLN:HG3	2.28	0.54
3:D:953:ASP:OD1	3:D:1020:LEU:HG	2.06	0.54
2:C:881:ASN:OD1	3:D:1034:GLN:NE2	2.40	0.54
3:D:1271:LYS:O	3:D:1272:ALA:C	2.46	0.54
2:C:159:ILE:HG21	2:C:306:THR:HG23	1.88	0.54
1:A:162:ILE:HG23	1:A:163:ASN:ND2	2.22	0.54
3:D:1148:VAL:O	3:D:1148:VAL:HG12	2.08	0.54
2:C:692:GLU:OE1	2:C:696:LYS:HE3	2.07	0.54
2:C:238:LEU:O	2:C:241:LEU:HB2	2.07	0.54
1:B:118:ALA:O	1:B:120:VAL:N	2.41	0.54
4:E:26:ARG:NH2	4:E:30:LEU:CD1	2.70	0.54
2:C:266:ARG:C	2:C:268:ASP:H	2.11	0.54
3:D:480:GLU:O	3:D:493:ARG:NH2	2.39	0.54
1:A:104:GLU:C	1:A:136:GLY:HA3	2.27	0.54
1:B:143:ARG:HD2	1:B:159:LYS:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:603:VAL:O	2:C:604:VAL:HG23	2.07	0.54
3:D:1069:GLU:O	3:D:1071:PHE:N	2.41	0.54
3:D:1331:ASP:O	3:D:1333:HIS:N	2.40	0.54
1:A:9:PRO:HG3	1:B:224:TYR:CG	2.43	0.54
1:B:188:GLN:CG	3:D:688:TRP:CD1	2.91	0.54
1:A:128:HIS:CE1	1:A:131:THR:OG1	2.61	0.54
3:D:969:ARG:NH2	3:D:970:LYS:HE3	2.22	0.54
2:C:908:GLY:O	2:C:909:ALA:HB3	2.07	0.54
2:C:328:LEU:C	2:C:484:VAL:HG11	2.28	0.54
2:C:831:ARG:O	2:C:832:LYS:C	2.46	0.54
3:D:1031:ASN:ND2	3:D:1034:GLN:HB2	2.23	0.54
3:D:957:PRO:CD	3:D:1007:VAL:HB	2.38	0.54
2:C:231:PRO:O	2:C:233:GLU:N	2.40	0.54
1:A:157:GLY:N	1:A:166:PRO:HB3	2.23	0.54
2:C:745:ILE:HD12	2:C:802:GLY:HA2	1.90	0.54
3:D:703:ASN:OD1	3:D:704:ARG:N	2.41	0.54
1:A:175:ARG:O	1:A:176:ARG:CB	2.56	0.54
2:C:958:SER:C	2:C:962:GLN:HE21	2.10	0.54
3:D:654:LYS:O	3:D:657:LEU:HB3	2.08	0.54
2:C:1001:VAL:HG11	3:D:724:GLN:CB	2.32	0.54
2:C:148:PHE:HE2	2:C:310:LEU:HA	1.73	0.54
2:C:289:THR:O	2:C:290:LEU:O	2.26	0.54
1:B:76:VAL:HA	1:B:79:ILE:HB	1.90	0.54
3:D:28:LYS:CB	3:D:548:ILE:HG23	2.38	0.54
1:B:47:SER:O	1:B:48:ILE:CG1	2.55	0.54
3:D:497:GLU:HG2	3:D:1389:LEU:HD21	1.88	0.54
2:C:949:LYS:C	2:C:951:GLY:H	2.11	0.54
2:C:115:LEU:HA	2:C:375:SER:OG	2.08	0.54
2:C:31:GLN:HG2	2:C:39:ARG:NE	2.23	0.54
2:C:586:ARG:O	2:C:588:VAL:N	2.40	0.54
3:D:760:ARG:HH12	4:E:59:ASN:ND2	2.06	0.54
2:C:198:ARG:HG3	2:C:228:ALA:HA	1.89	0.54
1:A:83:LYS:CE	1:A:168:ASP:HB2	2.38	0.54
1:B:221:HIS:HA	1:B:224:TYR:CE1	2.43	0.54
1:B:220:GLU:O	1:B:223:ASN:HB2	2.08	0.54
2:C:722:ILE:HA	2:C:758:ARG:HB2	1.90	0.54
3:D:1213:ARG:HG3	3:D:1214:PRO:CD	2.38	0.54
3:D:558:LEU:HD11	3:D:567:ILE:HD11	1.90	0.54
3:D:832:ARG:HG2	3:D:832:ARG:O	2.07	0.54
2:C:1115:LEU:HD23	2:C:1115:LEU:N	2.23	0.54
3:D:82:ARG:O	3:D:84:ILE:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:640:ARG:HG3	2:C:641:PRO:HD2	1.89	0.53
3:D:1009:ASN:OD1	3:D:1009:ASN:O	2.25	0.53
3:D:1264:GLU:O	3:D:1265:ALA:HB3	2.08	0.53
3:D:723:GLY:C	3:D:724:GLN:HE21	2.12	0.53
1:B:177:VAL:HG13	1:B:199:ILE:HD12	1.90	0.53
2:C:915:LYS:O	2:C:919:ALA:N	2.41	0.53
3:D:117:ASP:C	3:D:119:SER:H	2.10	0.53
3:D:149:LYS:O	3:D:151:GLN:N	2.41	0.53
3:D:876:SER:O	3:D:877:PRO:C	2.46	0.53
3:D:879:ARG:HE	3:D:904:VAL:H	1.56	0.53
2:C:520:GLU:N	2:C:521:PRO:HD3	2.22	0.53
2:C:959:PRO:HG2	2:C:960:GLU:N	2.18	0.53
3:D:1479:ASP:C	3:D:1481:VAL:N	2.61	0.53
2:C:555:ALA:O	2:C:558:ALA:HB3	2.08	0.53
3:D:1281:VAL:HG22	3:D:1315:ASP:H	1.73	0.53
2:C:13:ILE:HG23	2:C:14:PRO:CD	2.38	0.53
2:C:363:SER:OG	2:C:364:PRO:HD2	2.08	0.53
2:C:466:PHE:HD1	2:C:467:ILE:CG1	2.22	0.53
2:C:493:ARG:NH1	3:D:1069:GLU:CD	2.62	0.53
2:C:566:THR:C	2:C:568:ALA:H	2.12	0.53
2:C:598:GLU:N	2:C:614:ARG:NH1	2.56	0.53
3:D:1033:GLN:HG3	3:D:1034:GLN:N	2.24	0.53
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.43	0.53
3:D:1363:LEU:O	3:D:1364:HIS:HB2	2.08	0.53
3:D:882:PHE:HA	3:D:885:ILE:CD1	2.35	0.53
1:A:22:GLU:HA	1:A:198:ARG:HA	1.89	0.53
2:C:854:PRO:HB2	2:C:856:GLU:HG3	1.91	0.53
3:D:1156:LEU:CD1	3:D:1177:ALA:HA	2.38	0.53
1:B:101:LEU:HD23	1:B:140:MET:HE2	1.89	0.53
1:B:53:VAL:HG23	1:B:85:LEU:HD23	1.90	0.53
3:D:702:LEU:O	3:D:713:ILE:O	2.26	0.53
3:D:8:VAL:HG12	3:D:1434:TRP:HH2	1.72	0.53
3:D:1465:ASN:HD21	3:D:1470:ARG:NH1	2.06	0.53
3:D:951:ILE:HG22	3:D:952:ASP:N	2.23	0.53
3:D:1409:ALA:O	3:D:1413:VAL:N	2.40	0.53
2:C:901:TYR:C	2:C:902:ILE:HD12	2.29	0.53
2:C:399:ASN:ND2	2:C:402:SER:H	2.06	0.53
2:C:478:VAL:C	2:C:479:VAL:HG22	2.29	0.53
2:C:613:VAL:HG22	2:C:620:LEU:N	2.24	0.53
2:C:801:VAL:HG23	2:C:828:ALA:HB2	1.88	0.53
2:C:882:LEU:HD11	2:C:884:GLN:NE2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1043:GLY:CA	3:D:1057:VAL:H	2.17	0.53
3:D:1420:LEU:HD12	3:D:1421:LEU:H	1.72	0.53
4:E:41:GLU:N	4:E:42:PRO:HD2	2.23	0.53
1:B:71:VAL:HA	1:B:132:LEU:HA	1.91	0.53
1:A:138:LEU:O	1:A:139:TYR:C	2.47	0.53
3:D:1434:TRP:HD1	3:D:1447:LEU:HD12	1.74	0.53
3:D:1459:LEU:HD12	3:D:1470:ARG:NH1	2.24	0.53
1:B:124:ASN:OD1	1:B:124:ASN:N	2.41	0.53
3:D:989:TYR:CZ	3:D:993:ILE:HG13	2.44	0.53
3:D:1224:VAL:HG12	3:D:1224:VAL:O	2.08	0.53
2:C:243:ARG:HG3	2:C:244:PRO:HA	1.89	0.53
2:C:100:LEU:HD23	2:C:372:LEU:HD12	1.90	0.53
2:C:1076:VAL:HG21	3:D:753:SER:CB	2.38	0.53
2:C:466:PHE:HD1	2:C:467:ILE:HG13	1.72	0.53
2:C:580:MET:O	2:C:581:THR:O	2.27	0.53
2:C:628:TYR:O	2:C:629:ALA:O	2.26	0.53
3:D:1041:MET:HG2	3:D:1042:ARG:N	2.24	0.53
3:D:715:ALA:O	3:D:764:LEU:HD12	2.07	0.53
3:D:949:ILE:O	3:D:949:ILE:HG22	2.08	0.53
1:B:109:VAL:HG21	1:B:138:LEU:HD23	1.91	0.53
3:D:571:LYS:C	3:D:573:MET:N	2.62	0.53
2:C:672:VAL:O	2:C:991:GLN:HA	2.08	0.53
1:A:6:LEU:C	1:A:8:ALA:N	2.62	0.53
3:D:916:TYR:CD2	3:D:917:GLN:N	2.76	0.53
3:D:879:ARG:NE	3:D:904:VAL:H	2.06	0.53
2:C:102:HIS:HD2	2:C:106:GLY:HA3	1.72	0.53
2:C:118:LEU:C	2:C:118:LEU:HD23	2.28	0.53
2:C:376:ARG:N	2:C:377:PRO:CD	2.62	0.53
2:C:440:PRO:HG3	2:C:454:SER:CA	2.38	0.53
2:C:839:LEU:O	2:C:994:ILE:HG22	2.08	0.53
3:D:1311:LEU:HD12	3:D:1311:LEU:H	1.73	0.53
3:D:1393:GLN:HE21	3:D:1420:LEU:HD21	1.74	0.53
3:D:643:GLY:CA	3:D:727:GLN:HB2	2.39	0.53
3:D:792:ILE:HG12	3:D:941:LEU:HG	1.91	0.53
1:B:33:GLY:HA3	1:B:181:VAL:HG21	1.90	0.53
2:C:1103:ASP:O	2:C:1104:GLU:C	2.47	0.53
2:C:892:LEU:HD23	2:C:893:ALA:N	2.22	0.53
2:C:449:ILE:O	2:C:451:LEU:N	2.41	0.53
1:A:31:GLY:N	1:A:193:ASP:OD2	2.37	0.53
3:D:876:SER:CA	3:D:879:ARG:HG3	2.38	0.53
2:C:1019:GLN:HB2	3:D:622:ARG:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:443:THR:H	2:C:444:PRO:CD	2.21	0.53
2:C:589:ARG:HH12	2:C:596:TYR:CB	2.22	0.53
3:D:1231:GLU:HB3	3:D:1232:PRO:CD	2.32	0.53
4:E:63:TRP:O	4:E:66:LYS:N	2.40	0.53
2:C:718:GLY:HA3	2:C:761:PHE:CG	2.43	0.53
3:D:89:ARG:O	3:D:520:LEU:HD21	2.07	0.53
1:A:131:THR:HG23	2:C:644:ARG:NE	2.23	0.53
3:D:542:ASP:O	3:D:544:TYR:N	2.42	0.53
3:D:634:GLY:O	3:D:636:GLN:N	2.42	0.53
2:C:987:ILE:HD11	3:D:946:GLY:CA	2.38	0.53
3:D:910:SER:O	3:D:911:LEU:C	2.46	0.53
2:C:841:ASN:HD21	2:C:845:ASN:H	1.55	0.53
2:C:144:PRO:HA	2:C:162:ILE:HG22	1.89	0.53
1:B:207:PRO:O	1:B:210:ALA:N	2.42	0.53
2:C:759:THR:HB	2:C:785:VAL:HG11	1.89	0.53
3:D:563:PRO:O	3:D:565:ILE:N	2.42	0.53
3:D:578:VAL:C	3:D:580:ALA:N	2.62	0.53
2:C:240:THR:O	2:C:240:THR:HG22	2.09	0.53
2:C:336:VAL:O	2:C:339:LEU:N	2.41	0.53
2:C:840:ALA:HB2	2:C:846:LYS:HA	1.91	0.53
2:C:552:HIS:CE1	3:D:1064:GLY:CA	2.92	0.53
2:C:218:VAL:O	2:C:221:LEU:N	2.42	0.53
3:D:809:PRO:C	3:D:811:GLU:N	2.62	0.53
3:D:1402:ALA:O	3:D:1404:ASN:N	2.42	0.53
2:C:811:PRO:O	2:C:813:VAL:N	2.41	0.53
3:D:468:LEU:O	3:D:471:GLU:HG2	2.09	0.53
2:C:111:ASP:O	2:C:113:VAL:N	2.34	0.53
3:D:1015:TYR:HA	3:D:1018:ASN:HD22	1.74	0.53
2:C:17:PRO:O	2:C:18:LEU:CB	2.56	0.53
2:C:564:MET:CE	2:C:846:LYS:HB3	2.39	0.53
2:C:577:PRO:HG2	2:C:580:MET:CB	2.38	0.53
3:D:1260:ILE:HG22	3:D:1261:GLU:N	2.23	0.53
2:C:257:LEU:O	2:C:260:LEU:N	2.41	0.53
2:C:290:LEU:HD12	2:C:291:VAL:N	2.21	0.53
2:C:308:ARG:O	2:C:310:LEU:N	2.42	0.53
1:A:225:PHE:HE1	1:B:36:LEU:HD13	1.73	0.53
1:A:41:ARG:CB	1:A:41:ARG:HH11	2.21	0.53
1:B:174:VAL:HA	1:B:201:THR:HB	1.90	0.53
1:A:41:ARG:HE	2:C:860:HIS:CE1	2.26	0.53
3:D:811:GLU:HA	3:D:814:ALA:CB	2.24	0.53
1:B:58:ILE:HA	1:B:139:TYR:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:VAL:CG2	1:B:85:LEU:HD23	2.40	0.53
2:C:1095:LEU:HD11	3:D:603:LEU:HB3	1.91	0.53
2:C:1017:THR:O	2:C:1018:GLN:CB	2.48	0.53
3:D:971:LEU:O	3:D:974:ILE:HG22	2.09	0.53
1:A:52:ALA:HB3	1:A:171:PHE:CD1	2.44	0.53
2:C:921:ALA:HA	2:C:924:LEU:HG	1.92	0.52
1:A:74:ASP:OD1	1:A:74:ASP:C	2.46	0.52
3:D:1043:GLY:O	3:D:1057:VAL:HG23	2.08	0.52
3:D:638:LYS:CB	3:D:932:ASP:OD1	2.57	0.52
4:E:3:GLU:HG3	4:E:6:ILE:HD11	1.91	0.52
2:C:163:ILE:HG21	2:C:169:GLY:CA	2.39	0.52
1:A:26:GLU:OE2	1:A:185:ARG:NH2	2.42	0.52
1:B:14:THR:HB	1:B:22:GLU:HB3	1.90	0.52
1:B:179:PHE:CB	1:B:197:LEU:HD12	2.39	0.52
3:D:542:ASP:O	3:D:545:ARG:N	2.41	0.52
3:D:509:PRO:HA	3:D:511:TRP:CD1	2.44	0.52
3:D:965:GLU:C	3:D:968:ASP:H	2.13	0.52
3:D:705:ALA:HB3	3:D:706:PRO:HD2	1.91	0.52
3:D:1192:LEU:CD2	3:D:1369:GLU:HB3	2.39	0.52
2:C:600:ASP:C	2:C:648:ARG:HB2	2.28	0.52
2:C:552:HIS:NE2	2:C:886:LEU:HD12	2.24	0.52
3:D:1223:VAL:O	3:D:1227:GLU:HG3	2.10	0.52
3:D:1439:SER:OG	3:D:1467:ILE:HD11	2.09	0.52
3:D:1216:SER:OG	4:E:16:LYS:N	2.42	0.52
4:E:25:LYS:HD3	4:E:25:LYS:O	2.08	0.52
1:A:162:ILE:HG12	1:A:163:ASN:CG	2.30	0.52
3:D:890:VAL:HG13	3:D:922:LEU:HD13	1.90	0.52
1:A:186:LEU:O	1:A:187:GLY:C	2.46	0.52
1:B:203:GLY:O	1:B:204:SER:CB	2.58	0.52
1:B:79:ILE:HG23	1:B:167:VAL:CG1	2.40	0.52
2:C:501:THR:N	2:C:502:PRO:CD	2.73	0.52
2:C:507:ARG:O	2:C:518:ARG:HA	2.09	0.52
3:D:502:PHE:HE1	3:D:1452:ILE:CG1	2.17	0.52
3:D:1119:SER:HA	3:D:1186:VAL:O	2.09	0.52
3:D:1082:ALA:O	3:D:1085:ALA:HB3	2.09	0.52
2:C:232:GLU:C	2:C:234:ALA:N	2.61	0.52
2:C:874:LEU:O	2:C:876:VAL:N	2.42	0.52
3:D:1274:ILE:HD11	3:D:1334:GLN:NE2	2.24	0.52
3:D:1365:ASP:C	3:D:1366:LYS:HG3	2.29	0.52
3:D:764:LEU:HD21	3:D:766:ALA:HB3	1.92	0.52
3:D:115:LEU:C	3:D:117:ASP:N	2.59	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:569:ASN:O	3:D:572:ARG:HG2	2.10	0.52
2:C:922:PHE:CD2	2:C:964:LYS:HG3	2.45	0.52
2:C:603:VAL:O	2:C:604:VAL:CB	2.58	0.52
1:A:76:VAL:HG21	2:C:628:TYR:OH	2.09	0.52
2:C:68:PHE:CD2	2:C:98:LEU:HD22	2.43	0.52
3:D:1202:GLN:O	3:D:1203:LYS:CB	2.57	0.52
3:D:1251:ASP:O	3:D:1253:THR:N	2.40	0.52
3:D:885:ILE:HG12	3:D:937:TYR:CE2	2.44	0.52
2:C:1045:ALA:CB	2:C:1048:THR:HB	2.28	0.52
1:A:101:LEU:O	1:A:139:TYR:HA	2.09	0.52
1:A:121:GLU:HB3	1:A:123:MET:HE3	1.91	0.52
2:C:953:VAL:HG23	2:C:966:LEU:HD13	1.91	0.52
2:C:642:ARG:O	2:C:643:VAL:HB	2.09	0.52
3:D:495:ARG:O	3:D:499:VAL:N	2.28	0.52
4:E:9:LEU:HD23	4:E:69:LEU:HD13	1.90	0.52
3:D:494:LYS:O	3:D:497:GLU:HB2	2.08	0.52
3:D:863:THR:C	3:D:864:VAL:HG23	2.30	0.52
2:C:626:ARG:NE	2:C:637:PHE:CZ	2.76	0.52
2:C:552:HIS:ND1	3:D:1064:GLY:HA2	2.25	0.52
3:D:927:THR:O	3:D:931:LEU:HD23	2.09	0.52
1:A:16:GLN:HE21	1:A:16:GLN:HA	1.75	0.52
1:A:9:PRO:HA	1:A:27:PRO:HD2	1.91	0.52
1:B:199:ILE:HG22	1:B:207:PRO:HB3	1.90	0.52
2:C:820:ARG:O	2:C:821:GLU:O	2.27	0.52
3:D:545:ARG:CG	3:D:546:ARG:N	2.72	0.52
2:C:959:PRO:CG	2:C:960:GLU:H	2.18	0.52
3:D:658:LEU:HA	3:D:661:MET:CE	2.39	0.52
3:D:1399:ASP:OD2	3:D:1417:TRP:HB3	2.10	0.52
2:C:146:VAL:HG22	2:C:161:SER:HA	1.91	0.52
3:D:1292:VAL:HG23	3:D:1305:LEU:HD23	1.91	0.52
2:C:568:ALA:O	2:C:569:VAL:HG12	2.10	0.52
3:D:783:ARG:O	3:D:784:ASP:CB	2.49	0.52
1:B:148:VAL:HG23	1:B:149:GLY:H	1.74	0.52
2:C:445:GLU:HG3	7:C:1640:RFP:H303	1.90	0.52
3:D:1437:ALA:HA	3:D:1440:PHE:CD1	2.45	0.52
2:C:141:HIS:HE1	2:C:334:ARG:HG3	1.75	0.52
2:C:613:VAL:HG22	2:C:621:VAL:N	2.24	0.52
2:C:671:ASN:HB3	2:C:993:PHE:HB2	1.92	0.52
3:D:1110:ALA:O	3:D:1112:CYS:N	2.42	0.52
3:D:1462:LEU:HD23	3:D:1473:PRO:CG	2.40	0.52
1:A:56:VAL:HG13	1:A:167:VAL:CG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:691:LEU:C	3:D:693:GLU:N	2.63	0.52
1:B:132:LEU:CD2	1:B:132:LEU:N	2.73	0.52
1:B:59:GLU:O	1:B:60:ASP:CB	2.58	0.52
2:C:911:GLU:N	2:C:912:PRO:HD2	2.25	0.52
3:D:774:SER:HA	3:D:1209:LEU:HD21	1.92	0.52
1:A:134:GLU:CB	2:C:606:VAL:HG23	2.40	0.52
3:D:1221:VAL:O	3:D:1222:GLY:C	2.46	0.52
3:D:1365:ASP:O	3:D:1366:LYS:HB2	2.09	0.52
3:D:699:VAL:HG12	3:D:717:GLN:HG3	1.92	0.52
3:D:885:ILE:HD13	3:D:937:TYR:HD2	1.75	0.52
1:B:38:ASN:HB3	1:B:39:PRO:CD	2.35	0.52
2:C:713:ARG:HB2	2:C:720:GLU:OE1	2.09	0.52
3:D:1147:ARG:HB3	3:D:1188:VAL:HG21	1.89	0.52
1:A:53:VAL:HG21	1:A:82:LEU:O	2.09	0.52
1:A:105:GLY:HA2	1:A:136:GLY:H	1.75	0.52
3:D:1304:LYS:H	3:D:1304:LYS:CD	2.23	0.52
3:D:1365:ASP:O	3:D:1366:LYS:CB	2.58	0.52
3:D:759:ALA:HA	3:D:763:MET:HG2	1.92	0.52
1:A:28:LEU:CD1	1:A:195:LEU:HB2	2.40	0.52
3:D:599:PRO:C	3:D:600:LEU:HD23	2.30	0.52
3:D:968:ASP:O	3:D:971:LEU:HB2	2.09	0.52
2:C:84:ARG:HA	2:C:131:GLY:CA	2.38	0.52
2:C:137:VAL:HG21	2:C:393:GLN:CD	2.29	0.52
1:B:74:ASP:O	1:B:75:VAL:C	2.48	0.52
2:C:65:VAL:HB	2:C:101:ILE:HG12	1.91	0.52
2:C:369:PRO:C	2:C:371:LYS:H	2.12	0.52
2:C:16:PRO:HB3	2:C:586:ARG:HH21	1.75	0.52
2:C:613:VAL:HG21	2:C:619:ARG:HE	1.75	0.52
3:D:1335:LEU:HD23	3:D:1344:VAL:CG2	2.40	0.52
3:D:1486:VAL:O	4:E:79:LEU:CD1	2.58	0.52
2:C:215:GLY:O	2:C:217:LEU:HG	2.10	0.52
1:A:222:LEU:O	1:A:225:PHE:HD1	1.92	0.52
3:D:518:PRO:HA	3:D:544:TYR:OH	2.09	0.52
1:A:122:ILE:O	1:A:124:ASN:N	2.43	0.52
1:A:124:ASN:ND2	1:A:127:LEU:HD22	2.25	0.52
2:C:52:PHE:HD1	2:C:52:PHE:O	1.93	0.52
2:C:586:ARG:O	2:C:589:ARG:N	2.43	0.51
2:C:399:ASN:OD1	2:C:668:LEU:HD22	2.11	0.51
2:C:845:ASN:HD21	2:C:876:VAL:HG11	1.75	0.51
2:C:325:ILE:O	2:C:327:HIS:N	2.43	0.51
1:A:108:GLU:HG2	2:C:644:ARG:NH2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:552:ASN:C	3:D:554:LEU:H	2.13	0.51
3:D:1443:THR:O	3:D:1447:LEU:HB2	2.09	0.51
3:D:1237:THR:O	3:D:1257:PRO:HD3	2.11	0.51
3:D:823:LEU:O	3:D:824:ASN:CB	2.58	0.51
2:C:690:ILE:O	2:C:852:ILE:HA	2.10	0.51
2:C:610:ARG:HA	2:C:623:HIS:O	2.11	0.51
2:C:662:GLU:O	2:C:662:GLU:HG3	2.10	0.51
2:C:73:ILE:HG22	2:C:74:GLY:N	2.26	0.51
3:D:643:GLY:HA3	3:D:727:GLN:N	2.16	0.51
1:A:125:PRO:O	1:A:127:LEU:N	2.43	0.51
1:A:59:GLU:HG2	1:A:137:LYS:CE	2.34	0.51
3:D:962:ARG:O	3:D:966:GLU:HG3	2.10	0.51
2:C:950:LEU:O	2:C:951:GLY:C	2.49	0.51
2:C:603:VAL:O	2:C:604:VAL:HB	2.11	0.51
2:C:601:GLY:HA3	2:C:647:GLN:C	2.31	0.51
2:C:873:PRO:O	2:C:874:LEU:C	2.47	0.51
3:D:1377:LYS:HG2	3:D:1378:TYR:CE1	2.45	0.51
3:D:617:ASN:OD1	3:D:621:LYS:HE3	2.11	0.51
4:E:30:LEU:C	4:E:32:ARG:N	2.64	0.51
2:C:184:MET:CG	2:C:193:LEU:HD23	2.40	0.51
1:B:56:VAL:HG13	1:B:142:VAL:HB	1.92	0.51
3:D:1403:LEU:HD12	3:D:1417:TRP:CZ3	2.43	0.51
2:C:577:PRO:HB3	2:C:993:PHE:CE2	2.44	0.51
2:C:874:LEU:HD21	3:D:784:ASP:N	2.25	0.51
3:D:639:LEU:O	3:D:641:GLN:N	2.41	0.51
2:C:163:ILE:CB	2:C:164:PRO:HD2	2.41	0.51
1:B:38:ASN:ND2	1:B:41:ARG:HD2	2.25	0.51
2:C:236:VAL:HG13	2:C:248:PRO:O	2.10	0.51
3:D:104:PHE:O	3:D:511:TRP:CZ3	2.62	0.51
2:C:282:GLY:O	2:C:283:VAL:HB	2.10	0.51
2:C:283:VAL:CG1	2:C:284:GLY:N	2.73	0.51
3:D:1475:GLY:O	3:D:1477:GLY:N	2.43	0.51
4:E:13:VAL:HG21	4:E:19:LEU:HB2	1.92	0.51
3:D:916:TYR:O	3:D:918:ALA:N	2.43	0.51
2:C:937:ASP:OD1	2:C:939:ARG:HD2	2.11	0.51
2:C:13:ILE:HG23	2:C:14:PRO:HD2	1.91	0.51
3:D:1330:ILE:O	3:D:1331:ASP:C	2.49	0.51
3:D:729:HIS:O	3:D:731:LEU:N	2.44	0.51
2:C:193:LEU:HD11	2:C:307:LEU:HD22	1.93	0.51
2:C:270:GLY:O	2:C:274:ARG:HG2	2.09	0.51
1:A:225:PHE:CE2	1:B:25:LEU:HD23	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:808:THR:O	3:D:808:THR:HG22	2.09	0.51
2:C:3:ILE:HD13	2:C:900:ARG:HB2	1.91	0.51
2:C:243:ARG:CG	2:C:244:PRO:HA	2.41	0.51
1:B:118:ALA:C	1:B:120:VAL:H	2.13	0.51
2:C:1034:GLU:O	2:C:1037:VAL:N	2.43	0.51
2:C:443:THR:H	2:C:444:PRO:HD3	1.76	0.51
2:C:15:LEU:HD21	2:C:461:VAL:CB	2.41	0.51
2:C:460:ARG:HG3	2:C:461:VAL:N	2.26	0.51
2:C:548:PRO:HG3	2:C:842:ARG:NH2	2.25	0.51
2:C:631:SER:OG	2:C:636:ALA:N	2.31	0.51
2:C:699:PHE:O	2:C:701:THR:N	2.43	0.51
3:D:1038:LEU:O	3:D:1060:SER:O	2.28	0.51
2:C:713:ARG:HH12	2:C:816:LYS:HG2	1.74	0.51
2:C:8:ARG:O	2:C:494:TYR:OH	2.27	0.51
3:D:486:ARG:CG	3:D:487:ALA:H	2.22	0.51
3:D:1397:LYS:HD2	3:D:1400:VAL:HB	1.92	0.51
2:C:976:ASP:O	2:C:978:ARG:N	2.44	0.51
3:D:999:THR:HG23	3:D:1000:THR:N	2.26	0.51
3:D:1110:ALA:HA	3:D:1202:GLN:O	2.10	0.51
2:C:874:LEU:CD2	3:D:784:ASP:CA	2.88	0.51
2:C:310:LEU:O	2:C:313:LEU:HB3	2.10	0.51
1:A:196:THR:OG1	1:A:196:THR:O	2.26	0.51
2:C:282:GLY:O	2:C:283:VAL:CB	2.59	0.51
3:D:1088:THR:O	3:D:1091:SER:HB3	2.10	0.51
2:C:430:VAL:O	2:C:431:HIS:C	2.49	0.51
3:D:1166:LEU:HD22	3:D:1166:LEU:H	1.75	0.51
3:D:879:ARG:CZ	3:D:904:VAL:CA	2.88	0.51
2:C:1034:GLU:OE2	3:D:1096:ARG:NH1	2.44	0.51
3:D:1251:ASP:C	3:D:1253:THR:N	2.62	0.51
4:E:41:GLU:N	4:E:42:PRO:CD	2.74	0.51
2:C:758:ARG:NH1	2:C:758:ARG:HG3	2.25	0.51
3:D:542:ASP:O	3:D:545:ARG:HG2	2.10	0.51
1:B:205:VAL:HG12	1:B:206:THR:N	2.26	0.51
2:C:925:TYR:OH	2:C:972:VAL:HG21	2.11	0.51
2:C:333:ILE:HG21	2:C:460:ARG:NH2	2.26	0.51
2:C:401:LEU:HD21	2:C:543:ASN:HB2	1.92	0.51
2:C:676:ILE:HG22	2:C:677:MET:N	2.25	0.51
3:D:1150:ALA:O	3:D:1151:ARG:HB2	2.10	0.51
3:D:1228:SER:O	3:D:1232:PRO:HD2	2.11	0.51
3:D:645:PRO:HB3	3:D:724:GLN:H	1.76	0.51
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ILE:HG13	1:A:161:ARG:CG	2.41	0.51
3:D:489:ARG:O	3:D:493:ARG:HG2	2.11	0.51
2:C:729:LEU:HD21	2:C:754:ILE:CD1	2.40	0.51
2:C:755:LEU:HD13	2:C:755:LEU:C	2.31	0.51
1:A:105:GLY:O	1:A:133:GLU:HA	2.10	0.51
2:C:1101:THR:HB	2:C:1110:ASP:CB	2.41	0.51
2:C:981:GLU:HB3	2:C:982:PRO:CD	2.41	0.51
1:B:97:THR:HG21	1:B:120:VAL:CG2	2.30	0.51
3:D:1277:ILE:CG2	3:D:1279:GLY:H	2.24	0.51
2:C:943:VAL:O	2:C:944:LEU:C	2.49	0.51
2:C:950:LEU:C	3:D:1018:ASN:HD21	2.14	0.51
3:D:905:PRO:HG2	3:D:906:GLN:N	2.26	0.51
1:A:72:LYS:O	1:A:73:GLU:O	2.29	0.51
2:C:115:LEU:CG	2:C:116:GLY:H	2.24	0.51
2:C:564:MET:HG3	2:C:997:LEU:CD1	2.39	0.51
2:C:1008:ARG:O	3:D:652:LEU:HD13	2.11	0.51
2:C:254:LEU:C	2:C:256:TYR:H	2.12	0.51
2:C:796:GLU:CG	3:D:681:ARG:HH22	2.24	0.51
3:D:1457:ASP:C	3:D:1459:LEU:H	2.14	0.51
4:E:17:TYR:N	4:E:17:TYR:CD1	2.77	0.51
2:C:428:ARG:O	2:C:429:ASP:CB	2.59	0.51
1:B:64:GLU:HA	1:B:75:VAL:HG11	1.93	0.51
2:C:1059:ASP:HA	2:C:1083:GLU:CB	2.41	0.51
3:D:795:VAL:HG12	3:D:796:ARG:H	1.75	0.50
2:C:139:GLN:NE2	2:C:334:ARG:NH2	2.59	0.50
2:C:354:GLY:O	2:C:357:GLU:HB3	2.11	0.50
2:C:637:PHE:HB2	2:C:659:PRO:CB	2.41	0.50
3:D:1107:VAL:HG12	3:D:1217:ILE:HD13	1.92	0.50
3:D:1353:GLN:O	3:D:1356:TYR:N	2.43	0.50
3:D:1105:ILE:HG21	3:D:1370:ILE:HG23	1.92	0.50
3:D:729:HIS:HE1	3:D:935:LYS:HD3	1.75	0.50
2:C:201:GLY:O	2:C:203:ASP:OD2	2.29	0.50
1:A:42:ARG:HD3	2:C:977:GLY:O	2.12	0.50
3:D:521:PRO:N	3:D:522:PRO:CD	2.73	0.50
1:B:114:PHE:O	1:B:116:PRO:N	2.44	0.50
3:D:1483:PHE:CE2	4:E:18:ARG:NE	2.79	0.50
3:D:117:ASP:C	3:D:119:SER:N	2.65	0.50
2:C:183:THR:CG2	2:C:190:LYS:HG3	2.40	0.50
4:E:77:GLU:OE1	4:E:77:GLU:HA	2.11	0.50
2:C:377:PRO:O	2:C:379:GLU:O	2.27	0.50
4:E:28:GLN:O	4:E:28:GLN:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:148:PHE:HE2	2:C:310:LEU:CA	2.23	0.50
3:D:690:ALA:O	3:D:694:VAL:HG23	2.11	0.50
2:C:743:VAL:HG13	2:C:744:ARG:N	2.26	0.50
2:C:796:GLU:HG2	3:D:681:ARG:NH1	2.25	0.50
4:E:48:MET:O	4:E:49:ARG:HG3	2.12	0.50
3:D:968:ASP:HA	3:D:971:LEU:HB2	1.94	0.50
1:A:6:LEU:O	1:A:8:ALA:N	2.45	0.50
2:C:35:PRO:C	2:C:37:GLU:H	2.12	0.50
2:C:415:PRO:O	2:C:416:GLY:O	2.29	0.50
2:C:15:LEU:HD22	2:C:471:TYR:OH	2.11	0.50
2:C:66:LEU:HD11	2:C:98:LEU:HB2	1.94	0.50
3:D:1252:ILE:C	3:D:1254:GLN:N	2.64	0.50
3:D:1273:VAL:H	3:D:1324:PRO:CG	2.22	0.50
2:C:1082:PRO:HG2	2:C:1085:PHE:HB3	1.93	0.50
3:D:1459:LEU:HD12	3:D:1470:ARG:HH11	1.76	0.50
2:C:137:VAL:HG12	2:C:411:SER:HB2	1.93	0.50
4:E:27:ALA:HB1	4:E:60:ALA:CB	2.41	0.50
2:C:492:ASP:H	2:C:532:MET:N	2.08	0.50
2:C:492:ASP:N	2:C:532:MET:H	2.05	0.50
3:D:908:LYS:HG3	3:D:1027:GLY:HA2	1.90	0.50
2:C:118:LEU:HD23	2:C:119:PRO:O	2.10	0.50
2:C:348:LEU:HA	2:C:351:LEU:HB3	1.93	0.50
2:C:613:VAL:CB	2:C:619:ARG:HG2	2.41	0.50
3:D:1008:PHE:HE1	3:D:1035:ILE:CG1	2.18	0.50
3:D:1322:GLY:O	3:D:1323:GLN:CB	2.58	0.50
2:C:186:VAL:HG11	2:C:258:PHE:CD2	2.47	0.50
2:C:263:ASP:CG	2:C:264:PRO:HD3	2.31	0.50
1:A:56:VAL:HG13	1:A:167:VAL:HG23	1.94	0.50
1:B:58:ILE:HG23	1:B:140:MET:CG	2.42	0.50
1:B:58:ILE:O	1:B:59:GLU:C	2.49	0.50
3:D:1118:ILE:CD1	3:D:1190:SER:H	2.24	0.50
3:D:492:ALA:O	3:D:495:ARG:HB2	2.11	0.50
3:D:824:ASN:O	3:D:825:ALA:C	2.50	0.50
2:C:407:LYS:C	2:C:409:ARG:H	2.13	0.50
1:B:68:ILE:N	1:B:68:ILE:HD12	2.27	0.50
3:D:795:VAL:HA	3:D:862:ASP:CB	2.41	0.50
3:D:879:ARG:NH2	3:D:904:VAL:CA	2.63	0.50
3:D:1363:LEU:O	3:D:1363:LEU:HD23	2.11	0.50
1:A:34:VAL:O	1:A:35:THR:C	2.48	0.50
1:B:199:ILE:O	1:B:199:ILE:CG2	2.59	0.50
2:C:502:PRO:O	2:C:507:ARG:CZ	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1118:ILE:HD11	3:D:1190:SER:H	1.76	0.50
3:D:1381:VAL:O	3:D:1382:THR:HG23	2.11	0.50
3:D:1449:GLU:O	3:D:1450:ALA:C	2.50	0.50
3:D:506:GLY:O	3:D:507:ASN:CB	2.59	0.50
2:C:7:GLY:O	2:C:8:ARG:HG3	2.12	0.50
1:B:49:PRO:HD2	1:B:213:GLN:HE21	1.76	0.50
2:C:393:GLN:HE22	7:C:1640:RFP:C8	2.25	0.50
1:B:144:VAL:HG12	1:B:145:ASP:H	1.76	0.50
3:D:1276:GLU:CD	3:D:1301:LYS:HE2	2.32	0.50
3:D:853:VAL:HG11	3:D:860:LEU:HB2	1.93	0.50
2:C:65:VAL:HB	2:C:101:ILE:CG1	2.42	0.50
2:C:342:ASP:N	2:C:345:ARG:HH11	2.10	0.50
2:C:352:ALA:HA	2:C:355:VAL:CG1	2.37	0.50
3:D:1004:THR:HG22	3:D:1005:GLN:N	2.27	0.50
3:D:1007:VAL:HG13	3:D:1008:PHE:N	2.26	0.50
3:D:1347:TYR:CZ	3:D:1351:GLU:HG2	2.46	0.50
3:D:885:ILE:CD1	3:D:937:TYR:HD2	2.24	0.50
1:A:218:LEU:O	1:A:222:LEU:HD23	2.12	0.50
1:B:202:ASP:C	1:B:204:SER:N	2.64	0.50
1:B:40:LEU:O	1:B:44:LEU:HB2	2.11	0.50
2:C:1106:ASP:C	2:C:1108:PRO:HD3	2.32	0.50
1:B:151:VAL:CG2	1:B:169:ALA:HB3	2.36	0.50
2:C:902:ILE:HG22	2:C:902:ILE:O	2.10	0.50
3:D:612:GLY:C	3:D:614:PHE:N	2.63	0.50
2:C:482:GLU:HA	2:C:486:MET:HE1	1.94	0.50
2:C:662:GLU:O	2:C:663:GLU:CB	2.58	0.50
2:C:798:GLY:O	2:C:827:VAL:HG13	2.12	0.50
3:D:1250:THR:HG23	3:D:1269:LYS:CD	2.39	0.50
3:D:1347:TYR:OH	3:D:1351:GLU:HG2	2.11	0.50
3:D:1436:SER:CB	3:D:1464:GLU:HG2	2.41	0.50
2:C:220:GLY:HA2	2:C:223:ASP:OD2	2.10	0.50
2:C:277:ALA:O	2:C:281:LEU:N	2.36	0.50
2:C:148:PHE:CE2	2:C:310:LEU:HA	2.47	0.50
1:B:23:PHE:CD1	1:B:211:LEU:HD22	2.47	0.50
2:C:710:ILE:HG21	2:C:758:ARG:HD2	1.92	0.50
2:C:755:LEU:HD23	2:C:792:VAL:HG23	1.92	0.50
1:A:108:GLU:HG3	2:C:644:ARG:HH22	1.77	0.50
3:D:1490:ARG:C	3:D:1492:LEU:H	2.15	0.50
1:A:67:THR:O	1:A:69:PRO:HD3	2.12	0.50
2:C:705:ILE:HG23	2:C:828:ALA:HA	1.94	0.50
2:C:180:GLY:O	2:C:181:VAL:HB	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:GLY:O	1:A:158:ILE:C	2.50	0.50
1:A:41:ARG:HB3	1:A:41:ARG:CZ	2.40	0.50
2:C:722:ILE:O	2:C:722:ILE:HG22	2.12	0.50
1:B:106:PRO:HA	1:B:132:LEU:O	2.12	0.50
2:C:250:LYS:HG3	2:C:250:LYS:O	2.12	0.50
3:D:1434:TRP:HB2	3:D:1450:ALA:HB2	1.94	0.50
3:D:1465:ASN:OD1	3:D:1470:ARG:HB3	2.11	0.50
3:D:1051:GLU:O	3:D:1052:THR:C	2.50	0.50
2:C:42:VAL:H	2:C:46:ALA:HB2	1.77	0.50
2:C:352:ALA:O	2:C:353:ARG:C	2.50	0.50
2:C:354:GLY:O	2:C:358:ARG:HG2	2.12	0.50
2:C:635:THR:CG2	2:C:636:ALA:N	2.74	0.50
2:C:704:HIS:ND1	2:C:831:ARG:HD2	2.26	0.50
3:D:1236:LEU:HD13	3:D:1259:VAL:HG21	1.92	0.50
3:D:1205:TYR:CD1	3:D:1366:LYS:HD2	2.47	0.50
2:C:159:ILE:HG13	2:C:310:LEU:HD13	1.89	0.50
1:A:158:ILE:HG12	1:A:159:LYS:N	2.27	0.50
2:C:712:ALA:HB3	2:C:820:ARG:O	2.12	0.50
2:C:768:SER:O	2:C:769:PRO:O	2.30	0.50
2:C:434:HIS:O	2:C:436:GLY:N	2.45	0.50
1:B:4:SER:O	1:B:5:LYS:CB	2.59	0.50
1:A:178:ALA:HB2	2:C:864:GLY:HA3	1.94	0.49
2:C:1043:TYR:CE2	3:D:710:ARG:HD3	2.47	0.49
2:C:845:ASN:HD22	2:C:884:GLN:CD	2.15	0.49
3:D:935:LYS:HG3	3:D:939:PHE:HE1	1.77	0.49
2:C:222:LEU:O	2:C:225:ALA:N	2.43	0.49
2:C:257:LEU:HB2	2:C:258:PHE:HD1	1.77	0.49
2:C:261:LEU:C	2:C:263:ASP:N	2.64	0.49
1:A:188:GLN:O	1:A:189:ARG:HB3	2.12	0.49
2:C:755:LEU:HD11	2:C:825:VAL:HB	1.94	0.49
1:A:127:LEU:HG	1:A:129:ILE:HD11	1.94	0.49
3:D:10:ILE:HG21	3:D:1450:ALA:CB	2.42	0.49
2:C:9:ILE:CG2	2:C:10:ARG:H	2.13	0.49
3:D:1403:LEU:HD21	3:D:1415:VAL:N	2.20	0.49
3:D:110:SER:C	3:D:112:ILE:H	2.15	0.49
2:C:1054:THR:HG22	2:C:1055:ILE:N	2.27	0.49
2:C:551:GLU:HG2	2:C:906:PHE:HA	1.94	0.49
3:D:1353:GLN:NE2	3:D:1368:ILE:HD11	2.08	0.49
3:D:732:VAL:O	3:D:733:CYS:C	2.49	0.49
3:D:936:TYR:CD2	3:D:936:TYR:C	2.86	0.49
1:A:167:VAL:HG12	1:A:168:ASP:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:HH11	1:A:42:ARG:N	2.10	0.49
2:C:712:ALA:HB2	2:C:722:ILE:CD1	2.41	0.49
1:A:108:GLU:CG	2:C:644:ARG:NH2	2.75	0.49
3:D:502:PHE:HD1	3:D:1452:ILE:HG23	1.77	0.49
3:D:40(U):UNK:O	3:D:41(U):UNK:O	2.30	0.49
1:A:77:GLU:O	1:A:80:LEU:N	2.45	0.49
2:C:483:VAL:O	2:C:485:TYR:N	2.46	0.49
2:C:571:LEU:CD2	2:C:670:GLN:HG3	2.40	0.49
3:D:1321:ALA:O	3:D:1324:PRO:HD2	2.12	0.49
3:D:935:LYS:HG3	3:D:939:PHE:CE1	2.48	0.49
2:C:181:VAL:CG1	2:C:182:VAL:HG23	2.40	0.49
2:C:474:VAL:HG22	2:C:530:GLU:CB	2.43	0.49
2:C:747:ALA:O	2:C:800:VAL:HG23	2.12	0.49
1:B:132:LEU:HD23	1:B:132:LEU:H	1.77	0.49
2:C:226:VAL:HG23	2:C:227:LEU:N	2.27	0.49
2:C:691:SER:O	2:C:692:GLU:C	2.49	0.49
3:D:9(U):UNK:O	3:D:10(U):UNK:CB	2.60	0.49
2:C:598:GLU:HG3	2:C:614:ARG:NH2	2.28	0.49
2:C:872:ASN:HD21	2:C:874:LEU:HB3	1.77	0.49
3:D:996:TRP:HA	3:D:999:THR:CG2	2.42	0.49
2:C:163:ILE:HG21	2:C:169:GLY:C	2.33	0.49
2:C:198:ARG:HD3	2:C:198:ARG:C	2.32	0.49
2:C:263:ASP:CB	2:C:264:PRO:HD3	2.42	0.49
2:C:727:PRO:C	2:C:729:LEU:H	2.14	0.49
1:A:150:TYR:HB2	2:C:696:LYS:HE2	1.93	0.49
3:D:973:GLN:O	3:D:977:ALA:HB2	2.13	0.49
3:D:633:VAL:HA	3:D:740:PHE:CZ	2.47	0.49
3:D:684:LYS:HE2	3:D:685:ASP:OD2	2.12	0.49
2:C:44:ILE:HG22	2:C:45:GLN:N	2.27	0.49
2:C:45:GLN:O	2:C:48:PHE:HB2	2.12	0.49
2:C:328:LEU:O	2:C:484:VAL:HG11	2.12	0.49
3:D:1327:ARG:CB	3:D:1327:ARG:HH11	2.25	0.49
3:D:1331:ASP:O	3:D:1334:GLN:N	2.28	0.49
2:C:164:PRO:HD3	2:C:267:TYR:CE2	2.48	0.49
1:A:111:ALA:HB2	1:A:127:LEU:HB3	1.93	0.49
3:D:1017:PHE:O	3:D:1019:PRO:N	2.46	0.49
3:D:864:VAL:HG12	3:D:874:GLU:O	2.13	0.49
3:D:879:ARG:HH22	3:D:905:PRO:HD2	1.78	0.49
3:D:764:LEU:HB3	3:D:767:HIS:CD2	2.48	0.49
1:A:38:ASN:HB3	1:A:39:PRO:HD3	1.95	0.49
1:B:14:THR:HG22	1:B:14:THR:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:687:VAL:O	3:D:690:ALA:CB	2.60	0.49
2:C:910:THR:CG2	2:C:912:PRO:HD2	2.40	0.49
3:D:739:ASP:O	3:D:741:ASP:N	2.46	0.49
2:C:100:LEU:CD1	2:C:369:PRO:HD3	2.42	0.49
2:C:89:THR:HG23	2:C:129:ILE:HG23	1.94	0.49
2:C:12:VAL:HG21	2:C:479:VAL:CG1	2.43	0.49
2:C:344:PHE:HE2	2:C:378:LEU:HD23	1.77	0.49
2:C:636:ALA:HB2	2:C:705:ILE:CD1	2.42	0.49
1:A:77:GLU:OE2	2:C:640:ARG:NH1	2.46	0.49
2:C:676:ILE:C	3:D:948:THR:HG22	2.32	0.49
2:C:1053:LEU:HD13	3:D:621:LYS:HD2	1.94	0.49
2:C:142:ARG:HG2	2:C:147:TYR:CE1	2.47	0.49
3:D:1156:LEU:HB3	3:D:1173:PHE:HE1	1.77	0.49
1:B:80:LEU:HB3	3:D:839:LEU:CB	2.42	0.49
3:D:552:ASN:C	3:D:554:LEU:N	2.66	0.49
3:D:97:THR:O	3:D:571:LYS:HE3	2.13	0.49
2:C:969:LEU:CD2	3:D:952:ASP:HB2	2.40	0.49
3:D:1429:LEU:HD13	3:D:1440:PHE:CD2	2.47	0.49
1:B:94:MET:HE1	1:B:119:ASP:O	2.13	0.49
2:C:559:LEU:C	2:C:559:LEU:CD1	2.80	0.49
2:C:875:GLY:HA2	2:C:879:ARG:CG	2.39	0.49
3:D:1034:GLN:HE22	3:D:1037:GLN:NE2	2.11	0.49
3:D:1324:PRO:CD	3:D:1325:LEU:H	2.25	0.49
3:D:1394:VAL:CG1	3:D:1395:LEU:N	2.75	0.49
2:C:1030:GLN:NE2	3:D:628:ARG:HD3	2.25	0.49
2:C:149:THR:HG23	2:C:323:ASP:CB	2.42	0.49
2:C:173:ASP:HB3	2:C:185:LYS:HE3	1.95	0.49
1:A:41:ARG:HG2	1:A:177:VAL:CB	2.43	0.49
1:A:41:ARG:NH2	2:C:860:HIS:CD2	2.81	0.49
3:D:583:ASP:O	3:D:585:GLY:N	2.46	0.49
2:C:889:HIS:HE1	3:D:951:ILE:N	2.03	0.49
1:B:46:SER:O	1:B:47:SER:C	2.50	0.49
3:D:794:GLN:OE1	3:D:794:GLN:HA	2.12	0.49
2:C:551:GLU:O	3:D:1065:LEU:HB3	2.13	0.49
2:C:705:ILE:HD12	2:C:705:ILE:N	2.26	0.49
3:D:648:MET:HE2	3:D:747:VAL:HG11	1.95	0.49
2:C:286:SER:O	2:C:288:ARG:N	2.46	0.49
2:C:325:ILE:C	2:C:327:HIS:N	2.66	0.49
1:A:15:THR:HG22	1:B:230:ALA:CB	2.34	0.49
1:A:9:PRO:HB2	1:A:25:LEU:HD13	1.93	0.49
2:C:803:ARG:HD2	2:C:803:ARG:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1171:VAL:HG12	3:D:1171:VAL:O	2.12	0.49
1:B:57:TYR:CD2	1:B:58:ILE:N	2.81	0.49
2:C:691:SER:O	2:C:693:GLU:N	2.45	0.49
2:C:421:GLU:O	2:C:422:ARG:C	2.50	0.49
3:D:1027:GLY:O	3:D:1028:ALA:HB2	2.13	0.49
2:C:1020:PRO:HD3	2:C:1057:SER:HA	1.94	0.49
2:C:129:ILE:HG22	2:C:130:ASN:ND2	2.28	0.49
2:C:556:ASN:O	2:C:559:LEU:HG	2.12	0.49
3:D:709:HIS:HA	3:D:1227:GLU:HB3	1.95	0.49
3:D:1272:ALA:HB1	3:D:1325:LEU:HA	1.95	0.49
2:C:159:ILE:HG21	2:C:306:THR:HG21	1.95	0.49
1:A:16:GLN:OE1	1:A:19:HIS:HE1	1.96	0.49
2:C:745:ILE:HG22	2:C:746:GLY:N	2.28	0.49
3:D:552:ASN:O	3:D:555:LYS:N	2.44	0.49
2:C:1091:GLU:OE1	3:D:613:ARG:HG3	2.13	0.49
1:B:143:ARG:CG	1:B:144:VAL:N	2.76	0.49
3:D:482:LYS:HE2	3:D:488:ARG:HB3	1.95	0.49
2:C:115:LEU:HD13	2:C:375:SER:OG	2.13	0.48
2:C:569:VAL:O	2:C:571:LEU:HD12	2.13	0.48
2:C:845:ASN:OD1	2:C:845:ASN:O	2.30	0.48
3:D:1065:LEU:C	3:D:1067:VAL:H	2.15	0.48
3:D:1071:PHE:CE2	3:D:1075:HIS:NE2	2.78	0.48
4:E:79:LEU:O	4:E:81:PRO:CD	2.61	0.48
2:C:256:TYR:CG	2:C:260:LEU:HD13	2.48	0.48
2:C:307:LEU:O	2:C:310:LEU:HB3	2.13	0.48
1:A:10:VAL:HB	1:A:26:GLU:HG2	1.90	0.48
2:C:473:ARG:HE	2:C:476:ASN:HA	1.77	0.48
1:B:77:GLU:O	1:B:81:ASN:ND2	2.46	0.48
3:D:1164:ARG:HG2	3:D:1165:TYR:N	2.28	0.48
3:D:664:LYS:O	3:D:665:ALA:HB3	2.13	0.48
3:D:1483:PHE:HZ	4:E:18:ARG:HG3	1.76	0.48
2:C:487:THR:O	2:C:488:ALA:C	2.51	0.48
3:D:1425:THR:C	3:D:1427:SER:H	2.15	0.48
3:D:1277:ILE:HG22	3:D:1278:ASP:H	1.76	0.48
2:C:342:ASP:HA	2:C:345:ARG:HD2	1.94	0.48
2:C:465:GLY:O	2:C:466:PHE:HB3	2.13	0.48
2:C:479:VAL:O	2:C:480:THR:C	2.52	0.48
2:C:836:GLY:O	2:C:837:ASP:O	2.31	0.48
1:A:162:ILE:CG2	1:A:163:ASN:N	2.73	0.48
1:A:55:SER:HG	1:A:164:ALA:HB1	1.78	0.48
1:A:195:LEU:CD2	1:A:196:THR:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:NH1	2:C:934:PHE:HE1	2.11	0.48
2:C:489:SER:O	2:C:490:GLU:CB	2.61	0.48
2:C:946:ARG:NH1	2:C:946:ARG:HG2	2.29	0.48
2:C:839:LEU:HD23	2:C:849:VAL:CG2	2.42	0.48
2:C:872:ASN:HD21	2:C:874:LEU:CB	2.26	0.48
3:D:1008:PHE:HD2	3:D:1008:PHE:O	1.96	0.48
3:D:1223:VAL:C	3:D:1225:ALA:H	2.16	0.48
3:D:626:SER:OG	3:D:748:HIS:N	2.46	0.48
1:A:62:LEU:CD1	2:C:745:ILE:HB	2.43	0.48
3:D:28:LYS:O	3:D:548:ILE:HG21	2.13	0.48
3:D:961:GLN:O	3:D:964:LEU:O	2.30	0.48
2:C:900:ARG:C	2:C:901:TYR:CD1	2.86	0.48
2:C:725:ASP:O	2:C:725:ASP:OD1	2.31	0.48
3:D:853:VAL:HG13	3:D:858:LEU:O	2.13	0.48
3:D:1102:ALA:O	3:D:1103:HIS:O	2.31	0.48
3:D:935:LYS:O	3:D:936:TYR:C	2.52	0.48
3:D:552:ASN:C	3:D:555:LYS:H	2.16	0.48
2:C:134:ARG:HB3	2:C:393:GLN:O	2.14	0.48
3:D:1476:THR:HG22	4:E:21:VAL:CG2	2.43	0.48
3:D:669:ASN:OD1	3:D:670:VAL:N	2.47	0.48
3:D:1278:ASP:HA	3:D:1318:TYR:CA	2.36	0.48
3:D:1316:GLY:O	3:D:1317:ASP:CB	2.61	0.48
1:A:80:LEU:HD11	2:C:572:ILE:HG21	1.96	0.48
2:C:493:ARG:NH1	3:D:1069:GLU:OE2	2.47	0.48
3:D:1311:LEU:O	3:D:1323:GLN:OE1	2.30	0.48
3:D:646:LYS:HB3	3:D:720:LEU:HD23	1.96	0.48
3:D:699:VAL:N	3:D:756:GLN:HE22	1.99	0.48
2:C:142:ARG:HD2	2:C:324:ASP:HA	1.95	0.48
2:C:304:LEU:H	2:C:305:PRO:CD	2.26	0.48
2:C:324:ASP:C	2:C:326:ASP:N	2.66	0.48
1:A:158:ILE:HG23	1:A:159:LYS:N	2.22	0.48
2:C:800:VAL:O	2:C:800:VAL:HG12	2.12	0.48
2:C:816:LYS:HB3	2:C:819:VAL:HG21	1.96	0.48
1:B:128:HIS:O	1:B:129:ILE:HB	2.13	0.48
2:C:674:VAL:CG2	2:C:675:ALA:H	2.26	0.48
2:C:278:GLU:HG3	2:C:284:GLY:N	2.22	0.48
2:C:1059:ASP:HA	2:C:1083:GLU:OE1	2.13	0.48
1:B:185:ARG:CB	1:B:190:THR:HA	2.43	0.48
1:A:152:PRO:O	1:A:154:GLU:N	2.44	0.48
3:D:793:THR:HG22	3:D:879:ARG:HH12	1.77	0.48
2:C:1054:THR:C	2:C:1056:LYS:N	2.64	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:574:ALA:O	2:C:575:GLN:HG3	2.14	0.48
2:C:648:ARG:O	2:C:653:ASP:HB2	2.14	0.48
2:C:573:ARG:O	2:C:670:GLN:HG2	2.13	0.48
2:C:705:ILE:HA	2:C:827:VAL:O	2.13	0.48
3:D:1250:THR:HA	3:D:1269:LYS:HZ3	1.77	0.48
3:D:1341:PRO:HD2	3:D:1342:GLU:OE1	2.14	0.48
2:C:208:VAL:HG12	2:C:209:ARG:N	2.29	0.48
2:C:208:VAL:HG21	2:C:218:VAL:CG1	2.43	0.48
2:C:255:ALA:O	2:C:298:PHE:HE2	1.97	0.48
1:B:184:THR:HG21	1:B:194:LYS:HD3	1.96	0.48
1:B:44:LEU:HG	1:B:199:ILE:CD1	2.40	0.48
1:B:44:LEU:CD2	1:B:199:ILE:HD11	2.44	0.48
2:C:860:HIS:HD2	2:C:977:GLY:HA3	1.77	0.48
2:C:476:ASN:O	2:C:477:GLY:C	2.51	0.48
2:C:948:GLU:HA	2:C:953:VAL:H	1.77	0.48
1:B:157:GLY:HA3	1:B:166:PRO:HB3	1.95	0.48
3:D:669:ASN:OD1	3:D:671:LYS:HG2	2.13	0.48
3:D:1129:THR:O	3:D:1130:ARG:C	2.52	0.48
3:D:795:VAL:CG2	3:D:904:VAL:HG21	2.44	0.48
2:C:466:PHE:CD1	2:C:467:ILE:CG1	2.96	0.48
3:D:1105:ILE:CG2	3:D:1200:VAL:CB	2.92	0.48
3:D:1253:THR:CA	3:D:1258:ARG:HD2	2.36	0.48
2:C:172:ILE:HD13	2:C:184:MET:SD	2.54	0.48
1:A:198:ARG:HH12	2:C:932:GLU:CD	2.17	0.48
2:C:95:TYR:HB3	2:C:114:PHE:HA	1.95	0.48
3:D:1147:ARG:O	3:D:1165:TYR:HA	2.14	0.48
2:C:1109:VAL:O	2:C:1109:VAL:HG13	2.13	0.48
3:D:1434:TRP:HZ3	3:D:1457:ASP:H	1.62	0.48
4:E:8:LYS:CE	4:E:69:LEU:HD21	2.43	0.48
3:D:1045:MET:HG2	3:D:1073:SER:HB3	1.94	0.48
2:C:87:ASP:CG	2:C:824:ARG:HH22	2.16	0.48
2:C:1020:PRO:O	2:C:1021:LEU:CB	2.62	0.48
2:C:91:GLN:HA	2:C:119:PRO:HA	1.96	0.48
2:C:14:PRO:HA	2:C:458:TYR:CE1	2.49	0.48
3:D:1336:LEU:HA	3:D:1340:GLY:O	2.14	0.48
3:D:1393:GLN:HE21	3:D:1420:LEU:CD2	2.27	0.48
3:D:716:PHE:CE2	3:D:765:SER:HB3	2.48	0.48
1:B:203:GLY:O	1:B:204:SER:HB3	2.14	0.48
2:C:745:ILE:C	2:C:747:ALA:H	2.16	0.48
2:C:761:PHE:O	2:C:762:LYS:O	2.31	0.48
1:A:128:HIS:C	1:A:128:HIS:CD2	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:THR:CG2	2:C:644:ARG:HH21	2.11	0.48
1:A:121:GLU:C	1:A:123:MET:H	2.16	0.48
2:C:1106:ASP:N	2:C:1108:PRO:HD3	2.29	0.48
3:D:8:VAL:CG1	3:D:1434:TRP:HH2	2.27	0.48
2:C:892:LEU:C	2:C:894:GLY:H	2.17	0.48
2:C:953:VAL:HG11	2:C:962:GLN:CB	2.42	0.48
2:C:1023:GLY:C	2:C:1024:LYS:HG3	2.34	0.48
2:C:427:VAL:O	2:C:430:VAL:HB	2.14	0.48
3:D:647:ARG:HA	3:D:647:ARG:HD2	1.63	0.48
3:D:836:VAL:HG11	3:D:858:LEU:CD1	2.44	0.48
3:D:905:PRO:HG2	3:D:906:GLN:H	1.78	0.48
2:C:13:ILE:HG13	2:C:14:PRO:HD2	1.96	0.48
2:C:44:ILE:CD1	2:C:44:ILE:H	2.26	0.48
2:C:328:LEU:HD23	2:C:468:ARG:HD2	1.95	0.48
2:C:880:MET:C	2:C:881:ASN:ND2	2.67	0.48
3:D:1103:HIS:H	3:D:1222:GLY:CA	2.27	0.48
2:C:254:LEU:O	2:C:257:LEU:HD12	2.14	0.48
1:B:25:LEU:HD12	1:B:26:GLU:N	2.28	0.48
1:B:31:GLY:O	1:B:35:THR:OG1	2.31	0.48
2:C:735:ARG:C	2:C:737:LEU:N	2.66	0.48
2:C:501:THR:O	2:C:501:THR:HG22	2.14	0.48
3:D:1238:MET:O	3:D:1238:MET:HG3	2.13	0.48
3:D:124:GLU:HA	3:D:456:MET:SD	2.54	0.48
3:D:632:VAL:HG12	3:D:633:VAL:O	2.13	0.48
2:C:929:ARG:C	2:C:931:GLY:N	2.66	0.48
3:D:1015:TYR:HB3	3:D:1018:ASN:CB	2.40	0.48
2:C:613:VAL:CG1	2:C:619:ARG:HA	2.44	0.48
2:C:74:GLY:O	2:C:76:PRO:N	2.47	0.48
2:C:668:LEU:HB2	2:C:995:MET:HE2	1.95	0.48
3:D:1071:PHE:HA	3:D:1074:SER:HB3	1.96	0.48
3:D:724:GLN:O	3:D:725:SER:O	2.31	0.48
2:C:156:GLY:O	2:C:157:ARG:O	2.32	0.48
3:D:1101:VAL:HG21	3:D:1424:VAL:CG2	2.24	0.48
3:D:500:ARG:O	3:D:504:ASP:HB2	2.14	0.48
1:A:43:ILE:CD1	1:B:32:PHE:CE1	2.97	0.48
3:D:1076:GLY:HA2	3:D:1079:LYS:HE2	1.96	0.48
3:D:1086:LEU:HD12	3:D:1089:ALA:CB	2.44	0.48
1:A:133:GLU:C	1:A:135:GLY:H	2.16	0.48
3:D:468:LEU:C	3:D:470:LEU:N	2.67	0.48
3:D:848:GLU:HA	3:D:851:LEU:HB3	1.96	0.48
3:D:879:ARG:HG2	3:D:879:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LYS:HB3	1:A:73:GLU:OE2	2.14	0.47
2:C:831:ARG:HH12	2:C:1002:GLU:CB	2.27	0.47
3:D:1274:ILE:H	3:D:1274:ILE:HD12	1.77	0.47
3:D:1344:VAL:O	3:D:1348:LEU:N	2.44	0.47
3:D:716:PHE:CE2	3:D:765:SER:CB	2.97	0.47
4:E:25:LYS:O	4:E:28:GLN:C	2.52	0.47
2:C:173:ASP:CB	2:C:185:LYS:HE3	2.44	0.47
1:A:13:ALA:O	1:A:15:THR:N	2.46	0.47
1:B:26:GLU:O	1:B:27:PRO:C	2.53	0.47
3:D:690:ALA:O	3:D:694:VAL:N	2.47	0.47
3:D:1140:ILE:HD13	3:D:1175:ILE:HG12	1.95	0.47
1:A:112:VAL:C	1:A:114:PHE:H	2.17	0.47
2:C:1103:ASP:O	2:C:1106:ASP:N	2.44	0.47
2:C:495:THR:O	2:C:496:ILE:CB	2.61	0.47
4:E:8:LYS:NZ	4:E:69:LEU:HD21	2.29	0.47
2:C:425:PHE:O	2:C:426:ASP:HB3	2.14	0.47
3:D:815:ALA:O	3:D:817:GLU:N	2.47	0.47
2:C:1008:ARG:HH12	2:C:1021:LEU:H	1.61	0.47
2:C:21:ILE:HD11	2:C:455:LEU:HD21	1.97	0.47
2:C:328:LEU:HD21	2:C:468:ARG:NH1	2.29	0.47
2:C:399:ASN:HD21	2:C:401:LEU:N	2.10	0.47
2:C:564:MET:CE	2:C:846:LYS:HG2	2.45	0.47
2:C:589:ARG:NH2	2:C:654:LEU:HD12	2.23	0.47
2:C:679:PHE:N	2:C:683:ASN:OD1	2.43	0.47
2:C:831:ARG:NH1	2:C:1002:GLU:CD	2.67	0.47
2:C:73:ILE:HD12	2:C:94:LEU:HD13	1.96	0.47
3:D:643:GLY:O	3:D:644:LEU:HB2	2.13	0.47
4:E:26:ARG:HH22	4:E:37:ASN:HB3	1.77	0.47
1:A:225:PHE:CE1	1:B:36:LEU:HD13	2.50	0.47
1:B:164:ALA:O	1:B:165:ILE:C	2.52	0.47
2:C:1082:PRO:HG2	2:C:1085:PHE:HB2	1.96	0.47
2:C:6:PHE:HD2	2:C:909:ALA:H	1.61	0.47
3:D:800:LYS:CB	3:D:821:VAL:H	2.26	0.47
3:D:1384:PRO:HG3	3:D:1389:LEU:O	2.14	0.47
2:C:1059:ASP:CG	2:C:1083:GLU:HB2	2.35	0.47
2:C:13:ILE:HG22	2:C:15:LEU:N	2.21	0.47
2:C:14:PRO:HA	2:C:458:TYR:CD1	2.48	0.47
2:C:831:ARG:NH1	2:C:1002:GLU:OE2	2.48	0.47
2:C:993:PHE:O	2:C:993:PHE:CD1	2.67	0.47
3:D:1065:LEU:C	3:D:1067:VAL:N	2.67	0.47
2:C:184:MET:CE	2:C:191:PHE:HZ	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:790:LEU:O	2:C:791:ARG:O	2.32	0.47
1:B:132:LEU:CD2	1:B:132:LEU:H	2.27	0.47
1:B:81:ASN:O	1:B:82:LEU:C	2.51	0.47
3:D:575:GLN:NE2	3:D:579:ASP:OD2	2.47	0.47
2:C:7:GLY:HA2	2:C:907:ASP:OD1	2.14	0.47
3:D:1481:VAL:O	3:D:1482:ARG:CG	2.60	0.47
3:D:21:TRP:C	3:D:23:TYR:H	2.18	0.47
2:C:405:ARG:HD2	2:C:543:ASN:ND2	2.29	0.47
2:C:601:GLY:HA3	2:C:648:ARG:N	2.30	0.47
2:C:657:ASP:OD1	2:C:663:GLU:HA	2.14	0.47
3:D:1053:PHE:CD1	3:D:1072:ILE:HG23	2.49	0.47
3:D:1274:ILE:HA	3:D:1322:GLY:N	2.30	0.47
3:D:707:THR:C	3:D:708:LEU:HG	2.34	0.47
2:C:184:MET:HE3	2:C:191:PHE:HZ	1.79	0.47
2:C:261:LEU:O	2:C:264:PRO:HD2	2.14	0.47
2:C:274:ARG:CG	2:C:275:TYR:N	2.78	0.47
1:A:10:VAL:O	1:A:12:THR:N	2.43	0.47
1:B:44:LEU:HG	1:B:199:ILE:CG1	2.44	0.47
3:D:654:LYS:O	3:D:657:LEU:N	2.47	0.47
2:C:83:CYS:SG	2:C:88:LEU:HB2	2.55	0.47
1:B:118:ALA:C	1:B:120:VAL:N	2.68	0.47
3:D:1277:ILE:HG22	3:D:1279:GLY:N	2.27	0.47
3:D:836:VAL:CG1	3:D:858:LEU:HD11	2.45	0.47
2:C:1036:GLU:O	2:C:1039:ALA:HB3	2.14	0.47
2:C:637:PHE:HE1	2:C:1639:GLN:HE21	1.61	0.47
2:C:23:VAL:HG12	2:C:24:GLU:N	2.30	0.47
2:C:408:ARG:NH1	2:C:455:LEU:HD23	2.29	0.47
2:C:333:ILE:CG2	2:C:460:ARG:HH22	2.25	0.47
3:D:1035:ILE:C	3:D:1037:GLN:N	2.68	0.47
3:D:1336:LEU:HD13	3:D:1340:GLY:C	2.35	0.47
2:C:159:ILE:CD1	2:C:310:LEU:HB2	2.34	0.47
1:A:79:ILE:CD1	1:A:165:ILE:HD12	2.38	0.47
1:A:18:ASP:O	1:A:19:HIS:HB3	2.15	0.47
1:B:219:LYS:O	1:B:222:LEU:HB2	2.14	0.47
3:D:1155:ALA:O	3:D:1156:LEU:C	2.53	0.47
1:A:108:GLU:CG	2:C:644:ARG:HH22	2.27	0.47
2:C:195:LEU:HD13	2:C:227:LEU:CD1	2.31	0.47
3:D:564:GLU:O	3:D:565:ILE:C	2.53	0.47
1:A:88:ARG:CB	1:A:121:GLU:HB2	2.38	0.47
2:C:1095:LEU:CD1	3:D:603:LEU:HD23	2.35	0.47
2:C:985:GLY:O	2:C:986:PRO:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:966:LEU:CD1	2:C:986:PRO:HG3	2.40	0.47
4:E:8:LYS:HB3	4:E:69:LEU:HD11	1.96	0.47
2:C:768:SER:CB	2:C:769:PRO:HD2	2.42	0.47
2:C:778:PHE:CD1	2:C:778:PHE:N	2.82	0.47
2:C:449:ILE:HG22	2:C:450:GLY:N	2.29	0.47
2:C:46:ALA:O	2:C:50:GLU:N	2.31	0.47
1:B:87:VAL:CG1	1:B:88:ARG:N	2.77	0.47
2:C:425:PHE:O	2:C:426:ASP:CB	2.62	0.47
1:B:119:ASP:C	1:B:120:VAL:HG23	2.35	0.47
3:D:859:ASP:OD1	3:D:861:GLN:NE2	2.48	0.47
2:C:1007:ALA:HB1	3:D:652:LEU:CD2	2.44	0.47
3:D:1071:PHE:O	3:D:1074:SER:N	2.46	0.47
3:D:899:LEU:H	3:D:899:LEU:HD22	1.79	0.47
1:A:41:ARG:HH12	1:A:42:ARG:HG2	1.80	0.47
1:A:35:THR:HG21	1:B:43:ILE:CG1	2.45	0.47
1:B:181:VAL:HG13	1:B:181:VAL:O	2.14	0.47
1:B:111:ALA:O	1:B:114:PHE:CD1	2.68	0.47
3:D:705:ALA:CB	3:D:706:PRO:HD3	2.44	0.47
3:D:464:LEU:O	3:D:468:LEU:CB	2.63	0.47
3:D:897:GLN:HE21	3:D:897:GLN:CA	2.27	0.47
3:D:497:GLU:HG2	3:D:1389:LEU:HD11	1.96	0.47
2:C:15:LEU:HD21	2:C:461:VAL:HB	1.96	0.47
2:C:30:LEU:HD12	2:C:44:ILE:HG12	1.97	0.47
2:C:881:ASN:CG	3:D:1034:GLN:CD	2.73	0.47
2:C:1034:GLU:OE2	3:D:1096:ARG:NH2	2.47	0.47
2:C:460:ARG:HB2	2:C:468:ARG:HA	1.97	0.47
2:C:547:ILE:HG23	2:C:843:HIS:CE1	2.50	0.47
2:C:875:GLY:O	2:C:876:VAL:C	2.53	0.47
3:D:1095:THR:O	3:D:1099:VAL:HG23	2.13	0.47
3:D:708:LEU:O	3:D:709:HIS:O	2.33	0.47
2:C:327:HIS:C	2:C:329:GLY:N	2.68	0.47
1:B:26:GLU:OE1	1:B:27:PRO:HD3	2.15	0.47
2:C:747:ALA:O	2:C:748:GLU:C	2.52	0.47
2:C:749:VAL:HG23	2:C:800:VAL:HG23	1.96	0.47
1:B:113:ASP:O	1:B:114:PHE:C	2.53	0.47
3:D:602:SER:O	3:D:606:ILE:HD12	2.15	0.47
3:D:1465:ASN:O	3:D:1470:ARG:HB2	2.15	0.47
3:D:1132:LEU:CD1	3:D:1184:ARG:HH12	2.20	0.47
2:C:1067:TYR:O	2:C:1071:ILE:HD13	2.15	0.47
3:D:962:ARG:O	3:D:966:GLU:CG	2.63	0.47
2:C:78:PHE:HB3	2:C:82:GLU:OE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1073:GLY:CA	3:D:659:LYS:HE3	2.44	0.47
3:D:1136:LYS:CG	3:D:1139:ASP:OD2	2.62	0.47
2:C:397:GLU:OE2	2:C:632:ASN:ND2	2.47	0.47
1:A:152:PRO:C	1:A:154:GLU:H	2.18	0.47
3:D:1055:VAL:O	3:D:1055:VAL:HG12	2.13	0.47
2:C:944:LEU:HD11	2:C:963:LEU:CD2	2.45	0.47
2:C:987:ILE:HG22	2:C:987:ILE:O	2.14	0.47
2:C:1034:GLU:O	2:C:1037:VAL:HB	2.15	0.47
3:D:1005:GLN:O	3:D:1009:ASN:HB3	2.15	0.47
3:D:947:ILE:CA	3:D:1020:LEU:HD13	2.43	0.47
3:D:1311:LEU:HD12	3:D:1311:LEU:N	2.30	0.47
2:C:1056:LYS:O	3:D:624:ASP:HB2	2.14	0.47
3:D:764:LEU:CD2	3:D:766:ALA:HB3	2.45	0.47
2:C:198:ARG:CZ	2:C:203:ASP:OD2	2.63	0.47
3:D:687:VAL:O	3:D:690:ALA:HB3	2.15	0.47
2:C:97:ARG:HG2	2:C:112:GLU:H	1.79	0.47
2:C:774:LEU:O	2:C:778:PHE:N	2.47	0.47
2:C:554:ASP:O	2:C:555:ALA:C	2.53	0.47
3:D:537:THR:O	3:D:537:THR:HG22	2.15	0.47
3:D:793:THR:HA	3:D:879:ARG:HH12	1.80	0.47
2:C:1055:ILE:N	2:C:1055:ILE:HD12	2.11	0.47
2:C:26:TYR:HE2	2:C:30:LEU:HD22	1.80	0.47
2:C:876:VAL:HB	2:C:877:PRO:HD3	1.94	0.47
3:D:1231:GLU:C	3:D:1233:GLY:N	2.67	0.47
3:D:1327:ARG:CB	3:D:1327:ARG:NH1	2.76	0.47
2:C:208:VAL:O	2:C:209:ARG:HB2	2.14	0.47
2:C:216:ASP:C	2:C:218:VAL:N	2.67	0.47
2:C:252:LYS:HE3	2:C:298:PHE:HE1	1.80	0.47
1:A:199:ILE:HD12	1:A:199:ILE:N	2.30	0.47
1:A:223:ASN:O	1:A:225:PHE:N	2.48	0.47
1:B:32:PHE:HA	1:B:35:THR:OG1	2.15	0.47
2:C:730:SER:O	2:C:731:GLU:O	2.33	0.47
1:A:111:ALA:O	1:A:112:VAL:C	2.53	0.47
2:C:1091:GLU:OE1	3:D:606:ILE:HG22	2.15	0.47
2:C:890:LEU:HD11	2:C:917:LEU:HD13	1.97	0.47
3:D:120:ALA:HB1	3:D:126:VAL:CB	2.45	0.47
2:C:794:PRO:HG2	2:C:1027:PHE:HB2	1.97	0.47
3:D:1134:LEU:N	3:D:1134:LEU:HD23	2.29	0.47
2:C:862:PRO:HG2	2:C:863:ASP:H	1.80	0.47
2:C:101:ILE:HG22	2:C:102:HIS:N	2.29	0.47
2:C:20:GLU:OE2	2:C:461:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1205:TYR:O	3:D:1206:GLY:O	2.32	0.47
3:D:1236:LEU:HB3	3:D:1256:LEU:N	2.30	0.47
3:D:937:TYR:O	3:D:941:LEU:HB2	2.14	0.47
2:C:175:GLU:O	2:C:182:VAL:HA	2.15	0.47
2:C:304:LEU:HD23	2:C:305:PRO:N	2.30	0.47
1:A:34:VAL:C	1:A:36:LEU:N	2.67	0.47
1:B:11:PHE:HA	1:B:25:LEU:HA	1.96	0.47
1:A:222:LEU:CD1	1:B:215:VAL:HG13	2.40	0.47
1:B:30:ARG:CZ	2:C:854:PRO:HB3	2.45	0.47
3:D:553:ARG:C	3:D:554:LEU:HD23	2.36	0.47
3:D:507:ASN:O	3:D:508:ARG:HG2	2.15	0.47
3:D:99:ALA:O	3:D:575:GLN:HB2	2.14	0.47
3:D:1081:GLY:HA2	3:D:1084:THR:HG23	1.97	0.47
4:E:13:VAL:HG21	4:E:19:LEU:CB	2.45	0.47
2:C:78:PHE:HB3	2:C:82:GLU:CD	2.36	0.47
2:C:78:PHE:HD2	2:C:82:GLU:OE2	1.98	0.47
3:D:706:PRO:HG2	3:D:706:PRO:O	2.15	0.47
2:C:706:GLU:O	2:C:826:PHE:HA	2.15	0.47
2:C:314:THR:O	2:C:315:ALA:HB3	2.15	0.47
2:C:1052:MET:HE1	3:D:748:HIS:CB	2.43	0.46
2:C:358:ARG:O	2:C:359:MET:C	2.53	0.46
2:C:115:LEU:HA	2:C:375:SER:CB	2.45	0.46
1:A:134:GLU:HB3	2:C:606:VAL:HG23	1.96	0.46
2:C:595:LEU:HG	2:C:655:LEU:HD23	1.97	0.46
2:C:846:LYS:HD2	2:C:846:LYS:O	2.16	0.46
3:D:1075:HIS:H	3:D:1075:HIS:CD2	2.33	0.46
3:D:1094:LEU:O	3:D:1095:THR:C	2.53	0.46
3:D:1251:ASP:O	3:D:1252:ILE:HB	2.15	0.46
3:D:1340:GLY:HA3	3:D:1342:GLU:OE1	2.15	0.46
3:D:789:LEU:CD1	3:D:934:LEU:HD22	2.44	0.46
2:C:149:THR:CB	2:C:158:TYR:HE1	2.22	0.46
3:D:1101:VAL:CG2	3:D:1424:VAL:HG22	2.24	0.46
1:A:195:LEU:C	1:A:196:THR:HG22	2.34	0.46
1:A:199:ILE:HG21	1:A:207:PRO:HA	1.97	0.46
2:C:796:GLU:HG2	3:D:681:ARG:NH2	2.28	0.46
2:C:674:VAL:HG23	2:C:869:VAL:O	2.15	0.46
2:C:890:LEU:HD11	2:C:901:TYR:CE2	2.50	0.46
1:B:24:VAL:O	1:B:24:VAL:HG12	2.13	0.46
3:D:149:LYS:C	3:D:151:GLN:N	2.68	0.46
2:C:127:PHE:N	2:C:127:PHE:CD1	2.83	0.46
2:C:928:LYS:O	2:C:931:GLY:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:65:VAL:HB	2:C:101:ILE:HB	1.97	0.46
1:A:70:GLY:HA2	2:C:606:VAL:HG22	1.97	0.46
2:C:613:VAL:HG13	2:C:620:LEU:N	2.15	0.46
2:C:215:GLY:O	2:C:216:ASP:O	2.34	0.46
1:A:198:ARG:HH12	2:C:932:GLU:CB	2.27	0.46
2:C:728:HIS:CD2	2:C:783:ARG:NH1	2.83	0.46
2:C:691:SER:HB2	2:C:858:MET:CE	2.45	0.46
3:D:1083:ASP:C	3:D:1085:ALA:N	2.69	0.46
2:C:166:PRO:HB3	2:C:417:GLY:N	2.27	0.46
4:E:55:TYR:O	4:E:56:ASP:C	2.54	0.46
4:E:86:GLN:HA	4:E:89:MET:HG2	1.97	0.46
2:C:434:HIS:C	2:C:436:GLY:N	2.69	0.46
3:D:794:GLN:HB3	3:D:1017:PHE:CZ	2.49	0.46
2:C:545:ASN:HA	2:C:905:VAL:HG21	1.98	0.46
3:D:638:LYS:CB	3:D:729:HIS:NE2	2.78	0.46
3:D:752:SER:O	3:D:753:SER:C	2.54	0.46
2:C:308:ARG:C	2:C:310:LEU:H	2.19	0.46
2:C:308:ARG:C	2:C:310:LEU:N	2.68	0.46
1:B:188:GLN:NE2	1:B:188:GLN:C	2.69	0.46
2:C:72:ARG:HH11	2:C:112:GLU:CD	2.17	0.46
3:D:631:ILE:HD11	3:D:743:ASP:CB	2.45	0.46
3:D:560:GLN:O	3:D:561:GLY:C	2.54	0.46
2:C:1099:VAL:HG22	3:D:10:ILE:CD1	2.42	0.46
3:D:1339:LYS:HD2	3:D:1339:LYS:HA	1.58	0.46
3:D:149:LYS:O	3:D:152:LEU:N	2.48	0.46
2:C:609:THR:HG23	2:C:609:THR:O	2.14	0.46
3:D:1290:LEU:O	3:D:1291:SER:C	2.54	0.46
3:D:855:HIS:N	3:D:855:HIS:CD2	2.66	0.46
2:C:100:LEU:HD23	2:C:372:LEU:CD1	2.45	0.46
2:C:437:ARG:O	2:C:437:ARG:HG3	2.14	0.46
2:C:461:VAL:O	2:C:481:GLU:HG2	2.16	0.46
3:D:709:HIS:HA	3:D:1227:GLU:CD	2.36	0.46
3:D:1273:VAL:O	3:D:1322:GLY:HA3	2.15	0.46
3:D:695:ILE:HG23	3:D:718:PRO:HD2	1.96	0.46
3:D:701:LEU:CD1	3:D:715:ALA:HB2	2.44	0.46
4:E:78:ASN:O	4:E:79:LEU:HB2	2.15	0.46
2:C:727:PRO:O	2:C:729:LEU:N	2.48	0.46
3:D:552:ASN:O	3:D:556:LYS:N	2.49	0.46
2:C:1108:PRO:O	2:C:1109:VAL:O	2.33	0.46
2:C:672:VAL:HG22	2:C:868:ASP:CG	2.36	0.46
3:D:660:LYS:O	3:D:664:LYS:N	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:15:SER:O	4:E:17:TYR:N	2.49	0.46
3:D:773:ALA:O	3:D:774:SER:CB	2.64	0.46
3:D:772:PRO:CB	3:D:778:LEU:HD23	2.46	0.46
2:C:460:ARG:CA	2:C:468:ARG:O	2.63	0.46
2:C:549:PHE:HA	2:C:551:GLU:OE1	2.15	0.46
2:C:641:PRO:HA	2:C:656:ALA:HA	1.96	0.46
3:D:1114:THR:CB	3:D:1189:ARG:HH11	2.27	0.46
2:C:258:PHE:N	2:C:258:PHE:CD1	2.83	0.46
2:C:186:VAL:HG11	2:C:258:PHE:HD2	1.79	0.46
1:A:30:ARG:HH11	1:A:192:LEU:HD23	1.80	0.46
1:B:211:LEU:C	1:B:215:VAL:HG23	2.33	0.46
3:D:1156:LEU:HB3	3:D:1173:PHE:CE1	2.50	0.46
3:D:99:ALA:HB3	3:D:458:ALA:CB	2.45	0.46
2:C:494:TYR:O	2:C:495:THR:CB	2.62	0.46
3:D:654:LYS:O	3:D:655:PRO:C	2.51	0.46
3:D:1089:ALA:C	3:D:1091:SER:H	2.19	0.46
2:C:684:PHE:O	2:C:686:ASP:N	2.49	0.46
2:C:946:ARG:CD	2:C:984:GLU:HB2	2.45	0.46
2:C:358:ARG:HB2	2:C:372:LEU:CD2	2.45	0.46
2:C:351:LEU:HA	2:C:377:PRO:HG3	1.98	0.46
2:C:1639:GLN:HG2	2:C:658:GLY:HA2	1.97	0.46
3:D:1109:GLU:O	3:D:1202:GLN:CB	2.64	0.46
3:D:700:VAL:N	3:D:716:PHE:O	2.48	0.46
2:C:756:VAL:O	2:C:790:LEU:N	2.48	0.46
2:C:805:ARG:NE	2:C:821:GLU:OE2	2.38	0.46
1:B:101:LEU:HD23	1:B:140:MET:CE	2.45	0.46
3:D:1435:LEU:CD2	3:D:1457:ASP:OD2	2.64	0.46
4:E:48:MET:HE2	4:E:57:ASP:HB3	1.98	0.46
3:D:1472:ILE:O	3:D:1477:GLY:HA3	2.15	0.46
2:C:122:THR:HG22	2:C:123:GLU:N	2.30	0.46
1:A:105:GLY:HA2	1:A:136:GLY:N	2.30	0.46
2:C:395:LYS:CG	2:C:397:GLU:HG3	2.44	0.46
1:B:144:VAL:HG12	1:B:145:ASP:N	2.30	0.46
3:D:467:GLU:O	3:D:468:LEU:O	2.34	0.46
3:D:31(U):UNK:O	3:D:32(U):UNK:CB	2.62	0.46
3:D:794:GLN:OE1	3:D:906:GLN:NE2	2.49	0.46
2:C:1038:TRP:CH2	3:D:1096:ARG:HA	2.50	0.46
2:C:1055:ILE:HG22	2:C:1055:ILE:O	2.16	0.46
2:C:66:LEU:N	2:C:100:LEU:HA	2.30	0.46
3:D:1377:LYS:HE2	3:D:1378:TYR:CZ	2.51	0.46
3:D:937:TYR:N	3:D:937:TYR:HD1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:760:ARG:NH2	4:E:3:GLU:OE2	2.38	0.46
2:C:143:SER:O	2:C:147:TYR:OH	2.27	0.46
1:A:30:ARG:NH1	1:A:192:LEU:CD2	2.79	0.46
1:A:194:LYS:HG2	1:A:194:LYS:O	2.16	0.46
1:B:22:GLU:O	1:B:23:PHE:HD2	1.98	0.46
1:A:198:ARG:NH2	2:C:932:GLU:OE1	2.32	0.46
2:C:525:ALA:O	2:C:527:GLU:N	2.48	0.46
2:C:816:LYS:O	2:C:819:VAL:HB	2.15	0.46
3:D:28:LYS:O	3:D:30:GLU:N	2.49	0.46
3:D:548:ILE:O	3:D:552:ASN:ND2	2.49	0.46
3:D:98:PRO:CB	3:D:574:LEU:HD23	2.46	0.46
2:C:1014:SER:O	2:C:1018:GLN:OE1	2.34	0.46
2:C:969:LEU:HD11	3:D:952:ASP:N	2.22	0.46
2:C:813:VAL:HG12	2:C:815:LEU:CG	2.46	0.46
2:C:912:PRO:O	2:C:915:LYS:HB2	2.16	0.46
3:D:23(U):UNK:CB	3:D:43(U):UNK:N	2.79	0.46
3:D:1166:LEU:HB2	3:D:1170:ASP:HB2	1.96	0.46
2:C:1059:ASP:HA	2:C:1083:GLU:CG	2.46	0.46
2:C:340:MET:SD	2:C:340:MET:O	2.73	0.46
2:C:682:TYR:CE1	2:C:851:LYS:HD2	2.51	0.46
3:D:1277:ILE:O	3:D:1317:ASP:O	2.33	0.46
1:A:74:ASP:OD1	1:A:76:VAL:HG23	2.16	0.46
2:C:12:VAL:CG1	2:C:13:ILE:H	1.96	0.46
2:C:462:ASP:O	2:C:464:LEU:N	2.48	0.46
3:D:1057:VAL:HG12	3:D:1067:VAL:HG21	1.98	0.46
4:E:26:ARG:NH2	4:E:30:LEU:HD12	2.30	0.46
4:E:26:ARG:HH22	4:E:37:ASN:CB	2.29	0.46
2:C:252:LYS:HE3	2:C:298:PHE:CE1	2.51	0.46
1:A:184:THR:HG23	1:A:184:THR:O	2.15	0.46
1:B:30:ARG:NH2	2:C:854:PRO:HB3	2.31	0.46
2:C:787:ASP:O	2:C:789:SER:N	2.49	0.46
3:D:1449:GLU:O	3:D:1452:ILE:N	2.49	0.46
2:C:672:VAL:HG13	2:C:673:LEU:N	2.31	0.46
3:D:968:ASP:HA	3:D:971:LEU:HD12	1.96	0.46
3:D:1084:THR:C	3:D:1086:LEU:N	2.69	0.46
3:D:6(U):UNK:CB	3:D:36(U):UNK:HA	2.46	0.46
3:D:75:ARG:O	3:D:77:ALA:N	2.49	0.46
3:D:538:SER:O	3:D:539:ASP:C	2.55	0.46
3:D:1441:GLN:O	3:D:1442:ASN:HB3	2.16	0.46
3:D:1489:GLN:CB	4:E:72:ARG:HD2	2.46	0.46
3:D:836:VAL:HB	3:D:858:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:26:ARG:HH21	4:E:30:LEU:CD1	2.29	0.46
2:C:197:LEU:HD22	2:C:202:TYR:CD1	2.43	0.46
1:A:164:ALA:O	1:A:165:ILE:HG12	2.15	0.46
1:B:26:GLU:CG	1:B:27:PRO:HD3	2.45	0.46
3:D:520:LEU:HB3	3:D:521:PRO:HD2	1.97	0.46
1:B:99:LEU:HD13	1:B:114:PHE:CD2	2.51	0.46
3:D:642:CYS:SG	3:D:702:LEU:CD2	3.04	0.46
1:A:125:PRO:O	1:A:126:ASP:C	2.52	0.46
3:D:1454:GLY:O	3:D:1455:LYS:HB2	2.15	0.46
3:D:1485:GLN:HA	4:E:75:PHE:HA	1.98	0.46
1:B:64:GLU:O	1:B:75:VAL:HG21	2.16	0.46
3:D:1278:ASP:CA	3:D:1317:ASP:O	2.64	0.46
3:D:859:ASP:C	3:D:861:GLN:H	2.19	0.46
3:D:901:GLN:O	3:D:905:PRO:HD3	2.16	0.46
2:C:94:LEU:HD21	2:C:344:PHE:HZ	1.81	0.46
2:C:599:GLU:O	2:C:600:ASP:O	2.33	0.46
2:C:570:PRO:CG	2:C:635:THR:HG23	2.46	0.46
2:C:640:ARG:O	2:C:657:ASP:N	2.49	0.46
2:C:679:PHE:HE2	2:C:978:ARG:NH2	2.14	0.46
3:D:709:HIS:CE1	3:D:1231:GLU:HG3	2.51	0.46
3:D:1347:TYR:CE1	3:D:1351:GLU:HB2	2.51	0.46
3:D:957:PRO:CG	3:D:1007:VAL:HB	2.45	0.46
2:C:162:ILE:N	2:C:162:ILE:HD12	2.31	0.46
2:C:203:ASP:O	2:C:204:GLN:C	2.55	0.46
3:D:690:ALA:O	3:D:693:GLU:N	2.43	0.46
2:C:474:VAL:HG12	2:C:474:VAL:O	2.16	0.46
2:C:737:LEU:O	2:C:738:ASP:C	2.53	0.46
1:B:101:LEU:HD11	1:B:113:ASP:HB2	1.98	0.46
3:D:1485:GLN:CB	4:E:75:PHE:HB3	2.46	0.46
3:D:989:TYR:C	3:D:991:GLN:H	2.18	0.46
2:C:684:PHE:O	2:C:685:GLU:HB2	2.16	0.46
3:D:75:ARG:C	3:D:77:ALA:H	2.19	0.46
3:D:791:TYR:CE1	3:D:1023:MET:HG3	2.51	0.45
3:D:836:VAL:HG11	3:D:858:LEU:HD11	1.98	0.45
2:C:589:ARG:NH1	2:C:596:TYR:CB	2.79	0.45
3:D:1007:VAL:HG13	3:D:1008:PHE:H	1.81	0.45
3:D:700:VAL:CG2	3:D:718:PRO:HG3	2.46	0.45
3:D:937:TYR:CD1	3:D:937:TYR:N	2.84	0.45
2:C:172:ILE:CG2	2:C:173:ASP:N	2.79	0.45
2:C:306:THR:O	2:C:310:LEU:N	2.49	0.45
2:C:157:ARG:NH1	2:C:321:GLU:HG2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ILE:HD12	1:B:218:LEU:HB2	1.97	0.45
1:B:57:TYR:CD2	1:B:57:TYR:C	2.88	0.45
3:D:1165:TYR:CE2	3:D:1214:PRO:HB3	2.51	0.45
1:A:126:ASP:O	1:A:127:LEU:C	2.54	0.45
1:A:175:ARG:HB2	1:A:201:THR:CB	2.46	0.45
2:C:1099:VAL:O	2:C:1099:VAL:HG12	2.16	0.45
3:D:508:ARG:HB2	3:D:510:GLU:OE2	2.15	0.45
1:B:213:GLN:O	1:B:216:ALA:HB3	2.16	0.45
2:C:692:GLU:O	2:C:693:GLU:C	2.53	0.45
3:D:1475:GLY:HA2	4:E:17:TYR:CE2	2.51	0.45
3:D:1346:ARG:NH1	3:D:1369:GLU:OE2	2.50	0.45
2:C:937:ASP:O	2:C:939:ARG:N	2.48	0.45
2:C:1004:LYS:O	2:C:1005:MET:HB3	2.15	0.45
2:C:574:ALA:O	2:C:575:GLN:O	2.34	0.45
2:C:880:MET:O	2:C:881:ASN:O	2.33	0.45
2:C:540:PHE:CE1	2:C:906:PHE:HE1	2.34	0.45
3:D:1333:HIS:HE1	3:D:1421:LEU:HB3	1.80	0.45
3:D:638:LYS:CB	3:D:729:HIS:CE1	2.99	0.45
3:D:762:GLN:HE21	4:E:20:THR:CB	2.28	0.45
2:C:289:THR:HG23	2:C:302:VAL:O	2.16	0.45
2:C:321:GLU:O	2:C:322:VAL:C	2.54	0.45
1:A:24:VAL:HG22	1:A:196:THR:HB	1.98	0.45
3:D:678:GLU:C	3:D:680:GLN:N	2.69	0.45
3:D:1148:VAL:HG22	3:D:1163:GLY:O	2.17	0.45
2:C:1108:PRO:O	2:C:1109:VAL:C	2.55	0.45
2:C:8:ARG:C	2:C:494:TYR:OH	2.55	0.45
2:C:6:PHE:CD2	2:C:909:ALA:HA	2.52	0.45
3:D:772:PRO:HG3	3:D:778:LEU:HD23	1.99	0.45
2:C:351:LEU:HG	2:C:352:ALA:N	2.31	0.45
2:C:380:ALA:O	2:C:384:GLU:CB	2.64	0.45
2:C:654:LEU:HG	2:C:655:LEU:N	2.32	0.45
3:D:1462:LEU:CD2	3:D:1473:PRO:HG2	2.46	0.45
3:D:729:HIS:ND1	3:D:730:PRO:HD2	2.30	0.45
2:C:218:VAL:O	2:C:219:GLN:C	2.54	0.45
2:C:257:LEU:HA	2:C:261:LEU:CD2	2.45	0.45
2:C:733:ALA:O	2:C:734:LEU:C	2.55	0.45
2:C:959:PRO:O	2:C:962:GLN:N	2.50	0.45
2:C:137:VAL:HG11	2:C:411:SER:HB2	1.97	0.45
3:D:632:VAL:HG12	3:D:633:VAL:N	2.30	0.45
3:D:1170:ASP:C	3:D:1172:HIS:N	2.70	0.45
3:D:78:VAL:N	3:D:81:THR:O	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:926:PHE:HE1	2:C:929:ARG:NH1	2.14	0.45
2:C:574:ALA:HB1	2:C:667:ALA:O	2.17	0.45
2:C:681:GLY:CA	3:D:939:PHE:CE2	2.99	0.45
2:C:881:ASN:HB2	3:D:1061:PHE:CE2	2.52	0.45
3:D:1065:LEU:HD12	3:D:1067:VAL:HG23	1.98	0.45
3:D:1075:HIS:N	3:D:1075:HIS:CD2	2.85	0.45
3:D:770:LEU:CD1	3:D:770:LEU:N	2.77	0.45
3:D:963:TYR:HE2	3:D:1002:LYS:HB3	1.81	0.45
4:E:63:TRP:O	4:E:67:GLU:N	2.41	0.45
2:C:152:PRO:O	2:C:153:ALA:O	2.35	0.45
2:C:215:GLY:O	2:C:216:ASP:C	2.54	0.45
1:A:17:GLY:O	1:A:18:ASP:HB2	2.16	0.45
2:C:762:LYS:HD2	2:C:786:LYS:CD	2.38	0.45
3:D:678:GLU:O	3:D:680:GLN:N	2.45	0.45
2:C:224:GLU:C	2:C:226:VAL:N	2.70	0.45
2:C:520:GLU:N	2:C:521:PRO:CD	2.80	0.45
1:A:121:GLU:C	1:A:123:MET:N	2.70	0.45
3:D:653:PHE:O	3:D:654:LYS:C	2.55	0.45
3:D:1237:THR:HG22	3:D:1239:ARG:H	1.81	0.45
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.98	0.45
1:A:50:GLY:HA3	1:A:171:PHE:O	2.15	0.45
3:D:153:LEU:C	3:D:155:ASP:H	2.19	0.45
3:D:1044:LEU:HD12	3:D:1044:LEU:HA	1.73	0.45
3:D:845:ASN:O	3:D:847:ASP:N	2.42	0.45
3:D:1283:ILE:CD1	3:D:1312:LEU:HA	2.47	0.45
2:C:64:LEU:HA	2:C:101:ILE:O	2.16	0.45
2:C:553:ASP:HA	2:C:882:LEU:HA	1.98	0.45
2:C:588:VAL:CG2	2:C:666:LEU:HD13	2.46	0.45
1:A:74:ASP:HB2	2:C:627:ARG:NH2	2.31	0.45
3:D:1069:GLU:C	3:D:1071:PHE:N	2.70	0.45
3:D:1271:LYS:O	3:D:1273:VAL:N	2.49	0.45
3:D:764:LEU:HG	3:D:766:ALA:N	2.29	0.45
1:B:173:PRO:HA	1:B:203:GLY:HA3	1.99	0.45
3:D:1118:ILE:HD11	3:D:1193:THR:CG2	2.46	0.45
3:D:1140:ILE:O	3:D:1144:LEU:N	2.49	0.45
3:D:631:ILE:HD11	3:D:743:ASP:HB2	1.97	0.45
3:D:1086:LEU:HD13	3:D:1238:MET:CB	2.38	0.45
3:D:1051:GLU:O	3:D:1052:THR:O	2.35	0.45
2:C:848:VAL:HG12	3:D:740:PHE:O	2.16	0.45
3:D:1130:ARG:NH1	3:D:1130:ARG:HG2	2.32	0.45
1:B:15:THR:C	1:B:17:GLY:H	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:92:HIS:O	3:D:94:GLU:N	2.50	0.45
3:D:601:ARG:HD2	3:D:605:ASP:OD2	2.16	0.45
2:C:374:ASN:O	2:C:376:ARG:HG2	2.17	0.45
2:C:630:ARG:HA	2:C:705:ILE:CD1	2.45	0.45
2:C:32:ALA:HB2	2:C:73:ILE:HD13	1.99	0.45
3:D:1106:VAL:HG12	3:D:1107:VAL:N	2.32	0.45
3:D:1268:PRO:HB2	3:D:1269:LYS:H	1.67	0.45
2:C:304:LEU:H	2:C:305:PRO:HD3	1.82	0.45
1:A:30:ARG:NH1	1:A:192:LEU:HD23	2.32	0.45
1:A:42:ARG:NH2	1:B:34:VAL:HB	2.26	0.45
3:D:91:ALA:CB	3:D:518:PRO:CG	2.95	0.45
1:A:126:ASP:OD1	1:A:126:ASP:N	2.49	0.45
3:D:1085:ALA:C	3:D:1087:ARG:H	2.19	0.45
2:C:406:HIS:ND1	2:C:406:HIS:O	2.50	0.45
2:C:78:PHE:N	2:C:78:PHE:CD1	2.83	0.45
1:B:12:THR:O	1:B:24:VAL:N	2.50	0.45
3:D:666:PHE:CZ	3:D:676:MET:SD	3.10	0.45
4:E:77:GLU:O	4:E:77:GLU:HG3	2.17	0.45
2:C:935:GLY:O	2:C:936:VAL:O	2.33	0.45
1:A:179:PHE:CD1	1:A:179:PHE:O	2.69	0.45
2:C:940:GLU:HA	2:C:973:VAL:CG2	2.45	0.45
3:D:860:LEU:HD12	3:D:878:GLY:CA	2.47	0.45
3:D:876:SER:O	3:D:878:GLY:N	2.50	0.45
2:C:33:ASP:O	2:C:33:ASP:CG	2.55	0.45
2:C:115:LEU:HD13	2:C:375:SER:CB	2.47	0.45
2:C:378:LEU:N	2:C:378:LEU:HD12	2.31	0.45
2:C:877:PRO:HG2	3:D:949:ILE:HD12	1.98	0.45
2:C:905:VAL:O	2:C:906:PHE:HB2	2.17	0.45
3:D:1352:ILE:O	3:D:1353:GLN:C	2.55	0.45
3:D:609:GLY:O	3:D:611:GLN:N	2.50	0.45
1:A:189:ARG:O	1:A:191:ASP:N	2.50	0.45
1:A:198:ARG:NH1	2:C:932:GLU:HB3	2.31	0.45
1:B:36:LEU:O	1:B:40:LEU:HD23	2.17	0.45
2:C:758:ARG:O	2:C:788:THR:O	2.35	0.45
3:D:1076:GLY:HA2	3:D:1079:LYS:HG2	1.97	0.45
3:D:106:LYS:O	3:D:109:PRO:N	2.50	0.45
3:D:1192:LEU:HG	3:D:1369:GLU:HB3	1.99	0.45
3:D:21:TRP:C	3:D:23:TYR:N	2.70	0.45
2:C:1035:MET:HB3	3:D:707:THR:HB	1.98	0.45
2:C:410:ILE:HG21	2:C:468:ARG:HH22	1.81	0.45
2:C:545:ASN:C	2:C:547:ILE:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:576:ALA:HB1	2:C:577:PRO:HD2	1.99	0.45
3:D:957:PRO:HG3	3:D:1007:VAL:CA	2.47	0.45
3:D:1060:SER:C	3:D:1062:ARG:N	2.69	0.45
3:D:1319:VAL:O	3:D:1320:GLU:C	2.54	0.45
3:D:695:ILE:HD13	3:D:718:PRO:HB2	1.98	0.45
2:C:299:LYS:O	2:C:299:LYS:CG	2.64	0.45
1:A:157:GLY:H	1:A:166:PRO:HB3	1.80	0.45
1:A:157:GLY:O	1:A:164:ALA:HB1	2.17	0.45
1:B:44:LEU:CG	1:B:199:ILE:HD11	2.43	0.45
1:A:173:PRO:O	1:A:202:ASP:CA	2.62	0.45
2:C:282:GLY:O	2:C:283:VAL:HG23	2.17	0.45
3:D:705:ALA:HB3	3:D:706:PRO:HD3	1.98	0.45
2:C:545:ASN:O	2:C:547:ILE:N	2.49	0.45
2:C:884:GLN:HG3	2:C:885:ILE:HD12	1.98	0.45
3:D:1266:ARG:C	3:D:1268:PRO:HD3	2.37	0.45
3:D:710:ARG:NH1	3:D:768:ASN:HD21	2.15	0.45
3:D:924:MET:N	4:E:7:ASP:OD2	2.50	0.45
2:C:202:TYR:C	2:C:203:ASP:CG	2.75	0.45
2:C:202:TYR:CE1	2:C:304:LEU:HD13	2.52	0.45
1:A:195:LEU:HD22	1:A:197:LEU:HD22	1.99	0.45
1:A:23:PHE:CZ	1:A:207:PRO:HB2	2.49	0.45
3:D:679:ARG:C	3:D:680:GLN:HG2	2.38	0.45
1:A:88:ARG:HD3	1:A:121:GLU:CD	2.37	0.45
2:C:246:ASP:O	2:C:248:PRO:HD3	2.17	0.45
3:D:511:TRP:CD1	3:D:511:TRP:N	2.84	0.45
3:D:1283:ILE:HD13	3:D:1312:LEU:CD2	2.47	0.45
2:C:491:GLU:HA	2:C:531:PHE:CA	2.21	0.45
2:C:491:GLU:O	2:C:510:THR:N	2.43	0.45
2:C:531:PHE:O	2:C:532:MET:CB	2.60	0.45
3:D:778:LEU:O	3:D:778:LEU:HD12	2.17	0.45
2:C:944:LEU:O	2:C:946:ARG:N	2.50	0.45
3:D:907:GLU:HG3	3:D:911:LEU:HD13	1.97	0.45
2:C:537:LYS:O	2:C:540:PHE:N	2.48	0.45
2:C:405:ARG:NH1	2:C:566:THR:OG1	2.48	0.45
2:C:840:ALA:CB	2:C:846:LYS:HA	2.47	0.45
3:D:1311:LEU:CD1	3:D:1311:LEU:H	2.29	0.45
3:D:1463:LYS:HA	3:D:1466:VAL:HB	1.99	0.45
3:D:924:MET:O	3:D:927:THR:N	2.49	0.45
3:D:924:MET:O	3:D:925:GLU:C	2.54	0.45
2:C:150:PRO:HD3	2:C:321:GLU:HB3	1.98	0.45
2:C:163:ILE:CG2	2:C:169:GLY:HA3	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:143:SER:OG	2:C:330:ASN:HA	2.17	0.45
1:A:225:PHE:CD2	1:B:11:PHE:CE1	3.05	0.45
1:B:188:GLN:HG2	3:D:688:TRP:HD1	1.77	0.45
3:D:1435:LEU:HD21	3:D:1468:LEU:CD2	2.47	0.45
2:C:674:VAL:HG21	2:C:871:LEU:HB2	1.99	0.45
3:D:1083:ASP:O	3:D:1086:LEU:CB	2.62	0.45
2:C:778:PHE:O	2:C:780:GLU:N	2.50	0.45
3:D:983:LEU:HA	3:D:983:LEU:HD23	1.73	0.45
1:B:94:MET:HE3	1:B:94:MET:CB	2.47	0.44
1:A:178:ALA:HB2	2:C:863:ASP:O	2.17	0.44
3:D:905:PRO:CG	3:D:906:GLN:N	2.80	0.44
2:C:1008:ARG:HH22	2:C:1020:PRO:HA	1.82	0.44
2:C:584:GLU:C	2:C:586:ARG:H	2.19	0.44
2:C:874:LEU:HD12	2:C:874:LEU:HA	1.66	0.44
3:D:1343:ALA:O	3:D:1344:VAL:C	2.55	0.44
3:D:638:LYS:O	3:D:639:LEU:O	2.34	0.44
1:B:19:HIS:HA	1:B:207:PRO:HG3	1.98	0.44
1:B:80:LEU:HD22	3:D:839:LEU:CB	2.48	0.44
4:E:9:LEU:C	4:E:11:GLY:H	2.20	0.44
3:D:663:GLU:C	3:D:665:ALA:N	2.69	0.44
2:C:691:SER:HB2	2:C:858:MET:HE2	1.98	0.44
3:D:1478:SER:O	3:D:1481:VAL:N	2.45	0.44
3:D:149:LYS:C	3:D:151:GLN:H	2.19	0.44
2:C:30:LEU:HD13	2:C:118:LEU:HD11	1.98	0.44
2:C:378:LEU:O	2:C:382:LEU:HB2	2.17	0.44
2:C:588:VAL:HG21	2:C:666:LEU:HA	1.99	0.44
2:C:641:PRO:HA	2:C:656:ALA:CB	2.47	0.44
2:C:677:MET:H	2:C:873:PRO:HD3	1.82	0.44
3:D:1007:VAL:HG11	3:D:1040:GLY:HA3	2.00	0.44
3:D:1094:LEU:HA	3:D:1094:LEU:HD12	1.63	0.44
3:D:1344:VAL:HG11	3:D:1421:LEU:HD11	1.99	0.44
3:D:890:VAL:HG13	3:D:926:LYS:CE	2.45	0.44
1:B:111:ALA:HA	1:B:114:PHE:CE1	2.52	0.44
1:B:99:LEU:O	1:B:141:GLU:HA	2.17	0.44
2:C:520:GLU:O	2:C:522:VAL:N	2.49	0.44
2:C:1104:GLU:HA	3:D:6:ARG:HG3	1.99	0.44
4:E:13:VAL:HB	4:E:18:ARG:HB3	1.99	0.44
2:C:897:LEU:O	2:C:899:GLN:HG3	2.17	0.44
2:C:23:VAL:C	2:C:25:SER:H	2.19	0.44
2:C:440:PRO:HD3	2:C:455:LEU:HA	1.96	0.44
2:C:493:ARG:NH2	3:D:1069:GLU:OE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1467:ILE:C	3:D:1469:GLY:H	2.20	0.44
3:D:792:ILE:N	3:D:792:ILE:CD1	2.79	0.44
3:D:948:THR:O	3:D:1020:LEU:CB	2.58	0.44
4:E:4:PRO:CG	4:E:66:LYS:HE2	2.47	0.44
2:C:182:VAL:HG12	2:C:193:LEU:CB	2.48	0.44
3:D:691:LEU:C	3:D:693:GLU:H	2.19	0.44
3:D:809:PRO:C	3:D:811:GLU:H	2.19	0.44
1:B:133:GLU:C	1:B:135:GLY:H	2.21	0.44
1:A:111:ALA:N	1:A:129:ILE:HG12	2.31	0.44
3:D:1400:VAL:HG12	3:D:1400:VAL:O	2.17	0.44
3:D:84:ILE:O	3:D:85:VAL:CB	2.65	0.44
2:C:103:LYS:HA	2:C:103:LYS:HD3	1.85	0.44
2:C:1070:ILE:HD12	2:C:1070:ILE:N	2.32	0.44
2:C:544:THR:O	2:C:545:ASN:C	2.54	0.44
1:A:74:ASP:OD2	2:C:627:ARG:NH2	2.50	0.44
3:D:947:ILE:HA	3:D:1020:LEU:HD13	1.99	0.44
1:A:160:ASP:O	1:A:161:ARG:C	2.55	0.44
1:A:185:ARG:NH2	1:A:194:LYS:CE	2.80	0.44
1:A:26:GLU:HB3	1:A:27:PRO:HD2	1.88	0.44
2:C:527:GLU:O	2:C:529:VAL:N	2.50	0.44
2:C:729:LEU:CB	2:C:734:LEU:HD21	2.48	0.44
2:C:754:ILE:HD13	2:C:791:ARG:NE	2.33	0.44
2:C:722:ILE:HD13	2:C:821:GLU:OE1	2.17	0.44
2:C:520:GLU:C	2:C:522:VAL:N	2.69	0.44
3:D:960:LYS:O	3:D:961:GLN:C	2.56	0.44
2:C:394:PHE:HB2	7:C:1640:RFP:O8	2.18	0.44
3:D:43(U):UNK:O	3:D:44(U):UNK:CB	2.66	0.44
2:C:413:LEU:HD11	2:C:448:ASN:OD1	2.17	0.44
3:D:22:SER:C	3:D:24:GLY:H	2.21	0.44
3:D:1133:ARG:HG3	3:D:1134:LEU:N	2.31	0.44
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.52	0.44
3:D:853:VAL:HG21	3:D:877:PRO:HB3	1.99	0.44
3:D:864:VAL:CG1	3:D:874:GLU:O	2.66	0.44
2:C:15:LEU:HD21	2:C:461:VAL:HG23	1.94	0.44
2:C:341:ALA:O	2:C:344:PHE:N	2.45	0.44
2:C:328:LEU:HB3	2:C:467:ILE:HG21	1.98	0.44
2:C:605:LYS:HA	2:C:612:ALA:N	2.30	0.44
2:C:648:ARG:HH11	2:C:648:ARG:CG	2.27	0.44
2:C:669:GLY:HA3	2:C:995:MET:HA	1.98	0.44
2:C:73:ILE:CD1	2:C:94:LEU:HD13	2.48	0.44
3:D:1047:LYS:CA	3:D:1053:PHE:CE1	2.92	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1353:GLN:O	3:D:1354:LYS:C	2.55	0.44
3:D:1461:GLY:N	3:D:1464:GLU:OE1	2.47	0.44
2:C:202:TYR:CB	2:C:207:LEU:HD13	2.47	0.44
2:C:267:TYR:HD1	2:C:273:GLY:HA3	1.81	0.44
1:A:43:ILE:O	1:A:44:LEU:C	2.56	0.44
1:B:29:GLU:O	1:B:30:ARG:C	2.55	0.44
2:C:520:GLU:O	2:C:521:PRO:C	2.55	0.44
3:D:98:PRO:O	3:D:514:LEU:HD13	2.18	0.44
1:A:82:LEU:HD23	1:A:129:ILE:HD12	1.98	0.44
2:C:8:ARG:HB3	2:C:494:TYR:OH	2.18	0.44
2:C:9:ILE:O	2:C:10:ARG:HB3	2.18	0.44
1:B:169:ALA:HB1	1:B:171:PHE:CE1	2.52	0.44
2:C:445:GLU:HG3	7:C:1640:RFP:C30	2.47	0.44
4:E:22:VAL:HG21	4:E:75:PHE:CD2	2.52	0.44
2:C:79:SER:O	2:C:82:GLU:HB3	2.16	0.44
2:C:121:MET:HA	2:C:126:SER:O	2.17	0.44
3:D:984:THR:O	3:D:988:ARG:N	2.48	0.44
3:D:633:VAL:CG2	3:D:634:GLY:N	2.80	0.44
3:D:776:GLU:HB3	3:D:777:PRO:HD2	1.98	0.44
3:D:879:ARG:NH1	3:D:904:VAL:HG13	2.32	0.44
3:D:911:LEU:HA	3:D:911:LEU:HD12	1.85	0.44
2:C:569:VAL:HA	2:C:570:PRO:HD2	1.77	0.44
2:C:605:LYS:CG	2:C:606:VAL:H	2.30	0.44
2:C:606:VAL:O	2:C:607:ASP:HB2	2.18	0.44
3:D:1069:GLU:HG3	3:D:1072:ILE:CG1	2.48	0.44
3:D:1093:TYR:HE2	3:D:1097:LYS:CE	2.31	0.44
3:D:629:SER:HB3	3:D:726:ILE:CD1	2.47	0.44
3:D:641:GLN:HB3	3:D:719:VAL:CG2	2.46	0.44
4:E:63:TRP:O	4:E:64:ALA:C	2.56	0.44
1:A:164:ALA:O	1:A:165:ILE:C	2.56	0.44
1:A:221:HIS:HA	1:A:224:TYR:CE2	2.52	0.44
2:C:713:ARG:HH12	2:C:816:LYS:CG	2.31	0.44
2:C:895:TYR:HD2	2:C:896:PHE:CE1	2.36	0.44
2:C:959:PRO:CG	2:C:960:GLU:N	2.80	0.44
3:D:1304:LYS:CD	3:D:1304:LYS:N	2.80	0.44
3:D:772:PRO:CG	3:D:778:LEU:HD23	2.47	0.44
3:D:791:TYR:HE1	3:D:1023:MET:HG3	1.82	0.44
3:D:906:GLN:O	3:D:907:GLU:HB2	2.18	0.44
2:C:1021:LEU:O	2:C:1022:GLY:C	2.56	0.44
2:C:12:VAL:CG1	2:C:13:ILE:N	2.62	0.44
2:C:141:HIS:CE1	2:C:334:ARG:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:399:ASN:HD21	2:C:401:LEU:CB	2.27	0.44
2:C:584:GLU:H	2:C:584:GLU:HG3	1.31	0.44
2:C:613:VAL:H	2:C:621:VAL:HA	1.83	0.44
2:C:628:TYR:HE2	2:C:703:ILE:HD13	1.81	0.44
2:C:705:ILE:HA	2:C:828:ALA:HA	2.00	0.44
3:D:1047:LYS:HA	3:D:1053:PHE:CZ	2.49	0.44
3:D:1114:THR:HA	3:D:1189:ARG:HH11	1.83	0.44
3:D:1231:GLU:O	3:D:1233:GLY:N	2.51	0.44
4:E:32:ARG:HG3	4:E:33:HIS:N	2.32	0.44
1:A:18:ASP:O	1:A:19:HIS:CB	2.66	0.44
1:A:225:PHE:HD2	1:B:11:PHE:CE1	2.36	0.44
3:D:88:TYR:C	3:D:520:LEU:CD1	2.85	0.44
1:A:201:THR:HG22	1:A:202:ASP:N	2.31	0.44
2:C:236:VAL:CG2	2:C:250:LYS:HA	2.47	0.44
2:C:688:ILE:CG2	2:C:869:VAL:HG23	2.48	0.44
3:D:1125:MET:HG2	3:D:1126:ASP:H	1.81	0.44
2:C:835:VAL:HG13	2:C:850:ALA:O	2.18	0.44
2:C:488:ALA:O	2:C:490:GLU:N	2.51	0.44
2:C:340:MET:C	2:C:340:MET:SD	2.96	0.44
1:B:160:ASP:O	1:B:162:ILE:N	2.50	0.44
3:D:143:ASP:O	3:D:145:VAL:N	2.51	0.44
2:C:714:ASP:O	2:C:715:THR:O	2.35	0.44
2:C:925:TYR:CE2	2:C:972:VAL:HG21	2.53	0.44
2:C:983:PHE:O	2:C:984:GLU:C	2.55	0.44
2:C:598:GLU:HB3	2:C:599:GLU:H	1.59	0.44
3:D:1236:LEU:HD12	3:D:1256:LEU:CD1	2.47	0.44
1:B:188:GLN:NE2	1:B:188:GLN:O	2.50	0.44
3:D:688:TRP:HE3	3:D:688:TRP:HA	1.82	0.44
3:D:680:GLN:C	3:D:681:ARG:HG3	2.38	0.44
3:D:1117:TYR:C	3:D:1118:ILE:HD12	2.38	0.44
1:A:86:VAL:HG13	1:A:123:MET:HB3	1.99	0.44
3:D:92:HIS:O	3:D:93:ILE:C	2.57	0.44
2:C:1038:TRP:CZ2	3:D:1096:ARG:HA	2.52	0.44
3:D:1047:LYS:HB3	3:D:1048:PRO:CD	2.45	0.44
3:D:1252:ILE:HG21	3:D:1261:GLU:OE1	2.18	0.44
3:D:1274:ILE:O	3:D:1275:SER:C	2.57	0.44
3:D:628:ARG:O	3:D:629:SER:HB2	2.18	0.44
4:E:3:GLU:HB3	4:E:4:PRO:HD2	1.99	0.44
2:C:172:ILE:HG22	2:C:173:ASP:N	2.32	0.44
3:D:896:ALA:HA	3:D:899:LEU:HD22	2.00	0.44
2:C:11:GLU:OE1	2:C:473:ARG:CD	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:11:GLU:OE1	2:C:473:ARG:CG	2.66	0.44
2:C:1088:LEU:HD23	3:D:1468:LEU:CD2	2.48	0.44
2:C:278:GLU:HA	2:C:283:VAL:HA	1.99	0.44
2:C:773:LEU:O	2:C:774:LEU:C	2.56	0.44
3:D:462:GLN:O	3:D:463:GLU:C	2.56	0.44
3:D:1220:ALA:O	3:D:1224:VAL:HG23	2.18	0.44
2:C:100:LEU:HD11	2:C:369:PRO:CD	2.46	0.43
2:C:64:LEU:N	2:C:101:ILE:O	2.51	0.43
2:C:881:ASN:HB2	3:D:1061:PHE:HE2	1.81	0.43
3:D:1251:ASP:N	3:D:1269:LYS:HZ2	1.84	0.43
2:C:710:ILE:CD1	2:C:710:ILE:N	2.74	0.43
2:C:738:ASP:HA	2:C:743:VAL:HA	2.00	0.43
2:C:754:ILE:O	2:C:754:ILE:HG22	2.18	0.43
1:B:59:GLU:OE1	1:B:60:ASP:N	2.50	0.43
3:D:564:GLU:HG3	3:D:568:ARG:NE	2.29	0.43
1:A:100:ILE:HG22	1:A:101:LEU:H	1.82	0.43
3:D:606:ILE:HD12	3:D:606:ILE:N	2.28	0.43
3:D:658:LEU:O	3:D:661:MET:N	2.51	0.43
1:B:95:ALA:O	1:B:96:SER:CB	2.60	0.43
2:C:343:GLN:HG2	2:C:385:PHE:HB2	2.00	0.43
2:C:794:PRO:HG2	2:C:1027:PHE:CB	2.48	0.43
2:C:104:ASP:N	2:C:104:ASP:OD1	2.50	0.43
3:D:1011:PHE:CE2	3:D:1022:VAL:CG1	3.01	0.43
3:D:905:PRO:CG	3:D:906:GLN:H	2.31	0.43
2:C:443:THR:O	2:C:444:PRO:O	2.36	0.43
2:C:54:ILE:HG13	2:C:55:GLU:O	2.18	0.43
2:C:626:ARG:CZ	2:C:637:PHE:CZ	3.00	0.43
2:C:836:GLY:C	2:C:837:ASP:OD2	2.55	0.43
3:D:1066:THR:C	3:D:1068:LEU:N	2.71	0.43
2:C:1042:ALA:CB	3:D:1227:GLU:OE1	2.66	0.43
3:D:931:LEU:HA	3:D:931:LEU:HD13	1.84	0.43
3:D:899:LEU:O	3:D:900:ILE:CG1	2.53	0.43
1:A:41:ARG:NH1	1:A:42:ARG:N	2.66	0.43
2:C:760:SER:OG	2:C:762:LYS:HG3	2.18	0.43
2:C:95:TYR:CD1	2:C:112:GLU:OE1	2.71	0.43
3:D:564:GLU:O	3:D:567:ILE:HG22	2.19	0.43
1:B:151:VAL:O	1:B:169:ALA:N	2.46	0.43
3:D:969:ARG:CZ	3:D:970:LYS:HE3	2.47	0.43
7:C:1640:RFP:N1	7:C:1640:RFP:N2	2.65	0.43
3:D:1192:LEU:HD21	3:D:1369:GLU:HA	2.00	0.43
3:D:851:LEU:O	3:D:851:LEU:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1034:GLU:HG3	2:C:1035:MET:N	2.33	0.43
2:C:380:ALA:O	2:C:384:GLU:N	2.38	0.43
2:C:605:LYS:HG2	2:C:606:VAL:N	2.33	0.43
3:D:1071:PHE:O	3:D:1075:HIS:HD2	2.01	0.43
3:D:1261:GLU:OE2	3:D:1268:PRO:HB3	2.18	0.43
3:D:1253:THR:HG21	3:D:1327:ARG:HG2	2.00	0.43
3:D:770:LEU:HD23	3:D:927:THR:CG2	2.49	0.43
4:E:40:LEU:HA	4:E:44:GLU:HG3	2.00	0.43
2:C:291:VAL:HB	2:C:299:LYS:O	2.19	0.43
3:D:899:LEU:N	3:D:899:LEU:CD1	2.78	0.43
3:D:805:ALA:O	3:D:806:PHE:CB	2.66	0.43
3:D:808:THR:O	3:D:809:PRO:O	2.36	0.43
2:C:85:GLU:O	2:C:806:LEU:HD11	2.18	0.43
3:D:513:ILE:CG2	3:D:514:LEU:N	2.81	0.43
4:E:9:LEU:C	4:E:11:GLY:N	2.72	0.43
3:D:816:TYR:HA	3:D:832:ARG:NH2	2.33	0.43
3:D:1292:VAL:CG2	3:D:1305:LEU:HD23	2.49	0.43
2:C:73:ILE:HD12	2:C:73:ILE:N	2.32	0.43
3:D:1235:GLN:C	3:D:1236:LEU:HD23	2.38	0.43
3:D:785:ILE:HD13	3:D:935:LYS:HA	2.00	0.43
4:E:25:LYS:HZ3	4:E:29:GLN:CD	2.21	0.43
2:C:203:ASP:H	2:C:207:LEU:HB2	1.83	0.43
1:A:165:ILE:O	1:A:165:ILE:CG1	2.60	0.43
1:B:11:PHE:HZ	1:B:211:LEU:HD21	1.83	0.43
1:A:222:LEU:HD21	1:B:218:LEU:HD23	2.00	0.43
3:D:687:VAL:O	3:D:688:TRP:C	2.56	0.43
1:A:86:VAL:HG13	1:A:86:VAL:O	2.18	0.43
3:D:1011:PHE:O	3:D:1013:GLU:N	2.51	0.43
2:C:1035:MET:HB2	2:C:1036:GLU:OE2	2.17	0.43
2:C:596:TYR:CD1	2:C:596:TYR:O	2.71	0.43
3:D:1331:ASP:C	3:D:1333:HIS:N	2.70	0.43
3:D:935:LYS:HG2	3:D:939:PHE:HD1	1.83	0.43
2:C:186:VAL:O	2:C:187:ASN:C	2.57	0.43
1:A:218:LEU:HD12	1:A:218:LEU:O	2.18	0.43
3:D:1175:ILE:O	3:D:1179:GLU:HG3	2.18	0.43
3:D:567:ILE:CA	3:D:570:GLU:HB2	2.49	0.43
2:C:236:VAL:CG1	2:C:248:PRO:O	2.67	0.43
1:B:214:ALA:HA	1:B:217:ILE:HG13	1.99	0.43
3:D:590:PRO:C	3:D:600:LEU:HD21	2.39	0.43
2:C:312:ALA:HB1	2:C:318:PRO:HG2	1.97	0.43
2:C:67:ASP:N	2:C:67:ASP:OD1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:491:GLU:CA	2:C:531:PHE:HA	2.21	0.43
2:C:398:THR:O	2:C:635:THR:HG21	2.19	0.43
2:C:539:VAL:HB	2:C:540:PHE:CD1	2.53	0.43
2:C:568:ALA:O	2:C:569:VAL:CG1	2.66	0.43
2:C:595:LEU:HD21	2:C:623:HIS:CB	2.47	0.43
3:D:1057:VAL:HG13	3:D:1067:VAL:HG11	2.01	0.43
3:D:1231:GLU:C	3:D:1233:GLY:H	2.21	0.43
3:D:1250:THR:HG22	3:D:1251:ASP:O	2.18	0.43
3:D:1323:GLN:H	3:D:1324:PRO:HD2	1.83	0.43
3:D:700:VAL:HG13	3:D:748:HIS:O	2.18	0.43
2:C:306:THR:HG22	2:C:307:LEU:N	2.34	0.43
1:B:133:GLU:HG2	1:B:134:GLU:N	2.33	0.43
3:D:1443:THR:O	3:D:1444:THR:C	2.57	0.43
2:C:724:ARG:C	2:C:726:ILE:HD12	2.38	0.43
2:C:428:ARG:O	2:C:429:ASP:HB2	2.18	0.43
3:D:669:ASN:O	3:D:672:ALA:N	2.50	0.43
3:D:1306:PRO:O	3:D:1308:ASP:N	2.52	0.43
2:C:944:LEU:C	2:C:946:ARG:N	2.71	0.43
3:D:853:VAL:O	3:D:854:ALA:O	2.35	0.43
3:D:836:VAL:CB	3:D:858:LEU:HD21	2.49	0.43
2:C:399:ASN:O	2:C:399:ASN:ND2	2.44	0.43
2:C:467:ILE:HG22	2:C:484:VAL:CG2	2.48	0.43
2:C:606:VAL:HG22	2:C:606:VAL:O	2.19	0.43
3:D:1258:ARG:HG3	3:D:1258:ARG:NH1	2.33	0.43
3:D:764:LEU:HD23	3:D:767:HIS:CD2	2.54	0.43
3:D:885:ILE:HG12	3:D:937:TYR:CD2	2.54	0.43
2:C:184:MET:HE2	2:C:196:LEU:HD22	1.99	0.43
1:A:28:LEU:O	1:A:192:LEU:HB3	2.19	0.43
1:B:188:GLN:HG3	3:D:688:TRP:HD1	1.84	0.43
3:D:806:PHE:N	3:D:827:ILE:HA	2.17	0.43
2:C:99:GLN:OE1	2:C:109:LYS:HE3	2.18	0.43
3:D:1480:PHE:HE2	4:E:15:SER:HB2	1.82	0.43
3:D:1481:VAL:HG12	4:E:21:VAL:HG21	1.98	0.43
2:C:15:LEU:CD1	2:C:461:VAL:HG21	2.37	0.43
2:C:89:THR:HA	2:C:130:ASN:H	1.84	0.43
3:D:1103:HIS:O	3:D:1105:ILE:HG12	2.19	0.43
4:E:38:THR:HG23	4:E:63:TRP:CZ3	2.53	0.43
2:C:163:ILE:CG2	2:C:265:LYS:HD2	2.48	0.43
1:B:177:VAL:HG13	1:B:199:ILE:CD1	2.49	0.43
2:C:788:THR:O	2:C:788:THR:HG23	2.19	0.43
2:C:1095:LEU:O	2:C:1096:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:491:LYS:HE2	3:D:495:ARG:HH21	1.84	0.43
2:C:84:ARG:HE	2:C:128:ILE:HG12	1.84	0.43
2:C:769:PRO:HG2	2:C:770:GLU:HG3	2.00	0.43
2:C:413:LEU:CD2	2:C:451:LEU:HD13	2.44	0.43
3:D:110:SER:O	3:D:112:ILE:N	2.48	0.43
3:D:916:TYR:C	3:D:918:ALA:N	2.72	0.43
1:A:71:VAL:HG22	1:A:132:LEU:HB3	2.00	0.43
1:B:61:VAL:O	1:B:62:LEU:O	2.36	0.43
2:C:974:LEU:HD23	2:C:987:ILE:HG21	2.01	0.43
2:C:110:GLU:HB2	2:C:369:PRO:HB2	2.00	0.43
2:C:648:ARG:CG	2:C:648:ARG:NH1	2.81	0.43
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.54	0.43
3:D:711:LEU:HD21	3:D:768:ASN:O	2.19	0.43
4:E:28:GLN:O	4:E:29:GLN:HB2	2.19	0.43
4:E:25:LYS:NZ	4:E:29:GLN:OE1	2.49	0.43
2:C:218:VAL:O	2:C:220:GLY:N	2.52	0.43
2:C:254:LEU:O	2:C:254:LEU:HD12	2.19	0.43
2:C:260:LEU:HD23	2:C:261:LEU:CB	2.45	0.43
3:D:483:HIS:N	3:D:484:PRO:CD	2.54	0.43
1:A:221:HIS:O	1:A:222:LEU:C	2.57	0.43
1:B:173:PRO:HA	1:B:203:GLY:CA	2.48	0.43
1:B:174:VAL:HG23	1:B:174:VAL:O	2.19	0.43
2:C:730:SER:CA	2:C:734:LEU:HD11	2.44	0.43
2:C:796:GLU:HA	3:D:681:ARG:NH2	2.33	0.43
1:B:70:GLY:O	1:B:132:LEU:HB2	2.18	0.43
2:C:967:PHE:C	2:C:969:LEU:H	2.22	0.43
2:C:5:ARG:NH2	2:C:10:ARG:NH1	2.66	0.43
2:C:397:GLU:HB2	2:C:632:ASN:HD22	1.83	0.43
3:D:15:PRO:O	3:D:19:ARG:HG3	2.19	0.43
3:D:793:THR:CA	3:D:879:ARG:HH12	2.31	0.43
3:D:901:GLN:O	3:D:903:ASP:N	2.52	0.43
2:C:631:SER:C	2:C:634:GLY:H	2.23	0.43
3:D:1114:THR:CB	3:D:1189:ARG:NH1	2.82	0.43
3:D:759:ALA:HA	3:D:763:MET:CG	2.47	0.43
2:C:148:PHE:HA	2:C:159:ILE:HA	2.01	0.43
2:C:182:VAL:HG11	2:C:307:LEU:HD11	2.01	0.43
2:C:205:GLU:OE2	2:C:209:ARG:HD2	2.19	0.43
1:B:41:ARG:HA	1:B:177:VAL:HG11	2.01	0.43
1:B:40:LEU:O	1:B:44:LEU:HD22	2.18	0.43
3:D:1154:GLU:O	3:D:1155:ALA:CB	2.63	0.43
3:D:1156:LEU:H	3:D:1182:GLU:CD	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:710:ILE:H	2:C:710:ILE:HD12	1.83	0.43
1:A:94:MET:HE1	1:A:119:ASP:HB2	1.95	0.43
3:D:952:ASP:C	3:D:954:ALA:N	2.71	0.43
1:B:171:PHE:O	1:B:172:SER:OG	2.33	0.43
3:D:1122:LEU:CD1	3:D:1186:VAL:HG23	2.49	0.43
2:C:424:GLY:O	2:C:427:VAL:HG23	2.18	0.43
3:D:472:LYS:O	3:D:473:LEU:C	2.58	0.43
3:D:772:PRO:CD	3:D:778:LEU:N	2.81	0.42
2:C:549:PHE:CE2	2:C:886:LEU:HB3	2.54	0.42
2:C:63:GLY:O	2:C:64:LEU:HB2	2.19	0.42
3:D:770:LEU:HD23	3:D:927:THR:HG21	2.00	0.42
3:D:936:TYR:C	3:D:936:TYR:HD2	2.22	0.42
3:D:957:PRO:HD3	3:D:1007:VAL:HG23	2.01	0.42
2:C:211:LEU:HG	2:C:212:SER:N	2.33	0.42
2:C:221:LEU:HG	2:C:221:LEU:O	2.18	0.42
2:C:310:LEU:O	2:C:313:LEU:N	2.44	0.42
1:A:162:ILE:CG2	1:A:163:ASN:H	2.30	0.42
3:D:694:VAL:O	3:D:696:HIS:N	2.52	0.42
2:C:745:ILE:C	2:C:747:ALA:N	2.71	0.42
2:C:754:ILE:CD1	2:C:791:ARG:NE	2.80	0.42
1:A:127:LEU:O	1:A:127:LEU:HG	2.19	0.42
2:C:953:VAL:HG12	2:C:954:SER:N	2.33	0.42
4:E:13:VAL:HG11	4:E:19:LEU:N	2.34	0.42
3:D:498:VAL:O	3:D:501:ALA:HB3	2.19	0.42
2:C:442:GLU:OE1	2:C:558:ALA:HB3	2.18	0.42
3:D:734:GLU:OE2	3:D:780:LYS:NZ	2.52	0.42
2:C:1112:PHE:O	2:C:1114:GLY:N	2.52	0.42
3:D:1303:TYR:O	3:D:1305:LEU:N	2.52	0.42
2:C:922:PHE:O	2:C:926:PHE:N	2.51	0.42
2:C:341:ALA:CB	2:C:345:ARG:HH12	2.32	0.42
2:C:676:ILE:N	2:C:676:ILE:HD12	2.33	0.42
3:D:1069:GLU:O	3:D:1070:TYR:C	2.58	0.42
3:D:1151:ARG:HA	3:D:1162:GLU:HG3	2.01	0.42
3:D:1252:ILE:HD12	3:D:1269:LYS:HB2	2.01	0.42
3:D:1275:SER:O	3:D:1319:VAL:HA	2.19	0.42
3:D:707:THR:HG23	3:D:712:GLY:HA3	2.00	0.42
3:D:752:SER:O	3:D:755:ALA:N	2.47	0.42
3:D:930:LEU:HD12	3:D:934:LEU:HG	2.01	0.42
2:C:164:PRO:CG	2:C:168:ARG:HG2	2.49	0.42
2:C:254:LEU:C	2:C:254:LEU:HD12	2.39	0.42
1:A:142:VAL:CG2	1:A:142:VAL:O	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:O	1:A:40:LEU:HG	2.19	0.42
1:B:34:VAL:O	1:B:36:LEU:N	2.52	0.42
1:B:76:VAL:O	1:B:79:ILE:HB	2.19	0.42
3:D:1149:LEU:HD23	3:D:1188:VAL:HG23	2.00	0.42
2:C:79:SER:OG	2:C:82:GLU:CB	2.64	0.42
3:D:468:LEU:C	3:D:470:LEU:H	2.21	0.42
2:C:1069:ALA:O	2:C:1075:ASP:O	2.37	0.42
1:A:118:ALA:O	1:A:120:VAL:N	2.48	0.42
2:C:739:GLU:O	2:C:739:GLU:HG3	2.19	0.42
3:D:795:VAL:CA	3:D:862:ASP:CB	2.97	0.42
3:D:907:GLU:O	3:D:908:LYS:CB	2.67	0.42
2:C:342:ASP:CA	2:C:345:ARG:HH11	2.32	0.42
2:C:348:LEU:C	2:C:350:ARG:N	2.71	0.42
2:C:349:ALA:O	2:C:350:ARG:HG3	2.20	0.42
2:C:515:ALA:CB	3:D:1069:GLU:OE2	2.67	0.42
2:C:574:ALA:O	2:C:669:GLY:O	2.37	0.42
2:C:74:GLY:O	2:C:75:ASP:C	2.57	0.42
3:D:1030:GLY:O	3:D:1031:ASN:CB	2.67	0.42
3:D:1004:THR:OG1	3:D:1036:ARG:HB2	2.19	0.42
3:D:1194:CYS:SG	3:D:1201:CYS:CB	3.06	0.42
3:D:1326:THR:O	3:D:1327:ARG:CB	2.65	0.42
3:D:1327:ARG:HG3	3:D:1327:ARG:O	2.19	0.42
3:D:1142:SER:C	3:D:1364:HIS:HD2	2.22	0.42
1:A:41:ARG:NE	2:C:860:HIS:CE1	2.85	0.42
2:C:816:LYS:HA	2:C:817:PRO:HD2	1.88	0.42
2:C:518:ARG:C	2:C:520:GLU:N	2.70	0.42
3:D:540:LEU:HD11	3:D:603:LEU:HD13	2.00	0.42
3:D:584:ASN:HB2	3:D:602:SER:HB3	2.01	0.42
2:C:1071:ILE:HD11	3:D:655:PRO:HB3	2.00	0.42
2:C:686:ASP:CG	3:D:739:ASP:OD2	2.57	0.42
3:D:1427:SER:C	3:D:1429:LEU:N	2.72	0.42
2:C:1059:ASP:HA	2:C:1083:GLU:HB2	2.01	0.42
1:B:183:ASP:HA	1:B:192:LEU:O	2.19	0.42
3:D:907:GLU:HB3	3:D:911:LEU:CD2	2.48	0.42
2:C:342:ASP:HA	2:C:345:ARG:HH11	1.83	0.42
2:C:547:ILE:HD12	2:C:550:LEU:HD13	2.00	0.42
2:C:603:VAL:O	2:C:604:VAL:CG2	2.66	0.42
2:C:676:ILE:H	2:C:676:ILE:HD12	1.84	0.42
3:D:1071:PHE:O	3:D:1072:ILE:C	2.56	0.42
3:D:1114:THR:CA	3:D:1189:ARG:HH11	2.32	0.42
3:D:937:TYR:O	3:D:938:GLY:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:26:ARG:NH2	4:E:30:LEU:HD13	2.35	0.42
4:E:64:ALA:O	4:E:68:LEU:N	2.52	0.42
2:C:268:ASP:HB2	2:C:269:LEU:H	1.54	0.42
1:A:63:HIS:HA	1:A:165:ILE:HG22	2.01	0.42
1:A:41:ARG:HG2	1:A:177:VAL:HG12	1.99	0.42
1:B:29:GLU:OE1	1:B:189:ARG:NH1	2.52	0.42
1:B:32:PHE:C	1:B:34:VAL:N	2.72	0.42
2:C:11:GLU:CD	2:C:473:ARG:NE	2.73	0.42
1:B:109:VAL:HG23	1:B:132:LEU:HD22	2.01	0.42
1:B:101:LEU:N	1:B:140:MET:O	2.52	0.42
2:C:517:ARG:CG	2:C:518:ARG:N	2.82	0.42
3:D:586:ARG:C	3:D:587:ARG:HD3	2.40	0.42
3:D:1471:LEU:O	3:D:1472:ILE:C	2.57	0.42
2:C:122:THR:HG22	2:C:123:GLU:H	1.83	0.42
3:D:632:VAL:CG1	3:D:633:VAL:N	2.81	0.42
2:C:923:ASN:N	2:C:924:LEU:HD23	2.35	0.42
2:C:534:VAL:N	2:C:538:GLN:HE22	2.17	0.42
2:C:549:PHE:CD1	2:C:886:LEU:O	2.71	0.42
3:D:1258:ARG:HH11	3:D:1258:ARG:HG3	1.84	0.42
3:D:1329:ALA:O	3:D:1330:ILE:C	2.57	0.42
3:D:1336:LEU:CD1	3:D:1340:GLY:C	2.88	0.42
3:D:1378:TYR:CD1	3:D:1378:TYR:N	2.88	0.42
3:D:609:GLY:HA2	3:D:615:ARG:NE	2.34	0.42
3:D:722:GLU:HB3	3:D:723:GLY:H	1.48	0.42
2:C:193:LEU:HD13	2:C:193:LEU:C	2.39	0.42
2:C:261:LEU:CD1	2:C:263:ASP:HB3	2.47	0.42
1:A:143:ARG:NH1	1:A:145:ASP:OD1	2.52	0.42
1:A:13:ALA:O	1:B:230:ALA:CB	2.68	0.42
1:B:202:ASP:O	1:B:204:SER:N	2.52	0.42
2:C:72:ARG:NE	2:C:95:TYR:HE1	2.17	0.42
1:B:73:GLU:HG3	1:B:77:GLU:HG2	2.01	0.42
3:D:558:LEU:HD21	3:D:567:ILE:CD1	2.49	0.42
2:C:9:ILE:O	2:C:10:ARG:CB	2.68	0.42
3:D:1476:THR:HG22	4:E:21:VAL:HG23	2.00	0.42
1:A:32:PHE:O	1:A:33:GLY:C	2.57	0.42
3:D:884:ARG:O	3:D:887:GLY:N	2.52	0.42
2:C:418:LEU:HG	2:C:418:LEU:O	2.19	0.42
2:C:1051:GLU:OE2	3:D:751:LEU:HB3	2.19	0.42
2:C:34:VAL:O	2:C:34:VAL:HG12	2.19	0.42
2:C:573:ARG:CG	2:C:573:ARG:HH11	2.29	0.42
2:C:586:ARG:O	2:C:587:VAL:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:613:VAL:CG2	2:C:619:ARG:HE	2.31	0.42
3:D:1201:CYS:SG	3:D:1204:CYS:HB2	2.60	0.42
3:D:1466:VAL:O	3:D:1467:ILE:C	2.57	0.42
3:D:935:LYS:HG2	3:D:939:PHE:CD1	2.54	0.42
4:E:6:ILE:HG22	4:E:10:PHE:CD1	2.54	0.42
4:E:38:THR:CG2	4:E:40:LEU:H	2.24	0.42
2:C:266:ARG:O	2:C:266:ARG:HG3	2.18	0.42
2:C:755:LEU:CD1	2:C:756:VAL:HG23	2.50	0.42
2:C:710:ILE:CG1	2:C:790:LEU:HB2	2.48	0.42
1:B:57:TYR:O	1:B:140:MET:HA	2.20	0.42
3:D:713:ILE:HG22	3:D:714:GLN:N	2.35	0.42
3:D:570:GLU:HA	3:D:573:MET:HE2	2.00	0.42
2:C:395:LYS:HG2	2:C:397:GLU:CD	2.40	0.42
1:B:206:THR:OG1	1:B:209:GLU:HG3	2.20	0.42
3:D:734:GLU:O	3:D:735:ALA:C	2.57	0.42
3:D:795:VAL:CG1	3:D:796:ARG:N	2.83	0.42
3:D:795:VAL:CG1	3:D:864:VAL:CG2	2.92	0.42
3:D:876:SER:O	3:D:879:ARG:N	2.53	0.42
3:D:905:PRO:CD	3:D:906:GLN:H	2.32	0.42
2:C:1055:ILE:HD11	2:C:1079:PRO:CG	2.49	0.42
2:C:561:GLY:HA3	2:C:842:ARG:O	2.20	0.42
2:C:603:VAL:HB	2:C:604:VAL:H	1.61	0.42
2:C:699:PHE:C	2:C:701:THR:H	2.22	0.42
3:D:953:ASP:OD1	3:D:1020:LEU:CG	2.66	0.42
3:D:638:LYS:O	3:D:639:LEU:C	2.55	0.42
3:D:729:HIS:CE1	3:D:935:LYS:HD3	2.54	0.42
3:D:953:ASP:OD1	3:D:1020:LEU:CB	2.68	0.42
3:D:999:THR:O	3:D:1000:THR:C	2.58	0.42
4:E:26:ARG:NH2	4:E:67:GLU:OE2	2.53	0.42
4:E:80:VAL:CB	4:E:81:PRO:CD	2.97	0.42
2:C:208:VAL:HG13	2:C:212:SER:OG	2.20	0.42
2:C:194:VAL:HG22	2:C:221:LEU:HD12	2.02	0.42
2:C:750:LYS:HE2	2:C:753:ASP:OD2	2.18	0.42
1:B:129:ILE:O	1:B:130:ALA:CB	2.68	0.42
1:A:90:LEU:HD21	1:A:121:GLU:OE2	2.20	0.42
2:C:985:GLY:O	2:C:986:PRO:C	2.57	0.42
2:C:1067:TYR:CE1	2:C:1071:ILE:HD11	2.55	0.42
3:D:654:LYS:HB3	3:D:655:PRO:CD	2.45	0.42
2:C:693:GLU:O	2:C:694:LEU:C	2.57	0.42
2:C:1113:GLU:C	2:C:1115:LEU:N	2.69	0.42
1:A:115:THR:CG2	1:A:115:THR:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:497:GLU:CG	3:D:1389:LEU:HD21	2.50	0.42
2:C:592:LEU:HA	2:C:592:LEU:HD23	1.80	0.42
2:C:772:ARG:HH11	2:C:776:SER:HB3	1.84	0.42
3:D:1276:GLU:HG3	3:D:1303:TYR:OH	2.20	0.42
3:D:876:SER:O	3:D:879:ARG:HG3	2.20	0.42
2:C:32:ALA:O	2:C:34:VAL:N	2.52	0.42
2:C:342:ASP:N	2:C:345:ARG:NH1	2.68	0.42
2:C:257:LEU:C	2:C:259:GLY:N	2.72	0.42
1:A:56:VAL:CG1	1:A:167:VAL:HG21	2.50	0.42
3:D:496:LEU:O	3:D:500:ARG:HB2	2.19	0.42
3:D:1145:TYR:CD2	3:D:1146:GLY:N	2.80	0.42
1:B:100:ILE:HG22	1:B:101:LEU:N	2.35	0.42
2:C:892:LEU:C	2:C:894:GLY:N	2.73	0.42
3:D:106:LYS:O	3:D:110:SER:N	2.53	0.42
3:D:1153:VAL:CG1	3:D:1153:VAL:O	2.64	0.42
3:D:984:THR:O	3:D:985:ASP:C	2.59	0.42
2:C:420:ARG:HD3	2:C:420:ARG:H	1.84	0.42
3:D:879:ARG:CZ	3:D:904:VAL:HG22	2.48	0.42
2:C:21:ILE:HD11	2:C:455:LEU:CD2	2.50	0.42
2:C:433:THR:HG21	3:D:1075:HIS:CD2	2.55	0.42
2:C:471:TYR:O	2:C:472:ARG:HG2	2.20	0.42
2:C:597:ALA:CA	2:C:614:ARG:HH11	2.26	0.42
2:C:885:ILE:HD12	2:C:885:ILE:N	2.34	0.42
3:D:1094:LEU:O	3:D:1097:LYS:N	2.53	0.42
3:D:732:VAL:HG22	3:D:769:LEU:HD11	2.01	0.42
2:C:874:LEU:CD1	3:D:787:LEU:HD22	2.47	0.42
1:A:25:LEU:HB3	1:A:26:GLU:H	1.61	0.42
1:B:21:GLY:O	1:B:23:PHE:CD2	2.73	0.42
2:C:892:LEU:HA	2:C:895:TYR:CB	2.50	0.42
3:D:964:LEU:O	3:D:965:GLU:HB3	2.20	0.42
2:C:897:LEU:O	2:C:898:GLY:C	2.58	0.42
1:B:159:LYS:O	1:B:161:ARG:N	2.40	0.42
3:D:69:GLU:O	3:D:70:ALA:CB	2.68	0.42
3:D:151:GLN:O	3:D:154:THR:N	2.53	0.42
2:C:822:VAL:HG12	2:C:822:VAL:O	2.19	0.42
2:C:1025:ALA:HB1	2:C:1026:GLN:NE2	2.35	0.42
3:D:1294:VAL:O	3:D:1301:LYS:N	2.53	0.42
2:C:937:ASP:OD1	2:C:939:ARG:CD	2.68	0.42
3:D:874:GLU:O	3:D:875:THR:O	2.38	0.42
2:C:34:VAL:O	2:C:35:PRO:C	2.58	0.42
2:C:358:ARG:HB2	2:C:372:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:415:PRO:O	2:C:416:GLY:C	2.58	0.42
2:C:332:ARG:NH1	2:C:465:GLY:O	2.53	0.42
2:C:539:VAL:HB	2:C:540:PHE:CE1	2.54	0.42
2:C:56:GLU:OE1	2:C:64:LEU:O	2.38	0.42
3:D:1108:ARG:O	3:D:1109:GLU:CG	2.65	0.42
3:D:710:ARG:HG3	3:D:711:LEU:N	2.35	0.42
3:D:638:LYS:CA	3:D:729:HIS:CD2	3.03	0.42
2:C:202:TYR:O	2:C:203:ASP:CG	2.58	0.42
2:C:252:LYS:HG2	2:C:256:TYR:HD1	1.83	0.42
2:C:148:PHE:CE1	2:C:309:TYR:HD2	2.38	0.42
1:A:27:PRO:HG2	1:A:27:PRO:O	2.19	0.42
2:C:278:GLU:O	2:C:283:VAL:HG22	2.19	0.42
2:C:421:GLU:O	2:C:423:ALA:N	2.53	0.42
4:E:54:LEU:O	4:E:55:TYR:CB	2.67	0.42
3:D:920:LEU:CD2	3:D:920:LEU:N	2.83	0.42
3:D:1011:PHE:C	3:D:1013:GLU:N	2.73	0.41
2:C:140:ILE:HD12	2:C:331:ARG:HD2	2.02	0.41
2:C:43:GLY:O	2:C:44:ILE:C	2.58	0.41
2:C:552:HIS:CD2	2:C:886:LEU:HD12	2.55	0.41
2:C:605:LYS:HD2	2:C:607:ASP:CG	2.40	0.41
2:C:873:PRO:CG	2:C:874:LEU:N	2.78	0.41
2:C:197:LEU:HD23	2:C:197:LEU:HA	1.92	0.41
2:C:200:LEU:HD21	2:C:290:LEU:HD22	2.02	0.41
1:B:222:LEU:O	1:B:223:ASN:C	2.57	0.41
1:B:41:ARG:HD3	1:B:41:ARG:C	2.40	0.41
2:C:728:HIS:C	2:C:730:SER:N	2.73	0.41
2:C:734:LEU:O	2:C:737:LEU:O	2.38	0.41
2:C:1105:LYS:C	2:C:1108:PRO:HD3	2.40	0.41
3:D:9:ARG:HA	3:D:1456:LYS:HA	2.02	0.41
3:D:583:ASP:OD1	3:D:604:THR:OG1	2.26	0.41
2:C:674:VAL:HG11	2:C:992:MET:HB2	2.02	0.41
3:D:1402:ALA:HB3	3:D:1415:VAL:HG11	2.01	0.41
3:D:974:ILE:CG2	3:D:975:GLU:N	2.83	0.41
3:D:1130:ARG:HG2	3:D:1130:ARG:HH11	1.85	0.41
1:B:15:THR:C	1:B:17:GLY:N	2.74	0.41
2:C:924:LEU:H	2:C:924:LEU:HD23	1.75	0.41
2:C:1020:PRO:O	2:C:1021:LEU:CG	2.68	0.41
2:C:355:VAL:CG1	2:C:356:ARG:N	2.83	0.41
2:C:560:MET:O	2:C:564:MET:HB2	2.20	0.41
2:C:614:ARG:CZ	2:C:623:HIS:HE1	2.33	0.41
2:C:575:GLN:C	2:C:667:ALA:HB1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:704:HIS:HD1	2:C:831:ARG:HD2	1.84	0.41
2:C:839:LEU:HD13	2:C:839:LEU:HA	1.76	0.41
3:D:1094:LEU:HB3	3:D:1095:THR:H	1.77	0.41
3:D:1110:ALA:O	3:D:1111:ASP:C	2.58	0.41
3:D:1436:SER:OG	3:D:1464:GLU:HG2	2.20	0.41
3:D:620:GLY:O	3:D:621:LYS:HG3	2.20	0.41
3:D:645:PRO:O	3:D:646:LYS:C	2.56	0.41
4:E:26:ARG:HD2	4:E:26:ARG:HA	1.79	0.41
2:C:167:LYS:O	2:C:168:ARG:HB2	2.19	0.41
3:D:496:LEU:CD1	3:D:500:ARG:HG2	2.48	0.41
1:B:109:VAL:HG23	1:B:132:LEU:CD2	2.49	0.41
2:C:224:GLU:O	2:C:227:LEU:N	2.46	0.41
2:C:521:PRO:O	2:C:522:VAL:C	2.58	0.41
3:D:566:ILE:O	3:D:570:GLU:HG3	2.20	0.41
3:D:962:ARG:O	3:D:966:GLU:HB2	2.19	0.41
2:C:137:VAL:CG2	2:C:406:HIS:HE1	2.33	0.41
2:C:769:PRO:C	2:C:771:GLU:N	2.74	0.41
1:B:51:THR:HA	1:B:145:ASP:O	2.19	0.41
3:D:471:GLU:HG3	3:D:471:GLU:O	2.20	0.41
3:D:887:GLY:C	3:D:889:ALA:H	2.23	0.41
3:D:12:LEU:HD12	3:D:12:LEU:HA	1.79	0.41
3:D:876:SER:H	3:D:879:ARG:CD	2.33	0.41
2:C:1001:VAL:O	2:C:1002:GLU:C	2.58	0.41
2:C:334:ARG:HA	2:C:338:GLU:OE2	2.20	0.41
2:C:542:LEU:HA	2:C:545:ASN:HD22	1.85	0.41
2:C:623:HIS:HA	2:C:624:PRO:HD3	1.89	0.41
3:D:963:TYR:CE2	3:D:1002:LYS:HB3	2.55	0.41
3:D:1331:ASP:O	3:D:1334:GLN:HB2	2.20	0.41
1:A:79:ILE:HG23	1:A:167:VAL:CG2	2.50	0.41
3:D:97:THR:O	3:D:571:LYS:CE	2.68	0.41
2:C:1023:GLY:O	2:C:1024:LYS:HG3	2.21	0.41
2:C:83:CYS:HB3	2:C:88:LEU:O	2.21	0.41
3:D:472:LYS:C	3:D:474:GLU:N	2.71	0.41
3:D:597:GLU:HG2	3:D:598:ARG:N	2.36	0.41
2:C:947:ALA:O	2:C:950:LEU:N	2.53	0.41
2:C:1034:GLU:HG3	2:C:1035:MET:H	1.86	0.41
2:C:30:LEU:O	2:C:31:GLN:C	2.58	0.41
2:C:333:ILE:HG22	2:C:333:ILE:O	2.19	0.41
3:D:1067:VAL:C	3:D:1069:GLU:N	2.74	0.41
3:D:1065:LEU:HD12	3:D:1067:VAL:CG2	2.50	0.41
3:D:1348:LEU:HD12	3:D:1348:LEU:HA	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1431:THR:HG23	3:D:1432:LYS:HG2	2.03	0.41
3:D:999:THR:O	3:D:1002:LYS:N	2.53	0.41
3:D:805:ALA:HB1	3:D:809:PRO:HD2	2.03	0.41
2:C:717:LEU:O	2:C:761:PHE:CB	2.68	0.41
2:C:758:ARG:HD3	2:C:788:THR:O	2.20	0.41
1:A:200:TRP:O	1:A:201:THR:O	2.38	0.41
3:D:1403:LEU:CG	3:D:1415:VAL:HB	2.46	0.41
3:D:965:GLU:O	3:D:968:ASP:CB	2.67	0.41
3:D:1192:LEU:CD1	3:D:1345:GLU:HB3	2.49	0.41
3:D:23:TYR:O	3:D:24:GLY:C	2.58	0.41
2:C:442:GLU:O	2:C:442:GLU:HG3	2.20	0.41
2:C:1112:PHE:C	2:C:1114:GLY:N	2.73	0.41
2:C:511:ASP:OD1	2:C:516:ARG:HB2	2.20	0.41
3:D:1282:ARG:HG2	3:D:1293:PHE:CB	2.44	0.41
3:D:794:GLN:O	3:D:795:VAL:CB	2.65	0.41
3:D:795:VAL:CG2	3:D:904:VAL:HG11	2.45	0.41
2:C:368:THR:O	2:C:371:LYS:HB2	2.21	0.41
2:C:115:LEU:HD11	2:C:378:LEU:HD22	2.01	0.41
2:C:588:VAL:HG21	2:C:666:LEU:HD13	2.02	0.41
2:C:657:ASP:HB3	2:C:658:GLY:H	1.46	0.41
2:C:575:GLN:HA	2:C:662:GLU:CD	2.40	0.41
2:C:679:PHE:C	2:C:681:GLY:N	2.73	0.41
3:D:710:ARG:NH2	3:D:1219:GLU:OE2	2.51	0.41
3:D:1394:VAL:HG11	3:D:1398:TRP:HE3	1.84	0.41
3:D:767:HIS:O	3:D:769:LEU:N	2.49	0.41
2:C:198:ARG:HG2	2:C:228:ALA:CA	2.37	0.41
2:C:218:VAL:C	2:C:220:GLY:N	2.73	0.41
3:D:891:GLY:H	3:D:926:LYS:NZ	2.17	0.41
3:D:1101:VAL:HG22	3:D:1424:VAL:O	2.20	0.41
3:D:809:PRO:O	3:D:811:GLU:N	2.53	0.41
2:C:806:LEU:O	2:C:821:GLU:HA	2.20	0.41
2:C:1085:PHE:CE1	3:D:1468:LEU:HD22	2.55	0.41
3:D:99:ALA:HB1	3:D:512:MET:O	2.20	0.41
2:C:1014:SER:O	2:C:1018:GLN:HA	2.20	0.41
2:C:889:HIS:O	2:C:891:GLY:N	2.53	0.41
3:D:1238:MET:HE3	3:D:1257:PRO:HG3	2.02	0.41
2:C:773:LEU:O	2:C:777:ILE:HG13	2.20	0.41
3:D:126:VAL:N	3:D:456:MET:CE	2.83	0.41
3:D:988:ARG:O	3:D:989:TYR:C	2.59	0.41
1:A:71:VAL:HA	1:A:132:LEU:HA	2.01	0.41
2:C:918:LEU:HD13	2:C:968:ASP:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:868:TYR:HA	3:D:871:ARG:O	2.20	0.41
1:B:122:ILE:HD12	1:B:122:ILE:N	2.35	0.41
1:B:110:ARG:C	1:B:112:VAL:H	2.23	0.41
3:D:904:VAL:HG12	3:D:906:GLN:NE2	2.36	0.41
2:C:29:ALA:O	2:C:44:ILE:HD13	2.20	0.41
2:C:648:ARG:NH1	2:C:653:ASP:HB3	2.35	0.41
3:D:956:ILE:HD11	3:D:1062:ARG:HB3	2.01	0.41
3:D:1113:GLY:O	3:D:1114:THR:O	2.38	0.41
1:B:128:HIS:HE1	1:B:131:THR:N	2.18	0.41
2:C:498:GLN:CB	2:C:503:LEU:H	2.34	0.41
3:D:1456:LYS:O	3:D:1457:ASP:C	2.58	0.41
4:E:47:LYS:CD	4:E:54:LEU:HD23	2.48	0.41
3:D:469:ASP:C	3:D:471:GLU:N	2.72	0.41
3:D:850:LEU:O	3:D:853:VAL:HB	2.20	0.41
2:C:1051:GLU:OE2	3:D:752:SER:OG	2.34	0.41
2:C:454:SER:O	2:C:455:LEU:HB2	2.21	0.41
2:C:460:ARG:N	2:C:468:ARG:O	2.54	0.41
2:C:550:LEU:HD23	2:C:905:VAL:CG1	2.51	0.41
3:D:1486:VAL:HG21	4:E:25:LYS:CE	2.50	0.41
3:D:697:GLY:O	3:D:760:ARG:NH1	2.53	0.41
3:D:626:SER:CB	3:D:748:HIS:HA	2.50	0.41
4:E:38:THR:HG22	4:E:39:VAL:H	1.84	0.41
2:C:147:TYR:O	2:C:148:PHE:CB	2.66	0.41
2:C:162:ILE:HG13	2:C:171:TRP:HZ3	1.77	0.41
2:C:202:TYR:O	2:C:203:ASP:OD2	2.39	0.41
2:C:216:ASP:O	2:C:218:VAL:N	2.54	0.41
1:B:174:VAL:CA	1:B:201:THR:HG22	2.48	0.41
3:D:521:PRO:CD	3:D:522:PRO:HD3	2.51	0.41
3:D:575:GLN:O	3:D:578:VAL:N	2.53	0.41
3:D:590:PRO:HA	3:D:600:LEU:CG	2.50	0.41
3:D:1079:LYS:C	3:D:1081:GLY:N	2.73	0.41
2:C:777:ILE:C	2:C:779:GLY:H	2.23	0.41
3:D:497:GLU:O	3:D:501:ALA:HB2	2.21	0.41
2:C:514:VAL:C	2:C:516:ARG:H	2.23	0.41
2:C:943:VAL:O	2:C:946:ARG:HB3	2.19	0.41
3:D:1011:PHE:CE2	3:D:1022:VAL:HG11	2.55	0.41
2:C:471:TYR:HB3	2:C:534:VAL:HG21	2.03	0.41
2:C:614:ARG:NH1	2:C:623:HIS:HE1	2.19	0.41
3:D:1321:ALA:C	3:D:1323:GLN:N	2.74	0.41
3:D:1141:GLU:OE1	3:D:1168:LEU:HD11	2.20	0.41
2:C:969:LEU:CD1	3:D:952:ASP:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:892:LEU:HA	2:C:895:TYR:HB2	2.03	0.41
2:C:959:PRO:HA	2:C:962:GLN:NE2	2.36	0.41
2:C:80:GLN:OE1	2:C:122:THR:HG23	2.21	0.41
3:D:659:LYS:O	3:D:662:GLU:HB3	2.20	0.41
3:D:1170:ASP:C	3:D:1172:HIS:H	2.24	0.41
1:B:205:VAL:HG13	1:B:209:GLU:OE1	2.20	0.41
1:A:14:THR:HG22	1:A:14:THR:O	2.21	0.41
3:D:1302:GLU:C	3:D:1303:TYR:CD1	2.94	0.41
3:D:776:GLU:H	3:D:776:GLU:HG2	1.47	0.41
3:D:1017:PHE:O	3:D:1018:ASN:C	2.58	0.41
3:D:879:ARG:CG	3:D:879:ARG:NH1	2.83	0.41
2:C:34:VAL:HG13	2:C:38:LYS:HG3	2.00	0.41
2:C:598:GLU:HG3	2:C:614:ARG:CZ	2.51	0.41
2:C:976:ASP:C	2:C:978:ARG:H	2.23	0.41
3:D:1007:VAL:C	3:D:1009:ASN:H	2.24	0.41
2:C:1052:MET:CE	3:D:748:HIS:HB3	2.50	0.41
4:E:26:ARG:CZ	4:E:67:GLU:OE2	2.68	0.41
2:C:13:ILE:HG23	2:C:14:PRO:N	2.36	0.41
2:C:352:ALA:C	2:C:355:VAL:HG12	2.41	0.41
2:C:432:ARG:CZ	3:D:1048:PRO:O	2.68	0.41
2:C:611:ILE:HD11	2:C:641:PRO:CB	2.51	0.41
2:C:841:ASN:ND2	2:C:842:ARG:N	2.69	0.41
3:D:1093:TYR:CE2	3:D:1097:LYS:HD2	2.56	0.41
3:D:1151:ARG:N	3:D:1162:GLU:HG3	2.35	0.41
3:D:701:LEU:HG	3:D:763:MET:CE	2.50	0.41
3:D:710:ARG:C	3:D:712:GLY:H	2.24	0.41
3:D:930:LEU:HD12	3:D:930:LEU:O	2.21	0.41
2:C:253:ALA:C	2:C:255:ALA:H	2.24	0.41
2:C:149:THR:CG2	2:C:150:PRO:HD2	2.50	0.41
2:C:313:LEU:HA	2:C:319:GLY:HA2	2.03	0.41
1:A:220:GLU:HA	1:A:223:ASN:HD22	1.85	0.41
1:A:43:ILE:O	1:A:46:SER:N	2.54	0.41
1:A:212:ASN:O	1:A:213:GLN:C	2.59	0.41
1:B:40:LEU:O	1:B:44:LEU:N	2.42	0.41
2:C:816:LYS:HD2	2:C:817:PRO:HG2	2.03	0.41
1:B:127:LEU:O	1:B:129:ILE:HG12	2.20	0.41
3:D:1382:THR:O	3:D:1383:ASP:C	2.58	0.41
3:D:631:ILE:HG21	3:D:745:MET:CE	2.47	0.41
3:D:1455:LYS:O	3:D:1456:LYS:HG2	2.21	0.41
3:D:1132:LEU:HD13	3:D:1184:ARG:NH1	2.20	0.41
2:C:695:LEU:O	2:C:696:LYS:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:137:VAL:HG23	2:C:393:GLN:HG3	2.03	0.41
2:C:445:GLU:HB3	2:C:446:GLY:H	1.67	0.41
4:E:75:PHE:N	4:E:75:PHE:CD1	2.89	0.41
3:D:816:TYR:HA	3:D:832:ARG:HH22	1.86	0.41
2:C:769:PRO:O	2:C:770:GLU:HB2	2.21	0.41
2:C:427:VAL:HG12	2:C:428:ARG:N	2.35	0.41
2:C:361:MET:O	2:C:362:GLY:O	2.39	0.41
3:D:989:TYR:O	3:D:991:GLN:N	2.53	0.41
1:B:205:VAL:CG1	1:B:206:THR:N	2.84	0.41
3:D:1137:ARG:N	3:D:1137:ARG:HD2	2.35	0.41
2:C:440:PRO:CD	2:C:455:LEU:N	2.80	0.41
2:C:705:ILE:CD1	2:C:705:ILE:N	2.84	0.41
3:D:1107:VAL:HG23	3:D:1221:VAL:HG23	2.03	0.41
3:D:1323:GLN:H	3:D:1324:PRO:CD	2.32	0.41
4:E:62:THR:O	4:E:63:TRP:C	2.58	0.41
2:C:152:PRO:HD2	2:C:158:TYR:HE2	1.84	0.41
1:A:198:ARG:HH22	2:C:932:GLU:CD	2.17	0.41
1:B:16:GLN:CB	1:B:20:TYR:HB3	2.51	0.41
2:C:750:LYS:HG2	2:C:753:ASP:OD1	2.21	0.41
3:D:558:LEU:C	3:D:560:GLN:N	2.73	0.41
3:D:976:GLN:C	3:D:978:TYR:N	2.71	0.41
3:D:782:SER:HA	3:D:786:ILE:HD11	2.03	0.41
2:C:1049:LEU:C	2:C:1051:GLU:H	2.24	0.40
2:C:1052:MET:HE3	2:C:1056:LYS:NZ	2.35	0.40
2:C:25:SER:O	2:C:28:LYS:HG2	2.20	0.40
2:C:566:THR:O	2:C:568:ALA:N	2.53	0.40
2:C:584:GLU:C	2:C:586:ARG:N	2.74	0.40
2:C:653:ASP:CG	2:C:653:ASP:O	2.60	0.40
3:D:1102:ALA:C	3:D:1103:HIS:O	2.59	0.40
2:C:151:ASP:N	2:C:157:ARG:HA	2.32	0.40
2:C:162:ILE:N	2:C:162:ILE:CD1	2.84	0.40
2:C:184:MET:CE	2:C:196:LEU:HD22	2.51	0.40
1:B:32:PHE:HA	1:B:35:THR:CB	2.51	0.40
3:D:675:ARG:CZ	3:D:675:ARG:HB2	2.50	0.40
3:D:1145:TYR:HA	3:D:1171:VAL:HG21	2.02	0.40
1:A:88:ARG:O	1:A:89:PHE:HD1	2.05	0.40
1:B:49:PRO:HB3	1:B:146:ARG:HH21	1.84	0.40
2:C:692:GLU:O	2:C:695:LEU:N	2.54	0.40
3:D:829:VAL:O	3:D:830:ALA:CB	2.69	0.40
2:C:935:GLY:O	2:C:936:VAL:C	2.60	0.40
2:C:1008:ARG:NH2	2:C:1020:PRO:CB	2.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:102:HIS:HB3	2:C:103:LYS:H	1.59	0.40
2:C:115:LEU:CD1	2:C:116:GLY:N	2.65	0.40
2:C:881:ASN:ND2	3:D:1034:GLN:CG	2.85	0.40
3:D:1066:THR:O	3:D:1067:VAL:C	2.59	0.40
3:D:1329:ALA:O	3:D:1330:ILE:O	2.39	0.40
3:D:709:HIS:CA	3:D:1227:GLU:HB3	2.51	0.40
2:C:216:ASP:C	2:C:218:VAL:H	2.24	0.40
2:C:222:LEU:O	2:C:223:ASP:C	2.60	0.40
1:A:187:GLY:HA3	1:A:192:LEU:HD11	2.03	0.40
1:B:223:ASN:O	1:B:224:TYR:C	2.60	0.40
2:C:734:LEU:HG	2:C:734:LEU:H	1.68	0.40
3:D:557:LEU:O	3:D:558:LEU:HG	2.21	0.40
3:D:655:PRO:O	3:D:656:PHE:C	2.58	0.40
4:E:15:SER:O	4:E:18:ARG:N	2.30	0.40
2:C:949:LYS:C	2:C:951:GLY:N	2.74	0.40
2:C:66:LEU:HB2	2:C:100:LEU:HB3	2.02	0.40
2:C:342:ASP:OD1	2:C:345:ARG:HD2	2.21	0.40
2:C:462:ASP:O	2:C:463:ALA:C	2.59	0.40
2:C:439:CYS:CB	2:C:468:ARG:NH1	2.84	0.40
2:C:840:ALA:CA	2:C:846:LYS:HA	2.52	0.40
3:D:1107:VAL:CG2	3:D:1215:VAL:HG11	2.43	0.40
3:D:733:CYS:O	3:D:737:ASN:N	2.47	0.40
3:D:767:HIS:C	3:D:769:LEU:H	2.24	0.40
2:C:182:VAL:CG1	2:C:307:LEU:HD11	2.51	0.40
1:A:12:THR:HG22	1:A:13:ALA:N	2.36	0.40
1:A:185:ARG:HH21	1:A:194:LYS:CE	2.32	0.40
3:D:694:VAL:C	3:D:696:HIS:N	2.73	0.40
2:C:498:GLN:CB	2:C:502:PRO:HA	2.52	0.40
1:A:122:ILE:O	1:A:123:MET:C	2.60	0.40
1:A:127:LEU:O	1:A:129:ILE:HG12	2.20	0.40
3:D:660:LYS:NZ	4:E:58:PRO:HG2	2.36	0.40
4:E:57:ASP:HA	4:E:58:PRO:HD3	1.84	0.40
3:D:958:GLU:C	3:D:960:LYS:H	2.23	0.40
2:C:124:ASP:OD1	2:C:407:LYS:NZ	2.39	0.40
3:D:776:GLU:HB3	3:D:912:LYS:HE2	2.02	0.40
1:A:178:ALA:HB2	2:C:864:GLY:CA	2.51	0.40
2:C:336:VAL:O	2:C:338:GLU:N	2.55	0.40
2:C:533:ASP:O	2:C:535:SER:N	2.54	0.40
2:C:552:HIS:O	2:C:553:ASP:C	2.59	0.40
2:C:875:GLY:CA	2:C:879:ARG:HD2	2.50	0.40
3:D:1258:ARG:C	3:D:1260:ILE:N	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1466:VAL:O	3:D:1469:GLY:CA	2.70	0.40
3:D:948:THR:HB	3:D:949:ILE:H	1.68	0.40
4:E:81:PRO:CG	4:E:84:ARG:HD2	2.49	0.40
2:C:207:LEU:HG	2:C:208:VAL:N	2.36	0.40
1:A:13:ALA:O	1:B:230:ALA:HB2	2.22	0.40
1:A:191:ASP:O	1:A:192:LEU:O	2.39	0.40
2:C:854:PRO:C	2:C:856:GLU:N	2.74	0.40
2:C:860:HIS:HD2	2:C:977:GLY:CA	2.34	0.40
2:C:729:LEU:CD1	2:C:791:ARG:NH2	2.85	0.40
2:C:750:LYS:CE	2:C:753:ASP:OD2	2.70	0.40
1:B:99:LEU:HB3	1:B:114:PHE:HD2	1.86	0.40
3:D:1457:ASP:OD1	3:D:1459:LEU:N	2.52	0.40
2:C:969:LEU:HD13	3:D:952:ASP:OD1	2.21	0.40
2:C:895:TYR:CD1	2:C:991:GLN:NE2	2.89	0.40
2:C:916:GLU:O	2:C:919:ALA:N	2.55	0.40
3:D:1153:VAL:HG11	3:D:1174:LEU:HD21	2.03	0.40
1:A:147:GLY:HA3	1:A:171:PHE:CZ	2.56	0.40
1:B:65:PHE:O	1:B:65:PHE:HD1	2.05	0.40
1:B:91:ASP:HA	1:B:92:PRO:HD3	1.96	0.40
2:C:535:SER:HA	2:C:536:PRO:HD3	1.91	0.40
2:C:580:MET:HB2	2:C:584:GLU:OE2	2.21	0.40
2:C:611:ILE:O	2:C:611:ILE:HG22	2.21	0.40
2:C:670:GLN:OE1	2:C:699:PHE:C	2.60	0.40
3:D:1232:PRO:HB3	3:D:1361:VAL:CG1	2.51	0.40
3:D:1431:THR:O	3:D:1432:LYS:CG	2.68	0.40
3:D:625:TYR:O	3:D:652:LEU:HD12	2.22	0.40
3:D:885:ILE:HD13	3:D:937:TYR:CD2	2.55	0.40
2:C:1078:GLU:CD	4:E:32:ARG:HH12	2.25	0.40
4:E:38:THR:CG2	4:E:63:TRP:HZ3	2.34	0.40
1:A:41:ARG:HD3	1:A:177:VAL:O	2.22	0.40
3:D:571:LYS:O	3:D:573:MET:N	2.53	0.40
2:C:1107:ASN:OD1	2:C:1107:ASN:O	2.40	0.40
3:D:121:THR:CB	3:D:461:ILE:HD11	2.51	0.40
2:C:9:ILE:HD13	2:C:494:TYR:CE1	2.57	0.40
1:B:178:ALA:CB	1:B:198:ARG:HE	2.28	0.40
3:D:1372:VAL:CG2	3:D:1375:MET:HE3	2.49	0.40
1:B:175:ARG:O	1:B:176:ARG:CB	2.69	0.40
3:D:1192:LEU:HD21	3:D:1369:GLU:CA	2.52	0.40
3:D:1425:THR:C	3:D:1427:SER:N	2.75	0.40
3:D:77:ALA:C	3:D:79:GLU:H	2.25	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	222/314 (71%)	111 (50%)	61 (28%)	50 (22%)	0	0
1	B	228/314 (73%)	123 (54%)	62 (27%)	43 (19%)	0	1
2	C	1111/1118 (99%)	591 (53%)	277 (25%)	243 (22%)	0	0
3	D	1126/1264 (89%)	588 (52%)	291 (26%)	247 (22%)	0	0
4	E	96/99 (97%)	50 (52%)	24 (25%)	22 (23%)	0	0
All	All	2783/3109 (90%)	1463 (53%)	715 (26%)	605 (22%)	0	0

All (605) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	19	HIS
1	A	26	GLU
1	A	59	GLU
1	A	73	GLU
1	A	92	PRO
1	A	105	GLY
1	A	107	LYS
1	A	113	ASP
1	A	125	PRO
1	A	143	ARG
1	A	144	VAL
1	A	153	ALA
1	A	158	ILE
1	A	162	ILE
1	A	176	ARG
1	A	187	GLY
1	A	192	LEU
1	A	201	THR
1	B	4	SER
1	B	5	LYS

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Mol	Chain	Res	Type
1	B	6	LEU
1	B	26	GLU
1	B	60	ASP
1	B	62	LEU
1	B	63	HIS
1	B	75	VAL
1	B	96	SER
1	B	126	ASP
1	B	138	LEU
1	B	156	HIS
1	B	158	ILE
1	B	160	ASP
1	B	161	ARG
1	B	176	ARG
1	B	204	SER
1	B	224	TYR
2	C	31	GLN
2	C	32	ALA
2	C	33	ASP
2	C	36	PRO
2	C	44	ILE
2	C	77	PRO
2	C	153	ALA
2	C	157	ARG
2	C	204	GLN
2	C	216	ASP
2	C	258	PHE
2	C	261	LEU
2	C	268	ASP
2	C	269	LEU
2	C	276	LYS
2	C	283	VAL
2	C	287	GLY
2	C	290	LEU
2	C	295	ASP
2	C	325	ILE
2	C	360	VAL
2	C	361	MET
2	C	375	SER
2	C	388	ARG
2	C	402	SER
2	C	416	GLY

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Mol	Chain	Res	Type
2	C	426	ASP
2	C	427	VAL
2	C	432	ARG
2	C	449	ILE
2	C	450	GLY
2	C	460	ARG
2	C	461	VAL
2	C	462	ASP
2	C	467	ILE
2	C	468	ARG
2	C	469	THR
2	C	476	ASN
2	C	477	GLY
2	C	479	VAL
2	C	480	THR
2	C	484	VAL
2	C	488	ALA
2	C	489	SER
2	C	495	THR
2	C	496	ILE
2	C	502	PRO
2	C	517	ARG
2	C	526	PRO
2	C	528	GLU
2	C	568	ALA
2	C	569	VAL
2	C	573	ARG
2	C	575	GLN
2	C	600	ASP
2	C	602	GLU
2	C	603	VAL
2	C	604	VAL
2	C	606	VAL
2	C	613	VAL
2	C	615	TYR
2	C	629	ALA
2	C	636	ALA
2	C	654	LEU
2	C	660	ALA
2	C	677	MET
2	C	680	ASP
2	C	700	TYR

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Mol	Chain	Res	Type
2	C	715	THR
2	C	730	SER
2	C	734	LEU
2	C	762	LYS
2	C	788	THR
2	C	791	ARG
2	C	796	GLU
2	C	811	PRO
2	C	821	GLU
2	C	832	LYS
2	C	837	ASP
2	C	840	ALA
2	C	876	VAL
2	C	881	ASN
2	C	887	GLU
2	C	936	VAL
2	C	943	VAL
2	C	973	VAL
2	C	992	MET
2	C	993	PHE
2	C	1001	VAL
2	C	1018	GLN
2	C	1021	LEU
2	C	1022	GLY
2	C	1034	GLU
2	C	1055	ILE
2	C	1080	SER
2	C	1104	GLU
2	C	1109	VAL
3	D	28	LYS
3	D	83	SER
3	D	84	ILE
3	D	85	VAL
3	D	86	ARG
3	D	93	ILE
3	D	98	PRO
3	D	104	PHE
3	D	112	ILE
3	D	113	ALA
3	D	127	LEU
3	D	130	ASN
3	D	133	ILE

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Mol	Chain	Res	Type
3	D	137	PRO
3	D	143	ASP
3	D	467	GLU
3	D	468	LEU
3	D	483	HIS
3	D	509	PRO
3	D	511	TRP
3	D	512	MET
3	D	513	ILE
3	D	515	GLU
3	D	539	ASP
3	D	564	GLU
3	D	583	ASP
3	D	584	ASN
3	D	587	ARG
3	D	610	LYS
3	D	638	LYS
3	D	657	LEU
3	D	658	LEU
3	D	680	GLN
3	D	682	ASP
3	D	689	ASP
3	D	705	ALA
3	D	709	HIS
3	D	722	GLU
3	D	725	SER
3	D	740	PHE
3	D	748	HIS
3	D	753	SER
3	D	774	SER
3	D	783	ARG
3	D	795	VAL
3	D	824	ASN
3	D	827	ILE
3	D	828	VAL
3	D	835	SER
3	D	838	ARG
3	D	839	LEU
3	D	854	ALA
3	D	856	GLY
3	D	869	LEU
3	D	875	THR

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Mol	Chain	Res	Type
3	D	892	ASP
3	D	902	MET
3	D	908	LYS
3	D	969	ARG
3	D	1015	TYR
3	D	1018	ASN
3	D	1028	ALA
3	D	1052	THR
3	D	1075	HIS
3	D	1076	GLY
3	D	1089	ALA
3	D	1111	ASP
3	D	1112	CYS
3	D	1114	THR
3	D	1137	ARG
3	D	1197	ARG
3	D	1203	LYS
3	D	1206	GLY
3	D	1268	PRO
3	D	1270	ALA
3	D	1271	LYS
3	D	1279	GLY
3	D	1281	VAL
3	D	1282	ARG
3	D	1307	LYS
3	D	1312	LEU
3	D	1313	VAL
3	D	1315	ASP
3	D	1317	ASP
3	D	1320	GLU
3	D	1322	GLY
3	D	1323	GLN
3	D	1325	LEU
3	D	1339	LYS
3	D	1364	HIS
3	D	1392	GLY
3	D	1403	LEU
3	D	1442	ASN
3	D	1472	ILE
3	D	1482	ARG
4	E	29	GLN
4	E	31	LEU

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Mol	Chain	Res	Type
4	E	34	ARG
4	E	35	PHE
4	E	43	GLU
4	E	51	LEU
4	E	55	TYR
4	E	80	VAL
4	E	94	PRO
1	A	14	THR
1	A	30	ARG
1	A	90	LEU
1	A	96	SER
1	A	123	MET
1	A	139	TYR
1	A	161	ARG
1	A	182	GLU
1	A	190	THR
1	A	200	TRP
1	A	224	TYR
1	B	35	THR
1	B	47	SER
1	B	105	GLY
1	B	107	LYS
1	B	116	PRO
1	B	119	ASP
1	B	120	VAL
1	B	130	ALA
1	B	152	PRO
1	B	195	LEU
1	B	196	THR
2	C	10	ARG
2	C	23	VAL
2	C	42	VAL
2	C	59	LYS
2	C	90	TYR
2	C	148	PHE
2	C	155	PRO
2	C	168	ARG
2	C	262	ALA
2	C	303	PHE
2	C	309	TYR
2	C	315	ALA
2	C	319	GLY

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Mol	Chain	Res	Type
2	C	320	HIS
2	C	322	VAL
2	C	362	GLY
2	C	435	TYR
2	C	444	PRO
2	C	474	VAL
2	C	482	GLU
2	C	524	VAL
2	C	529	VAL
2	C	534	VAL
2	C	546	LEU
2	C	567	GLN
2	C	581	THR
2	C	587	VAL
2	C	643	VAL
2	C	657	ASP
2	C	663	GLU
2	C	713	ARG
2	C	728	HIS
2	C	731	GLU
2	C	769	PRO
2	C	777	ILE
2	C	779	GLY
2	C	812	GLY
2	C	874	LEU
2	C	886	LEU
2	C	922	PHE
2	C	938	LYS
2	C	945	ALA
2	C	969	LEU
2	C	970	GLY
2	C	975	TYR
2	C	977	GLY
2	C	1002	GLU
2	C	1025	ALA
2	C	1059	ASP
2	C	1074	GLU
2	C	1110	ASP
3	D	9	ARG
3	D	22	SER
3	D	29	PRO
3	D	72	VAL

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Mol	Chain	Res	Type
3	D	76	CYS
3	D	78	VAL
3	D	87	ARG
3	D	89	ARG
3	D	95	LEU
3	D	111	LYS
3	D	126	VAL
3	D	144	ALA
3	D	150	ARG
3	D	453	ASP
3	D	561	GLY
3	D	567	ILE
3	D	590	PRO
3	D	613	ARG
3	D	617	ASN
3	D	643	GLY
3	D	668	PRO
3	D	730	PRO
3	D	733	CYS
3	D	747	VAL
3	D	773	ALA
3	D	784	ASP
3	D	799	LYS
3	D	806	PHE
3	D	822	ALA
3	D	825	ALA
3	D	855	HIS
3	D	858	LEU
3	D	917	GLN
3	D	935	LYS
3	D	946	GLY
3	D	983	LEU
3	D	995	LEU
3	D	1070	TYR
3	D	1103	HIS
3	D	1109	GLU
3	D	1130	ARG
3	D	1151	ARG
3	D	1155	ALA
3	D	1156	LEU
3	D	1200	VAL
3	D	1220	ALA

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Mol	Chain	Res	Type
3	D	1272	ALA
3	D	1291	SER
3	D	1304	LYS
3	D	1316	GLY
3	D	1324	PRO
3	D	1330	ILE
3	D	1354	LYS
3	D	1366	LYS
3	D	1367	HIS
3	D	1408	ILE
3	D	1470	ARG
4	E	16	LYS
4	E	70	THR
1	A	20	TYR
1	A	48	ILE
1	A	112	VAL
1	A	160	ASP
1	A	199	ILE
1	B	90	LEU
1	B	207	PRO
2	C	55	GLU
2	C	75	ASP
2	C	103	LYS
2	C	156	GLY
2	C	203	ASP
2	C	210	GLU
2	C	264	PRO
2	C	328	LEU
2	C	420	ARG
2	C	457	ALA
2	C	463	ALA
2	C	512	ARG
2	C	527	GLU
2	C	531	PHE
2	C	551	GLU
2	C	555	ALA
2	C	610	ARG
2	C	692	GLU
2	C	732	ALA
2	C	738	ASP
2	C	857	ASP
2	C	873	PRO

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Mol	Chain	Res	Type
2	C	875	GLY
2	C	966	LEU
2	C	986	PRO
2	C	998	TYR
2	C	1043	TYR
2	C	1061	GLU
2	C	1072	LYS
2	C	1105	LYS
2	C	1112	PHE
2	C	1113	GLU
3	D	11	ALA
3	D	125	GLN
3	D	486	ARG
3	D	507	ASN
3	D	543	LEU
3	D	652	LEU
3	D	711	LEU
3	D	714	GLN
3	D	734	GLU
3	D	768	ASN
3	D	793	THR
3	D	809	PRO
3	D	816	TYR
3	D	840	LYS
3	D	862	ASP
3	D	893	GLU
3	D	905	PRO
3	D	953	ASP
3	D	959	GLU
3	D	968	ASP
3	D	990	ASP
3	D	1090	ASP
3	D	1152	GLU
3	D	1251	ASP
3	D	1252	ILE
3	D	1283	ILE
3	D	1309	ALA
3	D	1319	VAL
3	D	1426	LYS
3	D	1452	ILE
3	D	1488	ASP
4	E	30	LEU

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Mol	Chain	Res	Type
1	A	67	THR
1	A	119	ASP
1	A	126	ASP
1	A	128	HIS
1	A	152	PRO
1	B	15	THR
1	B	202	ASP
2	C	9	ILE
2	C	51	THR
2	C	58	ASP
2	C	66	LEU
2	C	105	THR
2	C	149	THR
2	C	181	VAL
2	C	187	ASN
2	C	232	GLU
2	C	324	ASP
2	C	326	ASP
2	C	380	ALA
2	C	425	PHE
2	C	431	HIS
2	C	499	ALA
2	C	626	ARG
2	C	685	GLU
2	C	699	PHE
2	C	781	LYS
2	C	890	LEU
2	C	894	GLY
2	C	1012	PRO
2	C	1044	GLY
3	D	522	PRO
3	D	599	PRO
3	D	629	SER
3	D	639	LEU
3	D	679	ARG
3	D	685	ASP
3	D	695	ILE
3	D	737	ASN
3	D	805	ALA
3	D	823	LEU
3	D	829	VAL
3	D	830	ALA

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Mol	Chain	Res	Type
3	D	904	VAL
3	D	906	GLN
3	D	907	GLU
3	D	961	GLN
3	D	1009	ASN
3	D	1031	ASN
3	D	1036	ARG
3	D	1060	SER
3	D	1061	PHE
3	D	1138	SER
3	D	1161	GLU
3	D	1207	TYR
3	D	1327	ARG
3	D	1344	VAL
4	E	2	ALA
4	E	12	MET
4	E	49	ARG
4	E	56	ASP
4	E	95	THR
1	A	64	GLU
1	A	111	ALA
1	A	118	ALA
1	A	122	ILE
1	A	134	GLU
1	A	189	ARG
1	A	196	THR
1	B	37	GLY
1	B	159	LYS
2	C	12	VAL
2	C	15	LEU
2	C	39	ARG
2	C	46	ALA
2	C	112	GLU
2	C	182	VAL
2	C	617	ASP
2	C	656	ALA
2	C	716	LYS
2	C	793	PRO
2	C	858	MET
2	C	877	PRO
2	C	898	GLY
2	C	921	ALA

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Mol	Chain	Res	Type
2	C	1077	PRO
3	D	94	GLU
3	D	132	TYR
3	D	134	VAL
3	D	145	VAL
3	D	540	LEU
3	D	558	LEU
3	D	572	ARG
3	D	582	ILE
3	D	644	LEU
3	D	654	LYS
3	D	673	ALA
3	D	861	GLN
3	D	894	LYS
3	D	1008	PHE
3	D	1321	ALA
3	D	1453	ALA
3	D	1476	THR
4	E	71	GLY
4	E	72	ARG
4	E	93	TYR
1	B	42	ARG
1	B	115	THR
1	B	128	HIS
1	B	134	GLU
2	C	35	PRO
2	C	376	ARG
2	C	856	GLU
2	C	1000	MET
2	C	1010	THR
2	C	1107	ASN
3	D	542	ASP
3	D	609	GLY
3	D	640	HIS
3	D	667	ALA
3	D	1332	PRO
3	D	1396	GLU
4	E	62	THR
1	A	109	VAL
1	A	203	GLY
2	C	113	VAL
2	C	164	PRO

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Mol	Chain	Res	Type
2	C	166	PRO
2	C	337	GLY
2	C	478	VAL
2	C	520	GLU
2	C	982	PRO
2	C	1011	GLY
3	D	771	SER
3	D	864	VAL
3	D	1043	GLY
3	D	1081	GLY
3	D	1381	VAL
1	B	24	VAL
1	B	125	PRO
1	B	136	GLY
2	C	54	ILE
2	C	144	PRO
2	C	819	VAL
3	D	1064	GLY
2	C	470	PRO
2	C	972	VAL
3	D	719	VAL
3	D	900	ILE
3	D	1267	ARG
2	C	535	SER
2	C	951	GLY
2	C	959	PRO
2	C	1079	PRO
3	D	136	ASP
3	D	1050	GLY
3	D	1222	GLY
4	E	41	GLU
1	A	136	GLY
1	B	71	VAL
2	C	443	THR
2	C	931	GLY
3	D	634	GLY
3	D	845	ASN
3	D	890	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	189/271 (70%)	161 (85%)	28 (15%)	4	17
1	B	190/271 (70%)	169 (89%)	21 (11%)	8	31
2	C	870/935 (93%)	770 (88%)	100 (12%)	7	29
3	D	782/1035 (76%)	671 (86%)	111 (14%)	4	19
4	E	67/88 (76%)	62 (92%)	5 (8%)	17	52
All	All	2098/2600 (81%)	1833 (87%)	265 (13%)	5	24

All (265) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	25	LEU
1	A	26	GLU
1	A	27	PRO
1	A	30	ARG
1	A	41	ARG
1	A	57	TYR
1	A	63	HIS
1	A	67	THR
1	A	74	ASP
1	A	77	GLU
1	A	91	ASP
1	A	97	THR
1	A	101	LEU
1	A	110	ARG
1	A	123	MET
1	A	126	ASP
1	A	132	LEU
1	A	142	VAL
1	A	143	ARG
1	A	144	VAL
1	A	192	LEU
1	A	195	LEU

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Mol	Chain	Res	Type
1	A	196	THR
1	A	197	LEU
1	A	200	TRP
1	A	213	GLN
1	A	222	LEU
1	B	19	HIS
1	B	20	TYR
1	B	25	LEU
1	B	38	ASN
1	B	41	ARG
1	B	44	LEU
1	B	51	THR
1	B	56	VAL
1	B	57	TYR
1	B	89	PHE
1	B	90	LEU
1	B	94	MET
1	B	123	MET
1	B	132	LEU
1	B	151	VAL
1	B	167	VAL
1	B	171	PHE
1	B	183	ASP
1	B	188	GLN
1	B	191	ASP
1	B	199	ILE
2	C	13	ILE
2	C	34	VAL
2	C	36	PRO
2	C	52	PHE
2	C	56	GLU
2	C	67	ASP
2	C	70	GLU
2	C	75	ASP
2	C	95	TYR
2	C	100	LEU
2	C	104	ASP
2	C	115	LEU
2	C	126	SER
2	C	129	ILE
2	C	135	VAL
2	C	138	SER

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Mol	Chain	Res	Type
2	C	142	ARG
2	C	147	TYR
2	C	157	ARG
2	C	158	TYR
2	C	163	ILE
2	C	176	VAL
2	C	194	VAL
2	C	198	ARG
2	C	203	ASP
2	C	214	TYR
2	C	232	GLU
2	C	251	ASP
2	C	254	LEU
2	C	258	PHE
2	C	261	LEU
2	C	263	ASP
2	C	267	TYR
2	C	285	LEU
2	C	303	PHE
2	C	304	LEU
2	C	306	THR
2	C	335	THR
2	C	344	PHE
2	C	351	LEU
2	C	356	ARG
2	C	393	GLN
2	C	399	ASN
2	C	407	LYS
2	C	425	PHE
2	C	433	THR
2	C	434	HIS
2	C	435	TYR
2	C	438	ILE
2	C	445	GLU
2	C	461	VAL
2	C	479	VAL
2	C	502	PRO
2	C	526	PRO
2	C	534	VAL
2	C	559	LEU
2	C	575	GLN
2	C	603	VAL

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Mol	Chain	Res	Type
2	C	630	ARG
2	C	633	GLN
2	C	635	THR
2	C	637	PHE
2	C	672	VAL
2	C	673	LEU
2	C	686	ASP
2	C	688	ILE
2	C	691	SER
2	C	698	ASP
2	C	699	PHE
2	C	705	ILE
2	C	710	ILE
2	C	714	ASP
2	C	723	THR
2	C	739	GLU
2	C	743	VAL
2	C	758	ARG
2	C	764	GLU
2	C	803	ARG
2	C	810	ASP
2	C	815	LEU
2	C	837	ASP
2	C	839	LEU
2	C	841	ASN
2	C	846	LYS
2	C	852	ILE
2	C	859	PRO
2	C	866	PRO
2	C	881	ASN
2	C	882	LEU
2	C	888	THR
2	C	892	LEU
2	C	924	LEU
2	C	981	GLU
2	C	1005	MET
2	C	1013	TYR
2	C	1018	GLN
2	C	1027	PHE
2	C	1031	ARG
2	C	1043	TYR
2	C	1115	LEU

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Mol	Chain	Res	Type
3	D	5	VAL
3	D	21	TRP
3	D	469	ASP
3	D	502	PHE
3	D	509	PRO
3	D	567	ILE
3	D	576	GLU
3	D	587	ARG
3	D	619	LEU
3	D	640	HIS
3	D	651	GLU
3	D	674	ARG
3	D	678	GLU
3	D	685	ASP
3	D	688	TRP
3	D	691	LEU
3	D	701	LEU
3	D	702	LEU
3	D	722	GLU
3	D	724	GLN
3	D	752	SER
3	D	754	PHE
3	D	762	GLN
3	D	769	LEU
3	D	772	PRO
3	D	776	GLU
3	D	778	LEU
3	D	791	TYR
3	D	794	GLN
3	D	796	ARG
3	D	798	GLU
3	D	834	THR
3	D	851	LEU
3	D	857	LEU
3	D	860	LEU
3	D	876	SER
3	D	879	ARG
3	D	886	VAL
3	D	899	LEU
3	D	904	VAL
3	D	906	GLN
3	D	911	LEU

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Mol	Chain	Res	Type
3	D	914	LEU
3	D	920	LEU
3	D	925	GLU
3	D	931	LEU
3	D	932	ASP
3	D	936	TYR
3	D	941	LEU
3	D	947	ILE
3	D	951	ILE
3	D	953	ASP
3	D	955	VAL
3	D	964	LEU
3	D	971	LEU
3	D	974	ILE
3	D	984	THR
3	D	989	TYR
3	D	1009	ASN
3	D	1031	ASN
3	D	1038	LEU
3	D	1041	MET
3	D	1042	ARG
3	D	1045	MET
3	D	1052	THR
3	D	1057	VAL
3	D	1061	PHE
3	D	1062	ARG
3	D	1068	LEU
3	D	1078	ARG
3	D	1093	TYR
3	D	1103	HIS
3	D	1104	GLU
3	D	1119	SER
3	D	1126	ASP
3	D	1130	ARG
3	D	1134	LEU
3	D	1137	ARG
3	D	1142	SER
3	D	1145	TYR
3	D	1154	GLU
3	D	1161	GLU
3	D	1166	LEU
3	D	1188	VAL

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Mol	Chain	Res	Type
3	D	1190	SER
3	D	1192	LEU
3	D	1194	CYS
3	D	1196	THR
3	D	1207	TYR
3	D	1210	SER
3	D	1213	ARG
3	D	1260	ILE
3	D	1273	VAL
3	D	1274	ILE
3	D	1278	ASP
3	D	1299	PHE
3	D	1304	LYS
3	D	1315	ASP
3	D	1327	ARG
3	D	1332	PRO
3	D	1348	LEU
3	D	1372	VAL
3	D	1373	ARG
3	D	1376	LEU
3	D	1390	LEU
3	D	1399	ASP
3	D	1424	VAL
3	D	1434	TRP
3	D	1447	LEU
3	D	1476	THR
3	D	1483	PHE
4	E	32	ARG
4	E	61	VAL
4	E	75	PHE
4	E	78	ASN
4	E	92	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	81	ASN
1	A	128	HIS
1	A	156	HIS
1	A	180	GLN
1	A	212	ASN

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Mol	Chain	Res	Type
1	A	223	ASN
1	A	227	ASN
1	B	38	ASN
1	B	81	ASN
1	B	156	HIS
1	B	188	GLN
1	B	213	GLN
1	B	221	HIS
1	B	223	ASN
2	C	22	GLN
2	C	102	HIS
2	C	141	HIS
2	C	320	HIS
2	C	343	GLN
2	C	393	GLN
2	C	399	ASN
2	C	538	GLN
2	C	545	ASN
2	C	565	GLN
2	C	623	HIS
2	C	632	ASN
2	C	1639	GLN
2	C	671	ASN
2	C	841	ASN
2	C	845	ASN
2	C	860	HIS
2	C	872	ASN
2	C	881	ASN
2	C	884	GLN
2	C	889	HIS
2	C	962	GLN
2	C	991	GLN
2	C	1026	GLN
2	C	1030	GLN
2	C	1107	ASN
3	D	507	ASN
3	D	549	ASN
3	D	551	ASN
3	D	552	ASN
3	D	636	GLN
3	D	640	HIS
3	D	696	HIS

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Mol	Chain	Res	Type
3	D	709	HIS
3	D	724	GLN
3	D	727	GLN
3	D	729	HIS
3	D	756	GLN
3	D	762	GLN
3	D	767	HIS
3	D	768	ASN
3	D	855	HIS
3	D	861	GLN
3	D	897	GLN
3	D	909	ASN
3	D	1018	ASN
3	D	1034	GLN
3	D	1333	HIS
3	D	1353	GLN
3	D	1364	HIS
3	D	1374	GLN
3	D	1393	GLN
3	D	1445	HIS
3	D	1465	ASN
4	E	33	HIS
4	E	59	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.



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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	RFP	C	1640	-	63,63,63	1.12	6 (9%)	82,94,94	1.02	6 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	RFP	C	1640	-	-	0/60/85/85	0/1/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1640	RFP	C42-N4	2.17	1.51	1.46
7	C	1640	RFP	C8-C9	2.46	1.51	1.43
7	C	1640	RFP	C5-C10	2.48	1.49	1.43
7	C	1640	RFP	O4-C11	2.64	1.27	1.21
7	C	1640	RFP	C39-N4	2.91	1.52	1.46
7	C	1640	RFP	O5-C29	2.93	1.48	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1640	RFP	C34-C26-C25	-2.26	107.15	111.38
7	C	1640	RFP	C5-C10-C9	-2.03	115.41	119.73
7	C	1640	RFP	C20-C21-C22	2.01	117.54	114.24
7	C	1640	RFP	C24-C23-C22	2.29	118.97	115.25
7	C	1640	RFP	C2-N1-C15	2.41	128.65	123.66
7	C	1640	RFP	O12-C4-C10	2.63	124.19	118.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1640	RFP	6	0

## 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 was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.