



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 03:26 AM UTC

PDB ID : 7O3M / pdb_00007o3m
Title : Crystal Structure of AcrB Single Mutant - 1
Authors : Ababou, A.
Deposited on : 2021-04-02
Resolution : 3.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

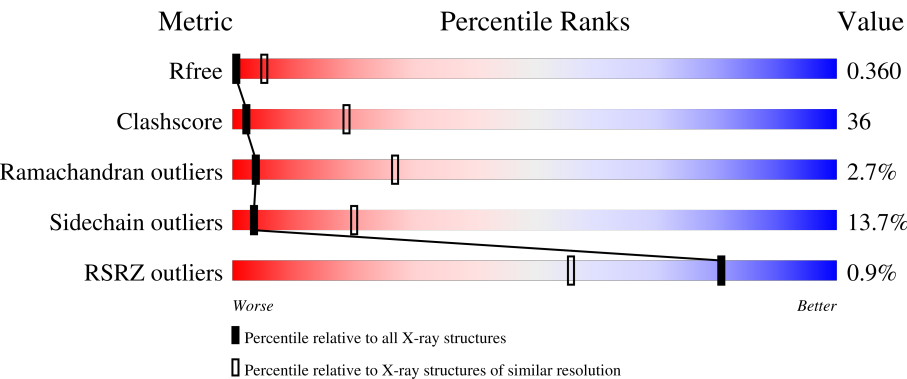
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1069	% 38%49%10%..
1	B	1069	39%47%11%.
1	C	1069	37%49%11%..
1	D	1069	% 37%48%12%..
1	E	1069	% 35%50%11%..

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Mol	Chain	Length	Quality of chain
1	F	1069	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LMT	A	2000	X	-	-	-
2	LMT	B	2000	X	-	-	-
2	LMT	C	2000	X	-	-	-
2	LMT	D	2000	X	-	-	-
2	LMT	E	2000	X	-	-	-
2	LMT	F	2000	X	-	-	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 47792 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 Efflux pump membrane transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1044	Total	C	N	O	S	0	0	0
			7936	5102	1312	1479	43			
1	B	1042	Total	C	N	O	S	0	0	0
			7919	5092	1308	1476	43			
1	C	1044	Total	C	N	O	S	0	0	0
			7936	5102	1312	1479	43			
1	D	1044	Total	C	N	O	S	0	0	0
			7936	5102	1312	1479	43			
1	E	1042	Total	C	N	O	S	0	0	0
			7919	5092	1308	1476	43			
1	F	1044	Total	C	N	O	S	0	0	0
			7936	5102	1312	1479	43			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP E2QH56
A	-18	GLY	-	expression tag	UNP E2QH56
A	-17	SER	-	expression tag	UNP E2QH56
A	-16	SER	-	expression tag	UNP E2QH56
A	-15	HIS	-	expression tag	UNP E2QH56
A	-14	HIS	-	expression tag	UNP E2QH56
A	-13	HIS	-	expression tag	UNP E2QH56
A	-12	HIS	-	expression tag	UNP E2QH56
A	-11	HIS	-	expression tag	UNP E2QH56
A	-10	HIS	-	expression tag	UNP E2QH56
A	-9	SER	-	expression tag	UNP E2QH56
A	-8	SER	-	expression tag	UNP E2QH56
A	-7	GLY	-	expression tag	UNP E2QH56
A	-6	LEU	-	expression tag	UNP E2QH56
A	-5	VAL	-	expression tag	UNP E2QH56
A	-4	PRO	-	expression tag	UNP E2QH56
A	-3	ARG	-	expression tag	UNP E2QH56

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP E2QH56
A	-1	SER	-	expression tag	UNP E2QH56
A	0	HIS	-	expression tag	UNP E2QH56
A	620	ALA	ARG	engineered mutation	UNP E2QH56
B	-19	MET	-	initiating methionine	UNP E2QH56
B	-18	GLY	-	expression tag	UNP E2QH56
B	-17	SER	-	expression tag	UNP E2QH56
B	-16	SER	-	expression tag	UNP E2QH56
B	-15	HIS	-	expression tag	UNP E2QH56
B	-14	HIS	-	expression tag	UNP E2QH56
B	-13	HIS	-	expression tag	UNP E2QH56
B	-12	HIS	-	expression tag	UNP E2QH56
B	-11	HIS	-	expression tag	UNP E2QH56
B	-10	HIS	-	expression tag	UNP E2QH56
B	-9	SER	-	expression tag	UNP E2QH56
B	-8	SER	-	expression tag	UNP E2QH56
B	-7	GLY	-	expression tag	UNP E2QH56
B	-6	LEU	-	expression tag	UNP E2QH56
B	-5	VAL	-	expression tag	UNP E2QH56
B	-4	PRO	-	expression tag	UNP E2QH56
B	-3	ARG	-	expression tag	UNP E2QH56
B	-2	GLY	-	expression tag	UNP E2QH56
B	-1	SER	-	expression tag	UNP E2QH56
B	0	HIS	-	expression tag	UNP E2QH56
B	620	ALA	ARG	engineered mutation	UNP E2QH56
C	-19	MET	-	initiating methionine	UNP E2QH56
C	-18	GLY	-	expression tag	UNP E2QH56
C	-17	SER	-	expression tag	UNP E2QH56
C	-16	SER	-	expression tag	UNP E2QH56
C	-15	HIS	-	expression tag	UNP E2QH56
C	-14	HIS	-	expression tag	UNP E2QH56
C	-13	HIS	-	expression tag	UNP E2QH56
C	-12	HIS	-	expression tag	UNP E2QH56
C	-11	HIS	-	expression tag	UNP E2QH56
C	-10	HIS	-	expression tag	UNP E2QH56
C	-9	SER	-	expression tag	UNP E2QH56
C	-8	SER	-	expression tag	UNP E2QH56
C	-7	GLY	-	expression tag	UNP E2QH56
C	-6	LEU	-	expression tag	UNP E2QH56
C	-5	VAL	-	expression tag	UNP E2QH56
C	-4	PRO	-	expression tag	UNP E2QH56
C	-3	ARG	-	expression tag	UNP E2QH56

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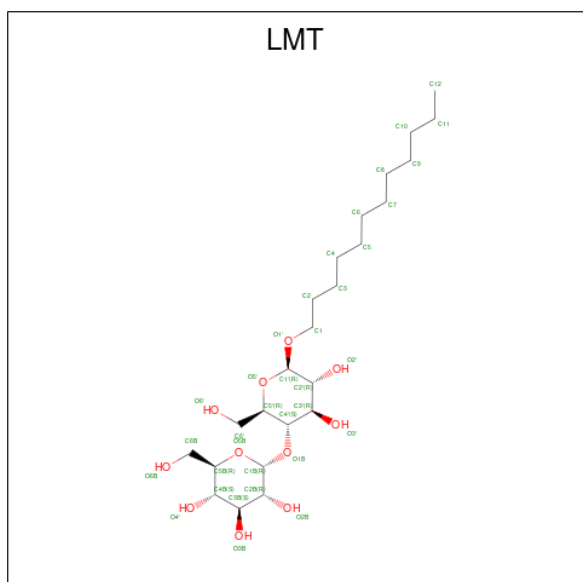
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP E2QH56
C	-1	SER	-	expression tag	UNP E2QH56
C	0	HIS	-	expression tag	UNP E2QH56
C	620	ALA	ARG	engineered mutation	UNP E2QH56
D	-19	MET	-	initiating methionine	UNP E2QH56
D	-18	GLY	-	expression tag	UNP E2QH56
D	-17	SER	-	expression tag	UNP E2QH56
D	-16	SER	-	expression tag	UNP E2QH56
D	-15	HIS	-	expression tag	UNP E2QH56
D	-14	HIS	-	expression tag	UNP E2QH56
D	-13	HIS	-	expression tag	UNP E2QH56
D	-12	HIS	-	expression tag	UNP E2QH56
D	-11	HIS	-	expression tag	UNP E2QH56
D	-10	HIS	-	expression tag	UNP E2QH56
D	-9	SER	-	expression tag	UNP E2QH56
D	-8	SER	-	expression tag	UNP E2QH56
D	-7	GLY	-	expression tag	UNP E2QH56
D	-6	LEU	-	expression tag	UNP E2QH56
D	-5	VAL	-	expression tag	UNP E2QH56
D	-4	PRO	-	expression tag	UNP E2QH56
D	-3	ARG	-	expression tag	UNP E2QH56
D	-2	GLY	-	expression tag	UNP E2QH56
D	-1	SER	-	expression tag	UNP E2QH56
D	0	HIS	-	expression tag	UNP E2QH56
D	620	ALA	ARG	engineered mutation	UNP E2QH56
E	-19	MET	-	initiating methionine	UNP E2QH56
E	-18	GLY	-	expression tag	UNP E2QH56
E	-17	SER	-	expression tag	UNP E2QH56
E	-16	SER	-	expression tag	UNP E2QH56
E	-15	HIS	-	expression tag	UNP E2QH56
E	-14	HIS	-	expression tag	UNP E2QH56
E	-13	HIS	-	expression tag	UNP E2QH56
E	-12	HIS	-	expression tag	UNP E2QH56
E	-11	HIS	-	expression tag	UNP E2QH56
E	-10	HIS	-	expression tag	UNP E2QH56
E	-9	SER	-	expression tag	UNP E2QH56
E	-8	SER	-	expression tag	UNP E2QH56
E	-7	GLY	-	expression tag	UNP E2QH56
E	-6	LEU	-	expression tag	UNP E2QH56
E	-5	VAL	-	expression tag	UNP E2QH56
E	-4	PRO	-	expression tag	UNP E2QH56
E	-3	ARG	-	expression tag	UNP E2QH56

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP E2QH56
E	-1	SER	-	expression tag	UNP E2QH56
E	0	HIS	-	expression tag	UNP E2QH56
E	620	ALA	ARG	engineered mutation	UNP E2QH56
F	-19	MET	-	initiating methionine	UNP E2QH56
F	-18	GLY	-	expression tag	UNP E2QH56
F	-17	SER	-	expression tag	UNP E2QH56
F	-16	SER	-	expression tag	UNP E2QH56
F	-15	HIS	-	expression tag	UNP E2QH56
F	-14	HIS	-	expression tag	UNP E2QH56
F	-13	HIS	-	expression tag	UNP E2QH56
F	-12	HIS	-	expression tag	UNP E2QH56
F	-11	HIS	-	expression tag	UNP E2QH56
F	-10	HIS	-	expression tag	UNP E2QH56
F	-9	SER	-	expression tag	UNP E2QH56
F	-8	SER	-	expression tag	UNP E2QH56
F	-7	GLY	-	expression tag	UNP E2QH56
F	-6	LEU	-	expression tag	UNP E2QH56
F	-5	VAL	-	expression tag	UNP E2QH56
F	-4	PRO	-	expression tag	UNP E2QH56
F	-3	ARG	-	expression tag	UNP E2QH56
F	-2	GLY	-	expression tag	UNP E2QH56
F	-1	SER	-	expression tag	UNP E2QH56
F	0	HIS	-	expression tag	UNP E2QH56
F	620	ALA	ARG	engineered mutation	UNP E2QH56

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).

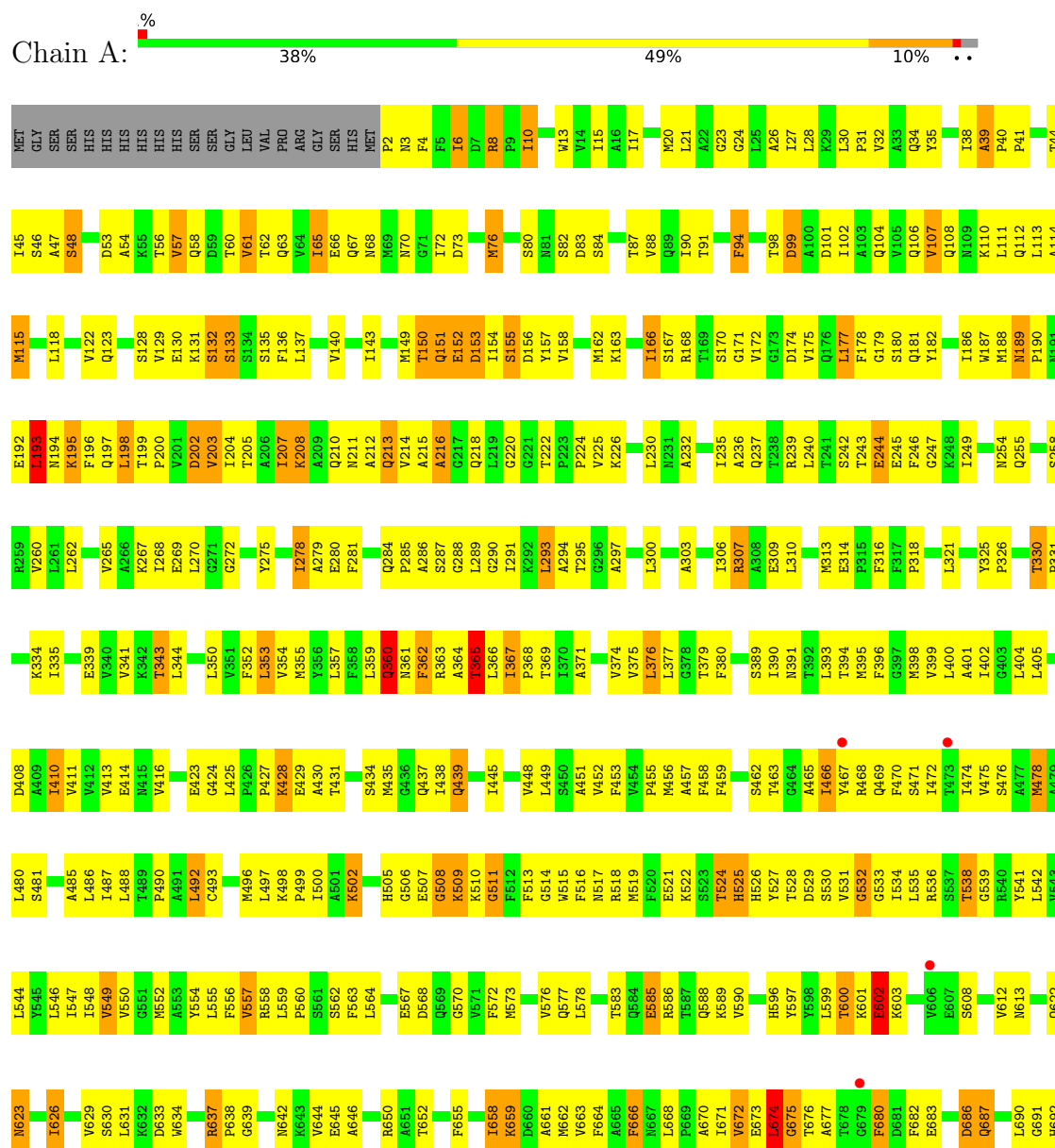


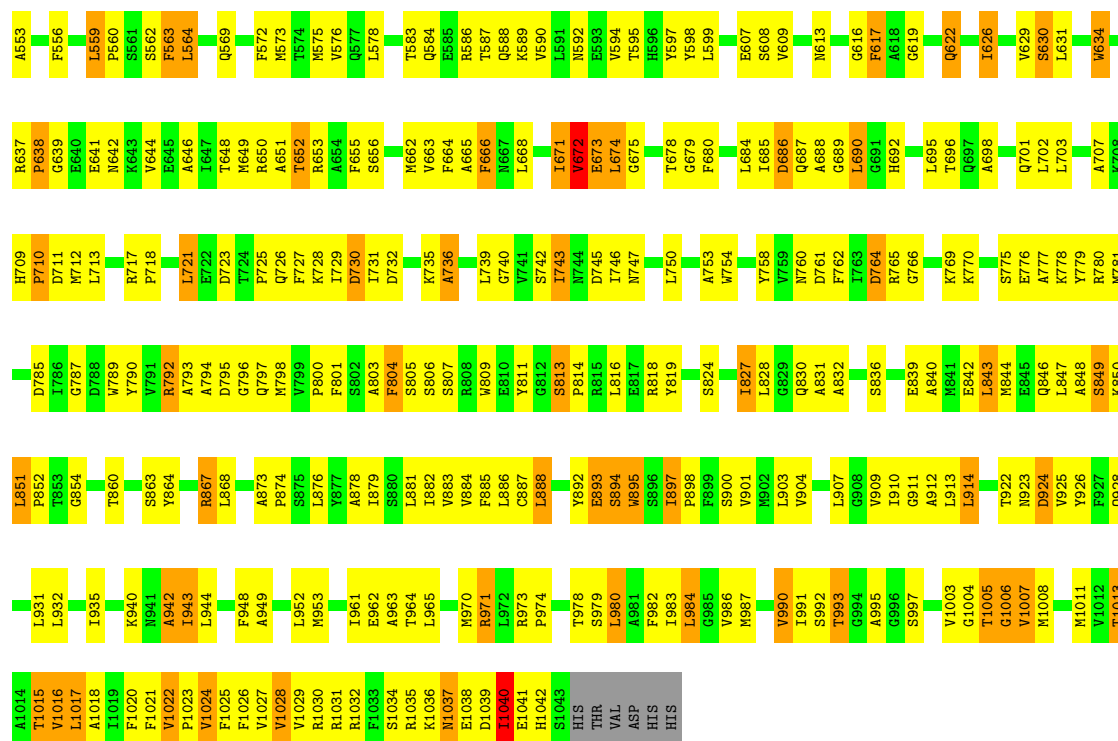
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	C	1	Total	C	O	0	0
			35	24	11		
2	D	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		
2	F	1	Total	C	O	0	0
			35	24	11		

3 Residue-property plots

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

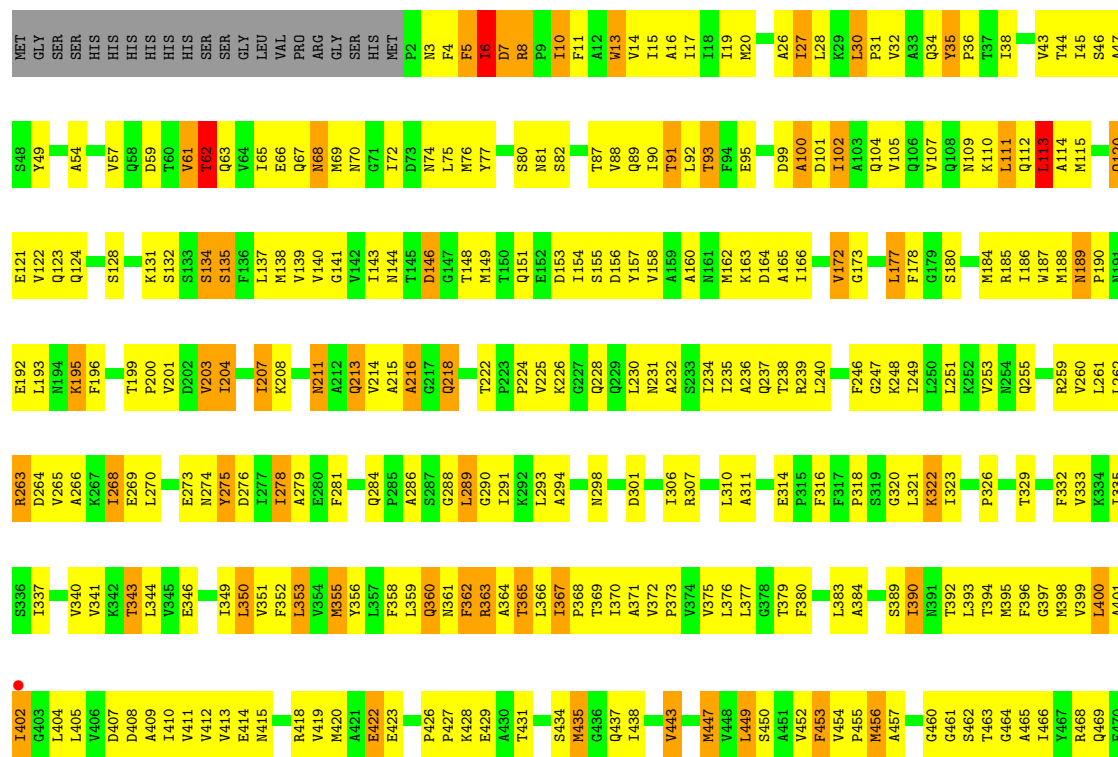
• Molecule 1: Efflux pump membrane transporter

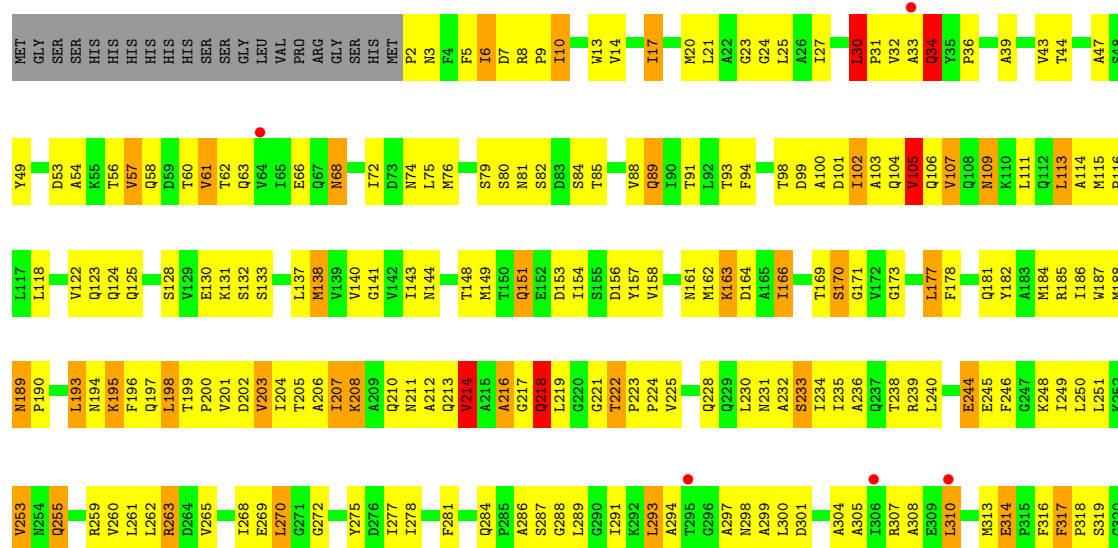


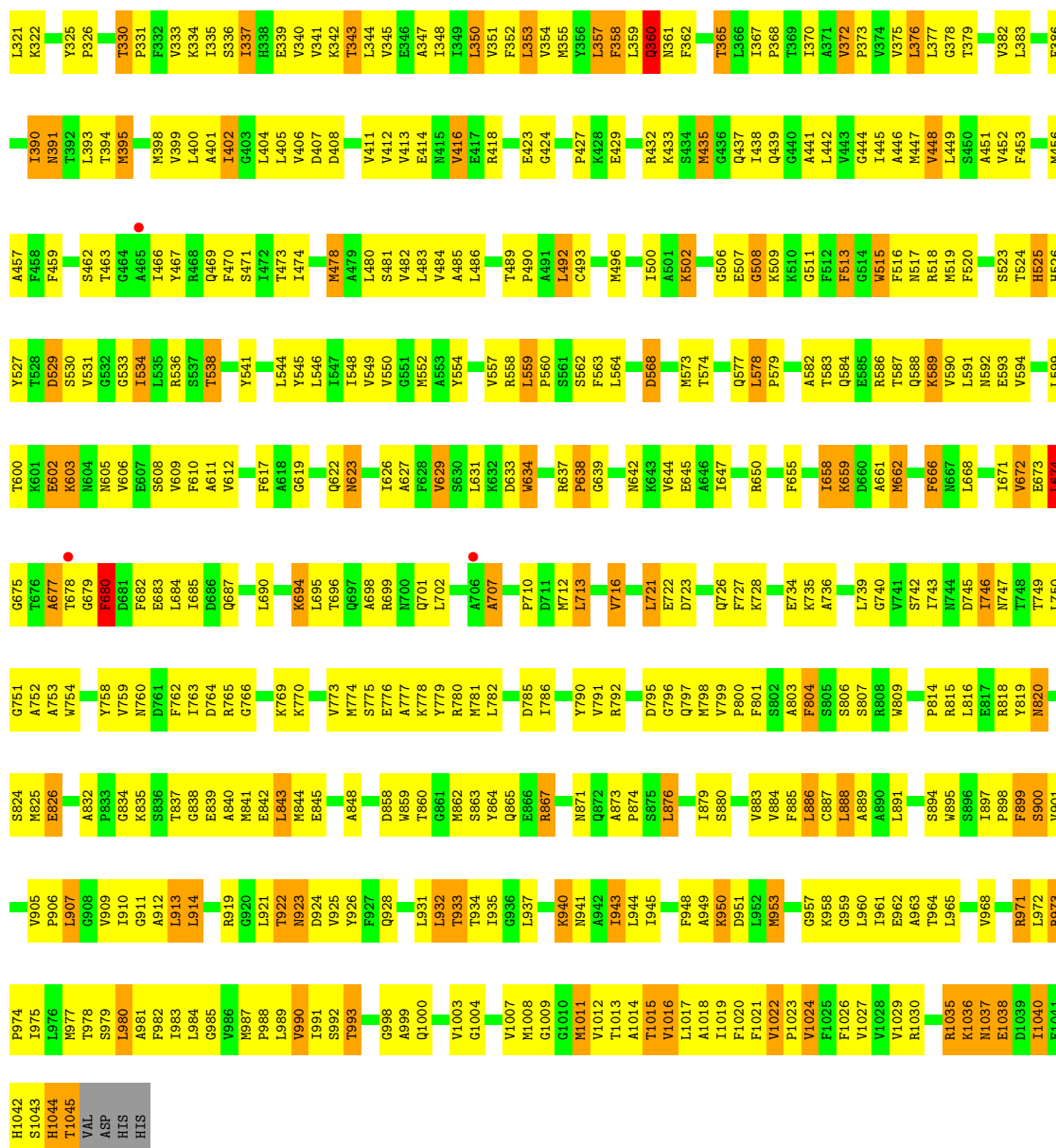


• Molecule 1: Efflux pump membrane transporter

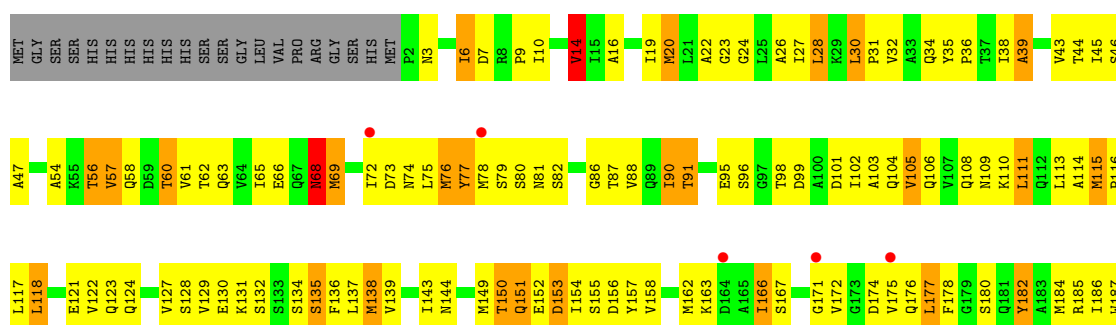
Chain C: 37% 49% 11% ..







● Molecule 1: Efflux pump membrane transporter



F1020	G957	A890	L816	T748	F680	E602	Q532	F459	F396	D328	Q255	M188
F1021	K958	L891	E817	T749	D881	V606	Q533	S462	G397	T329	Q255	M189
F1022	K959	L892	R818	L750	F682	V606	Q534	S462	K398	T330	R259	P190
F1023	L960	E893	Y819	F753	E683	V609	L535	I466	V399	P331	V260	N191
F1024	L961	S894	N820	A754	L684	V609	B536	I466	L400	F332	L261	E192
F1025				A754	L685	V609	S537	Y467	A401	V333	L262	L193
F1026	T964	L897	E826	T758	D886	N613	T538	R488	L402	S336	V265	K195
F1027	L965	P898	I827	Y759	G691	N614	Q539	Q469	L405	I337	T268	F196
F1028	D966	F899	A831	N760	H691	F615	Q540	F470	V406	H338	I268	
F1029	V967	S900	A832	D761	E698	F615	R540	S471	D407	E339	E269	
F1030	V968	V901	A832	F762	K694	Q622	L542	A477	D408	V340	L270	
R1031		M902		F762	K694	Q622		N478	A409	V341	G271	P200
R1032		L903	K835	L763	L695	T626	Y645	L474	D408	V340	L270	
F1033	L972	V904	L905	L763	L695	A627	Y645	L474	A409	V341	G271	
S1034	R973	V905	A840	R765	T696	F628	L546	V475	D407	V340	L270	
R1035	P974	P906	A840	R765	Q697	F628	L547	V475	D407	V340	L270	
K1036	T975	P906	E841	G766	A698	V629	L548	A477	V411	K342	G272	
N1037	L976	L907	E842	R767	R699	S630	V549	N478	V412	K343	E273	
N1038			L843	V768	N700	L631	V550		V413	L344	N274	
E1039	R977	I910	L844	V768	N700	L631	V550		E414	V345	T275	
D1039	T978	G911	E845	K769	Q701	K632	G551	S481	E414	D976	A206	
N1040	S979	A912	Q846	K770	L702	A632	H552	V482	M415	I277	A207	
E1041	L980	L913	L847	V771	L703	W634	H552	V482		I278	K208	
H1042	A981	L914	A848	V772	A704	W634		V484	V419	F352		
S1043	F982	A915	S849	V773	E705	R637	L555	A485	M420	V354		
HIS	L983	A916	K850	V774	A706	P638	V557		A421	K355	A286	
THR	L984		L851	S775		G639	R558	L488	E422	Y356	S287	
ASP	R919	R919	L851	A776	H709	E640	L559	T489	E423	A215	A216	
N987	G920	G920	G854	K778	P710	E641	P560	P490	G424	F358	L289	
P988	L921	L921	R855	V779	M712	N642	S561	A491	L425	L359	G290	
N989	T922	T922	G856	R780	L713	W643	S562	L492	P426	Q360	L291	
N990	N923	N923	L857	V781	L714	E645	F563	C493	P427	N361	K292	
N991	D924	D924	L858	V782	S715	A646	L564	A494	K428	L293	K292	
N992	L925	L925	W859	L782	V716	A647		T495	E429	R363	A294	
S993	V926	V926	M862	D785	R717	L647	Q569	N496		P224	V225	
G994	F927	F927	L863	T786	P718	N649	G570	L497	R432	T365		
A995	Q928	Q928	S863	G787	P718	R650	F572	P499	K433	L366	A297	
G996	N929	N929	L864	D788	L721	A651	L590	F500	S434	I367	T302	
S997	L931	G930	Q865	V789	E722	M652	M573	A501	M435	P368	A303	
G998	L932	L931	Q866	V790	D723	R653	T574	R502	Q436	T369	Q229	
A999	T933	L932	R867	V791	D723	R653	M575	K502	Q437	L230	G229	
Q1000	T934	T933	L868	R792	T724	A654	V576	H505	Q437	A371	N231	
N1001	L935	L934	L868	A793	P725	F655	Q577		Q439	V372	A232	
A1002	Q872	N871		A794	Q726	K659	L578	G596	C440	P373	I235	
V1003	Q873	Q872		D795	F727	D660	F579	E507	A441	P373	T235	
G1004	A873	A873	R874	G796	I729	A661	T583	G508	L442	V375	A236	
T1005	P874	P874	Q875	Q797	D730	A662	M584	K509	V443	L376	Q237	
G1006	S875	S875	M798	V798	I731	V663	Q584	K510	G444	L377	R239	
V1007	L876	L876	V799	V799	T731	F663	T587	F516	I445	G378	L240	
N1008	Y877	Y877	P800	V799		F664		A446	A446	T379		
M1011	A878	A878	A665	P800	A736	A665	Q588	N517	M447	F380	G247	
V1012	L879	L879	F666	F801	Q737	F667	R518	R518	V448	A381	F246	
T1013	S880	S880	S880	S802	A738	N667	V590	M519	L449	V382	G247	
A1014	L876	L876	L876	A803	L739	L668			S450	L383	F247	
T1015	Y877	Y877	F803	F804	G740		V594		A451	G319	G247	
L1016	V883	V883	S805	S805	V741	L671	T595	S523	A451	S319	F247	
V1017	F884	F884	S805	S805	V741	L671	T595	T594	V452	L321	K248	
A1018	V885	V885	V809	S742	V741	L671	T595	H525	F453	L321	K248	
L1019	L886	L886	W809	I743	V741	L671	T595	H525	F453	L321	K248	
L1020	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1021	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1022	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1023	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1024	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1025	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1026	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1027	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1028	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1029	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1030	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1031	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1032	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1033	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1034	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1035	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1036	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1037	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1038	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1039	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1040	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1041	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1042	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1043	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1044	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1045	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1046	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1047	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1048	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1049	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1050	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1051	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1052	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1053	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1054	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1055	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1056	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1057	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1058	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1059	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1060	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1061	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1062	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1063	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1064	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1065	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1066	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1067	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1068	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1069	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1070	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1071	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1072	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1073	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1074	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1075	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1076	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1077	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1078	C887	C887	L886	V743	V741	L671	T595	H525	F453	L321	K248	
L1079	C887	C887	L886	V743	V741	L67						

• Molecule 1: Efflux pump membrane transporter



A1014	K940	R867	F801	L739	A685	T587	A457	I390	F317	F246	G179	A114	S48
T1015	H941	G870	F804	G740	F686	Q588	S523	N391	P318	F247	S180	M115	Y49
V1016	A942	G871		V741	I687	K589	T524	T392	S319	K248	Q181	L116	D53
L1017	I943	N870		S742	L688	H525	H525	L393	G320	L249	Y182	L117	A54
A1018		K871	R808	I743	F689	L591	H526	T395	L321	L250	M184	L118	K55
L1019	V946	A873	R809	N744	A670	N592	Y527	M395		L251	M185	P119	T56
F1020	F947			D745	A671	E593	T528	G397	P326	L252	I186	E121	V57
F1021	F948	S880	S813	I746	V672	V594	D529	G398	Y327	V253	W187	V122	Q58
P1023	A949	V883	P814	N747	E673	T595	S520	M398	T330	G257	M188	Q123	D59
V1024	K950	R871	R815	T748	L674	H596	F470	V399	F331	Q258	M189	Q124	T60
F1025	L952	F885	R816	T749	G675		F471	L400	P190	Q125	P190	G126	V61
F1026	K953	L886	R818	L750	T676	L559	G533	A401	F332	R259	S258	G126	T62
V1027	H954	C887	Y819	G751	A677	T600	L534	I402	V333	R259	G126	V127	G63
V1028	K955	L888	N820	A752	T678	K601	L555	G403	K334	V260	E192		V64
R1030		A889	G821	A753	F680	K603	R536	L405	I337	L262	L193	S132	L65
R1031	G959	A890	L822	W754	F681	D681	T538	V406	H338	L261	K195		
R1032	L960	A891	P823	Y758	F682	S608	G539	V407	F339	V265	F196	S135	N68
F1033	R961	Y892	S824	W759	E683	V609	R540	D408	V340	F136		F136	M69
S1034	E962	E893	M825	N760	L684	F610	Y541	A409	V341	L137		L137	N70
R1035	A963	S894	E826	D761	T685	A611	L542	L480	K342	M138		G71	G71
K1036		S896	L828	F762	D686	V612	V543	S481	L343	L270		V139	L72
N1037	V968	I897	I827	I763		N613	L544	V482	L344	G271		V140	D73
	K970	P898	Q830	D764	G691	F617	Y545	E414	L350	G272		G141	N74
	R971	P899	Q830	R765	H692	A618	L546	L483	L350	E273		V140	L75
	L972	S900	A831	G766	E693	G619	I547	A485	V351	N274		I143	M76
	R973	V901	P833	V768	K694		L548	L486	F352	Y275		N144	Y77
P974	P974	M902	G834	K769	T696	Q622	V549	M420	L353	L207		I144	M78
		L903	K835	K770	G697	M623	M552	A421	V354	L278		G147	S79
	K977	V904	S836	W771	A698	L631	L559	E422	M355	F281		M149	S80
VAL	T978	V905	T837	V772	R699	L626	Y554	E423	Y356			T211	N81
ASP	S979	P906	G838	V773	N700	A627	L555	E424	L357	Q284		M149	S82
HIS	L980	L907	E839	M774	F628	V629	F557	L425	P285	T214		T150	D83
	A981	G908	A840	S775	Q701	F629	V567	P427	A286	A216		Q151	
	F982	V909	E776	E776	L702	S630	R558	P499	G287	E152		D153	T87
	I983	I910	E842	A777	L703	L631	L559	I500	F362	G217		I154	I90
	L984	G911	L843	K778	W712	K632	P560	A501	R363	Q218		S155	T91
	G985	A912	M844	Y779	L713	D633	S561	K498	A364	L219		D156	T92
	V986	L913	E945	R780	W716	W634	S562	P499	T365	G220		V157	L92
	N987	L914	Q846	M781	R717	P638	L564	I500	L366	G221		V158	T93
	P988		L847	L782	P718		L564	A501	L293	T222		A159	F94
		L921	A848	P783	W719	K644	G502	M435	P368	P223		G161	E95
	V990	T922	K850	D785	G720	E645	G503		T369	P224		A160	S96
	I991	N923	L851	I786	L721	E645		I438	V370	G97		M162	G97
		V925		G787	E722	M649	V571	Q439	A371	V225		M162	T98
	A995	Y926		D788	D723	R650	F572	A299	A299	Q228		K163	D99
	G996	F927	G854	W789	G726		G508	L300	L300	Q229		D164	A100
	S997	Q928	G856	Y790	S656	R653	M573	P373	D301	L230		A165	D101
	G998	V929	Y857	V791	A654	A654	T574	V374	T302	N231		I166	D101
	A999	G930	D858	R792	K659	K659	G511	L376	A232	A232		S167	A103
		L931	W859	A793	K728		F512	R307	S233	G237		R168	Q104
	V1007	L932	T860	A794	L731	F655	V576	L310	T234	A236		S170	V105
	M1008	T933	G861	G795	Q732	S656	Q577	A311	G173	Q108		G173	Q106
	G1009	T934	M862	G796	Q733	A654	L578	F380	A236	V107		D174	V107
	G1010	I835	S863	Q797	Q733	F516	W515	A451	A236	A236		V175	Q108
	M1011	G936	Y864	M798	A736	M517	F516	A381	K312	G174		G174	N109
	V1012	L937	Q865	V799	Q737	M519	M519	V382	K313	V175		Q176	K110
	T1013		E866	P800	A738	F664	R586	M456	L383	E314		F178	L111

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	152.37Å 156.80Å 218.65Å 90.00° 92.48° 90.00°	Depositor
Resolution (Å)	19.95 – 3.55 19.95 – 3.55	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.95-3.55) 99.0 (19.95-3.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 3.52Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.277 , 0.359 0.278 , 0.360	Depositor DCC
R_{free} test set	6185 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	101.9	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.074 for -k,-h,-l 0.095 for k,h,-l 0.089 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	47792	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.4003e-05.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.88	5/8088 (0.1%)	1.29	60/10983 (0.5%)
1	B	0.93	5/8070 (0.1%)	1.32	68/10958 (0.6%)
1	C	0.92	5/8088 (0.1%)	1.33	83/10983 (0.8%)
1	D	0.84	2/8088 (0.0%)	1.26	55/10983 (0.5%)
1	E	0.87	4/8070 (0.0%)	1.29	62/10958 (0.6%)
1	F	0.87	3/8088 (0.0%)	1.33	93/10983 (0.8%)
All	All	0.89	24/48492 (0.0%)	1.30	421/65848 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
All	All	0	2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1022	VAL	CA-CB	8.15	1.58	1.54
1	A	905	VAL	CA-CB	7.38	1.57	1.54
1	F	897	ILE	CA-CB	6.93	1.58	1.54
1	C	676	THR	CA-CB	6.12	1.62	1.53
1	F	150	THR	CA-CB	6.11	1.62	1.53
1	C	372	VAL	CA-C	6.06	1.59	1.52
1	A	897	ILE	CA-C	5.97	1.59	1.52
1	B	942	ALA	CA-CB	-5.84	1.44	1.53
1	B	894	SER	CA-C	-5.58	1.45	1.52
1	D	678	THR	CA-CB	5.55	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	482	VAL	CA-CB	5.47	1.60	1.54
1	A	879	ILE	CA-CB	5.47	1.60	1.54
1	E	1022	VAL	CA-CB	5.45	1.56	1.54
1	B	169	THR	CA-C	-5.38	1.50	1.53
1	A	1019	ILE	CA-CB	-5.29	1.47	1.54
1	C	905	VAL	CA-CB	5.27	1.56	1.54
1	C	954	ASP	CA-C	-5.24	1.47	1.53
1	E	534	ILE	CA-CB	5.22	1.60	1.54
1	B	1013	THR	CA-CB	-5.16	1.45	1.53
1	B	1022	VAL	CA-CB	5.14	1.56	1.54
1	C	402	ILE	CA-CB	5.07	1.60	1.54
1	E	214	VAL	CA-CB	-5.07	1.48	1.54
1	E	445	ILE	CA-CB	5.05	1.60	1.54
1	A	889	ALA	CA-CB	-5.03	1.44	1.53

All (421) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	8	ARG	CA-C-N	13.77	133.55	119.64
1	F	8	ARG	C-N-CA	13.77	133.55	119.64
1	A	35	TYR	CA-C-N	-11.16	108.98	120.03
1	A	35	TYR	C-N-CA	-11.16	108.98	120.03
1	E	325	TYR	CA-C-N	10.95	130.69	119.64
1	E	325	TYR	C-N-CA	10.95	130.69	119.64
1	B	679	GLY	N-CA-C	10.89	126.50	110.60
1	C	616	GLY	N-CA-C	-10.44	100.26	112.79
1	F	838	GLY	N-CA-C	10.33	125.99	112.77
1	D	30	LEU	CA-C-N	10.05	130.15	119.90
1	D	30	LEU	C-N-CA	10.05	130.15	119.90
1	A	1038	GLU	N-CA-C	-9.97	95.59	111.04
1	B	3	ASN	N-CA-C	-9.38	102.34	113.88
1	C	365	THR	N-CA-C	-9.12	101.59	112.89
1	D	513	PHE	N-CA-C	-9.03	102.03	113.23
1	F	30	LEU	CA-C-N	8.87	128.95	119.90
1	F	30	LEU	C-N-CA	8.87	128.95	119.90
1	F	40	PRO	CA-C-N	8.83	128.77	119.85
1	F	40	PRO	C-N-CA	8.83	128.77	119.85
1	F	717	ARG	CA-C-N	8.61	130.60	119.84
1	F	717	ARG	C-N-CA	8.61	130.60	119.84
1	E	492	LEU	N-CA-C	-8.56	101.89	111.14
1	A	115	MET	CA-C-N	-8.53	109.18	119.84
1	A	115	MET	C-N-CA	-8.53	109.18	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	189	ASN	CA-C-N	8.45	128.43	119.05
1	D	189	ASN	C-N-CA	8.45	128.43	119.05
1	C	135	SER	N-CA-C	8.30	121.10	109.15
1	D	534	ILE	N-CA-C	-8.24	102.85	111.58
1	A	39	ALA	CA-C-N	8.14	128.77	120.38
1	A	39	ALA	C-N-CA	8.14	128.77	120.38
1	E	1004	GLY	N-CA-C	8.10	122.44	112.64
1	B	680	PHE	N-CA-C	8.07	120.41	108.14
1	F	95	GLU	N-CA-C	8.06	121.87	110.50
1	D	317	PHE	CA-C-N	8.01	129.86	119.84
1	D	317	PHE	C-N-CA	8.01	129.86	119.84
1	F	115	MET	CA-C-N	-8.01	109.83	119.84
1	F	115	MET	C-N-CA	-8.01	109.83	119.84
1	D	85	THR	N-CA-C	-7.96	103.14	113.17
1	A	973	ARG	CA-C-N	-7.88	110.00	119.84
1	A	973	ARG	C-N-CA	-7.88	110.00	119.84
1	D	679	GLY	N-CA-C	7.83	122.03	110.60
1	D	680	PHE	N-CA-C	7.82	118.91	107.88
1	D	922	THR	N-CA-C	7.80	121.24	108.99
1	C	486	LEU	N-CA-C	-7.79	101.89	111.40
1	E	496	MET	N-CA-C	-7.79	103.78	113.28
1	E	132	SER	N-CA-C	7.78	122.29	109.06
1	F	685	ILE	N-CA-C	7.70	119.57	108.48
1	D	113	LEU	N-CA-C	-7.60	104.53	113.88
1	F	897	ILE	CB-CA-C	-7.60	104.04	114.00
1	E	505	HIS	N-CA-C	7.58	122.11	112.86
1	C	492	LEU	N-CA-C	7.58	120.64	111.40
1	F	691	GLY	N-CA-C	7.54	122.15	110.91
1	D	525	HIS	N-CA-C	-7.52	102.77	110.97
1	A	132	SER	N-CA-C	7.52	119.95	108.52
1	F	27	ILE	N-CA-C	-7.51	103.62	111.58
1	D	763	ILE	N-CA-C	7.50	118.28	106.88
1	D	34	GLN	N-CA-C	-7.38	103.16	111.14
1	E	28	LEU	N-CA-C	7.38	119.33	111.28
1	C	498	LYS	CA-C-N	-7.37	112.16	119.90
1	C	498	LYS	C-N-CA	-7.37	112.16	119.90
1	C	676	THR	N-CA-C	-7.33	104.86	113.88
1	D	314	GLU	CA-C-N	-7.28	113.40	120.83
1	D	314	GLU	C-N-CA	-7.28	113.40	120.83
1	E	563	PHE	N-CA-C	-7.28	103.50	113.18
1	A	189	ASN	CA-C-N	7.26	127.11	119.05
1	A	189	ASN	C-N-CA	7.26	127.11	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	LEU	CA-C-N	7.26	127.31	119.90
1	B	30	LEU	C-N-CA	7.26	127.31	119.90
1	C	567	GLU	N-CA-C	7.26	121.24	109.40
1	B	666	PHE	N-CA-C	7.23	119.74	108.96
1	B	489	THR	CA-C-N	-7.21	110.99	118.85
1	B	489	THR	C-N-CA	-7.21	110.99	118.85
1	B	897	ILE	CB-CA-C	-7.21	106.71	114.35
1	A	945	ILE	N-CA-C	7.21	117.34	110.42
1	E	644	VAL	N-CA-C	7.16	117.87	110.36
1	C	172	VAL	N-CA-C	7.15	118.12	108.11
1	E	674	LEU	N-CA-C	7.13	120.58	110.23
1	C	367	ILE	CA-C-N	-7.11	112.46	119.64
1	C	367	ILE	C-N-CA	-7.11	112.46	119.64
1	C	189	ASN	CA-C-N	7.10	126.94	119.05
1	C	189	ASN	C-N-CA	7.10	126.94	119.05
1	B	115	MET	CA-C-N	-7.06	111.02	119.84
1	B	115	MET	C-N-CA	-7.06	111.02	119.84
1	C	964	THR	N-CA-C	-7.03	103.55	111.07
1	A	498	LYS	CA-C-N	7.03	126.79	119.76
1	A	498	LYS	C-N-CA	7.03	126.79	119.76
1	A	367	ILE	CA-C-N	-7.01	112.47	120.04
1	A	367	ILE	C-N-CA	-7.01	112.47	120.04
1	F	487	ILE	N-CA-C	7.01	117.12	110.53
1	B	710	PRO	N-CA-C	-6.99	104.83	114.27
1	E	897	ILE	CB-CA-C	-6.98	106.96	114.35
1	B	513	PHE	N-CA-C	6.97	121.79	113.28
1	A	1040	ILE	N-CA-C	6.94	119.12	109.55
1	A	94	PHE	N-CA-C	6.91	120.39	109.81
1	F	617	PHE	N-CA-C	-6.91	105.00	113.50
1	B	813	SER	CA-C-N	6.90	127.86	120.47
1	B	813	SER	C-N-CA	6.90	127.86	120.47
1	B	897	ILE	N-CA-CB	6.89	114.84	110.50
1	F	108	GLN	N-CA-C	-6.89	103.79	111.71
1	C	10	ILE	N-CA-C	-6.88	104.29	111.58
1	E	679	GLY	N-CA-C	6.85	120.60	110.60
1	A	972	LEU	N-CA-C	-6.84	103.75	111.07
1	A	8	ARG	CA-C-N	6.81	126.52	119.64
1	A	8	ARG	C-N-CA	6.81	126.52	119.64
1	F	362	PHE	N-CA-C	6.81	118.36	111.07
1	D	39	ALA	N-CA-C	6.80	118.22	109.65
1	C	1043	SER	N-CA-C	6.80	117.45	108.07
1	F	49	TYR	CA-CB-CG	6.78	126.11	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	232	ALA	N-CA-C	6.75	118.46	108.60
1	C	619	GLY	N-CA-C	-6.75	101.50	110.74
1	F	867	ARG	N-CA-C	-6.74	104.02	111.36
1	F	164	ASP	N-CA-C	-6.72	104.56	112.89
1	F	973	ARG	CA-C-N	-6.71	111.45	119.84
1	F	973	ARG	C-N-CA	-6.71	111.45	119.84
1	A	513	PHE	N-CA-C	-6.71	105.06	113.18
1	B	132	SER	N-CA-C	6.70	119.83	108.90
1	E	629	VAL	N-CA-C	6.70	117.49	108.11
1	F	243	THR	N-CA-C	-6.68	104.61	112.89
1	E	877	TYR	CA-CB-CG	-6.68	101.88	113.90
1	B	851	LEU	CA-C-N	6.67	126.65	119.78
1	B	851	LEU	C-N-CA	6.67	126.65	119.78
1	C	622	GLN	N-CA-C	-6.67	104.04	111.71
1	C	897	ILE	CA-C-N	-6.66	111.66	119.05
1	C	897	ILE	C-N-CA	-6.66	111.66	119.05
1	B	532	GLY	N-CA-C	-6.64	104.80	112.50
1	E	894	SER	N-CA-C	6.64	119.26	109.24
1	C	453	PHE	N-CA-C	-6.55	105.28	113.28
1	E	367	ILE	CA-C-N	-6.55	113.03	119.64
1	E	367	ILE	C-N-CA	-6.55	113.03	119.64
1	B	421	ALA	N-CA-C	-6.55	105.17	113.02
1	F	136	PHE	N-CA-C	-6.50	100.27	109.96
1	F	107	VAL	N-CA-C	6.49	117.12	110.82
1	B	644	VAL	N-CA-C	6.46	117.98	110.62
1	E	445	ILE	N-CA-C	-6.46	104.03	110.62
1	A	826	GLU	N-CA-C	6.44	119.02	108.52
1	A	672	VAL	N-CA-C	-6.44	100.34	108.84
1	D	899	PHE	N-CA-C	-6.43	104.19	111.07
1	F	454	VAL	CA-C-N	-6.41	112.39	119.19
1	F	454	VAL	C-N-CA	-6.41	112.39	119.19
1	F	211	ASN	N-CA-C	6.39	119.12	108.20
1	B	189	ASN	CA-C-N	6.37	126.12	119.05
1	B	189	ASN	C-N-CA	6.37	126.12	119.05
1	C	1031	ARG	N-CA-C	-6.34	106.25	112.97
1	E	189	ASN	CA-C-N	6.34	126.09	119.05
1	E	189	ASN	C-N-CA	6.34	126.09	119.05
1	E	673	GLU	CA-C-N	6.32	129.68	120.71
1	E	673	GLU	C-N-CA	6.32	129.68	120.71
1	E	39	ALA	N-CA-C	6.31	118.76	109.42
1	A	113	LEU	N-CA-C	-6.31	106.12	113.88
1	C	259	ARG	N-CA-C	6.31	118.86	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	964	THR	N-CA-C	-6.31	104.32	111.07
1	C	49	TYR	CA-C-N	6.28	126.65	119.93
1	C	49	TYR	C-N-CA	6.28	126.65	119.93
1	C	756	GLY	N-CA-C	-6.28	105.73	112.08
1	B	379	THR	N-CA-C	-6.27	104.50	111.71
1	C	62	THR	N-CA-C	6.27	117.78	111.07
1	D	214	VAL	N-CA-C	6.26	116.87	108.11
1	C	1022	VAL	CB-CA-C	-6.24	107.77	113.70
1	D	826	GLU	N-CA-C	6.23	118.89	108.73
1	E	964	THR	N-CA-C	-6.22	104.41	111.07
1	F	220	GLY	N-CA-C	-6.21	105.52	115.08
1	B	711	ASP	N-CA-C	-6.19	105.82	113.19
1	D	806	SER	N-CA-C	-6.19	101.37	108.49
1	E	77	TYR	N-CA-C	6.19	118.26	108.79
1	E	448	VAL	N-CA-C	6.18	116.97	110.72
1	B	268	ILE	N-CA-C	6.18	116.92	107.77
1	B	425	LEU	CA-C-N	-6.18	114.02	120.38
1	B	425	LEU	C-N-CA	-6.18	114.02	120.38
1	E	1006	GLY	N-CA-C	-6.17	105.30	112.83
1	F	492	LEU	N-CA-C	6.16	118.91	111.40
1	D	707	ALA	N-CA-C	-6.16	105.77	113.28
1	C	921	LEU	N-CA-C	6.13	119.35	109.79
1	B	325	TYR	CA-C-N	6.12	127.48	119.84
1	B	325	TYR	C-N-CA	6.12	127.48	119.84
1	B	529	ASP	N-CA-C	-6.11	104.68	111.71
1	C	35	TYR	CA-C-N	-6.11	113.98	120.03
1	C	35	TYR	C-N-CA	-6.11	113.98	120.03
1	B	424	GLY	N-CA-C	-6.10	106.22	115.00
1	E	302	THR	N-CA-C	-6.10	104.63	111.28
1	B	453	PHE	N-CA-C	6.10	120.89	112.90
1	F	180	SER	N-CA-C	6.07	117.75	108.52
1	C	8	ARG	CA-C-N	6.06	127.42	119.84
1	C	8	ARG	C-N-CA	6.06	127.42	119.84
1	B	168	ARG	CA-C-N	-6.06	116.49	123.04
1	B	168	ARG	C-N-CA	-6.06	116.49	123.04
1	F	488	LEU	N-CA-C	6.04	120.75	112.04
1	A	198	LEU	N-CA-C	6.03	119.32	109.06
1	D	515	TRP	N-CA-C	-6.02	104.04	111.75
1	F	18	ILE	CB-CA-C	-6.02	104.26	111.97
1	B	622	GLN	N-CA-C	-6.00	104.80	111.71
1	F	829	GLY	N-CA-C	6.00	119.33	110.63
1	C	617	PHE	N-CA-C	-6.00	106.13	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	218	GLN	N-CA-C	5.98	118.50	109.23
1	B	218	GLN	N-CA-C	5.98	119.23	109.06
1	B	233	SER	N-CA-C	5.98	118.99	109.24
1	C	337	ILE	N-CA-C	5.97	116.15	110.42
1	D	740	GLY	N-CA-C	-5.97	107.09	115.32
1	F	83	ASP	N-CA-C	5.94	119.50	109.76
1	A	557	VAL	N-CA-C	5.92	116.11	110.42
1	F	137	LEU	N-CA-C	-5.92	104.82	111.28
1	F	894	SER	N-CA-C	5.91	118.40	109.23
1	B	964	THR	N-CA-C	-5.91	104.84	111.28
1	F	873	ALA	N-CA-C	5.90	121.56	113.77
1	E	303	ALA	N-CA-C	5.90	117.51	111.14
1	A	602	GLU	N-CA-C	-5.90	103.81	111.71
1	F	79	SER	N-CA-C	5.89	118.03	108.26
1	A	434	SER	N-CA-C	-5.88	104.78	111.07
1	C	211	ASN	N-CA-C	5.88	118.25	108.20
1	C	945	ILE	N-CA-C	5.87	116.06	110.42
1	F	1022	VAL	CB-CA-C	-5.87	108.13	113.70
1	A	1032	ARG	N-CA-C	-5.86	101.52	109.54
1	E	232	ALA	N-CA-C	5.84	117.73	108.79
1	E	666	PHE	N-CA-C	5.84	116.80	108.74
1	E	68	ASN	N-CA-C	5.83	120.51	113.17
1	F	353	LEU	N-CA-C	5.82	117.30	111.07
1	D	489	THR	CA-C-N	-5.79	112.53	118.85
1	D	489	THR	C-N-CA	-5.79	112.53	118.85
1	F	666	PHE	N-CA-C	5.79	116.73	108.74
1	C	724	THR	CA-C-N	5.77	125.96	119.90
1	C	724	THR	C-N-CA	5.77	125.96	119.90
1	F	644	VAL	N-CA-C	5.77	116.42	110.36
1	F	1043	SER	N-CA-C	5.76	116.02	108.07
1	E	998	GLY	N-CA-C	-5.75	105.40	112.77
1	C	435	MET	N-CA-C	5.75	117.22	111.07
1	D	105	VAL	N-CA-C	5.74	115.93	110.53
1	C	542	LEU	N-CA-C	-5.74	104.93	111.07
1	A	330	THR	CA-C-N	-5.74	113.71	119.56
1	A	330	THR	C-N-CA	-5.74	113.71	119.56
1	D	905	VAL	CA-C-N	-5.74	112.68	119.05
1	D	905	VAL	C-N-CA	-5.74	112.68	119.05
1	F	365	THR	N-CA-C	-5.74	105.00	112.23
1	C	449	LEU	N-CA-C	5.73	117.61	111.36
1	D	330	THR	CA-C-N	-5.73	113.78	119.56
1	D	330	THR	C-N-CA	-5.73	113.78	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	799	VAL	CA-C-N	5.72	125.63	119.85
1	F	799	VAL	C-N-CA	5.72	125.63	119.85
1	C	43	VAL	N-CA-C	5.71	116.08	107.75
1	F	101	ASP	N-CA-C	-5.71	104.26	111.11
1	F	122	VAL	N-CA-C	-5.71	104.76	110.30
1	A	1003	VAL	CA-C-N	5.71	126.42	120.03
1	A	1003	VAL	C-N-CA	5.71	126.42	120.03
1	F	42	ALA	N-CA-C	5.70	117.94	108.99
1	D	529	ASP	N-CA-C	-5.70	105.16	111.71
1	E	531	VAL	N-CA-C	5.70	116.34	110.36
1	B	671	ILE	N-CA-C	-5.69	102.19	109.30
1	A	314	GLU	CA-C-N	-5.69	115.03	120.83
1	A	314	GLU	C-N-CA	-5.69	115.03	120.83
1	A	357	LEU	CA-C-N	-5.68	113.12	122.79
1	A	357	LEU	C-N-CA	-5.68	113.12	122.79
1	C	165	ALA	N-CA-C	-5.67	106.71	113.97
1	F	214	VAL	N-CA-C	5.67	116.44	108.17
1	F	623	ASN	N-CA-C	5.66	117.45	111.28
1	C	763	ILE	N-CA-C	5.66	115.49	106.88
1	E	211	ASN	N-CA-C	5.66	117.88	108.20
1	E	214	VAL	N-CA-C	5.66	116.43	108.17
1	C	32	VAL	N-CA-C	5.65	116.13	107.77
1	A	525	HIS	N-CA-C	-5.64	104.83	110.97
1	E	103	ALA	N-CA-C	-5.63	105.04	111.07
1	E	710	PRO	N-CA-C	-5.63	107.11	114.03
1	C	487	ILE	N-CA-C	5.63	116.68	111.45
1	B	392	THR	N-CA-C	5.62	117.09	111.07
1	C	967	ALA	N-CA-C	-5.62	105.06	111.07
1	C	460	GLY	N-CA-C	5.61	121.75	112.89
1	D	998	GLY	N-CA-C	-5.61	105.86	113.37
1	A	466	ILE	N-CA-C	5.60	115.80	110.42
1	E	851	LEU	CA-C-N	5.60	125.55	119.78
1	E	851	LEU	C-N-CA	5.60	125.55	119.78
1	B	59	ASP	N-CA-C	5.59	120.38	113.50
1	A	532	GLY	N-CA-C	-5.59	106.01	112.50
1	B	1040	ILE	N-CA-C	5.57	120.93	109.34
1	D	336	SER	N-CA-C	5.56	117.03	110.97
1	D	953	MET	CB-CG-SD	-5.56	96.01	112.70
1	F	520	PHE	N-CA-C	-5.56	105.22	111.28
1	F	851	LEU	CA-C-N	5.56	125.51	119.78
1	F	851	LEU	C-N-CA	5.56	125.51	119.78
1	C	867	ARG	N-CA-C	-5.55	105.14	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	329	THR	N-CA-C	-5.55	106.51	113.28
1	B	1005	THR	N-CA-C	5.54	117.01	110.97
1	F	907	LEU	N-CA-C	-5.54	105.24	111.28
1	C	919	ARG	N-CA-C	-5.54	99.01	110.80
1	B	402	ILE	N-CA-C	5.53	116.92	110.62
1	C	644	VAL	N-CA-C	5.53	116.93	110.62
1	F	330	THR	N-CA-C	5.53	119.69	112.17
1	B	559	LEU	CA-C-N	5.53	126.75	119.84
1	B	559	LEU	C-N-CA	5.53	126.75	119.84
1	C	730	ASP	N-CA-C	5.52	118.63	108.58
1	F	124	GLN	N-CA-C	5.51	120.07	113.23
1	C	134	SER	CA-C-N	5.50	130.24	121.66
1	C	134	SER	C-N-CA	5.50	130.24	121.66
1	B	707	ALA	N-CA-C	-5.49	106.56	113.20
1	A	881	LEU	N-CA-C	5.48	117.33	111.36
1	F	498	LYS	CA-C-N	-5.47	114.16	119.90
1	F	498	LYS	C-N-CA	-5.47	114.16	119.90
1	F	897	ILE	N-CA-CB	5.47	114.72	110.45
1	C	515	TRP	N-CA-C	-5.46	104.75	111.75
1	E	532	GLY	N-CA-C	-5.45	106.19	112.73
1	E	559	LEU	CA-C-N	5.43	126.91	120.23
1	E	559	LEU	C-N-CA	5.43	126.91	120.23
1	B	39	ALA	N-CA-C	5.43	116.49	109.65
1	F	104	GLN	N-CA-C	-5.43	105.75	112.38
1	F	542	LEU	N-CA-C	-5.43	105.26	111.07
1	D	746	ILE	CB-CA-C	-5.42	105.03	111.97
1	C	837	THR	N-CA-C	-5.40	105.47	111.36
1	F	515	TRP	N-CA-C	-5.40	104.84	111.75
1	A	521	GLU	N-CA-C	-5.39	105.40	111.28
1	E	115	MET	CA-C-N	-5.39	114.19	119.64
1	E	115	MET	C-N-CA	-5.39	114.19	119.64
1	F	65	ILE	N-CA-C	5.39	116.05	110.82
1	C	701	GLN	N-CA-C	-5.38	105.31	111.07
1	C	30	LEU	CA-C-N	5.38	125.39	119.90
1	C	30	LEU	C-N-CA	5.38	125.39	119.90
1	D	319	SER	N-CA-C	5.38	117.98	109.96
1	C	624	THR	N-CA-C	5.38	118.58	109.76
1	A	706	ALA	N-CA-C	-5.37	106.41	113.17
1	B	117	LEU	N-CA-C	-5.37	107.04	113.21
1	B	516	PHE	N-CA-C	5.37	122.23	110.80
1	B	743	ILE	N-CA-C	-5.35	105.28	110.42
1	A	511	GLY	N-CA-C	5.34	123.59	115.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	68	ASN	N-CA-C	-5.34	106.44	113.17
1	F	856	GLY	N-CA-C	5.34	120.93	112.06
1	C	583	THR	N-CA-C	5.33	118.27	109.85
1	E	929	VAL	N-CA-C	-5.32	105.19	110.62
1	C	113	LEU	N-CA-C	-5.31	107.35	113.88
1	E	1007	VAL	N-CA-C	5.31	115.45	110.30
1	F	193	LEU	N-CA-C	-5.31	106.97	113.50
1	E	30	LEU	CA-C-N	5.30	125.31	119.90
1	E	30	LEU	C-N-CA	5.30	125.31	119.90
1	F	93	THR	N-CA-C	5.30	118.12	109.59
1	A	905	VAL	CB-CA-C	-5.29	108.67	113.70
1	C	973	ARG	CA-C-N	-5.29	113.08	118.85
1	C	973	ARG	C-N-CA	-5.29	113.08	118.85
1	E	240	LEU	N-CA-C	5.29	118.56	110.36
1	C	213	GLN	N-CA-C	-5.28	102.17	110.36
1	F	484	VAL	N-CA-C	5.28	115.49	110.53
1	E	180	SER	N-CA-C	5.28	116.43	108.46
1	D	809	TRP	N-CA-C	5.28	117.25	108.02
1	E	56	THR	N-CA-C	5.27	116.83	111.14
1	A	365	THR	N-CA-C	-5.26	105.60	112.23
1	D	233	SER	N-CA-C	5.26	118.20	109.46
1	F	149	MET	N-CA-C	-5.26	102.73	110.52
1	E	14	VAL	N-CA-C	-5.26	105.26	110.62
1	C	422	GLU	N-CA-C	-5.25	107.25	113.97
1	B	84	SER	N-CA-C	-5.25	107.17	113.21
1	F	6	ILE	N-CA-C	-5.25	104.69	112.04
1	E	260	VAL	N-CA-C	5.24	115.32	107.51
1	C	838	GLY	N-CA-C	5.24	119.48	112.77
1	C	590	VAL	CB-CA-C	-5.23	105.27	111.81
1	E	1022	VAL	CA-C-N	-5.23	113.24	119.05
1	E	1022	VAL	C-N-CA	-5.23	113.24	119.05
1	A	971	ARG	N-CA-C	5.23	119.21	112.41
1	C	100	ALA	N-CA-C	5.23	116.67	110.97
1	B	895	TRP	N-CA-C	-5.22	105.19	112.45
1	D	435	MET	N-CA-C	-5.22	105.49	111.07
1	F	562	SER	N-CA-C	5.20	115.41	108.23
1	C	400	LEU	CA-CB-CG	5.19	134.46	116.30
1	F	622	GLN	N-CA-C	-5.18	105.76	111.71
1	B	77	TYR	N-CA-C	5.17	116.15	108.60
1	B	848	ALA	N-CA-C	-5.17	106.95	113.20
1	A	991	ILE	N-CA-C	-5.17	106.86	113.22
1	D	68	ASN	N-CA-C	5.17	119.55	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	583	THR	N-CA-C	5.17	118.16	109.95
1	D	710	PRO	N-CA-C	-5.16	107.68	114.03
1	F	317	PHE	N-CA-C	5.16	117.44	110.31
1	F	382	VAL	N-CA-C	-5.16	104.64	111.09
1	C	218	GLN	N-CA-C	5.16	117.22	109.23
1	F	54	ALA	N-CA-C	5.16	116.59	111.07
1	F	548	ILE	N-CA-C	-5.15	105.52	110.72
1	C	482	VAL	N-CA-CB	5.15	116.57	110.55
1	C	559	LEU	CA-C-N	5.15	126.28	119.84
1	C	559	LEU	C-N-CA	5.15	126.28	119.84
1	A	851	LEU	CA-C-N	5.15	125.08	119.78
1	A	851	LEU	C-N-CA	5.15	125.08	119.78
1	B	220	GLY	N-CA-C	-5.14	107.16	115.08
1	B	1041	GLU	N-CA-C	-5.14	104.71	112.99
1	E	243	THR	N-CA-C	-5.13	106.17	112.90
1	C	360	GLN	N-CA-C	5.13	121.73	110.80
1	B	273	GLU	N-CA-C	-5.13	106.98	113.18
1	D	310	LEU	N-CA-C	5.12	116.94	111.36
1	F	837	THR	CA-C-N	5.11	125.62	120.00
1	F	837	THR	C-N-CA	5.11	125.62	120.00
1	C	545	TYR	N-CA-C	-5.11	105.60	111.07
1	F	367	ILE	CA-C-N	-5.11	114.52	120.04
1	F	367	ILE	C-N-CA	-5.11	114.52	120.04
1	D	666	PHE	N-CA-C	5.11	116.57	108.96
1	E	1039	ASP	CA-C-N	5.10	131.16	121.97
1	E	1039	ASP	C-N-CA	5.10	131.16	121.97
1	D	148	THR	N-CA-C	-5.10	105.91	111.82
1	A	776	GLU	N-CA-C	-5.10	103.20	110.59
1	F	1042	HIS	N-CA-C	5.10	121.66	110.80
1	A	213	GLN	N-CA-C	-5.09	103.21	110.59
1	C	515	TRP	CA-CB-CG	5.09	123.27	113.60
1	B	127	VAL	N-CA-C	-5.09	101.08	108.97
1	F	511	GLY	N-CA-C	5.08	125.21	113.18
1	B	607	GLU	N-CA-C	-5.08	106.18	112.93
1	D	839	GLU	N-CA-C	-5.07	105.75	111.28
1	B	169	THR	CB-CA-C	-5.07	109.77	117.07
1	B	1028	VAL	N-CA-C	5.07	117.42	111.09
1	D	9	PRO	CA-C-O	5.06	125.59	118.86
1	B	1006	GLY	N-CA-C	-5.06	106.66	112.83
1	C	705	GLU	N-CA-C	-5.05	106.62	112.89
1	C	28	LEU	N-CA-C	5.05	117.52	111.71
1	D	993	THR	N-CA-C	-5.05	101.87	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	700	ASN	N-CA-C	-5.05	105.96	111.82
1	D	198	LEU	N-CA-C	5.05	117.64	109.06
1	C	821	GLY	N-CA-C	5.03	121.75	115.21
1	D	322	LYS	N-CA-C	-5.02	102.08	110.17
1	A	193	LEU	N-CA-C	-5.02	107.00	113.23
1	B	474	ILE	N-CA-C	5.02	115.69	110.82
1	C	935	ILE	CB-CA-C	-5.02	105.46	112.04
1	A	202	ASP	N-CA-C	-5.02	106.67	112.89
1	B	637	ARG	CA-C-N	5.02	126.11	119.84
1	B	637	ARG	C-N-CA	5.02	126.11	119.84
1	F	218	GLN	N-CA-C	5.01	117.59	109.06
1	F	943	ILE	CB-CA-C	-5.01	105.55	111.97
1	F	1030	ARG	N-CA-C	-5.01	106.42	112.54
1	A	970	MET	CA-C-N	-5.00	114.63	122.49
1	A	970	MET	C-N-CA	-5.00	114.63	122.49
1	D	820	ASN	N-CA-C	5.00	121.46	110.80
1	A	637	ARG	CA-C-N	5.00	126.09	119.84
1	A	637	ARG	C-N-CA	5.00	126.09	119.84
1	E	138	MET	N-CA-C	5.00	116.44	108.79

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1038	GLU	Peptide
1	F	7	ASP	Peptide

5.2 Too-close contacts [i](#)

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	7936	0	8072	552	0
1	B	7919	0	8058	537	0
1	C	7936	0	8072	569	0
1	D	7936	0	8072	582	0
1	E	7919	0	8058	637	0
1	F	7936	0	8072	710	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	35	0	46	1	0
2	B	35	0	46	12	0
2	C	35	0	46	5	0
2	D	35	0	46	3	0
2	E	35	0	46	6	0
2	F	35	0	46	2	0
All	All	47792	0	48680	3466	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 36.

All (3466) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ILE:HD11	1:B:726:GLN:HB2	1.41	1.03
1:F:559:LEU:HD22	1:F:560:PRO:HD2	1.40	1.00
1:F:74:ASN:HB3	1:F:95:GLU:HB2	1.41	0.99
1:D:971:ARG:HG2	1:D:974:PRO:HG2	1.47	0.96
1:C:559:LEU:HD22	1:C:560:PRO:HD2	1.47	0.95
1:B:376:LEU:O	1:B:378:GLY:N	1.99	0.95
1:D:23:GLY:HA3	1:D:377:LEU:HB3	1.48	0.94
1:A:359:LEU:O	1:A:361:ASN:N	2.00	0.94
1:C:897:ILE:HG23	1:C:946:VAL:HG11	1.49	0.94
1:C:298:ASN:HB3	1:C:301:ASP:HB2	1.50	0.93
1:D:158:VAL:HA	1:D:162:MET:HE3	1.50	0.93
1:E:427:PRO:HD3	1:E:499:PRO:HB3	1.49	0.93
1:B:225:VAL:HG22	1:C:781:MET:HE3	1.51	0.93
1:D:214:VAL:HG21	1:D:236:ALA:HB3	1.48	0.93
1:D:236:ALA:O	1:E:728:LYS:NZ	2.02	0.93
1:F:586:ARG:HA	1:F:589:LYS:HD2	1.50	0.93
1:F:359:LEU:HD21	1:F:977:MET:HE1	1.48	0.93
1:A:511:GLY:HA2	1:A:515:TRP:HE1	1.33	0.92
1:D:359:LEU:O	1:D:361:ASN:N	2.02	0.92
1:D:832:ALA:HB3	1:D:835:LYS:HD2	1.51	0.92
1:A:236:ALA:O	1:B:728:LYS:NZ	2.03	0.92
1:C:945:ILE:HG13	1:C:971:ARG:HH22	1.35	0.92
1:B:236:ALA:O	1:C:728:LYS:NZ	2.02	0.92
1:F:38:ILE:HG23	1:F:462:SER:HB3	1.51	0.92
1:B:519:MET:O	1:B:523:SER:OG	1.89	0.91
1:C:971:ARG:HH21	1:C:975:ILE:HD11	1.33	0.91
1:A:832:ALA:HB3	1:A:835:LYS:HD2	1.50	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:THR:HG22	1:C:239:ARG:HH21	1.33	0.90
1:F:359:LEU:O	1:F:361:ASN:N	2.04	0.90
1:B:703:LEU:HD11	1:B:718:PRO:HD3	1.54	0.90
1:B:156:ASP:OD2	1:B:769:LYS:NZ	2.06	0.89
1:E:156:ASP:OD2	1:E:769:LYS:NZ	2.05	0.89
1:A:73:ASP:OD2	1:A:106:GLN:NE2	2.05	0.89
1:D:559:LEU:HD22	1:D:560:PRO:HD2	1.55	0.89
1:E:541:TYR:HH	2:E:2000:LMT:H6'	1.08	0.88
1:F:576:VAL:HG23	1:F:663:VAL:HG22	1.55	0.88
1:E:446:ALA:HB2	1:E:482:VAL:HG21	1.54	0.88
1:F:104:GLN:NE2	1:F:108:GLN:OE1	2.07	0.88
1:E:355:MET:HE1	1:E:410:ILE:HG13	1.57	0.87
1:E:359:LEU:O	1:E:361:ASN:N	2.07	0.87
1:D:582:ALA:HA	1:D:586:ARG:HH21	1.39	0.87
1:E:23:GLY:HA3	1:E:377:LEU:HB3	1.55	0.87
1:A:790:TYR:HB3	1:A:798:MET:HB3	1.56	0.87
1:B:350:LEU:HD13	1:B:984:LEU:HB3	1.57	0.87
1:E:197:GLN:NE2	1:E:796:GLY:O	2.08	0.86
1:C:160:ALA:O	1:C:767:ARG:NH1	2.09	0.86
1:A:945:ILE:HG13	1:A:971:ARG:HH12	1.41	0.85
1:F:74:ASN:O	1:F:95:GLU:N	2.07	0.85
1:C:618:ALA:O	1:C:815:ARG:NH2	2.10	0.85
1:E:444:GLY:HA3	1:E:891:LEU:HD22	1.58	0.85
1:B:924:ASP:O	1:B:928:GLN:HG3	1.77	0.85
1:D:451:ALA:HB1	1:D:883:VAL:HG23	1.59	0.85
1:F:49:TYR:CE1	1:F:60:THR:HG21	2.11	0.85
1:C:151:GLN:NE2	1:C:279:ALA:O	2.09	0.84
1:A:414:GLU:OE1	1:A:973:ARG:NH1	2.10	0.84
1:F:184:MET:HB3	1:F:771:VAL:HG13	1.59	0.84
1:B:583:THR:HG22	1:B:586:ARG:HE	1.43	0.84
1:D:182:TYR:HB2	1:D:769:LYS:HZ3	1.40	0.84
1:D:318:PRO:HD2	1:D:321:LEU:HD12	1.59	0.84
1:D:262:LEU:HD12	1:D:268:ILE:HD11	1.57	0.84
1:D:945:ILE:HG13	1:D:971:ARG:HH22	1.43	0.84
1:F:453:PHE:HE2	1:F:474:ILE:HG21	1.42	0.84
1:D:960:LEU:HD21	1:D:1027:VAL:HG22	1.59	0.84
1:F:156:ASP:OD2	1:F:769:LYS:NZ	2.09	0.83
1:A:318:PRO:HD2	1:A:321:LEU:HD12	1.60	0.83
1:E:174:ASP:OD2	1:E:176:GLN:NE2	2.11	0.83
1:E:960:LEU:H	1:E:1039:ASP:HB3	1.43	0.83
1:F:375:VAL:O	1:F:379:THR:OG1	1.95	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:728:LYS:HB3	1:F:808:ARG:HG3	1.58	0.83
1:D:400:LEU:HD11	1:D:933:THR:HG21	1.60	0.83
1:C:144:ASN:O	1:C:284:GLN:NE2	2.12	0.82
1:D:671:ILE:HG22	1:D:673:GLU:H	1.44	0.82
1:D:435:MET:SD	1:D:490:PRO:HB3	2.19	0.82
1:F:380:PHE:HA	1:F:383:LEU:HD12	1.60	0.82
1:B:422:GLU:O	1:B:502:LYS:NZ	2.12	0.82
1:E:186:ILE:HG12	1:E:268:ILE:HG12	1.62	0.82
1:B:1040:ILE:HG22	1:B:1042:HIS:H	1.45	0.82
1:C:151:GLN:HG2	1:C:278:ILE:HG22	1.62	0.82
1:A:108:GLN:NE2	1:B:109:ASN:O	2.13	0.82
1:E:340:VAL:HG11	1:E:395:MET:HB3	1.59	0.82
1:E:907:LEU:HD23	1:E:1017:LEU:HB3	1.62	0.82
1:F:587:THR:OG1	1:F:622:GLN:O	1.97	0.82
1:D:959:GLY:HA2	1:D:1040:ILE:HG23	1.63	0.81
1:E:3:ASN:HA	1:E:6:ILE:HD13	1.62	0.81
1:C:587:THR:OG1	1:C:622:GLN:O	1.97	0.81
1:E:764:ASP:OD2	1:E:765:ARG:NH2	2.14	0.81
1:B:54:ALA:HB1	1:B:816:LEU:HG	1.63	0.81
1:B:427:PRO:HD3	1:B:499:PRO:HB3	1.63	0.81
1:D:399:VAL:HG11	1:D:989:LEU:HD11	1.62	0.81
1:F:713:LEU:HD11	1:F:843:LEU:HD12	1.63	0.81
1:E:171:GLY:O	1:E:302:THR:OG1	1.96	0.81
1:C:649:MET:SD	1:C:653:ARG:NH2	2.54	0.80
1:D:414:GLU:OE1	1:D:973:ARG:NH1	2.14	0.80
1:C:940:LYS:HZ3	1:C:978:THR:HG21	1.46	0.80
1:C:343:THR:HG21	1:C:989:LEU:HD21	1.62	0.80
1:C:1043:SER:OG	1:C:1044:HIS:N	2.14	0.80
1:A:909:VAL:HA	1:A:931:LEU:HD11	1.64	0.80
1:D:612:VAL:HB	1:D:626:ILE:HG22	1.64	0.80
1:B:508:GLY:O	1:B:510:LYS:N	2.13	0.80
1:C:158:VAL:HA	1:C:162:MET:HE3	1.64	0.79
1:C:186:ILE:HB	1:C:773:VAL:HG22	1.63	0.79
1:C:393:LEU:HD22	1:C:469:GLN:HB2	1.64	0.79
1:C:428:LYS:HG2	1:C:494:ALA:HB1	1.62	0.79
1:D:859:TRP:HB3	1:D:863:SER:HB3	1.64	0.79
1:B:211:ASN:O	1:B:760:ASN:ND2	2.15	0.79
1:C:15:ILE:O	1:C:19:ILE:HG13	1.81	0.79
1:F:527:TYR:CE2	1:F:972:LEU:HD13	2.16	0.79
1:A:555:LEU:HD11	1:A:914:LEU:HD12	1.63	0.79
1:B:408:ASP:OD1	1:B:940:LYS:NZ	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:THR:HA	1:C:90:ILE:HD11	1.64	0.79
1:B:457:ALA:HB2	1:B:471:SER:HB3	1.65	0.79
1:E:453:PHE:O	1:E:471:SER:OG	2.01	0.79
1:B:534:ILE:HG22	2:B:2000:LMT:H3'	1.64	0.78
1:F:486:LEU:HD12	1:F:487:ILE:HG13	1.62	0.78
1:A:623:ASN:OD1	1:A:623:ASN:N	2.16	0.78
1:D:492:LEU:HB3	1:D:496:MET:HE2	1.63	0.78
1:E:44:THR:HG1	1:E:91:THR:HG1	1.22	0.78
1:E:562:SER:HB3	1:E:924:ASP:HB3	1.64	0.78
1:B:507:GLU:HG2	1:B:518:ARG:HG2	1.66	0.78
1:A:211:ASN:O	1:A:760:ASN:ND2	2.15	0.78
1:A:599:LEU:O	1:A:603:LYS:NZ	2.14	0.78
1:D:781:MET:HE2	1:F:225:VAL:HG22	1.63	0.78
1:C:359:LEU:O	1:C:361:ASN:N	2.17	0.78
1:C:740:GLY:O	1:C:794:ALA:N	2.15	0.78
1:E:924:ASP:O	1:E:928:GLN:HG3	1.83	0.78
1:F:790:TYR:HB3	1:F:798:MET:HB3	1.64	0.78
1:E:641:GLU:O	1:E:650:ARG:NH2	2.15	0.78
1:F:344:LEU:HD23	1:F:399:VAL:HG22	1.64	0.78
1:D:754:TRP:NE1	1:D:780:ARG:HB3	1.98	0.78
1:B:907:LEU:HB3	1:B:1017:LEU:HD11	1.65	0.78
1:C:713:LEU:HD11	1:C:843:LEU:HD12	1.64	0.78
1:D:144:ASN:O	1:D:284:GLN:NE2	2.16	0.78
1:E:484:VAL:HG13	1:E:488:LEU:HD22	1.65	0.78
1:F:376:LEU:O	1:F:379:THR:N	2.15	0.78
1:A:367:ILE:HD11	1:A:496:MET:HG3	1.64	0.78
1:A:747:ASN:ND2	1:C:237:GLN:OE1	2.14	0.77
1:C:455:PRO:HG2	1:C:880:SER:HA	1.66	0.77
1:D:376:LEU:O	1:D:379:THR:N	2.18	0.77
1:E:228:GLN:NE2	1:E:230:LEU:O	2.16	0.77
1:A:158:VAL:HA	1:A:162:MET:HE3	1.64	0.77
1:D:372:VAL:HG23	1:D:373:PRO:HD3	1.66	0.77
1:F:23:GLY:HA2	1:F:381:ALA:HB2	1.66	0.77
1:A:213:GLN:HG2	1:A:239:ARG:HG3	1.66	0.77
1:B:1013:THR:O	1:B:1017:LEU:HD12	1.85	0.77
1:E:115:MET:HA	1:E:118:LEU:HD22	1.66	0.77
1:A:62:THR:OG1	1:A:88:VAL:HG21	1.83	0.77
1:D:182:TYR:HB2	1:D:769:LYS:NZ	1.99	0.77
1:C:680:PHE:HB2	1:C:859:TRP:HZ3	1.48	0.77
1:C:1033:PHE:O	1:C:1035:ARG:N	2.18	0.77
1:D:137:LEU:HD13	1:D:293:LEU:HD13	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:507:GLU:HA	1:E:518:ARG:HG3	1.67	0.77
1:A:424:GLY:HA3	1:A:502:LYS:HG2	1.65	0.76
1:A:459:PHE:O	1:A:468:ARG:NH2	2.18	0.76
1:B:372:VAL:HG23	1:B:373:PRO:HD3	1.65	0.76
1:D:141:GLY:HA2	1:D:288:GLY:HA2	1.67	0.76
1:A:293:LEU:HD22	1:A:294:ALA:H	1.49	0.76
1:D:584:GLN:HG2	1:D:622:GLN:HG2	1.68	0.76
1:D:743:ILE:HA	1:D:746:ILE:HD12	1.67	0.76
1:E:448:VAL:HG13	1:E:884:VAL:HG22	1.68	0.76
1:A:945:ILE:HA	1:A:971:ARG:HH22	1.51	0.76
1:B:907:LEU:HG	1:B:1017:LEU:HD21	1.67	0.76
1:D:375:VAL:O	1:D:379:THR:OG1	2.03	0.76
1:C:195:LYS:HB3	1:C:196:PHE:CD2	2.19	0.76
1:A:405:LEU:HD22	1:A:481:SER:HB3	1.67	0.76
1:B:652:THR:HG23	1:B:665:ALA:H	1.50	0.76
1:C:982:PHE:O	1:C:985:GLY:N	2.18	0.76
1:E:453:PHE:HE1	1:E:474:ILE:HG21	1.51	0.76
1:E:54:ALA:HB1	1:E:816:LEU:HG	1.66	0.76
1:F:514:GLY:O	1:F:517:ASN:ND2	2.19	0.76
1:F:870:GLY:O	1:F:872:GLN:N	2.19	0.76
1:B:186:ILE:HG12	1:B:268:ILE:HG12	1.68	0.75
1:B:223:PRO:HG3	1:C:275:TYR:CD2	2.20	0.75
1:C:801:PHE:HA	1:C:804:PHE:HE2	1.51	0.75
1:F:99:ASP:O	1:F:103:ALA:N	2.18	0.75
1:E:248:LYS:HA	1:E:261:LEU:HD13	1.66	0.75
1:E:950:LYS:HA	1:E:953:MET:HE2	1.67	0.75
1:E:944:LEU:HB3	1:E:971:ARG:HD3	1.67	0.75
1:F:95:GLU:O	1:F:98:THR:OG1	2.04	0.75
1:F:141:GLY:HA2	1:F:288:GLY:HA2	1.69	0.75
1:A:34:GLN:NE2	1:A:670:ALA:O	2.19	0.75
1:B:446:ALA:HB2	1:B:482:VAL:HG21	1.69	0.75
1:C:588:GLN:HG3	1:C:592:ASN:HD21	1.51	0.75
1:D:945:ILE:HA	1:D:971:ARG:HH12	1.51	0.75
1:A:65:ILE:HD13	1:A:90:ILE:HD12	1.68	0.75
1:B:139:VAL:O	1:B:326:PRO:HD2	1.86	0.75
1:C:38:ILE:HG23	1:C:462:SER:HB3	1.69	0.75
1:A:23:GLY:HA3	1:A:377:LEU:HB3	1.68	0.74
1:E:200:PRO:HG2	1:E:749:THR:HG23	1.68	0.74
1:F:77:TYR:O	1:F:93:THR:HB	1.87	0.74
1:F:959:GLY:HA2	1:F:1041:GLU:H	1.49	0.74
1:A:754:TRP:NE1	1:A:780:ARG:HB3	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LEU:O	1:B:123:GLN:NE2	2.20	0.74
1:D:591:LEU:HD13	1:D:611:ALA:HB1	1.69	0.74
1:B:61:VAL:HG11	1:B:88:VAL:HG21	1.69	0.74
1:C:393:LEU:HD11	1:C:466:ILE:HA	1.69	0.74
1:F:394:THR:HG23	1:F:469:GLN:HB3	1.69	0.74
1:B:867:ARG:HH21	1:B:868:LEU:HD23	1.50	0.74
1:E:412:VAL:HG22	1:E:438:ILE:HD11	1.70	0.74
1:A:207:ILE:HG13	1:A:759:VAL:HG11	1.68	0.74
1:B:764:ASP:OD2	1:B:765:ARG:NH2	2.20	0.74
1:F:186:ILE:HG12	1:F:268:ILE:HG12	1.69	0.74
1:F:792:ARG:NH1	1:F:793:ALA:O	2.20	0.74
1:E:307:ARG:NH2	1:E:328:ASP:OD2	2.19	0.74
1:A:511:GLY:HA2	1:A:515:TRP:NE1	2.03	0.73
1:C:281:PHE:HD1	1:C:610:PHE:HD1	1.35	0.73
1:C:520:PHE:O	1:C:524:THR:OG1	2.05	0.73
1:E:372:VAL:O	1:E:375:VAL:N	2.21	0.73
1:A:115:MET:O	1:A:123:GLN:NE2	2.21	0.73
1:F:340:VAL:HG11	1:F:395:MET:HB3	1.70	0.73
1:A:427:PRO:HD3	1:A:499:PRO:HB3	1.69	0.73
1:E:7:ASP:OD2	1:E:432:ARG:NH2	2.21	0.73
1:F:64:VAL:HG11	1:F:118:LEU:HG	1.67	0.73
1:E:730:ASP:OD1	1:E:730:ASP:N	2.15	0.73
1:F:563:PHE:HB2	1:F:866:GLU:HB2	1.70	0.73
1:B:527:TYR:O	1:B:530:SER:OG	2.06	0.73
1:C:944:LEU:HB3	1:C:971:ARG:CZ	2.19	0.73
1:D:577:GLN:HE22	1:D:721:LEU:HD21	1.53	0.73
1:F:158:VAL:HA	1:F:162:MET:HE3	1.70	0.73
1:F:195:LYS:HD2	1:F:196:PHE:CE1	2.23	0.73
1:F:649:MET:SD	1:F:653:ARG:NH2	2.57	0.73
1:A:244:GLU:HG3	1:A:245:GLU:N	2.02	0.73
1:A:952:LEU:HD11	1:A:970:MET:HE1	1.68	0.73
1:D:138:MET:HE1	1:D:307:ARG:HH22	1.53	0.73
1:D:171:GLY:O	1:D:294:ALA:HB2	1.89	0.73
1:E:703:LEU:HG	1:E:716:VAL:HG12	1.71	0.73
1:E:139:VAL:O	1:E:326:PRO:HD2	1.88	0.73
1:E:559:LEU:HD23	1:E:923:ASN:HB2	1.69	0.73
1:F:493:CYS:O	1:F:497:LEU:HB3	1.89	0.73
1:D:345:VAL:HA	1:D:348:ILE:HD12	1.71	0.73
1:E:157:TYR:OH	1:E:316:PHE:O	2.07	0.73
1:A:800:PRO:HG2	1:A:803:ALA:HB2	1.68	0.72
1:B:250:LEU:HD13	1:B:261:LEU:HD23	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:ASP:OD2	1:D:769:LYS:NZ	2.22	0.72
1:A:137:LEU:HD22	1:A:293:LEU:HD23	1.69	0.72
1:B:231:ASN:OD1	1:C:622:GLN:NE2	2.22	0.72
1:E:576:VAL:HG12	1:E:663:VAL:HG13	1.71	0.72
1:B:362:PHE:O	1:B:365:THR:HG22	1.90	0.72
1:B:801:PHE:HA	1:B:804:PHE:CE2	2.23	0.72
1:B:800:PRO:HG2	1:B:803:ALA:HB2	1.70	0.72
1:A:583:THR:HA	1:A:622:GLN:OE1	1.90	0.72
1:C:27:ILE:HA	1:C:30:LEU:HD22	1.71	0.72
1:F:684:LEU:HB3	1:F:825:MET:O	1.90	0.72
1:B:762:PHE:CE1	1:B:764:ASP:HB3	2.25	0.72
1:C:172:VAL:HG13	1:C:291:ILE:HG23	1.71	0.72
1:F:562:SER:OG	1:F:563:PHE:N	2.22	0.72
1:C:82:SER:HB2	1:C:816:LEU:HB2	1.71	0.72
1:C:137:LEU:HD22	1:C:293:LEU:HD23	1.70	0.72
1:C:141:GLY:HA2	1:C:288:GLY:HA2	1.72	0.72
1:F:139:VAL:HG22	1:F:290:GLY:HA2	1.72	0.72
1:A:713:LEU:HD21	1:A:843:LEU:HD12	1.71	0.71
1:B:30:LEU:HD12	1:B:31:PRO:HD2	1.71	0.71
1:E:971:ARG:O	1:E:975:ILE:HG12	1.89	0.71
1:C:63:GLN:O	1:C:67:GLN:NE2	2.22	0.71
1:F:686:ASP:HB3	1:F:823:PRO:O	1.89	0.71
1:B:45:ILE:HG12	1:B:129:VAL:HG22	1.72	0.71
1:B:375:VAL:O	1:B:379:THR:OG1	2.06	0.71
1:C:455:PRO:HB3	1:C:879:ILE:HG22	1.72	0.71
1:B:4:PHE:HE2	1:B:8:ARG:HH11	1.37	0.71
1:B:376:LEU:C	1:B:378:GLY:H	1.98	0.71
1:D:188:MET:HE1	1:D:200:PRO:HG3	1.73	0.71
1:D:298:ASN:HB3	1:D:301:ASP:HB2	1.72	0.71
1:D:637:ARG:HA	1:D:642:ASN:HD22	1.55	0.71
1:D:790:TYR:HB3	1:D:798:MET:HB3	1.73	0.71
1:A:728:LYS:NZ	1:C:236:ALA:O	2.19	0.71
1:B:457:ALA:HB2	1:B:471:SER:CB	2.20	0.71
1:D:272:GLY:N	1:D:275:TYR:OH	2.22	0.71
1:D:511:GLY:HA2	1:D:515:TRP:CD1	2.26	0.71
1:E:600:THR:HB	1:E:601:LYS:HD2	1.71	0.71
1:D:408:ASP:OD2	1:D:940:LYS:NZ	2.21	0.71
1:D:61:VAL:HG12	1:D:118:LEU:HD22	1.72	0.71
1:D:143:ILE:HG22	1:D:286:ALA:HB2	1.72	0.71
1:F:366:LEU:O	1:F:370:ILE:HG12	1.90	0.71
1:E:867:ARG:HH11	1:E:868:LEU:HA	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101:ASP:O	1:F:105:VAL:HG23	1.91	0.71
1:B:17:ILE:HD13	1:B:20:MET:HE2	1.72	0.71
1:B:641:GLU:O	1:B:650:ARG:NH2	2.24	0.71
1:D:21:LEU:O	1:D:25:LEU:HB2	1.90	0.71
1:B:196:PHE:O	1:B:252:LYS:NZ	2.21	0.71
1:D:3:ASN:O	1:D:6:ILE:HG23	1.90	0.71
1:A:922:THR:O	1:A:924:ASP:N	2.24	0.70
1:E:352:PHE:HD2	1:E:353:LEU:HD23	1.55	0.70
1:B:193:LEU:HD22	1:B:265:VAL:HG22	1.73	0.70
1:C:658:ILE:O	1:C:659:LYS:NZ	2.19	0.70
1:C:971:ARG:CZ	1:C:971:ARG:HB3	2.20	0.70
1:D:447:MET:HB3	1:D:887:CYS:SG	2.31	0.70
1:B:139:VAL:HB	1:B:327:TYR:HB3	1.72	0.70
1:B:228:GLN:NE2	1:B:230:LEU:O	2.24	0.70
1:C:184:MET:HB3	1:C:771:VAL:HG13	1.73	0.70
1:E:982:PHE:HD2	1:E:1011:MET:HG3	1.54	0.70
1:C:151:GLN:O	1:C:155:SER:OG	2.05	0.70
1:A:352:PHE:HD2	1:A:353:LEU:HD23	1.56	0.70
1:C:363:ARG:CZ	1:C:363:ARG:H	2.04	0.70
1:D:33:ALA:HA	1:D:299:ALA:HB3	1.72	0.70
1:D:344:LEU:HD21	1:D:399:VAL:HA	1.73	0.70
1:B:3:ASN:HA	1:B:6:ILE:HD13	1.72	0.70
1:C:363:ARG:HB3	1:C:363:ARG:HH11	1.57	0.70
1:C:1034:SER:HB3	1:C:1037:ASN:HB3	1.74	0.70
1:E:135:SER:OG	1:E:673:GLU:OE1	2.08	0.70
1:A:841:MET:HE1	1:A:867:ARG:HG3	1.73	0.70
1:C:437:GLN:HG3	1:C:438:ILE:HG23	1.74	0.70
1:E:867:ARG:NH1	1:E:868:LEU:HA	2.06	0.70
1:E:82:SER:HB3	1:E:816:LEU:HB2	1.74	0.69
1:A:696:THR:O	1:A:700:ASN:ND2	2.24	0.69
1:F:758:TYR:CE1	1:F:770:LYS:HG3	2.27	0.69
1:D:357:LEU:HG	1:D:357:LEU:O	1.90	0.69
1:F:12:ALA:HB1	1:F:487:ILE:HG23	1.74	0.69
1:F:455:PRO:HG2	1:F:880:SER:HB2	1.74	0.69
1:B:354:VAL:HG22	1:B:980:LEU:HD23	1.75	0.69
1:F:676:THR:HG22	1:F:681:ASP:HB3	1.74	0.69
1:A:781:MET:HB3	1:C:228:GLN:OE1	1.93	0.69
1:C:375:VAL:O	1:C:379:THR:OG1	2.06	0.69
1:D:513:PHE:O	1:D:516:PHE:HB3	1.91	0.69
1:D:662:MET:HA	1:D:662:MET:HE3	1.74	0.69
1:F:400:LEU:HD21	1:F:933:THR:OG1	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ILE:HG13	1:A:20:MET:HE2	1.73	0.69
1:A:193:LEU:HD22	1:A:265:VAL:HB	1.75	0.69
1:A:453:PHE:O	1:A:471:SER:OG	2.08	0.69
1:A:951:ASP:O	1:A:955:LYS:N	2.25	0.69
1:A:988:PRO:O	1:A:992:SER:OG	2.09	0.69
1:D:372:VAL:HA	1:D:375:VAL:HG12	1.74	0.69
1:F:159:ALA:HA	1:F:163:LYS:HB3	1.75	0.69
1:F:506:GLY:C	1:F:508:GLY:H	2.00	0.69
1:A:801:PHE:HA	1:A:804:PHE:HE2	1.58	0.69
1:B:648:THR:O	1:B:652:THR:OG1	2.10	0.69
1:E:368:PRO:HG3	1:E:413:VAL:HG21	1.73	0.69
1:E:372:VAL:HG23	1:E:373:PRO:HD3	1.74	0.69
1:F:401:ALA:HB2	1:F:474:ILE:HG12	1.73	0.69
1:A:953:MET:HB3	1:A:1040:ILE:HG21	1.75	0.69
1:B:778:LYS:HE3	1:B:779:TYR:CZ	2.29	0.68
1:C:36:PRO:O	1:C:38:ILE:HG13	1.94	0.68
1:C:185:ARG:HB3	1:C:187:TRP:HE1	1.57	0.68
1:D:923:ASN:OD1	1:D:928:GLN:NE2	2.27	0.68
1:E:343:THR:HG21	1:E:989:LEU:HD21	1.73	0.68
1:F:30:LEU:HD12	1:F:31:PRO:HD2	1.75	0.68
1:F:137:LEU:HD13	1:F:293:LEU:HD13	1.73	0.68
1:F:897:ILE:HG23	1:F:946:VAL:HG11	1.75	0.68
1:C:74:ASN:HB3	1:C:95:GLU:HB2	1.76	0.68
1:E:832:ALA:HB3	1:E:835:LYS:HD3	1.76	0.68
1:A:961:ILE:HD11	1:A:1031:ARG:HH22	1.58	0.68
1:B:82:SER:HB2	1:B:816:LEU:HB2	1.75	0.68
1:B:717:ARG:HE	1:B:828:LEU:HB2	1.56	0.68
1:E:974:PRO:O	1:E:977:MET:N	2.26	0.68
1:F:428:LYS:HG2	1:F:494:ALA:HB1	1.76	0.68
1:C:588:GLN:O	1:C:592:ASN:ND2	2.26	0.68
1:D:712:MET:HE2	1:D:840:ALA:HB2	1.75	0.68
1:F:698:ALA:O	1:F:701:GLN:HB3	1.94	0.68
1:F:907:LEU:HD23	1:F:1017:LEU:HB3	1.75	0.68
1:B:218:GLN:HG3	1:B:221:GLY:HA2	1.75	0.68
1:C:196:PHE:HD1	1:C:260:VAL:HG13	1.57	0.68
1:A:1025:PHE:O	1:A:1029:VAL:HG13	1.92	0.68
1:B:174:ASP:OD2	1:B:176:GLN:NE2	2.26	0.68
1:B:203:VAL:O	1:B:207:ILE:HG13	1.94	0.68
1:D:634:TRP:CD1	1:D:634:TRP:H	2.11	0.68
1:E:340:VAL:HG22	1:E:396:PHE:CE2	2.28	0.68
1:E:536:ARG:NH1	2:E:2000:LMT:O3B	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ASP:OD2	1:A:769:LYS:NZ	2.24	0.68
1:A:507:GLU:O	1:A:509:LYS:N	2.27	0.68
1:B:69:MET:HE1	1:B:111:LEU:HB2	1.76	0.68
1:C:30:LEU:HD23	1:C:390:ILE:HD11	1.76	0.68
1:D:680:PHE:HD1	1:D:859:TRP:HZ3	1.42	0.68
1:C:222:THR:HA	1:C:224:PRO:HD3	1.76	0.68
1:F:163:LYS:HZ2	1:F:177:LEU:HB2	1.59	0.68
1:E:186:ILE:HD13	1:E:262:LEU:HD21	1.74	0.68
1:F:452:VAL:HG23	1:F:453:PHE:CD1	2.28	0.68
1:E:418:ARG:HH21	1:E:419:VAL:HG23	1.60	0.67
1:E:649:MET:HE3	1:E:653:ARG:HH11	1.58	0.67
1:F:405:LEU:HB2	1:F:481:SER:HB3	1.76	0.67
1:A:163:LYS:HD2	1:A:177:LEU:HD23	1.74	0.67
1:A:354:VAL:HG21	1:A:981:ALA:HA	1.76	0.67
1:C:833:PRO:C	1:C:835:LYS:H	2.01	0.67
1:F:60:THR:HG23	1:F:61:VAL:HG23	1.76	0.67
1:F:623:ASN:N	1:F:623:ASN:OD1	2.23	0.67
1:F:1043:SER:OG	1:F:1044:HIS:N	2.25	0.67
1:B:175:VAL:HG22	1:C:70:ASN:HD22	1.60	0.67
1:E:114:ALA:HA	1:E:117:LEU:HD13	1.74	0.67
1:E:356:TYR:HD1	1:E:365:THR:HG21	1.59	0.67
1:E:596:HIS:O	1:E:600:THR:OG1	2.12	0.67
1:C:185:ARG:HB3	1:C:187:TRP:NE1	2.10	0.67
1:D:444:GLY:HA3	1:D:891:LEU:HD22	1.77	0.67
1:E:609:VAL:HG13	1:E:629:VAL:HG22	1.75	0.67
1:F:218:GLN:HG3	1:F:221:GLY:HA2	1.74	0.67
1:B:535:LEU:HD22	1:B:1027:VAL:HG11	1.76	0.67
1:C:340:VAL:HG21	1:C:392:THR:HG23	1.77	0.67
1:A:20:MET:HG2	1:A:374:VAL:HG13	1.77	0.67
1:A:150:THR:OG1	1:A:151:GLN:N	2.26	0.67
1:B:533:GLY:HA3	2:B:2000:LMT:H6E	1.75	0.67
1:B:888:LEU:HD11	1:B:943:ILE:HD11	1.75	0.67
1:C:187:TRP:HB3	1:C:776:GLU:HG2	1.76	0.67
1:D:453:PHE:O	1:D:471:SER:OG	2.11	0.67
1:F:186:ILE:HB	1:F:773:VAL:HG12	1.75	0.67
1:B:986:VAL:HG21	1:B:1007:VAL:HG11	1.77	0.67
1:C:156:ASP:OD2	1:C:769:LYS:NZ	2.27	0.67
1:D:354:VAL:HG22	1:D:980:LEU:HD23	1.76	0.67
1:D:405:LEU:HD22	1:D:481:SER:HB2	1.75	0.67
1:E:801:PHE:HA	1:E:804:PHE:CE2	2.30	0.67
1:E:108:GLN:HE21	1:F:112:GLN:NE2	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:GLN:NE2	1:F:112:GLN:HE21	1.91	0.67
1:E:425:LEU:HD13	1:E:429:GLU:HG2	1.76	0.67
1:C:398:MET:HG2	1:C:473:THR:HG21	1.77	0.67
1:D:441:ALA:HA	1:D:891:LEU:HD21	1.77	0.67
1:E:382:VAL:HG21	1:E:476:SER:HB3	1.77	0.67
1:E:435:MET:O	1:E:439:GLN:HB2	1.95	0.67
1:D:196:PHE:HD1	1:D:260:VAL:HG13	1.60	0.67
1:E:579:PRO:HD3	1:E:661:ALA:HB2	1.75	0.67
1:E:885:PHE:CD1	1:E:886:LEU:HD22	2.30	0.67
1:C:959:GLY:HA2	1:C:1041:GLU:H	1.59	0.66
1:E:162:MET:HG2	1:E:317:PHE:HZ	1.60	0.66
1:E:905:VAL:HG22	1:E:935:ILE:HD12	1.77	0.66
1:B:146:ASP:OD2	1:B:148:THR:OG1	2.12	0.66
1:C:411:VAL:O	1:C:415:ASN:ND2	2.26	0.66
1:D:907:LEU:HG	1:D:1017:LEU:HB3	1.77	0.66
1:E:239:ARG:NH1	1:E:761:ASP:O	2.25	0.66
1:F:42:ALA:O	1:F:132:SER:OG	2.14	0.66
1:A:612:VAL:HB	1:A:626:ILE:HG22	1.78	0.66
1:B:393:LEU:HD13	1:B:466:ILE:HG23	1.78	0.66
1:D:187:TRP:NE1	1:D:269:GLU:OE2	2.29	0.66
1:A:343:THR:HG21	1:A:989:LEU:HD21	1.77	0.66
1:A:913:LEU:HD23	1:A:927:PHE:HZ	1.61	0.66
1:E:817:GLU:OE1	1:E:826:GLU:N	2.26	0.66
1:A:573:MET:HG3	1:A:666:PHE:HE1	1.60	0.66
1:B:162:MET:HE3	1:B:310:LEU:HD11	1.78	0.66
1:D:44:THR:HG22	1:D:91:THR:HG22	1.77	0.66
1:F:76:MET:HE2	1:F:864:TYR:HE2	1.60	0.66
1:F:391:ASN:ND2	1:F:469:GLN:OE1	2.29	0.66
1:B:197:GLN:O	1:B:792:ARG:HD3	1.96	0.66
1:B:649:MET:HE3	1:B:653:ARG:HH11	1.61	0.66
1:C:13:TRP:HH2	1:C:370:ILE:HG21	1.59	0.66
1:D:574:THR:HG23	1:D:627:ALA:HB3	1.77	0.66
1:F:186:ILE:HD13	1:F:262:LEU:HD21	1.76	0.66
1:A:2:PRO:HA	1:A:486:LEU:HD23	1.77	0.66
1:A:781:MET:HE2	1:C:225:VAL:HG22	1.75	0.66
1:A:895:TRP:O	1:A:898:PRO:HD2	1.96	0.66
1:E:475:VAL:HA	1:E:478:MET:HE3	1.78	0.66
1:C:393:LEU:HD13	1:C:469:GLN:HG3	1.77	0.66
1:F:94:PHE:CZ	1:F:107:VAL:HG21	2.31	0.66
1:A:225:VAL:HG13	1:B:781:MET:HE1	1.77	0.65
1:B:926:TYR:HB3	1:B:1003:VAL:HG22	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1019:ILE:HG13	1:C:1020:PHE:CD1	2.31	0.65
1:D:563:PHE:HB2	1:D:677:ALA:HB2	1.77	0.65
1:E:136:PHE:HA	1:E:292:LYS:HG2	1.78	0.65
1:E:400:LEU:HD11	1:E:1007:VAL:HG21	1.77	0.65
1:E:441:ALA:O	1:E:445:ILE:HG23	1.96	0.65
1:A:712:MET:HE3	1:A:832:ALA:H	1.61	0.65
1:B:792:ARG:NH1	1:B:793:ALA:O	2.30	0.65
1:C:733:GLN:HE22	1:C:743:ILE:HD13	1.61	0.65
1:E:547:ILE:HG13	1:E:548:ILE:N	2.10	0.65
1:B:7:ASP:OD2	1:B:432:ARG:NH2	2.28	0.65
1:B:200:PRO:HA	1:B:203:VAL:HG23	1.79	0.65
1:F:904:VAL:HG21	1:F:942:ALA:HB2	1.77	0.65
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.79	0.65
1:B:712:MET:O	1:B:832:ALA:N	2.25	0.65
1:B:903:LEU:HB3	1:B:1025:PHE:CZ	2.32	0.65
1:C:885:PHE:HA	1:C:902:MET:HE1	1.78	0.65
1:F:599:LEU:O	1:F:603:LYS:HG2	1.97	0.65
1:F:686:ASP:OD2	1:F:823:PRO:HD2	1.97	0.65
1:F:961:ILE:HD12	1:F:961:ILE:H	1.61	0.65
1:A:56:THR:O	1:A:60:THR:OG1	2.15	0.65
1:A:680:PHE:HB2	1:A:863:SER:OG	1.95	0.65
1:A:696:THR:OG1	1:A:825:MET:SD	2.49	0.65
1:E:684:LEU:HD12	1:E:856:GLY:O	1.96	0.65
1:A:743:ILE:O	1:A:746:ILE:HG12	1.97	0.65
1:E:61:VAL:HG21	1:E:122:VAL:HG21	1.78	0.65
1:F:1026:PHE:CZ	1:F:1030:ARG:HG3	2.31	0.65
1:B:114:ALA:HA	1:B:117:LEU:HD13	1.78	0.65
1:B:163:LYS:HD2	1:B:177:LEU:HD22	1.77	0.65
1:C:376:LEU:O	1:C:379:THR:N	2.29	0.65
1:E:108:GLN:HE21	1:F:112:GLN:HE21	1.42	0.65
1:F:4:PHE:HA	1:F:7:ASP:HB2	1.77	0.65
1:F:482:VAL:HG22	1:F:483:LEU:HD23	1.77	0.65
1:F:819:TYR:C	1:F:821:GLY:H	2.05	0.65
1:D:225:VAL:HG22	1:E:781:MET:HE2	1.79	0.65
1:B:536:ARG:HH11	2:B:2000:LMT:H5B	1.61	0.65
1:C:310:LEU:HD23	1:C:323:ILE:HD13	1.77	0.65
1:D:582:ALA:HA	1:D:586:ARG:NH2	2.11	0.65
1:F:900:SER:HB2	1:F:1029:VAL:HG11	1.78	0.65
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.79	0.64
1:A:168:ARG:HG2	1:B:70:ASN:HA	1.80	0.64
1:F:56:THR:O	1:F:60:THR:HB	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:GLN:NE2	1:F:230:LEU:O	2.30	0.64
1:F:393:LEU:HD22	1:F:393:LEU:H	1.62	0.64
1:A:744:ASN:O	1:A:748:THR:HG22	1.97	0.64
1:B:246:PHE:HB3	1:B:268:ILE:HD13	1.79	0.64
1:B:469:GLN:O	1:B:473:THR:OG1	2.11	0.64
1:C:311:ALA:HA	1:C:314:GLU:HG3	1.79	0.64
1:D:795:ASP:OD2	1:D:796:GLY:N	2.29	0.64
1:F:372:VAL:O	1:F:375:VAL:N	2.29	0.64
1:F:676:THR:HG21	1:F:828:LEU:HD22	1.78	0.64
1:B:844:MET:HE2	1:B:844:MET:HA	1.80	0.64
1:C:200:PRO:HA	1:C:203:VAL:HG23	1.80	0.64
1:C:913:LEU:HD23	1:C:927:PHE:HZ	1.61	0.64
1:D:351:VAL:HG22	1:D:981:ALA:HB1	1.77	0.64
1:E:393:LEU:HD13	1:E:466:ILE:HG23	1.80	0.64
1:E:415:ASN:CG	1:E:418:ARG:HH22	2.04	0.64
1:F:65:ILE:HD11	1:F:111:LEU:HG	1.79	0.64
1:F:75:LEU:HD12	1:F:93:THR:O	1.97	0.64
1:B:195:LYS:HD3	1:B:196:PHE:CE1	2.33	0.64
1:B:251:LEU:HD11	1:B:262:LEU:HA	1.78	0.64
1:C:945:ILE:HA	1:C:971:ARG:HH12	1.63	0.64
1:E:138:MET:HG2	1:E:291:ILE:HB	1.80	0.64
1:E:375:VAL:O	1:E:379:THR:OG1	2.13	0.64
1:F:453:PHE:O	1:F:471:SER:OG	2.16	0.64
1:F:1026:PHE:CE2	1:F:1030:ARG:HG3	2.31	0.64
1:B:418:ARG:HH21	1:B:419:VAL:HG23	1.63	0.64
1:B:456:MET:O	1:B:467:TYR:HB3	1.98	0.64
1:D:14:VAL:HG22	1:E:886:LEU:HD12	1.78	0.64
1:D:115:MET:O	1:D:123:GLN:NE2	2.30	0.64
1:D:199:THR:HG23	1:D:792:ARG:H	1.61	0.64
1:D:340:VAL:HG11	1:D:395:MET:HB3	1.79	0.64
1:E:26:ALA:O	1:E:30:LEU:HD22	1.98	0.64
1:E:294:ALA:HB3	1:E:297:ALA:HB3	1.80	0.64
1:E:535:LEU:HD22	1:E:1027:VAL:HG11	1.78	0.64
1:F:584:GLN:HB2	1:F:622:GLN:HG2	1.78	0.64
1:F:801:PHE:HA	1:F:804:PHE:HE2	1.61	0.64
1:A:456:MET:HG3	1:A:932:LEU:HD21	1.80	0.64
1:A:562:SER:OG	1:A:563:PHE:N	2.29	0.64
1:C:363:ARG:HG3	1:C:496:MET:HG2	1.79	0.64
1:C:465:ALA:O	1:C:469:GLN:HG2	1.98	0.64
1:C:682:PHE:HD1	1:C:683:GLU:N	1.96	0.64
1:D:563:PHE:HZ	1:D:865:GLN:HE21	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:PRO:HG3	1:B:779:TYR:HB3	1.78	0.64
1:D:13:TRP:NE1	1:D:492:LEU:HD21	2.12	0.64
1:D:195:LYS:HB3	1:D:196:PHE:CD2	2.33	0.64
1:D:441:ALA:O	1:D:445:ILE:HG23	1.98	0.64
1:F:409:ALA:HA	1:F:485:ALA:HB2	1.80	0.64
1:A:3:ASN:O	1:A:6:ILE:HG23	1.96	0.64
1:C:945:ILE:HG13	1:C:971:ARG:NH2	2.10	0.64
1:D:562:SER:OG	1:D:563:PHE:N	2.29	0.64
1:E:186:ILE:HG22	1:E:773:VAL:HG23	1.80	0.64
1:E:448:VAL:HG21	1:E:888:LEU:HG	1.80	0.64
1:F:634:TRP:CD1	1:F:634:TRP:H	2.14	0.64
1:F:908:GLY:HA2	1:F:1014:ALA:HB2	1.78	0.64
1:A:225:VAL:HG22	1:B:781:MET:SD	2.38	0.64
1:A:913:LEU:HD23	1:A:927:PHE:CZ	2.33	0.64
1:B:108:GLN:NE2	1:C:112:GLN:HB2	2.11	0.64
1:B:344:LEU:HD22	1:B:402:ILE:HD11	1.78	0.64
1:B:1020:PHE:HZ	2:B:2000:LMT:H42	1.61	0.64
1:C:393:LEU:O	1:C:396:PHE:HB2	1.98	0.64
1:E:222:THR:HA	1:E:224:PRO:HD3	1.79	0.64
1:E:246:PHE:HB3	1:E:268:ILE:HD13	1.80	0.64
1:F:250:LEU:HD13	1:F:261:LEU:HD23	1.79	0.64
1:A:712:MET:HE1	1:A:835:LYS:HB3	1.80	0.64
1:C:5:PHE:C	1:C:7:ASP:H	2.04	0.64
1:C:298:ASN:HD22	1:C:301:ASP:CG	2.06	0.64
1:D:400:LEU:HD21	1:D:933:THR:OG1	1.98	0.64
1:E:259:ARG:H	1:E:259:ARG:HD3	1.63	0.64
1:E:885:PHE:HD1	1:E:886:LEU:HD22	1.63	0.64
1:A:901:VAL:HG11	1:A:943:ILE:HG13	1.80	0.63
1:B:668:LEU:HD23	1:B:668:LEU:H	1.63	0.63
1:B:992:SER:O	1:B:997:SER:OG	2.11	0.63
1:C:507:GLU:HG2	1:C:518:ARG:HG3	1.80	0.63
1:C:1003:VAL:HG13	1:C:1004:GLY:H	1.62	0.63
1:E:795:ASP:OD2	1:E:797:GLN:HG2	1.98	0.63
1:F:94:PHE:CE2	1:F:107:VAL:HG21	2.32	0.63
1:A:532:GLY:O	1:A:536:ARG:HG2	1.97	0.63
1:A:562:SER:HB3	1:A:924:ASP:HB3	1.80	0.63
1:D:452:VAL:HG23	1:D:453:PHE:CD1	2.33	0.63
1:E:3:ASN:O	1:E:6:ILE:HB	1.98	0.63
1:E:598:TYR:CE2	1:E:629:VAL:HG21	2.34	0.63
1:E:776:GLU:HB3	1:E:779:TYR:CE1	2.32	0.63
1:A:905:VAL:HG22	1:A:935:ILE:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:TRP:HA	1:B:13:TRP:CE3	2.32	0.63
1:B:907:LEU:CB	1:B:1017:LEU:HD11	2.28	0.63
1:C:908:GLY:HA2	1:C:1014:ALA:HB2	1.79	0.63
1:C:971:ARG:HG2	1:C:974:PRO:HG3	1.80	0.63
1:E:201:VAL:HA	1:E:204:ILE:HD12	1.80	0.63
1:E:393:LEU:HD23	1:E:393:LEU:H	1.62	0.63
1:B:1026:PHE:HD2	1:B:1026:PHE:O	1.82	0.63
1:E:982:PHE:CD2	1:E:1011:MET:HG3	2.32	0.63
1:A:344:LEU:HD21	1:A:399:VAL:HA	1.79	0.63
1:A:712:MET:HE2	1:A:840:ALA:HB2	1.79	0.63
1:C:527:TYR:O	1:C:530:SER:OG	2.16	0.63
1:C:577:GLN:O	1:C:661:ALA:HB1	1.99	0.63
1:F:284:GLN:NE2	1:F:285:PRO:O	2.32	0.63
1:A:61:VAL:O	1:A:65:ILE:HG22	1.99	0.63
1:A:175:VAL:HG11	1:A:289:LEU:HD22	1.80	0.63
1:A:806:SER:O	1:A:807:SER:OG	2.15	0.63
1:A:1035:ARG:HE	1:A:1036:LYS:HG2	1.63	0.63
1:B:447:MET:HB3	1:B:887:CYS:SG	2.37	0.63
1:F:612:VAL:HB	1:F:626:ILE:HG22	1.81	0.63
1:A:172:VAL:HG22	1:A:306:ILE:HD11	1.81	0.63
1:A:577:GLN:O	1:A:661:ALA:HB1	1.99	0.63
1:E:405:LEU:HD22	1:E:481:SER:HB3	1.80	0.63
1:F:75:LEU:HA	1:F:94:PHE:HA	1.81	0.63
1:A:114:ALA:O	1:A:118:LEU:HG	1.99	0.63
1:B:790:TYR:CD1	1:B:800:PRO:HA	2.34	0.63
1:C:602:GLU:OE1	1:C:650:ARG:HD2	1.99	0.63
1:C:982:PHE:HD2	1:C:1011:MET:HG2	1.63	0.63
1:D:886:LEU:HD21	1:F:17:ILE:HG23	1.81	0.63
1:E:214:VAL:HG21	1:E:236:ALA:HB3	1.80	0.63
1:F:47:ALA:HB1	1:F:122:VAL:HG13	1.80	0.63
1:F:102:ILE:O	1:F:105:VAL:HB	1.97	0.63
1:F:185:ARG:HB3	1:F:187:TRP:HE1	1.64	0.63
1:F:527:TYR:O	1:F:531:VAL:HG23	1.98	0.63
1:B:598:TYR:HE2	1:B:629:VAL:HG11	1.64	0.63
1:D:54:ALA:HB2	1:D:84:SER:HB3	1.81	0.63
1:E:379:THR:HA	1:E:382:VAL:HG13	1.80	0.63
1:F:795:ASP:OD2	1:F:796:GLY:N	2.32	0.63
1:A:84:SER:HB3	1:A:814:PRO:HA	1.80	0.62
1:B:662:MET:HE3	1:B:663:VAL:H	1.64	0.62
1:C:38:ILE:CG2	1:C:462:SER:HB3	2.28	0.62
1:D:531:VAL:O	1:D:534:ILE:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:350:LEU:HG	1:F:984:LEU:HD12	1.81	0.62
1:F:847:LEU:HA	1:F:850:LYS:HE3	1.79	0.62
1:A:428:LYS:CD	1:A:428:LYS:H	2.08	0.62
1:B:1015:THR:O	1:B:1017:LEU:N	2.32	0.62
1:C:507:GLU:HG2	1:C:518:ARG:CG	2.28	0.62
1:C:623:ASN:OD1	1:C:623:ASN:N	2.24	0.62
1:E:214:VAL:HG11	1:E:237:GLN:HB3	1.80	0.62
1:A:187:TRP:NE1	1:A:269:GLU:OE2	2.32	0.62
1:E:790:TYR:CD1	1:E:800:PRO:HA	2.34	0.62
1:F:554:TYR:CE1	1:F:558:ARG:HG3	2.34	0.62
1:C:443:VAL:HG12	1:C:891:LEU:HD21	1.82	0.62
1:E:366:LEU:HA	1:E:369:THR:HB	1.82	0.62
1:F:157:TYR:O	1:F:161:ASN:ND2	2.28	0.62
1:F:1033:PHE:O	1:F:1035:ARG:N	2.30	0.62
1:C:17:ILE:HD13	1:C:20:MET:HE2	1.81	0.62
1:C:434:SER:O	1:C:437:GLN:HG2	1.99	0.62
1:D:131:LYS:HZ1	1:E:73:ASP:CG	2.08	0.62
1:D:351:VAL:HG21	1:D:406:VAL:HG11	1.81	0.62
1:E:130:GLU:HG2	1:F:113:LEU:HD21	1.80	0.62
1:A:622:GLN:CD	1:C:231:ASN:HD22	2.07	0.62
1:A:712:MET:HB3	1:A:713:LEU:HD22	1.81	0.62
1:C:680:PHE:HB2	1:C:859:TRP:CZ3	2.34	0.62
1:D:62:THR:OG1	1:D:88:VAL:HG21	1.99	0.62
1:D:1019:ILE:HG13	1:D:1020:PHE:HD1	1.64	0.62
1:E:405:LEU:HD11	1:E:477:ALA:HB1	1.80	0.62
1:F:905:VAL:HG22	1:F:935:ILE:HG13	1.81	0.62
1:A:23:GLY:HA2	1:A:377:LEU:O	2.00	0.62
1:A:364:ALA:HA	1:A:367:ILE:HD13	1.80	0.62
1:C:363:ARG:HA	1:C:366:LEU:HG	1.80	0.62
1:D:203:VAL:O	1:D:207:ILE:HG13	1.99	0.62
1:D:208:LYS:HG3	1:D:759:VAL:HG13	1.80	0.62
1:D:978:THR:O	1:D:982:PHE:N	2.29	0.62
1:E:58:GLN:O	1:E:63:GLN:HG3	1.99	0.62
1:E:943:ILE:O	1:E:947:GLU:HB3	1.99	0.62
1:F:375:VAL:HG13	1:F:480:LEU:HB2	1.81	0.62
1:F:429:GLU:OE1	1:F:430:ALA:N	2.32	0.62
1:A:135:SER:HB3	1:A:672:VAL:HG12	1.80	0.62
1:A:776:GLU:HB3	1:A:779:TYR:CE1	2.34	0.62
1:B:559:LEU:HD22	1:B:923:ASN:HB2	1.82	0.62
1:D:707:ALA:HB2	1:D:716:VAL:HG21	1.81	0.62
1:F:211:ASN:ND2	1:F:760:ASN:HD21	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:462:SER:N	1:F:865:GLN:OE1	2.32	0.62
1:F:509:LYS:HB3	1:F:514:GLY:HA3	1.81	0.62
1:B:418:ARG:NH1	1:B:970:MET:HE2	2.15	0.62
1:E:231:ASN:OD1	1:F:622:GLN:NE2	2.32	0.62
1:F:372:VAL:HG12	1:F:405:LEU:HD11	1.82	0.62
1:A:188:MET:HE1	1:A:200:PRO:HG3	1.82	0.62
1:A:300:LEU:HD23	1:A:334:LYS:HE3	1.81	0.62
1:A:1019:ILE:HG13	1:A:1020:PHE:CD1	2.35	0.62
1:B:182:TYR:HB2	1:B:769:LYS:NZ	2.15	0.62
1:C:5:PHE:HE1	1:C:8:ARG:HH11	1.46	0.62
1:E:251:LEU:HD11	1:E:262:LEU:HA	1.81	0.62
1:F:540:ARG:HD3	1:F:541:TYR:CE1	2.34	0.62
1:B:616:GLY:HA2	1:B:626:ILE:HB	1.82	0.61
1:D:2:PRO:HB3	1:D:486:LEU:HD23	1.82	0.61
1:D:211:ASN:O	1:D:760:ASN:ND2	2.32	0.61
1:D:668:LEU:H	1:D:668:LEU:HD23	1.65	0.61
1:F:564:LEU:HD23	1:F:565:PRO:HD2	1.81	0.61
1:F:600:THR:O	1:F:603:LYS:HG3	2.00	0.61
1:A:404:LEU:HD12	1:A:937:LEU:HD21	1.82	0.61
1:B:58:GLN:HA	1:B:62:THR:HB	1.82	0.61
1:B:214:VAL:CG2	1:B:237:GLN:HB3	2.30	0.61
1:D:408:ASP:OD1	1:D:481:SER:OG	2.16	0.61
1:D:577:GLN:O	1:D:661:ALA:HB1	2.00	0.61
1:E:356:TYR:HA	1:E:365:THR:HG21	1.82	0.61
1:E:418:ARG:CZ	1:E:418:ARG:HB3	2.31	0.61
1:A:508:GLY:HA2	1:A:514:GLY:HA3	1.82	0.61
1:A:945:ILE:HA	1:A:971:ARG:NH2	2.15	0.61
1:B:309:GLU:HG2	1:B:313:MET:HE3	1.82	0.61
1:B:1020:PHE:CZ	2:B:2000:LMT:H42	2.35	0.61
1:F:49:TYR:HE1	1:F:60:THR:HG21	1.63	0.61
1:F:184:MET:HG2	1:F:246:PHE:CE2	2.35	0.61
1:A:508:GLY:O	1:A:510:LYS:N	2.28	0.61
1:C:61:VAL:HB	1:C:88:VAL:HG11	1.81	0.61
1:D:101:ASP:OD2	1:D:101:ASP:N	2.32	0.61
1:D:776:GLU:OE1	1:D:778:LYS:NZ	2.32	0.61
1:E:110:LYS:HD3	1:E:113:LEU:HD12	1.81	0.61
1:E:407:ASP:OD1	1:E:978:THR:HG21	2.00	0.61
1:F:676:THR:HG23	1:F:677:ALA:H	1.64	0.61
1:F:703:LEU:HD21	1:F:827:ILE:HG23	1.83	0.61
1:A:70:ASN:O	1:A:110:LYS:NZ	2.31	0.61
1:A:895:TRP:C	1:A:898:PRO:HD2	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:LEU:O	1:B:361:ASN:N	2.33	0.61
1:B:1027:VAL:HG22	1:B:1031:ARG:HD2	1.82	0.61
1:C:870:GLY:O	1:C:872:GLN:N	2.33	0.61
1:D:622:GLN:NE2	1:F:231:ASN:OD1	2.34	0.61
1:E:344:LEU:HD21	1:E:399:VAL:HA	1.81	0.61
1:F:45:ILE:HD13	1:F:111:LEU:HD12	1.82	0.61
1:F:218:GLN:HA	1:F:234:ILE:HD13	1.81	0.61
1:F:801:PHE:HA	1:F:804:PHE:CE2	2.36	0.61
1:A:971:ARG:CG	1:A:974:PRO:HG2	2.31	0.61
1:D:414:GLU:CD	1:D:974:PRO:HG3	2.25	0.61
1:C:493:CYS:O	1:C:497:LEU:HB3	2.00	0.61
1:E:376:LEU:O	1:E:379:THR:N	2.33	0.61
1:B:352:PHE:HD2	1:B:353:LEU:HD23	1.66	0.61
1:B:418:ARG:HD2	1:B:422:GLU:OE1	2.01	0.61
1:C:186:ILE:HD13	1:C:262:LEU:HD21	1.82	0.61
1:D:922:THR:O	1:D:924:ASP:N	2.33	0.61
1:E:380:PHE:HD2	1:E:383:LEU:HD12	1.66	0.61
1:E:447:MET:HB3	1:E:887:CYS:SG	2.40	0.61
1:E:493:CYS:O	1:E:497:LEU:HB3	2.01	0.61
1:F:298:ASN:HB3	1:F:301:ASP:HB2	1.83	0.61
1:F:450:SER:O	1:F:454:VAL:HG23	2.01	0.61
1:F:476:SER:O	1:F:480:LEU:HG	1.99	0.61
1:F:846:GLN:O	1:F:849:SER:OG	2.18	0.61
1:C:366:LEU:HA	1:C:369:THR:HB	1.83	0.61
1:D:1013:THR:O	1:D:1017:LEU:HB2	2.00	0.61
1:E:69:MET:HG2	1:E:110:LYS:HB3	1.83	0.61
1:F:137:LEU:HD22	1:F:293:LEU:HD13	1.83	0.61
1:F:200:PRO:HA	1:F:203:VAL:HG23	1.83	0.61
1:B:222:THR:HA	1:B:224:PRO:HD3	1.83	0.61
1:B:792:ARG:NH1	1:B:792:ARG:O	2.34	0.61
1:C:634:TRP:CD1	1:C:634:TRP:H	2.19	0.61
1:D:776:GLU:HB3	1:D:779:TYR:CD1	2.36	0.61
1:D:990:VAL:HG22	1:D:1004:GLY:HA3	1.83	0.61
1:A:362:PHE:O	1:A:365:THR:HG22	2.01	0.60
1:E:457:ALA:HB1	1:E:468:ARG:HG3	1.82	0.60
1:E:775:SER:OG	1:E:780:ARG:HG2	2.00	0.60
1:E:801:PHE:HA	1:E:804:PHE:HE2	1.66	0.60
1:F:291:ILE:HD13	1:F:306:ILE:HD13	1.81	0.60
1:F:453:PHE:CE2	1:F:474:ILE:HG21	2.29	0.60
1:B:189:ASN:HB3	1:B:192:GLU:HB2	1.82	0.60
1:B:727:PHE:HB2	1:B:809:TRP:HE1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:LEU:HD13	1:C:384:ALA:HB2	1.83	0.60
1:D:452:VAL:HA	1:D:880:SER:OG	2.00	0.60
1:D:884:VAL:O	1:D:888:LEU:HD22	2.01	0.60
1:E:104:GLN:HE22	1:F:109:ASN:HB3	1.65	0.60
1:E:562:SER:OG	1:E:563:PHE:N	2.34	0.60
1:F:376:LEU:HD22	1:F:398:MET:HE2	1.83	0.60
1:F:583:THR:HA	1:F:622:GLN:OE1	2.00	0.60
1:F:795:ASP:OD2	1:F:797:GLN:HG2	2.01	0.60
1:A:897:ILE:HD11	1:A:1030:ARG:HH21	1.66	0.60
1:B:278:ILE:HG13	1:B:613:ASN:HB3	1.82	0.60
1:C:910:ILE:O	1:C:914:LEU:HB2	2.01	0.60
1:D:587:THR:OG1	1:D:622:GLN:O	2.18	0.60
1:A:72:ILE:HD13	1:A:107:VAL:HG22	1.83	0.60
1:A:622:GLN:HE21	1:C:222:THR:HG22	1.66	0.60
1:A:790:TYR:CD1	1:A:800:PRO:HA	2.36	0.60
1:C:186:ILE:HG12	1:C:268:ILE:HG22	1.84	0.60
1:C:971:ARG:O	1:C:975:ILE:HG12	2.01	0.60
1:E:193:LEU:HD22	1:E:265:VAL:HB	1.83	0.60
1:F:352:PHE:HD2	1:F:353:LEU:HD23	1.66	0.60
1:F:758:TYR:HE1	1:F:770:LYS:HG3	1.65	0.60
1:A:971:ARG:O	1:A:975:ILE:HG12	2.01	0.60
1:B:307:ARG:NH2	1:B:328:ASP:OD2	2.34	0.60
1:B:536:ARG:HD2	2:B:2000:LMT:H5B	1.84	0.60
1:C:527:TYR:O	1:C:531:VAL:HG23	2.01	0.60
1:E:996:GLY:O	1:E:999:ALA:N	2.34	0.60
1:F:358:PHE:CG	1:F:977:MET:HE2	2.37	0.60
1:F:680:PHE:CE2	1:F:682:PHE:HB2	2.36	0.60
1:F:833:PRO:C	1:F:835:LYS:H	2.10	0.60
1:E:744:ASN:O	1:E:748:THR:HG23	2.02	0.60
1:E:867:ARG:NH1	1:E:867:ARG:O	2.34	0.60
1:A:524:THR:O	1:A:528:THR:HG23	2.02	0.60
1:B:702:LEU:HD22	1:B:851:LEU:HD11	1.83	0.60
1:B:904:VAL:O	1:B:907:LEU:HB2	2.02	0.60
1:D:102:ILE:O	1:D:106:GLN:HG2	2.02	0.60
1:D:623:ASN:OD1	1:D:623:ASN:N	2.34	0.60
1:F:45:ILE:HD12	1:F:90:ILE:HG23	1.84	0.60
1:F:207:ILE:HG22	1:F:249:ILE:HD13	1.82	0.60
1:F:368:PRO:HG3	1:F:413:VAL:HG21	1.82	0.60
1:E:901:VAL:HG22	1:E:946:VAL:HG21	1.82	0.60
1:F:669:PRO:HD3	1:F:676:THR:O	2.01	0.60
1:F:684:LEU:O	1:F:824:SER:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:982:PHE:O	1:F:985:GLY:N	2.34	0.60
1:B:983:ILE:HG23	1:B:1008:MET:HE2	1.83	0.60
1:C:326:PRO:O	1:C:630:SER:HB2	2.01	0.60
1:E:519:MET:O	1:E:523:SER:OG	2.17	0.60
1:E:557:VAL:C	1:E:559:LEU:H	2.10	0.60
1:E:685:ILE:HD11	1:E:819:TYR:CD1	2.36	0.60
1:E:944:LEU:HD13	1:E:971:ARG:HH11	1.67	0.60
1:F:533:GLY:HA2	1:F:536:ARG:NH1	2.17	0.60
1:A:909:VAL:HG22	1:A:931:LEU:HD21	1.83	0.60
1:B:80:SER:HB2	1:B:818:ARG:HB2	1.84	0.60
1:D:559:LEU:HD12	1:D:923:ASN:HB2	1.82	0.60
1:F:144:ASN:CG	1:F:320:GLY:HA3	2.26	0.60
1:F:922:THR:O	1:F:924:ASP:N	2.35	0.60
1:A:467:TYR:CE2	1:A:925:VAL:HG23	2.37	0.59
1:B:195:LYS:HD3	1:B:196:PHE:CZ	2.36	0.59
1:B:576:VAL:HG22	1:B:663:VAL:HG13	1.84	0.59
1:B:598:TYR:CE2	1:B:629:VAL:HG11	2.37	0.59
1:C:65:ILE:HG13	1:C:111:LEU:HD23	1.82	0.59
1:D:390:ILE:O	1:D:394:THR:OG1	2.19	0.59
1:D:1011:MET:HE2	1:D:1014:ALA:HB3	1.84	0.59
1:E:428:LYS:HG2	1:E:494:ALA:HB1	1.82	0.59
1:E:958:LYS:NZ	1:E:966:ASP:OD2	2.35	0.59
1:E:1041:GLU:O	1:E:1042:HIS:HB2	2.00	0.59
1:B:894:SER:HB2	1:B:897:ILE:HG13	1.84	0.59
1:C:99:ASP:OD2	1:C:102:ILE:HB	2.02	0.59
1:C:380:PHE:HD2	1:C:383:LEU:HD12	1.66	0.59
1:D:34:GLN:HG2	1:D:333:VAL:HG22	1.83	0.59
1:A:211:ASN:OD1	1:A:240:LEU:HG	2.02	0.59
1:B:293:LEU:HD21	1:B:297:ALA:O	2.02	0.59
1:C:892:TYR:HD1	1:C:897:ILE:HG21	1.67	0.59
1:F:404:LEU:HD11	1:F:449:LEU:HD22	1.84	0.59
1:A:687:GLN:N	1:A:854:GLY:O	2.33	0.59
1:B:119:PRO:O	1:B:123:GLN:HG3	2.03	0.59
1:C:363:ARG:HB3	1:C:363:ARG:NH1	2.17	0.59
1:C:572:PHE:HD1	1:C:631:LEU:HD11	1.67	0.59
1:D:75:LEU:HB3	1:F:169:THR:O	2.02	0.59
1:D:754:TRP:CE2	1:D:780:ARG:HB3	2.37	0.59
1:D:945:ILE:HG13	1:D:971:ARG:NH2	2.15	0.59
1:F:418:ARG:O	1:F:422:GLU:HB2	2.02	0.59
1:B:344:LEU:HD23	1:B:399:VAL:HG22	1.85	0.59
1:D:394:THR:HB	1:D:473:THR:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:GLN:O	1:E:792:ARG:HD3	2.03	0.59
1:F:187:TRP:HA	1:F:774:MET:O	2.03	0.59
1:F:465:ALA:O	1:F:469:GLN:HG2	2.02	0.59
1:A:795:ASP:OD2	1:A:796:GLY:N	2.36	0.59
1:C:590:VAL:O	1:C:593:GLU:HB2	2.02	0.59
1:D:395:MET:HE2	1:D:398:MET:HG3	1.84	0.59
1:D:416:VAL:HG11	1:D:493:CYS:SG	2.43	0.59
1:D:1019:ILE:HG13	1:D:1020:PHE:CD1	2.38	0.59
1:E:102:ILE:HA	1:E:105:VAL:HG23	1.84	0.59
1:F:64:VAL:HG21	1:F:118:LEU:HD23	1.83	0.59
1:A:428:LYS:H	1:A:428:LYS:HD2	1.67	0.59
1:B:414:GLU:OE1	1:B:973:ARG:NH1	2.36	0.59
1:C:137:LEU:HB2	1:C:293:LEU:HB2	1.83	0.59
1:C:596:HIS:O	1:C:600:THR:OG1	2.21	0.59
1:E:184:MET:HB2	1:E:762:PHE:CE2	2.37	0.59
1:E:365:THR:O	1:E:368:PRO:HD2	2.03	0.59
1:F:420:MET:HE2	1:F:427:PRO:HG3	1.84	0.59
1:B:520:PHE:HE1	1:B:973:ARG:HD2	1.67	0.59
1:B:634:TRP:H	1:B:634:TRP:CD1	2.18	0.59
1:E:162:MET:HG2	1:E:317:PHE:CZ	2.37	0.59
1:F:163:LYS:NZ	1:F:177:LEU:HB2	2.17	0.59
1:A:709:HIS:CE1	1:A:847:LEU:HD11	2.37	0.59
1:A:1018:ALA:O	1:A:1022:VAL:HG13	2.03	0.59
1:B:13:TRP:HA	1:B:13:TRP:HE3	1.68	0.59
1:C:187:TRP:HA	1:C:774:MET:O	2.01	0.59
1:E:149:MET:HB2	1:E:153:ASP:HB2	1.84	0.59
1:E:905:VAL:HG22	1:E:935:ILE:HG23	1.84	0.59
1:A:518:ARG:O	1:A:522:LYS:HG3	2.03	0.59
1:B:910:ILE:O	1:B:914:LEU:HB2	2.03	0.59
1:D:637:ARG:NH1	1:D:642:ASN:O	2.35	0.59
1:D:971:ARG:C	1:D:974:PRO:HD2	2.28	0.59
1:E:102:ILE:CG2	1:E:106:GLN:HE22	2.16	0.59
1:F:185:ARG:HB3	1:F:187:TRP:NE1	2.18	0.59
1:B:730:ASP:OD1	1:B:730:ASP:N	2.24	0.58
1:C:99:ASP:O	1:C:102:ILE:HG22	2.02	0.58
1:C:944:LEU:HB3	1:C:971:ARG:NE	2.16	0.58
1:F:588:GLN:HG3	1:F:592:ASN:HD21	1.68	0.58
1:A:163:LYS:O	1:A:163:LYS:HG2	2.02	0.58
1:A:658:ILE:O	1:A:659:LYS:NZ	2.25	0.58
1:A:776:GLU:HB3	1:A:779:TYR:CD1	2.38	0.58
1:A:974:PRO:HA	1:A:977:MET:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1036:LYS:HB3	1:A:1040:ILE:HD13	1.85	0.58
1:C:139:VAL:HG22	1:C:290:GLY:HA2	1.85	0.58
1:D:124:GLN:CD	1:D:758:TYR:HD2	2.11	0.58
1:D:983:ILE:HD11	1:D:1011:MET:HB3	1.85	0.58
1:F:358:PHE:CD1	1:F:977:MET:HG2	2.38	0.58
1:A:634:TRP:CD1	1:A:634:TRP:H	2.22	0.58
1:A:715:SER:HB3	1:A:717:ARG:HD2	1.85	0.58
1:B:182:TYR:HB2	1:B:769:LYS:HZ2	1.67	0.58
1:C:240:LEU:HB2	1:C:246:PHE:CZ	2.38	0.58
1:E:24:GLY:N	1:E:377:LEU:HD12	2.18	0.58
1:E:947:GLU:HG3	1:E:948:PHE:CD2	2.38	0.58
1:F:913:LEU:HD23	1:F:927:PHE:HZ	1.67	0.58
1:A:58:GLN:O	1:A:63:GLN:HG3	2.03	0.58
1:B:280:GLU:OE1	1:B:588:GLN:NE2	2.35	0.58
1:B:448:VAL:HG13	1:B:884:VAL:HG13	1.84	0.58
1:B:790:TYR:HD1	1:B:800:PRO:HA	1.67	0.58
1:C:379:THR:HG23	1:C:476:SER:OG	2.02	0.58
1:D:511:GLY:HA2	1:D:515:TRP:HD1	1.68	0.58
1:F:57:VAL:HA	1:F:60:THR:HG22	1.85	0.58
1:F:166:ILE:HG21	1:F:289:LEU:HD13	1.86	0.58
1:A:801:PHE:HA	1:A:804:PHE:CE2	2.39	0.58
1:C:143:ILE:HG22	1:C:286:ALA:HB2	1.85	0.58
1:E:1013:THR:O	1:E:1017:LEU:HB2	2.04	0.58
1:B:108:GLN:HE21	1:C:112:GLN:NE2	2.01	0.58
1:B:262:LEU:HD12	1:B:265:VAL:HG12	1.85	0.58
1:C:100:ALA:HB1	1:C:131:LYS:HE3	1.85	0.58
1:C:924:ASP:O	1:C:928:GLN:HG3	2.04	0.58
1:D:442:LEU:O	1:D:445:ILE:HG13	2.03	0.58
1:D:538:THR:HG22	1:D:1024:VAL:HG13	1.85	0.58
1:E:203:VAL:O	1:E:207:ILE:HG13	2.03	0.58
1:A:452:VAL:HA	1:A:880:SER:OG	2.04	0.58
1:A:467:TYR:HE2	1:A:925:VAL:HG23	1.69	0.58
1:A:844:MET:HA	1:A:844:MET:HE2	1.86	0.58
1:A:1043:SER:OG	1:A:1044:HIS:N	2.35	0.58
1:D:335:ILE:O	1:D:339:GLU:HG2	2.04	0.58
1:E:982:PHE:CE2	1:E:1007:VAL:HG13	2.39	0.58
1:F:6:ILE:HG21	1:F:487:ILE:HG12	1.85	0.58
1:F:97:GLY:C	1:F:99:ASP:H	2.09	0.58
1:F:668:LEU:H	1:F:668:LEU:HD22	1.69	0.58
1:F:790:TYR:CE1	1:F:800:PRO:HA	2.39	0.58
1:A:262:LEU:HA	1:A:265:VAL:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:VAL:HA	1:B:204:ILE:HD12	1.86	0.58
1:C:414:GLU:HA	1:C:973:ARG:HH22	1.67	0.58
1:D:199:THR:CG2	1:D:792:ARG:H	2.17	0.58
1:D:860:THR:H	1:D:863:SER:HB2	1.67	0.58
1:D:940:LYS:O	1:D:943:ILE:N	2.36	0.58
1:D:1003:VAL:HG13	1:D:1004:GLY:H	1.68	0.58
1:E:81:ASN:O	1:E:88:VAL:HA	2.04	0.58
1:F:671:ILE:H	1:F:862:MET:HE2	1.69	0.58
1:B:36:PRO:O	1:B:38:ILE:HG13	2.04	0.58
1:C:578:LEU:CD2	1:C:579:PRO:HD2	2.34	0.58
1:D:446:ALA:HB2	1:D:482:VAL:HG21	1.86	0.58
1:D:982:PHE:O	1:D:985:GLY:N	2.34	0.58
1:D:1026:PHE:O	1:D:1026:PHE:HD2	1.87	0.58
1:F:160:ALA:O	1:F:767:ARG:NH1	2.37	0.58
1:F:187:TRP:HB3	1:F:776:GLU:HG2	1.86	0.58
1:F:272:GLY:N	1:F:275:TYR:OH	2.36	0.58
1:A:544:LEU:O	1:A:548:ILE:HG13	2.04	0.58
1:B:795:ASP:OD2	1:B:796:GLY:N	2.37	0.58
1:B:953:MET:HE2	1:B:963:ALA:HB3	1.85	0.58
1:D:47:ALA:HB3	1:D:88:VAL:HG13	1.86	0.58
1:D:178:PHE:HB2	1:D:288:GLY:H	1.69	0.58
1:F:214:VAL:HG11	1:F:236:ALA:HB3	1.85	0.58
1:F:350:LEU:HD23	1:F:984:LEU:O	2.03	0.58
1:C:193:LEU:HD22	1:C:265:VAL:HB	1.85	0.57
1:E:987:MET:O	1:E:990:VAL:HG22	2.04	0.57
1:F:691:GLY:O	1:F:694:LYS:HG2	2.03	0.57
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.86	0.57
1:A:1035:ARG:O	1:A:1037:ASN:N	2.37	0.57
1:D:3:ASN:OD1	1:D:6:ILE:HD12	2.03	0.57
1:D:30:LEU:HD22	1:D:31:PRO:HD2	1.87	0.57
1:D:75:LEU:O	1:F:170:SER:OG	2.23	0.57
1:D:408:ASP:O	1:D:411:VAL:HG12	2.04	0.57
1:E:587:THR:OG1	1:E:622:GLN:O	2.14	0.57
1:E:790:TYR:HB3	1:E:798:MET:HB3	1.85	0.57
1:B:239:ARG:NH1	1:B:761:ASP:O	2.37	0.57
1:B:433:LYS:O	1:B:437:GLN:HG3	2.03	0.57
1:C:394:THR:HG22	1:C:469:GLN:HB3	1.85	0.57
1:C:944:LEU:HD13	1:C:971:ARG:HE	1.69	0.57
1:D:350:LEU:HD23	1:D:985:GLY:HA2	1.85	0.57
1:D:600:THR:O	1:D:603:LYS:HG3	2.04	0.57
1:D:734:GLU:O	1:D:736:ALA:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:344:LEU:HG	1:E:399:VAL:HG22	1.86	0.57
1:E:452:VAL:C	1:E:455:PRO:HD2	2.28	0.57
1:A:723:ASP:OD2	1:A:813:SER:OG	2.21	0.57
1:B:909:VAL:O	1:B:912:ALA:N	2.37	0.57
1:C:5:PHE:O	1:C:7:ASP:N	2.37	0.57
1:C:414:GLU:HG2	1:C:973:ARG:NH1	2.18	0.57
1:C:484:VAL:O	1:C:488:LEU:N	2.32	0.57
1:D:367:ILE:HB	1:D:368:PRO:HD3	1.85	0.57
1:D:619:GLY:HA3	1:D:815:ARG:HH12	1.69	0.57
1:F:462:SER:HB2	1:F:865:GLN:HG2	1.86	0.57
1:F:527:TYR:CD2	1:F:972:LEU:HD22	2.39	0.57
1:A:235:ILE:HD11	1:B:726:GLN:CB	2.26	0.57
1:B:66:GLU:CD	1:B:818:ARG:HE	2.12	0.57
1:B:189:ASN:OD1	1:B:190:PRO:HD2	2.04	0.57
1:C:149:MET:HG3	1:C:154:ILE:HD11	1.87	0.57
1:D:154:ILE:HG22	1:D:287:SER:HB3	1.86	0.57
1:D:202:ASP:O	1:D:206:ALA:HB2	2.04	0.57
1:D:932:LEU:O	1:D:935:ILE:HB	2.05	0.57
1:E:293:LEU:HD13	1:E:294:ALA:O	2.04	0.57
1:F:4:PHE:O	1:F:7:ASP:HB2	2.05	0.57
1:A:278:ILE:HG23	1:A:613:ASN:HB3	1.86	0.57
1:B:843:LEU:O	1:B:847:LEU:HG	2.05	0.57
1:C:45:ILE:HA	1:C:128:SER:O	2.05	0.57
1:C:203:VAL:O	1:C:207:ILE:HG12	2.05	0.57
1:C:335:ILE:HG23	1:C:995:ALA:HB1	1.87	0.57
1:C:465:ALA:HA	1:C:468:ARG:NH1	2.20	0.57
1:C:926:TYR:HE2	1:C:999:ALA:HB1	1.69	0.57
1:D:367:ILE:HG23	1:D:496:MET:HE3	1.86	0.57
1:D:594:VAL:HG22	1:D:655:PHE:CE2	2.39	0.57
1:D:698:ALA:O	1:D:701:GLN:HB3	2.03	0.57
1:E:195:LYS:HD2	1:E:196:PHE:CE1	2.39	0.57
1:F:682:PHE:HB3	1:F:827:ILE:O	2.05	0.57
1:F:691:GLY:HA3	1:F:694:LYS:HE2	1.87	0.57
1:A:189:ASN:HB3	1:A:192:GLU:HG2	1.87	0.57
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.86	0.57
1:A:971:ARG:C	1:A:974:PRO:HD2	2.30	0.57
1:A:971:ARG:HG2	1:A:974:PRO:HG2	1.87	0.57
1:B:76:MET:HG2	1:B:864:TYR:HE2	1.68	0.57
1:C:366:LEU:O	1:C:370:ILE:HG13	2.04	0.57
1:D:10:ILE:HB	1:E:893:GLU:HG3	1.87	0.57
1:D:801:PHE:HA	1:D:804:PHE:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:ALA:HB3	1:E:297:ALA:CB	2.34	0.57
1:F:379:THR:O	1:F:383:LEU:HG	2.04	0.57
1:A:527:TYR:CE2	1:A:972:LEU:HD13	2.39	0.57
1:C:412:VAL:HG13	1:C:435:MET:HE1	1.85	0.57
1:D:231:ASN:HD22	1:E:622:GLN:CD	2.13	0.57
1:D:919:ARG:HH12	1:D:990:VAL:HG12	1.70	0.57
1:E:790:TYR:HD1	1:E:800:PRO:HA	1.70	0.57
1:A:408:ASP:OD2	1:A:940:LYS:NZ	2.38	0.57
1:D:186:ILE:HB	1:D:773:VAL:HG12	1.85	0.57
1:D:924:ASP:O	1:D:928:GLN:HG2	2.04	0.57
1:D:931:LEU:O	1:D:935:ILE:HG13	2.04	0.57
1:A:400:LEU:HD23	1:A:474:ILE:HD11	1.85	0.57
1:B:671:ILE:HB	1:B:674:LEU:HB2	1.87	0.57
1:C:375:VAL:HG13	1:C:480:LEU:HB2	1.85	0.57
1:D:841:MET:O	1:D:845:GLU:HG3	2.04	0.57
1:E:356:TYR:HE1	1:E:362:PHE:HA	1.70	0.57
1:F:572:PHE:HD2	1:F:631:LEU:HD11	1.69	0.57
1:B:100:ALA:O	1:B:103:ALA:N	2.38	0.56
1:E:153:ASP:OD1	1:E:153:ASP:N	2.37	0.56
1:E:225:VAL:HG12	1:F:781:MET:HE3	1.87	0.56
1:E:572:PHE:HD2	1:E:631:LEU:HD21	1.70	0.56
1:B:26:ALA:O	1:B:30:LEU:HB2	2.05	0.56
1:B:671:ILE:HD12	1:B:674:LEU:HG	1.87	0.56
1:C:746:ILE:HG22	1:C:791:VAL:HG11	1.87	0.56
1:C:900:SER:HB3	1:C:1029:VAL:HG21	1.86	0.56
1:E:214:VAL:CG1	1:E:237:GLN:HB3	2.34	0.56
1:E:696:THR:HG23	1:E:699:ARG:HH12	1.70	0.56
1:F:165:ALA:HB3	1:F:313:MET:HE1	1.86	0.56
1:F:948:PHE:O	1:F:952:LEU:HG	2.06	0.56
1:B:175:VAL:HG22	1:C:70:ASN:ND2	2.20	0.56
1:B:559:LEU:HD23	1:B:560:PRO:HD2	1.86	0.56
1:C:352:PHE:HD2	1:C:353:LEU:HD23	1.70	0.56
1:C:702:LEU:HD22	1:C:827:ILE:HD13	1.87	0.56
1:D:57:VAL:HG13	1:D:88:VAL:HB	1.86	0.56
1:D:100:ALA:O	1:D:103:ALA:N	2.37	0.56
1:D:157:TYR:O	1:D:161:ASN:ND2	2.27	0.56
1:D:186:ILE:HG12	1:D:268:ILE:HG12	1.87	0.56
1:D:459:PHE:CE2	1:D:876:LEU:HD12	2.40	0.56
1:F:372:VAL:HG23	1:F:373:PRO:HD3	1.88	0.56
1:F:407:ASP:OD2	1:F:940:LYS:HD2	2.05	0.56
1:F:723:ASP:HA	1:F:813:SER:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:974:PRO:O	1:F:978:THR:HG22	2.06	0.56
1:C:743:ILE:HA	1:C:746:ILE:HG12	1.87	0.56
1:D:838:GLY:O	1:D:841:MET:HB2	2.05	0.56
1:E:236:ALA:O	1:F:728:LYS:NZ	2.30	0.56
1:F:985:GLY:O	1:F:988:PRO:HD2	2.06	0.56
1:A:190:PRO:HB3	1:A:789:TRP:CZ2	2.40	0.56
1:A:596:HIS:O	1:A:600:THR:HG22	2.05	0.56
1:A:690:LEU:O	1:A:694:LYS:HB2	2.05	0.56
1:A:979:SER:OG	1:A:1015:THR:HG21	2.06	0.56
1:B:151:GLN:OE1	1:B:278:ILE:HG22	2.05	0.56
1:B:575:MET:CE	1:B:617:PHE:HB2	2.36	0.56
1:C:983:ILE:HD11	1:C:1011:MET:HG3	1.88	0.56
1:D:781:MET:HB2	1:D:782:LEU:HD12	1.88	0.56
1:F:727:PHE:HD1	1:F:809:TRP:CD1	2.23	0.56
1:B:961:ILE:HG13	1:B:962:GLU:H	1.70	0.56
1:D:58:GLN:HG3	1:D:818:ARG:HD2	1.88	0.56
1:D:526:HIS:CD2	2:D:2000:LMT:H41	2.40	0.56
1:F:273:GLU:OE2	1:F:770:LYS:HD3	2.05	0.56
1:F:897:ILE:CG2	1:F:946:VAL:HG11	2.36	0.56
1:A:352:PHE:HD1	1:A:369:THR:OG1	1.89	0.56
1:B:344:LEU:HD22	1:B:402:ILE:CD1	2.35	0.56
1:B:530:SER:HA	2:B:2000:LMT:H6D	1.87	0.56
1:D:170:SER:OG	1:E:75:LEU:N	2.39	0.56
1:D:568:ASP:CG	1:D:637:ARG:HH22	2.14	0.56
1:D:776:GLU:HG2	1:D:777:ALA:H	1.71	0.56
1:E:36:PRO:O	1:E:38:ILE:HG13	2.05	0.56
1:E:47:ALA:O	1:E:87:THR:HA	2.05	0.56
1:E:987:MET:HG3	1:E:1008:MET:SD	2.46	0.56
1:F:3:ASN:O	1:F:7:ASP:N	2.38	0.56
1:A:272:GLY:N	1:A:275:TYR:OH	2.38	0.56
1:B:844:MET:HE1	1:B:847:LEU:HD12	1.88	0.56
1:D:578:LEU:HD12	1:D:579:PRO:HD2	1.88	0.56
1:E:190:PRO:HG3	1:E:779:TYR:HB3	1.88	0.56
1:E:246:PHE:O	1:E:249:ILE:HG23	2.06	0.56
1:E:435:MET:SD	1:E:490:PRO:HB3	2.46	0.56
1:E:831:ALA:HB2	1:E:840:ALA:HB2	1.88	0.56
1:F:594:VAL:HG22	1:F:655:PHE:CE2	2.40	0.56
1:F:983:ILE:HG23	1:F:1008:MET:HE2	1.88	0.56
1:A:230:LEU:HD11	1:B:809:TRP:HH2	1.71	0.56
1:B:21:LEU:O	1:B:25:LEU:HB2	2.06	0.56
1:D:526:HIS:HD2	2:D:2000:LMT:H41	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:894:SER:OG	1:D:897:ILE:HG12	2.06	0.56
1:E:555:LEU:HD11	1:E:914:LEU:HD12	1.88	0.56
1:F:404:LEU:HD12	1:F:937:LEU:HD23	1.88	0.56
1:F:423:GLU:O	1:F:502:LYS:HB2	2.06	0.56
1:F:564:LEU:CD2	1:F:565:PRO:HD2	2.35	0.56
1:F:792:ARG:HG2	1:F:792:ARG:HH11	1.71	0.56
1:F:898:PRO:HA	1:F:901:VAL:HG12	1.87	0.56
1:A:181:GLN:HG2	1:A:769:LYS:HZ2	1.70	0.55
1:A:586:ARG:O	1:A:589:LYS:HB3	2.07	0.55
1:A:696:THR:HG23	1:A:699:ARG:NH1	2.21	0.55
1:C:565:PRO:HG3	1:C:999:ALA:HA	1.87	0.55
1:D:244:GLU:HG3	1:D:245:GLU:N	2.20	0.55
1:E:423:GLU:O	1:E:502:LYS:HB2	2.05	0.55
1:E:426:PRO:HG2	1:E:429:GLU:HB2	1.87	0.55
1:E:584:GLN:HB2	1:E:622:GLN:HG2	1.87	0.55
1:F:49:TYR:CD1	1:F:57:VAL:HG12	2.41	0.55
1:A:189:ASN:O	1:A:193:LEU:HB2	2.07	0.55
1:A:712:MET:O	1:A:832:ALA:N	2.39	0.55
1:A:953:MET:SD	1:A:960:LEU:HA	2.45	0.55
1:B:372:VAL:O	1:B:375:VAL:N	2.38	0.55
1:C:240:LEU:HB2	1:C:246:PHE:CE1	2.41	0.55
1:D:344:LEU:HD11	1:D:398:MET:HB3	1.87	0.55
1:D:435:MET:O	1:D:439:GLN:HB2	2.07	0.55
1:E:379:THR:O	1:E:382:VAL:HG22	2.06	0.55
1:E:703:LEU:HD11	1:E:718:PRO:HD3	1.88	0.55
1:F:420:MET:SD	1:F:500:ILE:HB	2.46	0.55
1:C:404:LEU:O	1:C:407:ASP:HB2	2.07	0.55
1:C:959:GLY:CA	1:C:1041:GLU:H	2.19	0.55
1:C:1026:PHE:CE1	1:C:1030:ARG:HG2	2.41	0.55
1:D:36:PRO:HG3	1:D:469:GLN:HG3	1.89	0.55
1:D:105:VAL:HG21	1:E:105:VAL:HB	1.88	0.55
1:D:605:ASN:HD22	1:D:647:ILE:HD11	1.70	0.55
1:E:96:SER:OG	1:E:865:GLN:NE2	2.40	0.55
1:F:119:PRO:HB2	1:F:122:VAL:HB	1.88	0.55
1:F:214:VAL:HG23	1:F:237:GLN:HB2	1.88	0.55
1:A:682:PHE:HD2	1:A:683:GLU:N	2.04	0.55
1:B:1015:THR:OG1	1:B:1016:VAL:N	2.40	0.55
1:C:190:PRO:HG3	1:C:779:TYR:HB3	1.89	0.55
1:C:572:PHE:HA	1:C:668:LEU:HD21	1.89	0.55
1:E:682:PHE:HE2	1:E:684:LEU:HB2	1.71	0.55
1:F:555:LEU:HD11	1:F:914:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:983:ILE:HD13	1:F:1012:VAL:HG22	1.88	0.55
1:A:740:GLY:O	1:A:793:ALA:HB1	2.06	0.55
1:B:904:VAL:HG21	1:B:942:ALA:CB	2.36	0.55
1:C:362:PHE:HB2	1:C:363:ARG:HH22	1.70	0.55
1:D:143:ILE:HG22	1:D:286:ALA:CB	2.36	0.55
1:D:149:MET:HE3	1:D:153:ASP:HB2	1.88	0.55
1:D:945:ILE:HA	1:D:971:ARG:NH1	2.20	0.55
1:F:262:LEU:HG	1:F:268:ILE:HD11	1.89	0.55
1:F:535:LEU:HD22	1:F:1027:VAL:HG21	1.89	0.55
1:B:979:SER:OG	1:B:1015:THR:HG21	2.06	0.55
1:C:139:VAL:O	1:C:326:PRO:HD2	2.05	0.55
1:C:320:GLY:O	1:C:322:LYS:N	2.39	0.55
1:C:414:GLU:HG2	1:C:973:ARG:CZ	2.37	0.55
1:C:562:SER:OG	1:C:924:ASP:HB3	2.05	0.55
1:D:728:LYS:HD2	1:F:235:ILE:O	2.07	0.55
1:D:826:GLU:HG3	1:D:826:GLU:O	2.06	0.55
1:E:76:MET:HG2	1:E:864:TYR:OH	2.07	0.55
1:E:598:TYR:HB3	1:E:606:VAL:HG21	1.89	0.55
1:E:1015:THR:O	1:E:1017:LEU:N	2.40	0.55
1:F:64:VAL:HG13	1:F:117:LEU:HB2	1.88	0.55
1:A:32:VAL:HG22	1:A:390:ILE:HB	1.89	0.55
1:D:619:GLY:N	1:D:815:ARG:HH22	2.05	0.55
1:E:167:SER:HB3	1:F:70:ASN:HD22	1.72	0.55
1:E:422:GLU:O	1:E:502:LYS:NZ	2.30	0.55
1:E:912:ALA:HB3	1:E:931:LEU:HD21	1.89	0.55
1:E:944:LEU:HD13	1:E:971:ARG:NH1	2.21	0.55
1:A:38:ILE:HG23	1:A:462:SER:HB3	1.89	0.55
1:A:555:LEU:HD12	1:A:910:ILE:HD12	1.89	0.55
1:A:942:ALA:O	1:A:946:VAL:HG12	2.06	0.55
1:C:684:LEU:HD22	1:C:695:LEU:HD11	1.88	0.55
1:D:261:LEU:HD13	1:D:263:ARG:HH21	1.71	0.55
1:D:563:PHE:HD1	1:D:677:ALA:HA	1.72	0.55
1:F:593:GLU:OE2	1:F:659:LYS:HE3	2.07	0.55
1:A:646:ALA:O	1:A:650:ARG:HG2	2.06	0.55
1:C:163:LYS:O	1:C:163:LYS:HG2	2.06	0.55
1:C:461:GLY:O	1:C:464:GLY:N	2.40	0.55
1:C:588:GLN:HG3	1:C:592:ASN:ND2	2.21	0.55
1:D:47:ALA:HB3	1:D:88:VAL:CG1	2.37	0.55
1:D:57:VAL:HG12	1:D:82:SER:HB3	1.89	0.55
1:D:261:LEU:CD1	1:D:263:ARG:HH21	2.20	0.55
1:D:407:ASP:OD1	1:D:978:THR:HG21	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:552:MET:HB2	1:D:910:ILE:HB	1.88	0.55
1:F:448:VAL:CG2	1:F:884:VAL:HG13	2.37	0.55
1:A:897:ILE:HD11	1:A:1030:ARG:HE	1.70	0.55
1:B:214:VAL:HG21	1:B:237:GLN:HB3	1.88	0.55
1:B:732:ASP:N	1:B:804:PHE:O	2.38	0.55
1:D:958:LYS:NZ	1:D:962:GLU:OE1	2.34	0.55
1:D:1026:PHE:HE2	1:D:1030:ARG:HE	1.54	0.55
1:E:675:GLY:HA2	1:E:862:MET:SD	2.46	0.55
1:F:343:THR:HG22	1:F:399:VAL:HG11	1.89	0.55
1:B:171:GLY:O	1:B:302:THR:OG1	2.17	0.54
1:C:563:PHE:HB2	1:C:866:GLU:HB2	1.89	0.54
1:D:530:SER:O	1:D:533:GLY:N	2.40	0.54
1:D:583:THR:HA	1:D:622:GLN:OE1	2.08	0.54
1:E:167:SER:HB3	1:F:70:ASN:HB3	1.89	0.54
1:E:637:ARG:NH1	1:E:643:LYS:HA	2.22	0.54
1:F:355:MET:HE1	1:F:368:PRO:HD2	1.89	0.54
1:A:280:GLU:OE2	1:A:588:GLN:NE2	2.40	0.54
1:B:775:SER:OG	1:B:776:GLU:N	2.40	0.54
1:B:904:VAL:HG21	1:B:942:ALA:HB2	1.88	0.54
1:C:172:VAL:HG12	1:C:173:GLY:O	2.07	0.54
1:D:481:SER:O	1:D:484:VAL:HG12	2.07	0.54
1:D:945:ILE:CA	1:D:971:ARG:HH12	2.18	0.54
1:E:871:ASN:OD1	1:E:871:ASN:N	2.40	0.54
1:F:147:GLY:O	1:F:149:MET:HG3	2.07	0.54
1:F:163:LYS:HD2	1:F:289:LEU:HD21	1.87	0.54
1:F:520:PHE:O	1:F:523:SER:OG	2.25	0.54
1:B:294:ALA:HB3	1:B:297:ALA:HB2	1.88	0.54
1:B:453:PHE:O	1:B:471:SER:OG	2.13	0.54
1:C:207:ILE:HG22	1:C:249:ILE:HD13	1.88	0.54
1:D:402:ILE:O	1:D:406:VAL:HG22	2.06	0.54
1:E:767:ARG:HG2	1:E:767:ARG:HH11	1.72	0.54
1:F:62:THR:HG21	1:F:818:ARG:HD3	1.88	0.54
1:F:281:PHE:HD1	1:F:610:PHE:HD1	1.55	0.54
1:F:364:ALA:HA	1:F:367:ILE:HD13	1.88	0.54
1:A:203:VAL:O	1:A:207:ILE:HG12	2.07	0.54
1:A:355:MET:SD	1:A:410:ILE:HD11	2.48	0.54
1:A:929:VAL:O	1:A:932:LEU:HB2	2.07	0.54
1:B:111:LEU:C	1:B:113:LEU:H	2.16	0.54
1:C:273:GLU:OE2	1:C:770:LYS:HD2	2.07	0.54
1:C:1031:ARG:HH22	1:C:1040:ILE:HD11	1.72	0.54
1:D:886:LEU:HD23	1:F:18:ILE:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:576:VAL:HG12	1:E:663:VAL:CG1	2.38	0.54
1:F:189:ASN:HB3	1:F:192:GLU:HB2	1.90	0.54
1:F:608:SER:OG	1:F:630:SER:OG	2.12	0.54
1:F:897:ILE:HB	1:F:898:PRO:HD3	1.89	0.54
1:A:335:ILE:O	1:A:339:GLU:HG2	2.07	0.54
1:B:686:ASP:HB2	1:B:695:LEU:HD13	1.89	0.54
1:B:692:HIS:NE2	1:B:813:SER:OG	2.23	0.54
1:D:84:SER:HB3	1:D:814:PRO:HA	1.89	0.54
1:D:968:VAL:HG11	1:D:1023:PRO:HG3	1.90	0.54
1:E:452:VAL:HA	1:E:880:SER:OG	2.07	0.54
1:E:714:THR:OG1	1:E:832:ALA:HA	2.07	0.54
1:E:762:PHE:CE1	1:E:764:ASP:HB2	2.43	0.54
1:E:778:LYS:HE3	1:E:779:TYR:CZ	2.42	0.54
1:E:892:TYR:O	1:E:893:GLU:HB2	2.06	0.54
1:F:149:MET:HB3	1:F:153:ASP:OD1	2.07	0.54
1:F:858:ASP:OD2	1:F:859:TRP:N	2.36	0.54
1:A:465:ALA:O	1:A:469:GLN:HG2	2.08	0.54
1:A:530:SER:O	1:A:533:GLY:N	2.40	0.54
1:A:948:PHE:O	1:A:952:LEU:HG	2.08	0.54
1:B:713:LEU:HD11	1:B:843:LEU:HD12	1.89	0.54
1:E:62:THR:OG1	1:E:88:VAL:HG21	2.08	0.54
1:E:545:TYR:HB2	1:E:1021:PHE:HE2	1.72	0.54
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.90	0.54
1:F:465:ALA:HA	1:F:468:ARG:HD2	1.90	0.54
1:F:479:ALA:O	1:F:483:LEU:HG	2.07	0.54
1:F:841:MET:HG3	1:F:859:TRP:CZ2	2.42	0.54
1:A:198:LEU:N	1:A:798:MET:HE1	2.22	0.54
1:B:383:LEU:CD2	1:B:472:ILE:HG22	2.36	0.54
1:C:412:VAL:HG13	1:C:435:MET:CE	2.38	0.54
1:D:24:GLY:N	1:D:377:LEU:HD22	2.23	0.54
1:D:211:ASN:ND2	1:D:240:LEU:HG	2.23	0.54
1:A:3:ASN:HA	1:A:6:ILE:HG23	1.89	0.54
1:B:394:THR:O	1:B:473:THR:HG21	2.08	0.54
1:B:961:ILE:HG12	1:B:1039:ASP:OD2	2.08	0.54
1:C:373:PRO:O	1:C:377:LEU:N	2.41	0.54
1:C:420:MET:SD	1:C:500:ILE:HB	2.47	0.54
1:D:515:TRP:HB3	1:D:519:MET:HE3	1.89	0.54
1:E:31:PRO:HB2	1:E:389:SER:HB3	1.90	0.54
1:F:378:GLY:O	1:F:382:VAL:HG23	2.07	0.54
1:F:462:SER:O	1:F:466:ILE:HG12	2.07	0.54
1:A:46:SER:HB2	1:A:128:SER:OG	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:530:SER:OG	1:C:531:VAL:N	2.39	0.54
1:C:743:ILE:O	1:C:746:ILE:HG12	2.08	0.54
1:D:979:SER:OG	1:D:1011:MET:SD	2.58	0.54
1:E:78:MET:HG3	1:E:90:ILE:HD11	1.89	0.54
1:E:910:ILE:O	1:E:914:LEU:HB2	2.07	0.54
1:E:972:LEU:HD22	1:E:976:LEU:HD13	1.90	0.54
1:A:210:GLN:O	1:A:237:GLN:NE2	2.40	0.54
1:A:459:PHE:CE2	1:A:876:LEU:HD12	2.43	0.54
1:C:776:GLU:HB2	1:C:779:TYR:CD1	2.43	0.54
1:D:375:VAL:HG23	1:D:480:LEU:CB	2.37	0.54
1:D:734:GLU:C	1:D:736:ALA:H	2.14	0.54
1:E:46:SER:HA	1:E:88:VAL:O	2.07	0.54
1:E:187:TRP:HA	1:E:774:MET:O	2.09	0.54
1:E:452:VAL:O	1:E:455:PRO:HD2	2.08	0.54
1:E:698:ALA:HA	1:E:701:GLN:HE21	1.72	0.54
1:F:530:SER:O	1:F:533:GLY:N	2.41	0.54
1:A:309:GLU:HG3	1:A:313:MET:HE3	1.90	0.53
1:B:184:MET:HE2	1:B:268:ILE:HG23	1.90	0.53
1:B:903:LEU:HB3	1:B:1025:PHE:CE2	2.42	0.53
1:C:208:LYS:HG3	1:C:759:VAL:CG1	2.38	0.53
1:C:531:VAL:O	1:C:534:ILE:HG12	2.08	0.53
1:C:801:PHE:HA	1:C:804:PHE:CE2	2.38	0.53
1:D:331:PRO:HA	1:D:334:LYS:HD2	1.89	0.53
1:A:1040:ILE:HG13	1:A:1041:GLU:N	2.21	0.53
1:B:327:TYR:C	1:B:327:TYR:CD2	2.87	0.53
1:C:120:GLN:HA	1:C:123:GLN:HB2	1.90	0.53
1:E:597:TYR:CD1	1:E:655:PHE:HZ	2.26	0.53
1:E:754:TRP:CZ2	1:E:780:ARG:HA	2.43	0.53
1:F:602:GLU:OE1	1:F:650:ARG:HD2	2.08	0.53
1:A:13:TRP:HE1	1:A:492:LEU:HD21	1.74	0.53
1:A:375:VAL:HG21	1:A:481:SER:HA	1.89	0.53
1:A:414:GLU:CD	1:A:974:PRO:HG3	2.34	0.53
1:C:957:GLY:HA3	1:C:1043:SER:HB2	1.91	0.53
1:D:189:ASN:OD1	1:D:190:PRO:HD2	2.09	0.53
1:D:362:PHE:O	1:D:365:THR:HG22	2.08	0.53
1:E:519:MET:SD	1:E:519:MET:N	2.80	0.53
1:F:571:VAL:O	1:F:668:LEU:HD21	2.08	0.53
1:A:890:ALA:HB2	1:C:14:VAL:HG11	1.89	0.53
1:A:945:ILE:HG13	1:A:971:ARG:NH1	2.19	0.53
1:A:957:GLY:O	1:A:1041:GLU:HA	2.08	0.53
1:C:401:ALA:HA	1:C:404:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:686:ASP:OD2	1:C:823:PRO:HD2	2.09	0.53
1:D:456:MET:O	1:D:467:TYR:HB3	2.08	0.53
1:E:375:VAL:HG22	1:E:484:VAL:HG21	1.89	0.53
1:F:144:ASN:OD1	1:F:320:GLY:HA3	2.08	0.53
1:F:190:PRO:HG3	1:F:779:TYR:HB3	1.90	0.53
1:F:352:PHE:CD2	1:F:353:LEU:HD23	2.43	0.53
1:A:986:VAL:HG21	1:A:1007:VAL:HG11	1.89	0.53
1:B:13:TRP:CZ3	1:B:488:LEU:HD11	2.43	0.53
1:B:46:SER:HA	1:B:88:VAL:O	2.08	0.53
1:B:157:TYR:OH	1:B:316:PHE:O	2.27	0.53
1:C:68:ASN:HB3	1:C:110:LYS:O	2.09	0.53
1:C:69:MET:HE3	1:C:92:LEU:HD21	1.90	0.53
1:C:960:LEU:H	1:C:1040:ILE:HG23	1.73	0.53
1:D:1003:VAL:HG13	1:D:1004:GLY:N	2.23	0.53
1:E:139:VAL:HG23	1:E:327:TYR:HD1	1.73	0.53
1:E:211:ASN:HB2	1:E:240:LEU:HD11	1.91	0.53
1:E:602:GLU:HB3	1:E:606:VAL:HG23	1.91	0.53
1:E:885:PHE:HB2	1:E:902:MET:SD	2.49	0.53
1:A:73:ASP:CG	1:A:106:GLN:HE22	2.14	0.53
1:A:475:VAL:HG13	1:A:478:MET:HE2	1.91	0.53
1:B:63:GLN:HE21	1:B:818:ARG:NH1	2.06	0.53
1:B:248:LYS:HA	1:B:261:LEU:HD13	1.90	0.53
1:D:222:THR:HA	1:D:224:PRO:HD3	1.91	0.53
1:D:250:LEU:HD23	1:E:737:GLN:OE1	2.09	0.53
1:D:781:MET:HB3	1:F:228:GLN:OE1	2.09	0.53
1:E:214:VAL:HG22	1:E:237:GLN:O	2.09	0.53
1:E:293:LEU:HD22	1:E:294:ALA:H	1.74	0.53
1:E:423:GLU:C	1:E:502:LYS:HB2	2.34	0.53
1:F:363:ARG:HB3	1:F:496:MET:HG2	1.91	0.53
1:F:509:LYS:HG3	1:F:513:PHE:HB2	1.90	0.53
1:A:958:LYS:HG2	1:A:962:GLU:OE1	2.09	0.53
1:B:224:PRO:HA	1:C:781:MET:HE1	1.90	0.53
1:D:844:MET:HA	1:D:844:MET:HE2	1.90	0.53
1:E:800:PRO:HG2	1:E:803:ALA:HB2	1.89	0.53
1:F:783:PRO:O	1:F:786:ILE:HG12	2.08	0.53
1:A:889:ALA:HA	1:A:894:SER:O	2.09	0.53
1:C:858:ASP:OD2	1:C:859:TRP:N	2.41	0.53
1:D:382:VAL:HG12	1:D:386:PHE:CE1	2.44	0.53
1:D:800:PRO:HG2	1:D:803:ALA:HB2	1.90	0.53
1:E:214:VAL:HG21	1:E:237:GLN:N	2.24	0.53
1:F:203:VAL:O	1:F:207:ILE:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:359:LEU:CD2	1:F:977:MET:HE1	2.29	0.53
1:F:452:VAL:CG1	1:F:884:VAL:HG21	2.39	0.53
1:F:586:ARG:O	1:F:589:LYS:HB2	2.08	0.53
1:F:1015:THR:O	1:F:1017:LEU:N	2.42	0.53
1:F:1030:ARG:C	1:F:1032:ARG:H	2.16	0.53
1:A:151:GLN:HG3	1:A:152:GLU:N	2.24	0.53
1:A:946:VAL:HG23	1:A:1026:PHE:CD2	2.43	0.53
1:B:61:VAL:CG1	1:B:88:VAL:HG21	2.39	0.53
1:B:949:ALA:HB3	1:B:1026:PHE:CE1	2.44	0.53
1:C:139:VAL:HA	1:C:289:LEU:O	2.09	0.53
1:C:157:TYR:OH	1:C:316:PHE:O	2.16	0.53
1:D:588:GLN:HE21	1:D:592:ASN:ND2	2.06	0.53
1:D:747:ASN:ND2	1:F:237:GLN:OE1	2.40	0.53
1:D:777:ALA:HB1	1:F:225:VAL:HG12	1.90	0.53
1:E:698:ALA:O	1:E:701:GLN:HB3	2.09	0.53
1:F:165:ALA:HA	1:F:168:ARG:HB2	1.89	0.53
1:A:559:LEU:HD23	1:A:560:PRO:HD2	1.90	0.53
1:A:597:TYR:HE1	1:A:601:LYS:HD2	1.73	0.53
1:A:674:LEU:HD22	1:A:675:GLY:N	2.24	0.53
1:F:297:ALA:HB1	1:F:302:THR:OG1	2.09	0.53
1:F:655:PHE:HB3	1:F:663:VAL:HB	1.91	0.53
1:B:327:TYR:C	1:B:327:TYR:HD2	2.16	0.52
1:B:543:VAL:O	1:B:547:ILE:HD13	2.09	0.52
1:B:982:PHE:HD2	1:B:1011:MET:HE2	1.74	0.52
1:E:531:VAL:HG11	1:E:968:VAL:HG21	1.91	0.52
1:F:23:GLY:CA	1:F:381:ALA:HB2	2.35	0.52
1:B:573:MET:HE2	1:B:666:PHE:CZ	2.45	0.52
1:C:582:ALA:HA	1:C:586:ARG:NH2	2.24	0.52
1:D:68:ASN:HB2	1:D:114:ALA:HB2	1.91	0.52
1:D:1035:ARG:O	1:D:1037:ASN:N	2.43	0.52
1:D:1038:GLU:CD	1:D:1038:GLU:H	2.16	0.52
1:A:725:PRO:O	1:C:232:ALA:HB1	2.09	0.52
1:A:729:ILE:HD13	1:C:234:ILE:HG23	1.90	0.52
1:A:804:PHE:CD2	1:A:804:PHE:N	2.75	0.52
1:C:449:LEU:HD21	1:C:937:LEU:HD23	1.92	0.52
1:D:358:PHE:CD2	1:D:977:MET:HE2	2.45	0.52
1:F:540:ARG:HD3	1:F:541:TYR:HE1	1.73	0.52
1:A:888:LEU:HB2	1:A:898:PRO:HB3	1.91	0.52
1:A:996:GLY:C	1:A:998:GLY:N	2.67	0.52
1:B:418:ARG:O	1:B:422:GLU:HG3	2.10	0.52
1:B:420:MET:HE1	1:B:498:LYS:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:PHE:O	1:C:11:PHE:HD2	1.93	0.52
1:C:574:THR:HG23	1:C:627:ALA:HB3	1.90	0.52
1:D:412:VAL:HG22	1:D:438:ILE:HD11	1.91	0.52
1:D:992:SER:OG	1:D:1000:GLN:OE1	2.22	0.52
1:E:302:THR:O	1:E:306:ILE:HB	2.09	0.52
1:E:485:ALA:O	1:E:490:PRO:HD3	2.09	0.52
1:F:682:PHE:HD1	1:F:683:GLU:N	2.08	0.52
1:A:400:LEU:HD21	1:A:933:THR:OG1	2.09	0.52
1:A:919:ARG:NH1	1:A:990:VAL:HG12	2.24	0.52
1:B:352:PHE:C	1:B:352:PHE:CD2	2.87	0.52
1:B:860:THR:HA	1:B:864:TYR:HB2	1.91	0.52
1:E:211:ASN:OD1	1:E:240:LEU:HG	2.10	0.52
1:E:634:TRP:H	1:E:634:TRP:CD1	2.26	0.52
1:F:4:PHE:C	1:F:7:ASP:HB2	2.35	0.52
1:F:69:MET:HB3	1:F:72:ILE:HD11	1.91	0.52
1:F:211:ASN:CG	1:F:240:LEU:HG	2.35	0.52
1:F:586:ARG:O	1:F:590:VAL:HG23	2.10	0.52
1:F:676:THR:HG23	1:F:677:ALA:N	2.25	0.52
1:F:739:LEU:HD13	1:F:799:VAL:HG11	1.91	0.52
1:F:994:GLY:O	1:F:997:SER:OG	2.28	0.52
1:B:66:GLU:OE2	1:B:80:SER:OG	2.24	0.52
1:B:486:LEU:O	1:B:490:PRO:HG3	2.10	0.52
2:B:2000:LMT:O6'	2:B:2000:LMT:O2B	2.25	0.52
1:C:72:ILE:HD12	1:C:75:LEU:HD13	1.91	0.52
1:C:562:SER:OG	1:C:563:PHE:N	2.41	0.52
1:C:1003:VAL:HG13	1:C:1004:GLY:N	2.24	0.52
1:E:155:SER:O	1:E:158:VAL:HB	2.10	0.52
1:E:574:THR:HG23	1:E:627:ALA:HB3	1.91	0.52
1:E:971:ARG:C	1:E:974:PRO:HD2	2.34	0.52
1:F:506:GLY:O	1:F:508:GLY:N	2.42	0.52
1:F:549:VAL:O	1:F:552:MET:HB3	2.08	0.52
1:A:196:PHE:HD1	1:A:260:VAL:HG13	1.75	0.52
1:A:414:GLU:HG3	1:A:974:PRO:HG3	1.92	0.52
1:B:35:TYR:CE2	1:B:671:ILE:HG12	2.44	0.52
1:B:36:PRO:HG3	1:B:469:GLN:HG3	1.90	0.52
1:C:251:LEU:HD11	1:C:262:LEU:HA	1.91	0.52
1:E:338:HIS:CE1	1:E:342:LYS:HE3	2.44	0.52
1:F:452:VAL:HA	1:F:880:SER:OG	2.09	0.52
1:F:924:ASP:O	1:F:928:GLN:HG3	2.09	0.52
1:A:987:MET:HA	1:A:1008:MET:HE1	1.92	0.52
1:B:191:ASN:O	1:B:194:ASN:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:662:MET:HE2	1:B:664:PHE:CE2	2.44	0.52
1:C:792:ARG:HG2	1:C:792:ARG:HH11	1.74	0.52
1:D:527:TYR:O	1:D:531:VAL:HG23	2.10	0.52
1:D:563:PHE:CZ	1:D:674:LEU:HD11	2.45	0.52
1:F:112:GLN:HA	1:F:115:MET:HG3	1.92	0.52
1:F:196:PHE:O	1:F:252:LYS:NZ	2.31	0.52
1:F:379:THR:HG23	1:F:476:SER:OG	2.09	0.52
1:F:543:VAL:O	1:F:546:LEU:HB2	2.10	0.52
1:A:1022:VAL:HA	1:A:1025:PHE:CD1	2.45	0.52
1:B:314:GLU:N	1:B:315:PRO:HD2	2.25	0.52
1:B:533:GLY:HA2	1:B:536:ARG:NH1	2.24	0.52
1:B:656:SER:HA	1:B:662:MET:HE1	1.91	0.52
1:C:44:THR:OG1	1:C:91:THR:OG1	2.25	0.52
1:C:414:GLU:OE1	1:C:974:PRO:HD3	2.10	0.52
1:C:833:PRO:C	1:C:835:LYS:N	2.68	0.52
1:D:355:MET:HE1	1:D:977:MET:HG2	1.92	0.52
1:D:358:PHE:HD2	1:D:977:MET:HE2	1.75	0.52
1:D:712:MET:HB3	1:D:713:LEU:HD22	1.92	0.52
1:D:758:TYR:CE1	1:D:770:LYS:HD3	2.45	0.52
1:D:949:ALA:O	1:D:953:MET:HE3	2.10	0.52
1:E:764:ASP:OD1	1:E:765:ARG:NE	2.25	0.52
1:E:1023:PRO:O	1:E:1027:VAL:HG12	2.10	0.52
1:F:394:THR:CG2	1:F:469:GLN:HB3	2.36	0.52
1:F:588:GLN:HG3	1:F:592:ASN:ND2	2.25	0.52
1:A:278:ILE:HG13	1:A:279:ALA:N	2.19	0.52
1:A:368:PRO:HA	1:A:371:ALA:HB2	1.92	0.52
1:A:525:HIS:O	1:A:526:HIS:C	2.53	0.52
1:A:572:PHE:HB2	1:A:666:PHE:O	2.09	0.52
1:A:764:ASP:C	1:A:766:GLY:H	2.18	0.52
1:A:790:TYR:HD1	1:A:800:PRO:HA	1.74	0.52
1:A:971:ARG:O	1:A:974:PRO:HD2	2.10	0.52
1:A:971:ARG:CZ	1:A:971:ARG:HB3	2.39	0.52
1:A:996:GLY:C	1:A:998:GLY:H	2.17	0.52
1:B:249:ILE:HD12	1:B:262:LEU:HD23	1.92	0.52
1:C:685:ILE:HD11	1:C:819:TYR:HB3	1.92	0.52
1:C:976:LEU:O	1:C:980:LEU:HB2	2.10	0.52
1:E:492:LEU:O	1:E:496:MET:HG2	2.10	0.52
1:E:776:GLU:HB3	1:E:779:TYR:CD1	2.44	0.52
1:F:354:VAL:HG12	1:F:980:LEU:HD23	1.91	0.52
1:F:415:ASN:O	1:F:419:VAL:HG13	2.10	0.52
1:A:157:TYR:OH	1:A:316:PHE:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ALA:HB1	1:C:122:VAL:HG13	1.92	0.51
1:C:610:PHE:HB3	1:C:628:PHE:HB2	1.92	0.51
1:D:448:VAL:HB	1:D:884:VAL:HG13	1.92	0.51
1:D:900:SER:HA	1:D:1029:VAL:HG21	1.91	0.51
1:F:408:ASP:OD1	1:F:478:MET:HE1	2.10	0.51
1:F:448:VAL:HA	1:F:451:ALA:HB3	1.92	0.51
1:F:971:ARG:HG2	1:F:974:PRO:HG3	1.92	0.51
1:F:1018:ALA:O	1:F:1022:VAL:HG23	2.09	0.51
1:A:57:VAL:HG21	1:A:83:ASP:O	2.11	0.51
1:A:449:LEU:O	1:A:453:PHE:HD1	1.94	0.51
1:A:451:ALA:HB1	1:A:883:VAL:CG1	2.40	0.51
1:A:964:THR:O	1:A:968:VAL:HG13	2.09	0.51
1:B:177:LEU:HD12	1:B:178:PHE:N	2.25	0.51
1:B:553:ALA:O	1:B:556:PHE:HB3	2.10	0.51
1:B:652:THR:HG22	1:B:664:PHE:CD2	2.45	0.51
1:E:359:LEU:C	1:E:361:ASN:H	2.15	0.51
1:E:850:LYS:HD3	1:E:850:LYS:N	2.24	0.51
1:F:6:ILE:HG23	1:F:12:ALA:HB2	1.91	0.51
1:F:925:VAL:HG12	1:F:926:TYR:CD2	2.46	0.51
1:A:826:GLU:O	1:A:826:GLU:HG3	2.10	0.51
1:C:47:ALA:O	1:C:87:THR:HA	2.10	0.51
1:D:170:SER:HB3	1:E:74:ASN:H	1.74	0.51
1:D:683:GLU:HG3	1:D:824:SER:OG	2.11	0.51
1:E:376:LEU:O	1:E:377:LEU:C	2.54	0.51
1:F:34:GLN:OE1	1:F:332:PHE:HD2	1.92	0.51
1:F:243:THR:OG1	1:F:268:ILE:HG22	2.10	0.51
1:F:892:TYR:HB3	1:F:897:ILE:HD12	1.92	0.51
1:F:912:ALA:N	1:F:1010:GLY:HA2	2.25	0.51
1:A:516:PHE:O	1:A:519:MET:N	2.43	0.51
1:A:563:PHE:O	1:A:564:LEU:HG	2.10	0.51
1:A:733:GLN:HE22	1:A:743:ILE:HG23	1.74	0.51
1:A:971:ARG:CZ	1:A:971:ARG:CB	2.83	0.51
1:B:108:GLN:OE1	1:B:129:VAL:HB	2.10	0.51
1:C:6:ILE:C	1:C:8:ARG:H	2.17	0.51
1:C:600:THR:O	1:C:603:LYS:HG2	2.09	0.51
1:C:746:ILE:HG13	1:C:747:ASN:N	2.26	0.51
1:C:804:PHE:CD2	1:C:804:PHE:N	2.79	0.51
1:D:452:VAL:HG13	1:D:884:VAL:HG21	1.92	0.51
1:A:1037:ASN:O	1:A:1037:ASN:ND2	2.39	0.51
1:B:251:LEU:HD21	1:B:262:LEU:HB2	1.93	0.51
1:B:638:PRO:HD2	1:B:642:ASN:HD22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:MET:HE2	1:C:864:TYR:HE2	1.75	0.51
1:C:479:ALA:O	1:C:483:LEU:HG	2.09	0.51
1:D:178:PHE:O	1:D:287:SER:OG	2.26	0.51
1:D:281:PHE:HB2	1:D:610:PHE:CD1	2.46	0.51
1:D:310:LEU:O	1:D:314:GLU:HG3	2.10	0.51
1:D:894:SER:CB	1:D:897:ILE:HG12	2.40	0.51
1:E:14:VAL:HG11	1:F:890:ALA:HB2	1.91	0.51
1:E:288:GLY:C	1:E:289:LEU:HD22	2.35	0.51
1:E:422:GLU:C	1:E:502:LYS:HG3	2.36	0.51
1:A:775:SER:OG	1:A:780:ARG:HG2	2.10	0.51
1:B:423:GLU:O	1:B:502:LYS:HB2	2.10	0.51
1:B:452:VAL:HG23	1:B:453:PHE:CD2	2.45	0.51
1:B:507:GLU:O	1:B:509:LYS:N	2.44	0.51
1:B:754:TRP:CZ2	1:B:780:ARG:HA	2.46	0.51
1:B:961:ILE:HG13	1:B:962:GLU:N	2.26	0.51
1:C:911:GLY:HA3	1:C:1013:THR:OG1	2.11	0.51
1:C:982:PHE:CD2	1:C:1011:MET:HG2	2.44	0.51
1:D:138:MET:HG3	1:D:291:ILE:HD12	1.93	0.51
1:D:400:LEU:HD11	1:D:933:THR:CG2	2.35	0.51
1:D:423:GLU:O	1:D:502:LYS:HB3	2.11	0.51
1:E:537:SER:HB3	1:E:540:ARG:HH22	1.75	0.51
1:E:546:LEU:HD13	1:E:547:ILE:N	2.25	0.51
1:F:36:PRO:HG2	1:F:38:ILE:CG1	2.41	0.51
1:F:351:VAL:HG22	1:F:981:ALA:HB1	1.92	0.51
1:A:535:LEU:HD21	1:A:1023:PRO:HB2	1.91	0.51
1:A:608:SER:OG	1:A:630:SER:HB3	2.10	0.51
1:A:987:MET:HB3	1:A:988:PRO:HD3	1.93	0.51
1:C:764:ASP:O	1:C:766:GLY:N	2.44	0.51
1:C:1015:THR:O	1:C:1017:LEU:N	2.44	0.51
1:D:313:MET:HB3	1:D:317:PHE:CE1	2.46	0.51
1:E:415:ASN:O	1:E:419:VAL:HG23	2.11	0.51
1:E:572:PHE:CD2	1:E:631:LEU:HD21	2.46	0.51
1:E:641:GLU:CD	1:E:641:GLU:H	2.16	0.51
1:E:671:ILE:HB	1:E:674:LEU:HG	1.93	0.51
1:E:742:SER:O	1:E:746:ILE:HG13	2.10	0.51
1:F:45:ILE:HD13	1:F:111:LEU:CD1	2.41	0.51
1:F:393:LEU:HG	1:F:466:ILE:HG23	1.93	0.51
1:F:574:THR:HG23	1:F:627:ALA:HB3	1.92	0.51
1:F:982:PHE:O	1:F:983:ILE:C	2.54	0.51
1:B:863:SER:O	1:B:867:ARG:HB2	2.11	0.51
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:988:PRO:HA	1:D:991:ILE:HD12	1.93	0.51
1:E:250:LEU:HD12	1:E:251:LEU:H	1.74	0.51
1:E:350:LEU:HD12	1:E:984:LEU:HD12	1.93	0.51
1:E:453:PHE:CE1	1:E:474:ILE:HG21	2.40	0.51
1:A:131:LYS:NZ	1:B:73:ASP:OD1	2.22	0.51
1:A:597:TYR:O	1:A:600:THR:HG23	2.11	0.51
1:A:971:ARG:HG3	1:A:974:PRO:HG2	1.93	0.51
1:B:235:ILE:O	1:C:728:LYS:HG3	2.11	0.51
1:B:892:TYR:O	1:B:893:GLU:HB2	2.10	0.51
1:C:457:ALA:HB2	1:C:471:SER:CB	2.41	0.51
1:C:612:VAL:HG11	1:C:615:PHE:HD1	1.76	0.51
1:C:885:PHE:CA	1:C:902:MET:HE1	2.39	0.51
1:C:971:ARG:HB3	1:C:971:ARG:NH1	2.26	0.51
1:D:300:LEU:O	1:D:304:ALA:HB2	2.11	0.51
1:E:240:LEU:HD12	1:E:246:PHE:CZ	2.46	0.51
1:E:988:PRO:HA	1:E:991:ILE:HB	1.91	0.51
1:F:62:THR:OG1	1:F:80:SER:HB3	2.11	0.51
1:F:685:ILE:HD13	1:F:824:SER:HB3	1.92	0.51
1:A:72:ILE:HD13	1:A:107:VAL:CG2	2.39	0.51
1:A:675:GLY:HA2	1:A:862:MET:HE2	1.93	0.51
1:B:420:MET:HE3	1:B:500:ILE:HB	1.93	0.51
1:C:355:MET:O	1:C:359:LEU:HG	2.11	0.51
1:C:960:LEU:N	1:C:1040:ILE:HG23	2.26	0.51
1:D:281:PHE:CE1	1:D:608:SER:HB2	2.46	0.51
1:D:375:VAL:HG23	1:D:480:LEU:HB2	1.92	0.51
1:E:185:ARG:HD2	1:E:187:TRP:CZ2	2.46	0.51
1:E:408:ASP:OD1	1:E:940:LYS:HE3	2.11	0.51
1:E:549:VAL:O	1:E:552:MET:HB3	2.11	0.51
1:E:922:THR:HG23	1:E:924:ASP:OD2	2.10	0.51
1:F:120:GLN:HA	1:F:123:GLN:HB2	1.92	0.51
1:F:358:PHE:CE1	1:F:977:MET:HG2	2.46	0.51
1:F:693:GLU:H	1:F:694:LYS:NZ	2.09	0.51
1:A:155:SER:OG	1:A:180:SER:O	2.28	0.50
1:A:212:ALA:C	1:A:239:ARG:HG2	2.36	0.50
1:A:451:ALA:HB1	1:A:883:VAL:HG13	1.93	0.50
1:A:944:LEU:O	1:A:947:GLU:HB3	2.11	0.50
1:B:62:THR:HG21	1:B:818:ARG:HD3	1.93	0.50
1:B:108:GLN:HE21	1:C:112:GLN:HE21	1.58	0.50
1:B:281:PHE:CE1	1:B:608:SER:HB2	2.47	0.50
1:B:468:ARG:HB2	1:B:468:ARG:CZ	2.40	0.50
1:B:575:MET:HA	1:B:626:ILE:HG13	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:944:LEU:HB3	1:B:971:ARG:NH1	2.26	0.50
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.94	0.50
1:C:730:ASP:OD1	1:C:808:ARG:NH1	2.43	0.50
1:C:926:TYR:CE2	1:C:999:ALA:HB1	2.46	0.50
1:D:376:LEU:O	1:D:377:LEU:C	2.53	0.50
1:D:932:LEU:O	1:D:935:ILE:N	2.44	0.50
1:E:211:ASN:O	1:E:760:ASN:ND2	2.44	0.50
1:E:239:ARG:HH12	1:E:762:PHE:HA	1.76	0.50
1:E:901:VAL:HG13	1:E:942:ALA:HB3	1.93	0.50
1:F:242:SER:O	1:F:246:PHE:CD1	2.64	0.50
1:A:108:GLN:O	1:A:112:GLN:HG2	2.12	0.50
1:A:247:GLY:HA2	1:A:268:ILE:HD12	1.93	0.50
1:A:672:VAL:O	1:A:673:GLU:HG2	2.11	0.50
1:B:34:GLN:O	1:B:392:THR:HG22	2.10	0.50
1:B:359:LEU:C	1:B:361:ASN:H	2.19	0.50
1:B:578:LEU:HD11	1:B:587:THR:N	2.26	0.50
1:B:668:LEU:HD12	1:B:672:VAL:HG13	1.93	0.50
1:C:5:PHE:C	1:C:7:ASP:N	2.70	0.50
1:C:238:THR:HG22	1:C:239:ARG:O	2.11	0.50
1:D:181:GLN:HG2	1:D:182:TYR:N	2.26	0.50
1:D:1018:ALA:O	1:D:1022:VAL:HG23	2.11	0.50
1:E:731:ILE:HA	1:E:805:SER:HA	1.93	0.50
1:F:151:GLN:OE1	1:F:151:GLN:N	2.37	0.50
1:F:360:GLN:NE2	1:F:513:PHE:O	2.45	0.50
1:F:380:PHE:O	1:F:383:LEU:HB2	2.12	0.50
1:F:445:ILE:HG13	1:F:943:ILE:HG21	1.93	0.50
1:F:473:THR:HG23	1:F:474:ILE:HG13	1.93	0.50
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.93	0.50
1:A:158:VAL:HG12	1:A:177:LEU:HD21	1.93	0.50
1:B:493:CYS:O	1:B:497:LEU:HB3	2.11	0.50
1:C:4:PHE:O	1:C:7:ASP:HB2	2.12	0.50
1:C:655:PHE:HB3	1:C:663:VAL:HG13	1.91	0.50
1:C:1020:PHE:CE2	2:C:2000:LMT:H32	2.46	0.50
1:D:200:PRO:HA	1:D:203:VAL:HG23	1.92	0.50
1:F:242:SER:O	1:F:246:PHE:HD1	1.94	0.50
1:F:375:VAL:HG13	1:F:480:LEU:CB	2.42	0.50
1:F:405:LEU:CD2	1:F:477:ALA:HB1	2.41	0.50
1:F:424:GLY:HA2	1:F:502:LYS:N	2.26	0.50
1:B:100:ALA:O	1:B:101:ASP:C	2.54	0.50
1:B:250:LEU:HD12	1:B:251:LEU:H	1.76	0.50
1:C:379:THR:HG23	1:C:476:SER:HG	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:843:LEU:HD22	1:C:846:GLN:HB2	1.92	0.50
1:C:982:PHE:O	1:C:983:ILE:C	2.55	0.50
1:D:7:ASP:CG	1:D:432:ARG:HH21	2.20	0.50
1:D:378:GLY:O	1:D:382:VAL:HG23	2.12	0.50
1:D:483:LEU:HA	1:D:486:LEU:HD13	1.94	0.50
1:D:726:GLN:HG2	1:F:233:SER:HB2	1.93	0.50
1:E:451:ALA:CB	1:E:883:VAL:HG12	2.41	0.50
1:A:45:ILE:HG23	1:A:129:VAL:HG22	1.94	0.50
1:A:242:SER:O	1:A:246:PHE:HD1	1.95	0.50
1:A:999:ALA:O	1:A:1002:ALA:HB3	2.11	0.50
1:B:63:GLN:HE21	1:B:818:ARG:HH12	1.60	0.50
1:B:320:GLY:O	1:B:322:LYS:HG2	2.11	0.50
1:B:572:PHE:CD2	1:B:631:LEU:HD11	2.46	0.50
1:B:792:ARG:HB3	1:B:798:MET:SD	2.51	0.50
1:C:356:TYR:C	1:C:358:PHE:H	2.18	0.50
1:C:527:TYR:OH	1:C:1019:ILE:O	2.12	0.50
1:E:940:LYS:O	1:E:943:ILE:HB	2.12	0.50
1:F:452:VAL:HG13	1:F:884:VAL:HG21	1.93	0.50
1:A:699:ARG:NH2	1:A:722:GLU:OE2	2.43	0.50
1:B:72:ILE:CD1	1:B:107:VAL:HG23	2.42	0.50
1:B:166:ILE:O	1:B:169:THR:OG1	2.28	0.50
1:B:340:VAL:HG22	1:B:396:PHE:CE2	2.47	0.50
1:C:121:GLU:O	1:C:124:GLN:HG2	2.12	0.50
1:C:841:MET:HG3	1:C:859:TRP:CZ2	2.47	0.50
1:D:98:THR:O	1:D:99:ASP:C	2.54	0.50
1:D:350:LEU:HG	1:D:984:LEU:HB3	1.93	0.50
1:D:832:ALA:O	1:D:835:LYS:HB2	2.12	0.50
1:D:888:LEU:HD11	1:D:943:ILE:HD11	1.93	0.50
1:E:34:GLN:HB2	1:E:333:VAL:HG22	1.92	0.50
1:F:537:SER:OG	1:F:540:ARG:HD2	2.11	0.50
1:F:544:LEU:O	1:F:548:ILE:HG12	2.12	0.50
1:A:404:LEU:HD12	1:A:937:LEU:CD2	2.41	0.50
1:A:514:GLY:HA2	1:A:517:ASN:OD1	2.12	0.50
1:A:527:TYR:CD2	1:A:972:LEU:HD22	2.46	0.50
1:B:559:LEU:HD23	1:B:560:PRO:CD	2.41	0.50
1:B:688:ALA:O	1:B:690:LEU:N	2.44	0.50
1:B:898:PRO:O	1:B:901:VAL:HG12	2.12	0.50
1:C:5:PHE:O	1:C:8:ARG:HG3	2.12	0.50
1:C:455:PRO:HB3	1:C:879:ILE:CG2	2.40	0.50
1:C:457:ALA:HB1	1:C:468:ARG:HG3	1.94	0.50
1:C:552:MET:HB2	1:C:910:ILE:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:790:TYR:HB3	1:C:798:MET:HB3	1.93	0.50
1:C:1034:SER:HB2	1:C:1038:GLU:HB2	1.92	0.50
1:D:845:GLU:OE1	1:D:867:ARG:NH1	2.44	0.50
1:F:358:PHE:HB3	1:F:977:MET:HE2	1.91	0.50
1:F:1027:VAL:O	1:F:1031:ARG:HG3	2.11	0.50
1:A:531:VAL:HA	1:A:534:ILE:HG12	1.93	0.50
1:B:186:ILE:HD13	1:B:262:LEU:HD21	1.94	0.50
1:B:418:ARG:CZ	1:B:970:MET:HE2	2.41	0.50
1:C:542:LEU:O	1:C:546:LEU:HD23	2.12	0.50
1:C:678:THR:O	1:C:830:GLN:HG2	2.12	0.50
1:C:974:PRO:O	1:C:978:THR:HG22	2.12	0.50
1:D:382:VAL:HG21	1:D:480:LEU:HD11	1.92	0.50
1:E:394:THR:HG22	1:E:469:GLN:HB3	1.94	0.50
1:E:424:GLY:HA2	1:E:501:ALA:HA	1.92	0.50
1:E:843:LEU:O	1:E:847:LEU:HG	2.12	0.50
1:F:144:ASN:ND2	1:F:319:SER:O	2.44	0.50
1:A:61:VAL:HG11	1:A:122:VAL:HG21	1.94	0.50
1:A:600:THR:OG1	1:A:601:LYS:N	2.43	0.50
1:B:383:LEU:HD11	1:B:473:THR:HA	1.93	0.50
1:B:762:PHE:HE1	1:B:764:ASP:HB3	1.74	0.50
1:D:104:GLN:HE21	1:D:131:LYS:HG2	1.77	0.50
1:D:181:GLN:OE1	1:D:769:LYS:HE2	2.11	0.50
1:D:222:THR:HG23	1:E:622:GLN:HE21	1.76	0.50
1:D:404:LEU:HD21	1:D:449:LEU:HD13	1.93	0.50
1:D:801:PHE:HA	1:D:804:PHE:HE2	1.76	0.50
1:E:80:SER:HB2	1:E:818:ARG:HD3	1.94	0.50
1:E:484:VAL:HG22	1:E:488:LEU:HD13	1.93	0.50
1:E:916:ALA:O	1:E:919:ARG:N	2.45	0.50
1:F:80:SER:HB2	1:F:818:ARG:HB2	1.94	0.50
1:F:405:LEU:HD22	1:F:477:ALA:HB1	1.94	0.50
1:F:427:PRO:HD3	1:F:499:PRO:HA	1.94	0.50
1:A:692:HIS:HD2	1:A:816:LEU:HD11	1.77	0.49
1:B:572:PHE:HD2	1:B:631:LEU:HD11	1.77	0.49
1:B:609:VAL:HG13	1:B:629:VAL:HG12	1.93	0.49
1:D:675:GLY:HA3	1:D:862:MET:SD	2.51	0.49
1:E:578:LEU:HD11	1:E:587:THR:N	2.26	0.49
1:E:841:MET:O	1:E:845:GLU:HG3	2.12	0.49
1:F:832:ALA:O	1:F:834:GLY:N	2.44	0.49
1:A:600:THR:HA	1:A:603:LYS:HE2	1.93	0.49
1:B:533:GLY:HA3	2:B:2000:LMT:C6'	2.42	0.49
1:C:356:TYR:HB2	1:C:365:THR:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:MET:HB3	1:C:876:LEU:HD21	1.93	0.49
1:E:80:SER:HB2	1:E:818:ARG:HB2	1.94	0.49
1:E:557:VAL:O	1:E:559:LEU:N	2.45	0.49
1:F:72:ILE:HD12	1:F:75:LEU:HD22	1.94	0.49
1:A:47:ALA:O	1:A:87:THR:HA	2.12	0.49
1:A:909:VAL:HA	1:A:931:LEU:CD1	2.40	0.49
1:B:116:PRO:C	1:B:118:LEU:H	2.19	0.49
1:B:184:MET:HB2	1:B:762:PHE:CE2	2.46	0.49
1:B:878:ALA:O	1:B:882:ILE:HB	2.12	0.49
1:C:584:GLN:HB2	1:C:622:GLN:HG2	1.94	0.49
1:C:1023:PRO:O	1:C:1027:VAL:HG22	2.12	0.49
1:D:971:ARG:NH1	1:D:971:ARG:HB3	2.28	0.49
1:E:150:THR:OG1	1:E:151:GLN:N	2.44	0.49
1:E:723:ASP:OD1	1:E:813:SER:OG	2.30	0.49
1:E:986:VAL:HG11	1:E:1007:VAL:HG12	1.94	0.49
1:F:183:ALA:HA	1:F:770:LYS:O	2.12	0.49
1:F:257:GLY:O	1:F:259:ARG:NH1	2.46	0.49
1:F:404:LEU:HA	1:F:937:LEU:HD21	1.94	0.49
1:A:686:ASP:HB3	1:A:695:LEU:HD13	1.94	0.49
1:A:696:THR:O	1:A:699:ARG:HB3	2.13	0.49
1:A:904:VAL:HG22	1:A:1025:PHE:CE1	2.47	0.49
1:B:1018:ALA:O	1:B:1022:VAL:HG23	2.12	0.49
1:C:409:ALA:O	1:C:413:VAL:HG23	2.13	0.49
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.95	0.49
1:C:1024:VAL:HA	1:C:1027:VAL:HG22	1.94	0.49
1:D:944:LEU:HB3	1:D:971:ARG:CZ	2.42	0.49
1:F:424:GLY:HA2	1:F:501:ALA:C	2.37	0.49
1:F:870:GLY:C	1:F:872:GLN:H	2.16	0.49
1:A:31:PRO:HB2	1:A:389:SER:CB	2.43	0.49
1:A:881:LEU:HD23	1:A:882:ILE:HD13	1.94	0.49
1:B:23:GLY:HA2	1:B:381:ALA:HB2	1.95	0.49
1:B:536:ARG:NH1	2:B:2000:LMT:H3B	2.27	0.49
1:B:787:GLY:C	1:B:789:TRP:H	2.20	0.49
1:C:888:LEU:CD1	1:C:901:VAL:HG11	2.43	0.49
1:D:586:ARG:O	1:D:589:LYS:HB3	2.12	0.49
1:D:1036:LYS:O	1:D:1038:GLU:N	2.45	0.49
1:E:19:ILE:HG22	1:E:378:GLY:HA2	1.95	0.49
1:E:375:VAL:HG11	1:E:405:LEU:HD13	1.93	0.49
1:E:459:PHE:CD1	1:E:876:LEU:HD12	2.47	0.49
1:F:40:PRO:HB2	1:F:94:PHE:O	2.12	0.49
1:F:60:THR:CG2	1:F:61:VAL:HG23	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:ILE:HG21	1:F:92:LEU:HD21	1.95	0.49
1:F:562:SER:HB3	1:F:924:ASP:HB3	1.94	0.49
1:F:602:GLU:OE2	1:F:650:ARG:NH1	2.46	0.49
1:A:727:PHE:HB2	1:A:809:TRP:NE1	2.27	0.49
1:B:361:ASN:OD1	1:B:363:ARG:HG3	2.13	0.49
1:B:1016:VAL:CG2	2:B:2000:LMT:H82	2.43	0.49
1:B:1024:VAL:HA	1:B:1027:VAL:HG12	1.95	0.49
1:C:101:ASP:O	1:C:105:VAL:HG23	2.13	0.49
1:C:344:LEU:HA	1:C:399:VAL:HG22	1.95	0.49
1:C:358:PHE:CD2	1:C:977:MET:HE2	2.47	0.49
1:D:637:ARG:HB3	1:D:642:ASN:HB3	1.95	0.49
1:D:764:ASP:C	1:D:766:GLY:H	2.21	0.49
1:D:895:TRP:O	1:D:898:PRO:HD2	2.13	0.49
1:E:104:GLN:NE2	1:F:109:ASN:HB3	2.27	0.49
1:E:310:LEU:HD23	1:E:323:ILE:HG21	1.93	0.49
1:E:455:PRO:HG2	1:E:880:SER:HA	1.93	0.49
1:E:537:SER:HB3	1:E:540:ARG:NH2	2.27	0.49
1:F:159:ALA:HB2	1:F:177:LEU:HD12	1.94	0.49
1:F:201:VAL:HG23	1:F:749:THR:HG23	1.93	0.49
1:F:396:PHE:HE1	1:F:999:ALA:HB1	1.78	0.49
1:F:677:ALA:HB1	1:F:830:GLN:HG2	1.94	0.49
1:F:932:LEU:O	1:F:935:ILE:HG22	2.13	0.49
1:A:428:LYS:HD2	1:A:428:LYS:N	2.28	0.49
1:B:13:TRP:CH2	1:B:492:LEU:HD21	2.48	0.49
1:B:155:SER:O	1:B:158:VAL:HB	2.13	0.49
1:B:455:PRO:O	1:B:876:LEU:HD11	2.13	0.49
1:B:867:ARG:NH2	1:B:868:LEU:HD23	2.22	0.49
1:C:187:TRP:HE3	1:C:775:SER:O	1.96	0.49
1:C:261:LEU:N	1:C:264:ASP:OD2	2.42	0.49
1:C:945:ILE:HA	1:C:971:ARG:NH1	2.27	0.49
1:D:200:PRO:HB2	1:D:749:THR:HG22	1.94	0.49
1:D:538:THR:HG22	1:D:1024:VAL:CG1	2.42	0.49
1:F:240:LEU:HD12	1:F:246:PHE:CE2	2.48	0.49
1:F:356:TYR:C	1:F:358:PHE:H	2.20	0.49
1:F:699:ARG:HH22	1:F:718:PRO:HB2	1.77	0.49
1:F:790:TYR:CD1	1:F:800:PRO:HA	2.48	0.49
1:B:143:ILE:HG22	1:B:286:ALA:HB2	1.93	0.49
1:B:376:LEU:C	1:B:378:GLY:N	2.63	0.49
1:B:764:ASP:C	1:B:766:GLY:H	2.21	0.49
1:C:3:ASN:C	1:C:5:PHE:N	2.69	0.49
1:C:686:ASP:HB3	1:C:823:PRO:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:699:ARG:HD3	1:C:825:MET:SD	2.53	0.49
1:D:251:LEU:HD12	1:D:260:VAL:HG12	1.93	0.49
1:D:305:ALA:O	1:D:308:ALA:HB3	2.13	0.49
1:D:858:ASP:OD1	1:D:859:TRP:N	2.42	0.49
1:F:240:LEU:HD12	1:F:246:PHE:CZ	2.48	0.49
1:F:787:GLY:C	1:F:789:TRP:H	2.20	0.49
1:F:819:TYR:O	1:F:821:GLY:N	2.46	0.49
1:F:913:LEU:HD23	1:F:927:PHE:CZ	2.47	0.49
1:A:199:THR:HG23	1:A:792:ARG:H	1.77	0.49
1:B:153:ASP:O	1:B:156:ASP:HB3	2.13	0.49
1:B:1015:THR:O	1:B:1018:ALA:N	2.46	0.49
1:C:362:PHE:HB2	1:C:363:ARG:NH2	2.27	0.49
1:D:554:TYR:CE2	1:D:558:ARG:HG3	2.48	0.49
1:D:682:PHE:HE2	1:D:684:LEU:HB2	1.77	0.49
1:E:184:MET:HG2	1:E:246:PHE:CZ	2.47	0.49
1:E:398:MET:HG2	1:E:473:THR:CG2	2.43	0.49
1:F:368:PRO:HA	1:F:371:ALA:HB2	1.94	0.49
1:F:376:LEU:O	1:F:377:LEU:C	2.56	0.49
1:F:693:GLU:N	1:F:694:LYS:HZ3	2.11	0.49
1:A:222:THR:HA	1:A:224:PRO:HD3	1.94	0.49
1:A:235:ILE:H	1:A:235:ILE:HD12	1.78	0.49
1:A:728:LYS:HD2	1:C:235:ILE:O	2.13	0.49
1:A:733:GLN:O	1:A:737:GLN:HB2	2.13	0.49
1:B:352:PHE:CE1	1:B:365:THR:HG23	2.48	0.49
1:B:776:GLU:HB3	1:B:779:TYR:CD1	2.48	0.49
1:C:368:PRO:O	1:C:371:ALA:HB3	2.13	0.49
1:D:214:VAL:O	1:D:216:ALA:N	2.45	0.49
1:D:244:GLU:O	1:D:248:LYS:HG2	2.12	0.49
1:D:690:LEU:HG	1:D:694:LYS:HE3	1.95	0.49
1:D:785:ASP:OD2	1:D:785:ASP:N	2.44	0.49
1:D:925:VAL:O	1:D:928:GLN:N	2.44	0.49
1:E:225:VAL:N	1:F:781:MET:HE1	2.28	0.49
1:E:364:ALA:O	1:E:368:PRO:HD3	2.13	0.49
1:E:792:ARG:NH1	1:E:793:ALA:O	2.45	0.49
1:E:982:PHE:O	1:E:983:ILE:C	2.56	0.49
1:F:64:VAL:O	1:F:114:ALA:HB1	2.12	0.49
1:A:135:SER:HB3	1:A:672:VAL:CG1	2.43	0.48
1:B:235:ILE:HD11	1:C:726:GLN:HB3	1.94	0.48
1:B:684:LEU:HB2	1:B:827:ILE:HD11	1.95	0.48
1:B:1005:THR:HG23	1:B:1006:GLY:N	2.28	0.48
1:C:189:ASN:OD1	1:C:190:PRO:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:GLN:NE2	1:C:230:LEU:O	2.41	0.48
1:C:804:PHE:H	1:C:804:PHE:HD2	1.59	0.48
1:D:230:LEU:HG	1:D:231:ASN:N	2.28	0.48
1:D:889:ALA:HB1	1:D:895:TRP:CE3	2.48	0.48
1:D:900:SER:CA	1:D:1029:VAL:HG21	2.43	0.48
1:D:919:ARG:HD3	1:D:921:LEU:HD13	1.95	0.48
1:E:108:GLN:NE2	1:F:112:GLN:HB2	2.28	0.48
1:E:121:GLU:N	1:E:121:GLU:OE2	2.44	0.48
1:E:691:GLY:H	1:E:694:LYS:HD3	1.78	0.48
1:E:764:ASP:C	1:E:766:GLY:H	2.21	0.48
1:F:175:VAL:CG1	1:F:289:LEU:HD22	2.42	0.48
1:F:446:ALA:HA	1:F:478:MET:HE2	1.93	0.48
1:F:754:TRP:CH2	1:F:780:ARG:HA	2.47	0.48
1:A:53:ASP:OD1	1:A:56:THR:OG1	2.22	0.48
1:D:457:ALA:HB2	1:D:471:SER:HB3	1.95	0.48
1:D:752:ALA:O	1:D:774:MET:HA	2.13	0.48
1:E:259:ARG:HD3	1:E:259:ARG:N	2.27	0.48
1:E:356:TYR:CD1	1:E:365:THR:HG21	2.43	0.48
1:E:527:TYR:CD2	1:E:972:LEU:HG	2.47	0.48
1:E:867:ARG:HH11	1:E:867:ARG:C	2.21	0.48
1:E:944:LEU:HD12	1:E:975:ILE:HD13	1.95	0.48
1:E:1007:VAL:HG12	1:E:1008:MET:N	2.28	0.48
1:F:281:PHE:CD1	1:F:610:PHE:HD1	2.31	0.48
1:F:506:GLY:C	1:F:508:GLY:N	2.68	0.48
1:F:676:THR:CG2	1:F:681:ASP:HB3	2.42	0.48
1:A:21:LEU:HD13	1:A:21:LEU:HA	1.75	0.48
1:A:132:SER:OG	1:A:133:SER:N	2.47	0.48
1:B:184:MET:HG2	1:B:246:PHE:CZ	2.48	0.48
1:B:578:LEU:HD11	1:B:586:ARG:HB2	1.95	0.48
1:C:111:LEU:C	1:C:113:LEU:H	2.21	0.48
1:C:560:PRO:O	1:C:922:THR:OG1	2.17	0.48
1:C:913:LEU:HD23	1:C:927:PHE:CZ	2.47	0.48
1:D:525:HIS:O	1:D:526:HIS:C	2.56	0.48
1:D:925:VAL:HA	1:D:928:GLN:HG2	1.95	0.48
1:E:767:ARG:NH2	1:F:117:LEU:HD11	2.29	0.48
1:F:4:PHE:CA	1:F:7:ASP:HB2	2.42	0.48
1:A:525:HIS:CE1	1:A:529:ASP:OD2	2.67	0.48
1:B:355:MET:HE3	1:B:355:MET:HA	1.95	0.48
1:B:546:LEU:HA	1:B:549:VAL:HG12	1.95	0.48
1:C:68:ASN:O	1:C:110:LYS:HD2	2.14	0.48
1:C:736:ALA:HB2	1:C:804:PHE:HD1	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:463:THR:HA	1:D:466:ILE:HD12	1.95	0.48
1:D:897:ILE:HB	1:D:898:PRO:HD3	1.94	0.48
1:D:987:MET:CA	1:D:1008:MET:HE1	2.43	0.48
1:E:362:PHE:CE2	1:E:366:LEU:HD21	2.48	0.48
1:F:194:ASN:CG	1:F:790:TYR:HD2	2.22	0.48
1:F:488:LEU:HD21	1:F:492:LEU:HG	1.96	0.48
1:F:683:GLU:OE1	1:F:685:ILE:HG12	2.13	0.48
1:A:54:ALA:HB1	1:A:816:LEU:HD23	1.93	0.48
1:A:194:ASN:HD22	1:A:798:MET:HE3	1.78	0.48
1:A:366:LEU:HA	1:A:369:THR:HB	1.96	0.48
1:A:1036:LYS:O	1:A:1038:GLU:N	2.45	0.48
1:B:104:GLN:CD	1:C:109:ASN:HD22	2.21	0.48
1:B:237:GLN:OE1	1:C:747:ASN:ND2	2.41	0.48
1:B:379:THR:HA	1:B:480:LEU:HD12	1.95	0.48
1:B:846:GLN:O	1:B:850:LYS:NZ	2.28	0.48
1:C:211:ASN:ND2	1:C:760:ASN:HD21	2.11	0.48
1:D:74:ASN:HA	1:F:170:SER:HB3	1.94	0.48
1:D:359:LEU:C	1:D:361:ASN:H	2.12	0.48
1:D:602:GLU:OE2	1:D:650:ARG:HD2	2.13	0.48
1:E:111:LEU:C	1:E:113:LEU:H	2.21	0.48
1:E:167:SER:CB	1:F:70:ASN:HD22	2.26	0.48
1:E:960:LEU:O	1:E:964:THR:HG23	2.13	0.48
1:F:101:ASP:OD1	1:F:101:ASP:N	2.45	0.48
1:F:542:LEU:O	1:F:546:LEU:HD23	2.13	0.48
1:F:565:PRO:O	1:F:670:ALA:HB2	2.13	0.48
1:A:380:PHE:CZ	1:A:398:MET:HE2	2.49	0.48
1:B:234:ILE:HD11	1:C:754:TRP:CE3	2.48	0.48
1:B:545:TYR:O	1:B:548:ILE:N	2.46	0.48
1:B:575:MET:HE3	1:B:617:PHE:HB2	1.94	0.48
1:B:595:THR:O	1:B:599:LEU:HG	2.13	0.48
1:B:736:ALA:HB2	1:B:804:PHE:HB3	1.94	0.48
1:E:211:ASN:CG	1:E:240:LEU:HG	2.39	0.48
1:E:536:ARG:HD2	2:E:2000:LMT:C3B	2.43	0.48
1:E:537:SER:OG	1:E:540:ARG:NH1	2.47	0.48
1:F:447:MET:HB3	1:F:887:CYS:SG	2.54	0.48
1:A:154:ILE:HG22	1:A:287:SER:HB3	1.96	0.48
1:B:182:TYR:O	1:B:769:LYS:HD3	2.12	0.48
1:B:211:ASN:CG	1:B:240:LEU:HG	2.39	0.48
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.94	0.48
1:B:617:PHE:O	1:B:619:GLY:N	2.45	0.48
1:B:678:THR:O	1:B:830:GLN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:710:PRO:C	1:B:712:MET:H	2.20	0.48
1:C:5:PHE:HE1	1:C:8:ARG:NH1	2.09	0.48
1:C:81:ASN:O	1:C:88:VAL:HG23	2.14	0.48
1:C:904:VAL:HG23	1:C:907:LEU:HD22	1.95	0.48
1:E:352:PHE:HD1	1:E:369:THR:OG1	1.96	0.48
1:E:382:VAL:HG21	1:E:476:SER:CB	2.44	0.48
1:E:408:ASP:OD2	1:E:445:ILE:HD11	2.14	0.48
1:E:888:LEU:HD11	1:E:943:ILE:HD11	1.95	0.48
1:F:137:LEU:HB2	1:F:293:LEU:HB2	1.96	0.48
1:F:163:LYS:HZ2	1:F:177:LEU:H	1.62	0.48
1:A:3:ASN:O	1:A:6:ILE:N	2.45	0.48
1:A:187:TRP:HA	1:A:774:MET:O	2.14	0.48
1:B:23:GLY:HA3	1:B:377:LEU:O	2.14	0.48
1:B:98:THR:O	1:B:99:ASP:C	2.57	0.48
1:B:776:GLU:HG2	1:B:777:ALA:H	1.78	0.48
1:C:427:PRO:O	1:C:431:THR:HG23	2.13	0.48
1:C:870:GLY:C	1:C:872:GLN:H	2.21	0.48
1:D:43:VAL:HG23	1:D:94:PHE:HE1	1.79	0.48
1:D:198:LEU:H	1:D:798:MET:HE1	1.77	0.48
1:D:444:GLY:O	1:D:447:MET:HB2	2.14	0.48
1:D:774:MET:HE3	1:D:780:ARG:HH21	1.79	0.48
1:D:900:SER:OG	1:D:1029:VAL:HG11	2.14	0.48
1:D:1035:ARG:HA	1:D:1035:ARG:HD2	1.68	0.48
1:E:182:TYR:HD2	1:E:765:ARG:HH22	1.61	0.48
1:E:1022:VAL:HA	1:E:1025:PHE:CD1	2.49	0.48
1:E:1035:ARG:HB3	1:E:1036:LYS:H	1.53	0.48
1:F:208:LYS:HG3	1:F:759:VAL:HG13	1.95	0.48
1:F:431:THR:HG21	1:F:490:PRO:HA	1.96	0.48
1:F:740:GLY:O	1:F:794:ALA:N	2.47	0.48
1:F:888:LEU:HD21	1:F:943:ILE:HD11	1.95	0.48
1:A:182:TYR:O	1:A:769:LYS:HD3	2.13	0.48
1:A:768:VAL:HG12	1:B:63:GLN:OE1	2.14	0.48
1:A:832:ALA:CB	1:A:835:LYS:HD2	2.35	0.48
1:D:137:LEU:HD22	1:D:293:LEU:HD13	1.95	0.48
1:D:736:ALA:HA	1:D:739:LEU:HD13	1.96	0.48
1:E:57:VAL:HG21	1:E:86:GLY:HA2	1.95	0.48
1:E:230:LEU:HG	1:E:231:ASN:N	2.27	0.48
1:E:571:VAL:O	1:E:668:LEU:HD21	2.14	0.48
1:E:957:GLY:O	1:E:1041:GLU:HA	2.13	0.48
1:F:478:MET:O	1:F:478:MET:HE3	2.13	0.48
1:A:736:ALA:HB2	1:A:804:PHE:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:974:PRO:O	1:A:977:MET:HG2	2.14	0.48
1:A:982:PHE:O	1:A:985:GLY:N	2.47	0.48
1:B:459:PHE:O	1:B:464:GLY:HA3	2.14	0.48
1:B:1023:PRO:O	1:B:1027:VAL:HG12	2.14	0.48
1:C:465:ALA:HA	1:C:468:ARG:HH12	1.78	0.48
1:C:895:TRP:HA	1:C:895:TRP:CE3	2.48	0.48
1:D:394:THR:HG22	1:D:469:GLN:HB3	1.96	0.48
1:D:584:GLN:NE2	1:F:222:THR:HG22	2.28	0.48
1:D:837:THR:O	1:D:840:ALA:HB3	2.14	0.48
1:F:74:ASN:HB3	1:F:95:GLU:CB	2.29	0.48
1:F:545:TYR:HB2	1:F:1021:PHE:HE2	1.79	0.48
1:F:703:LEU:HD13	1:F:718:PRO:HB3	1.95	0.48
1:F:754:TRP:CZ2	1:F:780:ARG:HA	2.49	0.48
1:A:355:MET:HE2	1:A:368:PRO:HG2	1.95	0.47
1:A:541:TYR:N	1:A:541:TYR:CD1	2.82	0.47
1:A:645:GLU:HG3	1:A:646:ALA:N	2.29	0.47
1:A:754:TRP:CE2	1:A:780:ARG:HB3	2.48	0.47
1:A:888:LEU:HD11	1:A:901:VAL:HB	1.96	0.47
1:B:154:ILE:HG22	1:B:287:SER:HB3	1.96	0.47
1:B:366:LEU:O	1:B:369:THR:HB	2.14	0.47
1:B:530:SER:HG	1:B:531:VAL:H	1.62	0.47
1:C:398:MET:HG2	1:C:473:THR:CG2	2.44	0.47
1:C:750:LEU:O	1:C:753:ALA:HB3	2.13	0.47
1:D:68:ASN:CB	1:D:114:ALA:HB2	2.44	0.47
1:D:196:PHE:CD2	1:D:196:PHE:N	2.80	0.47
1:D:438:ILE:O	1:D:441:ALA:HB3	2.14	0.47
1:E:95:GLU:HB2	1:E:98:THR:OG1	2.14	0.47
1:E:188:MET:HE1	1:E:200:PRO:HG3	1.96	0.47
1:E:219:LEU:HA	1:F:754:TRP:HZ3	1.79	0.47
1:E:877:TYR:HD2	1:E:877:TYR:HA	1.33	0.47
1:F:36:PRO:HG2	1:F:38:ILE:HG13	1.95	0.47
1:F:312:LYS:O	1:F:312:LYS:HE3	2.14	0.47
1:F:467:TYR:HE1	1:F:925:VAL:HG22	1.78	0.47
1:A:462:SER:O	1:A:466:ILE:HG12	2.14	0.47
1:A:674:LEU:HD22	1:A:675:GLY:H	1.79	0.47
1:B:8:ARG:HB3	1:C:893:GLU:CD	2.39	0.47
1:B:971:ARG:CG	1:B:971:ARG:HH11	2.27	0.47
1:C:66:GLU:OE2	1:C:821:GLY:HA2	2.14	0.47
1:C:1016:VAL:HG12	1:C:1016:VAL:O	2.14	0.47
1:D:177:LEU:HD13	1:D:178:PHE:C	2.39	0.47
1:D:235:ILE:O	1:E:728:LYS:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:GLU:OE1	1:D:433:LYS:HE2	2.14	0.47
1:D:926:TYR:HE1	1:D:999:ALA:CB	2.27	0.47
1:E:66:GLU:CD	1:E:818:ARG:HH21	2.21	0.47
1:E:166:ILE:HD13	1:E:310:LEU:HD13	1.95	0.47
1:E:175:VAL:HG22	1:F:70:ASN:CG	2.39	0.47
1:E:273:GLU:CD	1:E:770:LYS:HD2	2.39	0.47
1:E:508:GLY:C	1:E:510:LYS:H	2.22	0.47
1:F:250:LEU:HD12	1:F:251:LEU:H	1.79	0.47
1:F:776:GLU:HB2	1:F:779:TYR:CE1	2.48	0.47
1:F:777:ALA:C	1:F:781:MET:HE2	2.39	0.47
1:F:1013:THR:O	1:F:1017:LEU:HB2	2.14	0.47
1:A:414:GLU:CG	1:A:974:PRO:HG3	2.44	0.47
1:A:602:GLU:OE2	1:A:650:ARG:NH2	2.47	0.47
1:A:736:ALA:O	1:A:741:VAL:HG12	2.13	0.47
1:B:368:PRO:HG3	1:B:413:VAL:HG21	1.96	0.47
1:B:953:MET:HB2	1:B:953:MET:HE3	1.39	0.47
1:C:452:VAL:O	1:C:455:PRO:HD2	2.15	0.47
1:C:608:SER:OG	1:C:630:SER:HB3	2.15	0.47
1:C:764:ASP:C	1:C:766:GLY:H	2.22	0.47
1:D:10:ILE:HG21	1:E:893:GLU:C	2.39	0.47
1:D:162:MET:HG2	1:D:313:MET:SD	2.54	0.47
1:D:360:GLN:NE2	1:D:517:ASN:HD21	2.11	0.47
1:D:776:GLU:HG2	1:D:777:ALA:N	2.28	0.47
1:D:950:LYS:HE2	1:D:950:LYS:HB2	1.62	0.47
1:D:987:MET:CB	1:D:1008:MET:HE1	2.43	0.47
1:E:31:PRO:O	1:E:390:ILE:HG12	2.13	0.47
1:E:206:ALA:HB1	1:E:249:ILE:HD11	1.95	0.47
1:E:244:GLU:OE1	1:E:248:LYS:NZ	2.29	0.47
1:E:641:GLU:OE1	1:E:641:GLU:N	2.39	0.47
1:F:24:GLY:O	1:F:27:ILE:HG12	2.13	0.47
1:F:189:ASN:OD1	1:F:190:PRO:HD2	2.14	0.47
1:A:242:SER:OG	1:A:245:GLU:HG3	2.14	0.47
1:B:166:ILE:HD12	1:B:166:ILE:HA	1.82	0.47
1:B:1011:MET:O	1:B:1015:THR:HG23	2.14	0.47
1:C:120:GLN:O	1:C:124:GLN:HB3	2.13	0.47
1:C:135:SER:HB3	1:C:673:GLU:HA	1.95	0.47
1:C:358:PHE:HB3	1:C:359:LEU:HD23	1.96	0.47
1:D:151:GLN:H	1:D:151:GLN:HG3	1.28	0.47
1:D:462:SER:O	1:D:466:ILE:HG13	2.15	0.47
1:E:219:LEU:HD23	1:F:754:TRP:CZ3	2.49	0.47
1:E:235:ILE:O	1:F:728:LYS:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:559:LEU:HD12	1:E:560:PRO:HD2	1.96	0.47
1:E:648:THR:HG23	1:E:665:ALA:O	2.13	0.47
1:E:885:PHE:HB2	1:E:902:MET:HE1	1.97	0.47
1:E:986:VAL:HG11	1:E:1007:VAL:CG1	2.45	0.47
1:F:100:ALA:O	1:F:101:ASP:C	2.57	0.47
1:F:502:LYS:O	1:F:503:GLY:C	2.57	0.47
1:C:34:GLN:HG3	1:C:333:VAL:HG22	1.96	0.47
1:C:190:PRO:HG3	1:C:779:TYR:CG	2.49	0.47
1:C:742:SER:O	1:C:746:ILE:HG23	2.14	0.47
1:D:515:TRP:O	1:D:519:MET:HG3	2.14	0.47
1:D:520:PHE:O	1:D:523:SER:OG	2.23	0.47
1:D:873:ALA:N	1:D:874:PRO:HD2	2.29	0.47
1:E:219:LEU:HD11	1:F:727:PHE:CD2	2.50	0.47
1:E:379:THR:O	1:E:382:VAL:N	2.47	0.47
1:E:536:ARG:HD2	2:E:2000:LMT:H4B	1.97	0.47
1:E:873:ALA:N	1:E:874:PRO:HD2	2.29	0.47
1:F:326:PRO:HA	1:F:630:SER:OG	2.15	0.47
1:F:414:GLU:OE2	1:F:973:ARG:NH1	2.48	0.47
1:F:492:LEU:HD22	1:F:496:MET:HE3	1.96	0.47
1:F:618:ALA:O	1:F:815:ARG:NH2	2.48	0.47
1:F:885:PHE:CE2	1:F:886:LEU:HD23	2.50	0.47
1:F:983:ILE:CD1	1:F:1012:VAL:HG22	2.44	0.47
1:F:1026:PHE:O	1:F:1030:ARG:HB2	2.15	0.47
1:A:294:ALA:HB3	1:A:297:ALA:HB3	1.97	0.47
1:A:785:ASP:OD1	1:A:785:ASP:N	2.46	0.47
1:B:201:VAL:HG21	1:B:745:ASP:OD2	2.14	0.47
1:B:372:VAL:CG2	1:B:373:PRO:HD3	2.40	0.47
1:B:726:GLN:NE2	1:B:811:TYR:O	2.47	0.47
1:B:971:ARG:HH11	1:B:971:ARG:HG3	1.79	0.47
1:C:356:TYR:C	1:C:358:PHE:N	2.73	0.47
1:C:1031:ARG:NH2	1:C:1040:ILE:HD11	2.29	0.47
1:D:72:ILE:HG21	1:D:107:VAL:HG23	1.96	0.47
1:D:214:VAL:HG22	1:D:216:ALA:N	2.30	0.47
1:E:166:ILE:HD12	1:E:166:ILE:HA	1.65	0.47
1:E:185:ARG:HB3	1:E:187:TRP:NE1	2.30	0.47
1:E:222:THR:HA	1:E:224:PRO:CD	2.44	0.47
1:E:451:ALA:HB1	1:E:883:VAL:HG12	1.96	0.47
1:F:62:THR:O	1:F:90:ILE:HD12	2.14	0.47
1:F:111:LEU:C	1:F:113:LEU:H	2.23	0.47
1:F:143:ILE:HG22	1:F:286:ALA:CB	2.45	0.47
1:F:162:MET:HG2	1:F:313:MET:SD	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:PHE:CE1	1:F:608:SER:HB2	2.50	0.47
1:F:372:VAL:C	1:F:374:VAL:N	2.69	0.47
1:F:563:PHE:CE2	1:F:564:LEU:HD12	2.49	0.47
1:F:774:MET:HE3	1:F:780:ARG:HH21	1.79	0.47
1:A:293:LEU:HD22	1:A:294:ALA:N	2.23	0.47
1:A:360:GLN:OE1	1:A:517:ASN:ND2	2.44	0.47
1:A:576:VAL:HA	1:A:663:VAL:HG22	1.97	0.47
1:A:888:LEU:CB	1:A:898:PRO:HB3	2.45	0.47
1:A:909:VAL:O	1:A:912:ALA:N	2.43	0.47
1:A:965:LEU:O	1:A:968:VAL:HG22	2.15	0.47
1:B:363:ARG:NH1	1:B:496:MET:O	2.48	0.47
1:B:584:GLN:HB2	1:B:622:GLN:HG2	1.96	0.47
1:B:742:SER:O	1:B:746:ILE:HG13	2.15	0.47
1:B:909:VAL:HG23	1:B:935:ILE:HD11	1.97	0.47
1:C:184:MET:HB2	1:C:762:PHE:CD2	2.50	0.47
1:C:318:PRO:HG2	1:C:321:LEU:HB2	1.96	0.47
1:C:536:ARG:HD2	2:C:2000:LMT:O4'	2.14	0.47
2:C:2000:LMT:O4'	2:C:2000:LMT:O6B	2.25	0.47
1:D:194:ASN:HA	1:D:798:MET:HE3	1.96	0.47
1:D:355:MET:CE	1:D:977:MET:HG2	2.45	0.47
1:D:895:TRP:CZ2	1:F:10:ILE:HD12	2.49	0.47
1:D:926:TYR:CE1	1:D:999:ALA:HB1	2.50	0.47
1:D:949:ALA:HB3	1:D:1026:PHE:CE1	2.50	0.47
1:E:23:GLY:HA2	1:E:377:LEU:O	2.14	0.47
1:E:139:VAL:HA	1:E:289:LEU:O	2.15	0.47
1:E:172:VAL:HG22	1:E:302:THR:HG23	1.97	0.47
1:E:185:ARG:HB3	1:E:187:TRP:CZ2	2.50	0.47
1:E:420:MET:SD	1:E:427:PRO:HA	2.55	0.47
1:E:536:ARG:HH11	2:E:2000:LMT:C3B	2.28	0.47
1:E:652:THR:HG22	1:E:665:ALA:H	1.79	0.47
1:E:750:LEU:O	1:E:753:ALA:HB3	2.14	0.47
1:E:926:TYR:HE1	1:E:999:ALA:HB1	1.78	0.47
1:E:961:ILE:HG22	1:E:965:LEU:HD12	1.97	0.47
1:F:596:HIS:O	1:F:600:THR:OG1	2.25	0.47
1:F:971:ARG:C	1:F:974:PRO:HD2	2.38	0.47
1:A:66:GLU:OE2	1:A:80:SER:OG	2.23	0.47
1:B:54:ALA:O	1:B:57:VAL:HG23	2.14	0.47
1:B:444:GLY:O	1:B:447:MET:HB2	2.15	0.47
1:C:140:VAL:HG11	1:C:310:LEU:HD21	1.95	0.47
1:C:507:GLU:HG2	1:C:518:ARG:HG2	1.95	0.47
1:C:524:THR:HG23	1:C:972:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1030:ARG:C	1:C:1032:ARG:H	2.21	0.47
1:D:281:PHE:HD1	1:D:610:PHE:HD1	1.62	0.47
1:D:418:ARG:HD2	1:D:418:ARG:C	2.39	0.47
1:E:313:MET:HB3	1:E:317:PHE:CE1	2.49	0.47
1:E:904:VAL:HA	1:E:907:LEU:HD13	1.96	0.47
1:F:163:LYS:O	1:F:163:LYS:HG2	2.15	0.47
1:F:776:GLU:HB2	1:F:779:TYR:CD1	2.50	0.47
1:F:911:GLY:HA3	1:F:1013:THR:OG1	2.15	0.47
1:A:84:SER:N	1:A:814:PRO:O	2.48	0.47
1:A:158:VAL:CG1	1:A:177:LEU:HD21	2.45	0.47
1:A:457:ALA:HB1	1:A:468:ARG:HG3	1.97	0.47
1:A:746:ILE:HG22	1:A:791:VAL:HG21	1.95	0.47
1:B:13:TRP:CE3	1:B:488:LEU:HD11	2.50	0.47
1:B:81:ASN:O	1:B:88:VAL:HA	2.14	0.47
1:B:535:LEU:HD23	1:B:535:LEU:HA	1.75	0.47
1:B:805:SER:OG	1:B:806:SER:N	2.48	0.47
1:C:101:ASP:OD1	1:C:101:ASP:N	2.47	0.47
1:C:712:MET:O	1:C:832:ALA:N	2.36	0.47
1:C:971:ARG:C	1:C:974:PRO:HD2	2.39	0.47
1:D:58:GLN:OE1	1:D:816:LEU:HB3	2.15	0.47
1:D:736:ALA:HB2	1:D:804:PHE:HB3	1.96	0.47
1:D:987:MET:HA	1:D:990:VAL:HG23	1.96	0.47
1:E:785:ASP:N	1:E:785:ASP:OD1	2.48	0.47
1:E:897:ILE:HD13	1:E:950:LYS:HD2	1.97	0.47
1:F:925:VAL:HA	1:F:928:GLN:OE1	2.15	0.47
1:F:1008:MET:HB2	1:F:1008:MET:HE3	1.82	0.47
1:A:166:ILE:HD12	1:A:166:ILE:HA	1.78	0.47
1:A:344:LEU:HD23	1:A:344:LEU:HA	1.55	0.47
1:A:909:VAL:HG22	1:A:931:LEU:HD11	1.95	0.47
1:A:914:LEU:O	1:A:918:PHE:HB2	2.15	0.47
1:B:105:VAL:HG22	1:C:109:ASN:OD1	2.15	0.47
1:B:213:GLN:HG2	1:B:239:ARG:HG3	1.97	0.47
1:B:1005:THR:HG23	1:B:1006:GLY:H	1.80	0.47
1:C:352:PHE:HD1	1:C:369:THR:OG1	1.98	0.47
1:C:435:MET:CE	1:C:438:ILE:HD11	2.45	0.47
1:C:565:PRO:HG3	1:C:999:ALA:CA	2.45	0.47
1:C:698:ALA:O	1:C:701:GLN:HB3	2.14	0.47
1:C:758:TYR:CE1	1:C:770:LYS:HD3	2.50	0.47
1:D:166:ILE:HD12	1:D:166:ILE:HA	1.70	0.47
1:D:228:GLN:NE2	1:D:230:LEU:O	2.42	0.47
1:D:337:ILE:HA	1:D:337:ILE:HD12	1.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:404:LEU:HD12	1:D:937:LEU:HD21	1.97	0.47
1:D:909:VAL:O	1:D:912:ALA:N	2.46	0.47
1:E:56:THR:O	1:E:60:THR:OG1	2.32	0.47
1:E:356:TYR:CE1	1:E:362:PHE:HA	2.50	0.47
1:E:462:SER:O	1:E:466:ILE:HG13	2.15	0.47
1:F:42:ALA:HB2	1:F:93:THR:HG23	1.97	0.47
1:F:121:GLU:O	1:F:124:GLN:HG2	2.15	0.47
1:F:588:GLN:O	1:F:592:ASN:ND2	2.48	0.47
1:F:750:LEU:O	1:F:753:ALA:HB3	2.15	0.47
1:B:778:LYS:HE3	1:B:779:TYR:CE2	2.49	0.46
1:C:26:ALA:HB1	1:C:384:ALA:HB3	1.97	0.46
1:C:69:MET:HG3	1:C:92:LEU:HD11	1.98	0.46
1:C:408:ASP:O	1:C:412:VAL:HG23	2.15	0.46
1:C:453:PHE:O	1:C:456:MET:HG3	2.15	0.46
1:C:684:LEU:HD12	1:C:827:ILE:HD11	1.97	0.46
1:C:987:MET:O	1:C:990:VAL:HG22	2.15	0.46
1:D:128:SER:HB3	1:D:130:GLU:OE2	2.15	0.46
1:D:218:GLN:HG2	1:D:233:SER:HA	1.95	0.46
1:D:573:MET:HE1	1:D:617:PHE:HE2	1.79	0.46
1:D:933:THR:HG22	1:D:934:THR:N	2.30	0.46
1:E:115:MET:O	1:E:123:GLN:NE2	2.48	0.46
1:E:590:VAL:HG11	1:E:663:VAL:HG21	1.97	0.46
1:E:987:MET:CB	1:E:1008:MET:HE1	2.44	0.46
1:F:137:LEU:N	1:F:291:ILE:O	2.48	0.46
1:F:467:TYR:O	1:F:470:PHE:HB2	2.15	0.46
1:A:425:LEU:HD22	1:A:429:GLU:OE1	2.15	0.46
1:A:463:THR:O	1:A:466:ILE:HB	2.15	0.46
1:A:800:PRO:O	1:A:803:ALA:HB3	2.16	0.46
1:B:135:SER:OG	1:B:673:GLU:OE1	2.33	0.46
1:B:174:ASP:HB3	1:B:292:LYS:HB2	1.97	0.46
1:B:340:VAL:HG11	1:B:395:MET:HB3	1.97	0.46
1:B:608:SER:O	1:B:630:SER:N	2.44	0.46
1:C:54:ALA:HB1	1:C:816:LEU:HG	1.97	0.46
1:C:298:ASN:HB3	1:C:301:ASP:CB	2.33	0.46
1:C:355:MET:HB3	1:C:365:THR:HG23	1.98	0.46
1:C:358:PHE:C	1:C:359:LEU:HD23	2.40	0.46
1:C:414:GLU:HG3	1:C:974:PRO:HB3	1.97	0.46
1:C:758:TYR:HB2	1:C:772:TYR:CE2	2.51	0.46
1:D:690:LEU:O	1:D:694:LYS:HD3	2.14	0.46
1:D:727:PHE:HE1	1:D:807:SER:OG	1.98	0.46
1:D:889:ALA:HB1	1:D:895:TRP:CZ3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:910:ILE:O	1:D:914:LEU:HB2	2.15	0.46
1:D:987:MET:HB3	1:D:988:PRO:HD3	1.97	0.46
1:E:291:ILE:HD13	1:E:306:ILE:HD13	1.96	0.46
1:F:184:MET:HB2	1:F:762:PHE:CE2	2.50	0.46
1:F:397:GLY:HA3	1:F:470:PHE:HD2	1.79	0.46
1:F:577:GLN:NE2	1:F:721:LEU:HD11	2.29	0.46
1:A:900:SER:HB3	1:A:1029:VAL:HG21	1.98	0.46
1:A:904:VAL:HG22	1:A:1025:PHE:CD1	2.50	0.46
1:B:95:GLU:O	1:B:98:THR:OG1	2.22	0.46
1:B:327:TYR:HE2	1:B:329:THR:HG23	1.80	0.46
1:B:405:LEU:HD22	1:B:481:SER:HB2	1.97	0.46
1:B:801:PHE:HA	1:B:804:PHE:HE2	1.76	0.46
1:D:169:THR:O	1:D:170:SER:OG	2.32	0.46
1:D:182:TYR:O	1:D:769:LYS:HD3	2.15	0.46
1:D:345:VAL:O	1:D:348:ILE:HB	2.15	0.46
1:E:150:THR:HG23	1:E:153:ASP:OD1	2.15	0.46
1:E:167:SER:OG	1:E:175:VAL:HG11	2.15	0.46
1:E:979:SER:HB3	1:E:1015:THR:HG21	1.95	0.46
1:F:372:VAL:HG23	1:F:373:PRO:CD	2.45	0.46
1:F:850:LYS:O	1:F:851:LEU:HD23	2.16	0.46
1:A:76:MET:HE3	1:A:864:TYR:CD2	2.50	0.46
1:A:549:VAL:O	1:A:552:MET:HB3	2.14	0.46
1:B:456:MET:HA	1:B:876:LEU:HD21	1.98	0.46
1:B:594:VAL:HG22	1:B:655:PHE:CZ	2.51	0.46
1:B:721:LEU:HB3	1:B:814:PRO:HG2	1.97	0.46
1:C:15:ILE:HD13	1:C:487:ILE:HD13	1.96	0.46
1:C:922:THR:O	1:C:924:ASP:N	2.47	0.46
1:D:17:ILE:O	1:D:20:MET:HB2	2.16	0.46
1:D:445:ILE:HG21	1:D:940:LYS:CD	2.45	0.46
1:D:695:LEU:HD23	1:D:825:MET:HG3	1.96	0.46
1:E:188:MET:SD	1:E:203:VAL:HG21	2.55	0.46
1:E:280:GLU:OE2	1:E:588:GLN:NE2	2.49	0.46
1:E:686:ASP:HA	1:E:854:GLY:O	2.16	0.46
1:E:992:SER:HB3	1:E:1000:GLN:OE1	2.15	0.46
1:F:58:GLN:OE1	1:F:818:ARG:HD2	2.15	0.46
1:F:509:LYS:CG	1:F:513:PHE:HB2	2.45	0.46
1:F:535:LEU:HD23	1:F:535:LEU:HA	1.66	0.46
1:F:717:ARG:HG3	1:F:828:LEU:HB2	1.97	0.46
1:F:744:ASN:O	1:F:748:THR:HG23	2.15	0.46
1:B:688:ALA:HB3	1:B:690:LEU:HD22	1.97	0.46
1:C:222:THR:HA	1:C:224:PRO:CD	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:576:VAL:HG21	1:C:591:LEU:HD21	1.97	0.46
1:C:785:ASP:N	1:C:785:ASP:OD1	2.47	0.46
1:C:888:LEU:HD21	1:C:943:ILE:HD11	1.97	0.46
1:D:400:LEU:HD23	1:D:474:ILE:HD13	1.98	0.46
1:E:340:VAL:HG11	1:E:395:MET:CB	2.39	0.46
1:E:575:MET:HB2	1:E:626:ILE:HD11	1.98	0.46
1:E:680:PHE:CG	1:E:859:TRP:CZ3	3.04	0.46
1:F:352:PHE:HE1	1:F:366:LEU:HD23	1.79	0.46
1:F:904:VAL:HG21	1:F:942:ALA:CB	2.43	0.46
1:F:949:ALA:O	1:F:953:MET:HE2	2.15	0.46
1:F:961:ILE:H	1:F:961:ILE:CD1	2.21	0.46
1:A:472:ILE:O	1:A:476:SER:HB3	2.15	0.46
1:A:637:ARG:HA	1:A:642:ASN:HD22	1.80	0.46
1:A:686:ASP:OD2	1:A:823:PRO:HB2	2.15	0.46
1:A:740:GLY:C	1:A:793:ALA:HB1	2.40	0.46
1:A:752:ALA:O	1:A:774:MET:HA	2.14	0.46
1:B:544:LEU:O	1:B:548:ILE:HG13	2.16	0.46
1:B:609:VAL:HG13	1:B:629:VAL:CG1	2.46	0.46
1:C:888:LEU:HD23	1:C:888:LEU:HA	1.67	0.46
1:C:926:TYR:HE2	1:C:999:ALA:CB	2.29	0.46
1:D:62:THR:O	1:D:66:GLU:HG3	2.15	0.46
1:D:317:PHE:HA	1:D:318:PRO:HD3	1.62	0.46
1:D:525:HIS:CE1	1:D:529:ASP:OD1	2.68	0.46
1:D:680:PHE:CD1	1:D:859:TRP:HZ3	2.29	0.46
1:D:702:LEU:HD11	1:D:848:ALA:HB2	1.97	0.46
1:E:45:ILE:HG12	1:E:129:VAL:HG22	1.97	0.46
1:E:185:ARG:HB3	1:E:187:TRP:CE2	2.51	0.46
1:E:219:LEU:N	1:E:232:ALA:O	2.45	0.46
1:E:558:ARG:HE	1:E:558:ARG:HB3	1.52	0.46
1:F:465:ALA:O	1:F:468:ARG:HG2	2.16	0.46
1:F:764:ASP:O	1:F:766:GLY:N	2.49	0.46
1:A:62:THR:O	1:A:66:GLU:HG3	2.16	0.46
1:A:197:GLN:HA	1:A:798:MET:HE2	1.98	0.46
1:A:198:LEU:HD22	1:A:202:ASP:HB2	1.97	0.46
1:A:200:PRO:HB2	1:A:749:THR:HG22	1.97	0.46
1:A:455:PRO:O	1:A:458:PHE:HB2	2.16	0.46
2:A:2000:LMT:H11	2:A:2000:LMT:H2'	1.64	0.46
1:B:33:ALA:O	1:B:391:ASN:HA	2.16	0.46
1:B:588:GLN:HB2	1:B:613:ASN:ND2	2.30	0.46
1:B:894:SER:CB	1:B:897:ILE:HG13	2.46	0.46
1:C:960:LEU:O	1:C:964:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:ASN:HD22	1:E:109:ASN:HD21	1.64	0.46
1:D:253:VAL:HG12	1:D:259:ARG:HG2	1.96	0.46
1:D:982:PHE:O	1:D:983:ILE:C	2.59	0.46
1:E:539:GLY:O	1:E:542:LEU:HB2	2.14	0.46
1:F:36:PRO:O	1:F:38:ILE:HG13	2.14	0.46
1:F:125:GLN:NE2	1:F:125:GLN:O	2.48	0.46
1:F:164:ASP:HB2	1:F:767:ARG:HH21	1.80	0.46
1:F:208:LYS:HG3	1:F:759:VAL:CG1	2.46	0.46
1:F:371:ALA:O	1:F:375:VAL:HG23	2.16	0.46
1:F:577:GLN:O	1:F:661:ALA:HB1	2.15	0.46
1:F:785:ASP:N	1:F:785:ASP:OD1	2.48	0.46
1:A:393:LEU:HD13	1:A:466:ILE:HA	1.97	0.46
1:A:712:MET:HG3	1:A:713:LEU:HD13	1.97	0.46
1:B:721:LEU:HA	1:B:721:LEU:HD13	1.64	0.46
1:C:543:VAL:O	1:C:546:LEU:HB2	2.16	0.46
1:D:672:VAL:HG23	1:D:673:GLU:OE2	2.16	0.46
1:F:34:GLN:HB2	1:F:333:VAL:HG22	1.97	0.46
1:F:144:ASN:HA	1:F:320:GLY:O	2.14	0.46
1:F:331:PRO:O	1:F:334:LYS:HB2	2.15	0.46
1:F:372:VAL:O	1:F:376:LEU:N	2.33	0.46
1:F:738:ALA:O	1:F:740:GLY:N	2.48	0.46
1:F:775:SER:OG	1:F:780:ARG:HG2	2.16	0.46
1:F:940:LYS:O	1:F:943:ILE:HB	2.15	0.46
1:F:953:MET:HE2	1:F:953:MET:HB2	1.47	0.46
1:A:239:ARG:NH1	1:A:761:ASP:H	2.14	0.46
1:A:391:ASN:OD1	1:A:393:LEU:HB2	2.16	0.46
1:B:242:SER:OG	1:B:245:GLU:HG3	2.16	0.46
1:B:1026:PHE:CD2	1:B:1026:PHE:C	2.94	0.46
1:C:26:ALA:HB1	1:C:384:ALA:CB	2.46	0.46
1:C:699:ARG:HE	1:C:718:PRO:HB3	1.81	0.46
1:C:751:GLY:C	1:C:753:ALA:N	2.74	0.46
1:C:902:MET:HB2	1:C:902:MET:HE3	1.47	0.46
1:D:138:MET:HB2	1:D:138:MET:HE3	1.66	0.46
1:E:39:ALA:HB2	1:E:673:GLU:HG3	1.97	0.46
1:E:79:SER:O	1:E:90:ILE:HA	2.16	0.46
1:E:1015:THR:OG1	1:E:1016:VAL:N	2.48	0.46
1:F:182:TYR:O	1:F:769:LYS:HB3	2.15	0.46
1:F:219:LEU:HG	1:F:234:ILE:HD11	1.97	0.46
1:F:354:VAL:HG21	1:F:981:ALA:HA	1.97	0.46
1:F:888:LEU:HD12	1:F:901:VAL:HG11	1.97	0.46
1:A:186:ILE:HB	1:A:773:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:THR:OG1	1:A:268:ILE:HG22	2.16	0.46
1:B:235:ILE:CD1	1:C:726:GLN:HB3	2.46	0.46
1:B:356:TYR:C	1:B:358:PHE:H	2.23	0.46
1:B:758:TYR:CD1	1:B:770:LYS:HD3	2.51	0.46
1:B:1036:LYS:O	1:B:1037:ASN:ND2	2.49	0.46
1:C:57:VAL:HG13	1:C:88:VAL:HB	1.98	0.46
1:C:787:GLY:C	1:C:789:TRP:H	2.22	0.46
1:D:124:GLN:NE2	1:D:758:TYR:HB3	2.31	0.46
1:D:157:TYR:OH	1:D:316:PHE:O	2.34	0.46
1:E:200:PRO:HA	1:E:203:VAL:HG23	1.98	0.46
1:E:343:THR:CG2	1:E:399:VAL:HG11	2.46	0.46
1:E:434:SER:O	1:E:437:GLN:HG2	2.15	0.46
1:E:442:LEU:O	1:E:445:ILE:HG13	2.16	0.46
1:E:960:LEU:HD23	1:E:961:ILE:N	2.31	0.46
1:E:979:SER:CB	1:E:1015:THR:HG21	2.45	0.46
1:F:27:ILE:HA	1:F:30:LEU:HB2	1.97	0.46
1:F:136:PHE:HB2	1:F:327:TYR:CE2	2.51	0.46
1:F:214:VAL:HG12	1:F:216:ALA:N	2.31	0.46
1:F:420:MET:CE	1:F:427:PRO:HG3	2.44	0.46
1:F:439:GLN:CG	1:F:440:GLY:H	2.28	0.46
1:F:470:PHE:CD1	1:F:929:VAL:HG21	2.51	0.46
1:F:885:PHE:CD1	1:F:898:PRO:HB2	2.51	0.46
1:F:984:LEU:HD22	1:F:984:LEU:HA	1.69	0.46
1:A:24:GLY:O	1:A:28:LEU:HD13	2.16	0.45
1:A:396:PHE:HE1	1:A:999:ALA:HB1	1.80	0.45
1:A:922:THR:HG23	1:A:924:ASP:OD2	2.16	0.45
1:B:192:GLU:HA	1:B:195:LYS:HD2	1.98	0.45
1:B:210:GLN:NE2	1:B:250:LEU:H	2.14	0.45
1:C:401:ALA:HB2	1:C:474:ILE:HD13	1.97	0.45
1:C:944:LEU:HB3	1:C:971:ARG:NH2	2.31	0.45
1:D:449:LEU:HB3	1:D:478:MET:HE2	1.98	0.45
1:E:447:MET:HB3	1:E:887:CYS:HB3	1.98	0.45
1:E:527:TYR:O	1:E:530:SER:HB3	2.16	0.45
1:E:546:LEU:HD13	1:E:547:ILE:HG22	1.98	0.45
1:F:112:GLN:HG2	1:F:115:MET:HE3	1.97	0.45
1:F:428:LYS:CG	1:F:494:ALA:HB1	2.45	0.45
1:F:431:THR:CG2	1:F:490:PRO:HA	2.46	0.45
1:F:514:GLY:C	1:F:516:PHE:N	2.73	0.45
1:F:991:ILE:HD12	1:F:991:ILE:HA	1.70	0.45
1:A:284:GLN:HG3	1:A:285:PRO:HD2	1.98	0.45
1:B:58:GLN:O	1:B:63:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:685:ILE:HG12	1:B:824:SER:HB2	1.97	0.45
1:B:1026:PHE:HD2	1:B:1026:PHE:C	2.25	0.45
1:C:44:THR:N	1:C:132:SER:OG	2.44	0.45
1:C:68:ASN:HB2	1:C:114:ALA:HB2	1.98	0.45
1:C:146:ASP:O	1:C:148:THR:N	2.49	0.45
1:C:730:ASP:CG	1:C:808:ARG:HH12	2.25	0.45
1:D:214:VAL:CG2	1:D:236:ALA:HB3	2.32	0.45
1:D:445:ILE:HD13	1:D:940:LYS:HE2	1.97	0.45
1:E:116:PRO:HD2	1:E:117:LEU:HD12	1.98	0.45
1:E:907:LEU:HD23	1:E:1017:LEU:CB	2.41	0.45
1:F:354:VAL:CG1	1:F:980:LEU:HD23	2.47	0.45
1:B:294:ALA:HB3	1:B:297:ALA:CB	2.46	0.45
1:B:344:LEU:CD2	1:B:399:VAL:HG22	2.47	0.45
1:C:46:SER:HA	1:C:88:VAL:O	2.17	0.45
1:C:549:VAL:O	1:C:552:MET:HB3	2.15	0.45
1:C:885:PHE:HB2	1:C:902:MET:SD	2.57	0.45
1:E:3:ASN:O	1:E:6:ILE:N	2.45	0.45
1:E:225:VAL:HB	1:F:777:ALA:HB1	1.99	0.45
1:F:23:GLY:HA3	1:F:377:LEU:O	2.17	0.45
1:F:310:LEU:O	1:F:314:GLU:HG3	2.16	0.45
1:F:952:LEU:HD11	1:F:970:MET:CE	2.47	0.45
1:A:61:VAL:CG1	1:A:122:VAL:HG21	2.46	0.45
1:A:401:ALA:O	1:A:405:LEU:HG	2.17	0.45
1:A:416:VAL:HG22	1:A:431:THR:HA	1.99	0.45
1:A:505:HIS:O	1:A:507:GLU:HG2	2.15	0.45
1:A:567:GLU:CD	1:A:996:GLY:HA2	2.40	0.45
1:A:578:LEU:HD23	1:A:661:ALA:HB2	1.98	0.45
1:B:5:PHE:CE1	1:B:487:ILE:HG13	2.51	0.45
1:B:888:LEU:HG	1:B:901:VAL:HG11	1.98	0.45
1:C:792:ARG:HG3	1:C:798:MET:SD	2.56	0.45
1:D:281:PHE:CD1	1:D:610:PHE:HD1	2.34	0.45
1:D:776:GLU:HB3	1:D:779:TYR:HD1	1.78	0.45
1:E:309:GLU:HA	1:E:312:LYS:HE3	1.98	0.45
1:F:434:SER:O	1:F:438:ILE:HG12	2.17	0.45
1:F:456:MET:HE1	1:F:470:PHE:HB2	1.98	0.45
1:A:177:LEU:HA	1:A:177:LEU:HD22	1.63	0.45
1:A:393:LEU:CD1	1:A:466:ILE:HA	2.47	0.45
1:A:455:PRO:HG2	1:A:880:SER:HB2	1.99	0.45
1:B:847:LEU:C	1:B:849:SER:H	2.25	0.45
1:C:404:LEU:HG	1:C:449:LEU:HD13	1.98	0.45
1:C:1030:ARG:HD3	1:C:1030:ARG:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:609:VAL:HG22	1:D:629:VAL:HG13	1.98	0.45
1:D:631:LEU:HD21	1:D:647:ILE:HD12	1.99	0.45
1:D:776:GLU:HB3	1:D:779:TYR:CE1	2.51	0.45
1:E:72:ILE:HG23	1:E:106:GLN:CB	2.46	0.45
1:E:1018:ALA:O	1:E:1022:VAL:HG23	2.16	0.45
1:F:415:ASN:ND2	1:F:948:PHE:HZ	2.14	0.45
1:F:885:PHE:HB2	1:F:902:MET:HE1	1.97	0.45
1:B:10:ILE:HB	1:C:893:GLU:OE1	2.16	0.45
1:B:203:VAL:HG12	1:B:207:ILE:HD11	1.98	0.45
1:C:390:ILE:HG23	1:C:395:MET:SD	2.57	0.45
1:C:655:PHE:HB3	1:C:663:VAL:CG1	2.47	0.45
1:C:738:ALA:O	1:C:740:GLY:N	2.50	0.45
1:D:44:THR:CG2	1:D:91:THR:HG22	2.45	0.45
1:D:462:SER:OG	1:D:674:LEU:HD12	2.17	0.45
1:D:584:GLN:HG2	1:D:622:GLN:CG	2.43	0.45
1:D:685:ILE:HD11	1:D:819:TYR:CD2	2.52	0.45
1:E:20:MET:HE3	1:E:373:PRO:HB2	1.98	0.45
1:E:24:GLY:O	1:E:28:LEU:HD13	2.16	0.45
1:E:344:LEU:HD23	1:E:344:LEU:HA	1.65	0.45
1:E:594:VAL:HG22	1:E:655:PHE:CE2	2.52	0.45
1:E:774:MET:HE3	1:E:780:ARG:HH21	1.80	0.45
1:E:947:GLU:HG3	1:E:948:PHE:N	2.30	0.45
1:F:394:THR:HG22	1:F:469:GLN:O	2.16	0.45
1:F:534:ILE:C	1:F:536:ARG:N	2.74	0.45
1:F:577:GLN:HE22	1:F:721:LEU:HD11	1.80	0.45
1:A:668:LEU:HD23	1:A:668:LEU:H	1.81	0.45
1:B:105:VAL:HG21	1:C:105:VAL:HG13	1.97	0.45
1:B:184:MET:HG2	1:B:246:PHE:CE2	2.52	0.45
1:B:310:LEU:HD12	1:B:310:LEU:HA	1.73	0.45
1:B:646:ALA:O	1:B:649:MET:HB3	2.17	0.45
1:B:836:SER:OG	1:B:839:GLU:HG3	2.17	0.45
1:B:1031:ARG:O	1:B:1032:ARG:HG3	2.16	0.45
1:C:80:SER:HB2	1:C:818:ARG:HB2	1.98	0.45
1:C:177:LEU:HD22	1:C:178:PHE:N	2.32	0.45
1:C:945:ILE:HD13	1:C:968:VAL:HG22	1.97	0.45
1:E:77:TYR:HE2	1:E:864:TYR:CD2	2.35	0.45
1:E:398:MET:HG2	1:E:473:THR:HG21	1.98	0.45
1:E:401:ALA:HB2	1:E:474:ILE:HG23	1.99	0.45
1:E:559:LEU:HA	1:E:560:PRO:HD2	1.66	0.45
1:E:900:SER:HB3	1:E:1026:PHE:HA	1.99	0.45
1:F:312:LYS:O	1:F:315:PRO:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:363:ARG:HB3	1:F:496:MET:CG	2.47	0.45
1:F:428:LYS:HG2	1:F:494:ALA:CB	2.46	0.45
1:F:452:VAL:O	1:F:455:PRO:HD2	2.16	0.45
1:A:167:SER:OG	1:B:70:ASN:HB2	2.16	0.45
1:A:485:ALA:O	1:A:490:PRO:HD3	2.17	0.45
1:A:790:TYR:CE1	1:A:800:PRO:HA	2.52	0.45
1:A:960:LEU:HD23	1:A:1031:ARG:CZ	2.47	0.45
1:A:1036:LYS:HE3	1:A:1040:ILE:CD1	2.46	0.45
1:B:114:ALA:O	1:B:118:LEU:HG	2.16	0.45
1:B:559:LEU:HD12	1:B:913:LEU:HD22	1.98	0.45
1:B:684:LEU:HD12	1:B:684:LEU:HA	1.86	0.45
1:B:690:LEU:HD21	1:B:854:GLY:HA3	1.99	0.45
1:B:781:MET:HE3	1:B:781:MET:HB2	1.86	0.45
1:C:13:TRP:CH2	1:C:370:ILE:HG21	2.47	0.45
1:C:551:GLY:O	1:C:555:LEU:HB2	2.17	0.45
1:D:58:GLN:O	1:D:63:GLN:HG3	2.17	0.45
1:D:347:ALA:HB1	1:D:402:ILE:HG21	1.99	0.45
1:E:448:VAL:HA	1:E:451:ALA:HB3	1.98	0.45
1:F:47:ALA:O	1:F:87:THR:HA	2.17	0.45
1:F:448:VAL:HG23	1:F:884:VAL:HG13	1.98	0.45
1:F:682:PHE:HD2	1:F:844:MET:HE3	1.82	0.45
1:F:721:LEU:HB3	1:F:814:PRO:HG2	1.97	0.45
1:A:401:ALA:O	1:A:402:ILE:C	2.60	0.45
1:B:452:VAL:HG13	1:B:884:VAL:HG21	1.98	0.45
1:B:528:THR:HG23	1:B:965:LEU:HD22	1.98	0.45
1:B:583:THR:HG22	1:B:586:ARG:NE	2.22	0.45
1:B:685:ILE:HD11	1:B:819:TYR:HB3	1.97	0.45
1:B:764:ASP:O	1:B:766:GLY:N	2.50	0.45
1:B:944:LEU:HG	1:B:971:ARG:NH2	2.32	0.45
1:C:213:GLN:HG2	1:C:239:ARG:HG3	1.98	0.45
1:C:351:VAL:HG21	1:C:402:ILE:HG22	1.98	0.45
1:D:79:SER:OG	1:D:91:THR:OG1	2.35	0.45
1:D:508:GLY:HA3	1:D:518:ARG:HD3	1.98	0.45
1:E:680:PHE:CG	1:E:859:TRP:HZ3	2.34	0.45
1:F:363:ARG:HB3	1:F:496:MET:SD	2.57	0.45
1:F:412:VAL:CG2	1:F:435:MET:HE1	2.46	0.45
1:F:462:SER:HB2	1:F:865:GLN:CG	2.47	0.45
1:F:540:ARG:HD3	1:F:541:TYR:CD1	2.51	0.45
1:A:131:LYS:H	1:A:131:LYS:HG2	1.52	0.45
1:A:597:TYR:CD2	1:A:655:PHE:CZ	3.05	0.45
1:B:226:LYS:NZ	1:B:226:LYS:HB3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:LEU:HD12	1:B:488:LEU:HA	1.81	0.45
1:B:1024:VAL:HA	1:B:1027:VAL:CG1	2.47	0.45
1:D:549:VAL:HG22	1:D:906:PRO:HG2	1.99	0.45
1:E:189:ASN:ND2	1:E:190:PRO:HD2	2.32	0.45
1:E:778:LYS:HE3	1:E:779:TYR:OH	2.17	0.45
1:E:792:ARG:HG2	1:E:792:ARG:HH11	1.82	0.45
1:F:58:GLN:O	1:F:58:GLN:HG2	2.16	0.45
1:F:65:ILE:HG13	1:F:111:LEU:HA	1.98	0.45
1:F:83:ASP:HB3	1:F:87:THR:O	2.17	0.45
1:F:157:TYR:HE2	1:F:317:PHE:CE1	2.35	0.45
1:F:228:GLN:NE2	1:F:230:LEU:H	2.15	0.45
1:F:247:GLY:C	1:F:249:ILE:H	2.25	0.45
1:A:151:GLN:HE22	1:A:179:GLY:HA2	1.81	0.44
1:A:488:LEU:HD13	1:A:488:LEU:C	2.42	0.44
1:A:972:LEU:HG	1:A:976:LEU:CD1	2.47	0.44
1:B:193:LEU:HD13	1:B:265:VAL:HG21	1.99	0.44
1:B:718:PRO:HA	1:B:827:ILE:HA	1.99	0.44
1:B:789:TRP:O	1:B:801:PHE:HD2	2.00	0.44
1:B:844:MET:CE	1:B:847:LEU:HD12	2.47	0.44
1:B:1017:LEU:HD13	1:B:1018:ALA:N	2.32	0.44
1:C:563:PHE:CG	1:C:866:GLU:HB2	2.51	0.44
1:C:930:GLY:HA2	1:C:1007:VAL:HG23	1.99	0.44
1:D:149:MET:HE3	1:D:153:ASP:CB	2.47	0.44
1:D:158:VAL:HG11	1:D:177:LEU:HD21	1.99	0.44
1:D:213:GLN:HG2	1:D:239:ARG:HG3	1.98	0.44
1:D:931:LEU:HD12	1:D:932:LEU:N	2.32	0.44
1:E:105:VAL:HG11	1:F:108:GLN:NE2	2.32	0.44
1:E:250:LEU:HD13	1:E:261:LEU:HD23	2.00	0.44
1:E:736:ALA:HB2	1:E:804:PHE:HB3	1.99	0.44
1:E:905:VAL:HG13	1:E:935:ILE:HD11	1.98	0.44
1:E:913:LEU:HD23	1:E:927:PHE:HZ	1.81	0.44
1:F:723:ASP:OD1	1:F:723:ASP:N	2.49	0.44
1:F:733:GLN:OE1	1:F:743:ILE:HG23	2.17	0.44
1:B:392:THR:HG23	1:B:393:LEU:N	2.32	0.44
1:C:483:LEU:O	1:C:487:ILE:HB	2.18	0.44
1:C:541:TYR:OH	2:C:2000:LMT:H2'	2.16	0.44
1:C:564:LEU:HD23	1:C:565:PRO:HD2	1.99	0.44
1:C:706:ALA:HA	1:C:847:LEU:HD21	1.99	0.44
1:C:790:TYR:CE2	1:C:800:PRO:HB3	2.53	0.44
1:E:101:ASP:O	1:E:104:GLN:HB3	2.17	0.44
1:E:482:VAL:O	1:E:485:ALA:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:764:ASP:CG	1:E:765:ARG:HH21	2.21	0.44
1:F:578:LEU:CD2	1:F:579:PRO:HD2	2.47	0.44
1:F:656:SER:HB3	1:F:664:PHE:HE1	1.82	0.44
1:F:751:GLY:C	1:F:753:ALA:N	2.73	0.44
1:F:762:PHE:CD2	1:F:771:VAL:HG22	2.52	0.44
1:B:459:PHE:HD2	1:B:459:PHE:HA	1.69	0.44
1:C:402:ILE:O	1:C:405:LEU:HG	2.17	0.44
1:D:184:MET:HB2	1:D:762:PHE:CE2	2.52	0.44
1:D:466:ILE:HG22	1:D:470:PHE:CE2	2.51	0.44
1:D:549:VAL:HG22	1:D:906:PRO:CG	2.47	0.44
1:D:913:LEU:N	1:D:913:LEU:HD23	2.32	0.44
1:D:945:ILE:CG1	1:D:971:ARG:HH12	2.30	0.44
1:D:1026:PHE:HE2	1:D:1030:ARG:NE	2.16	0.44
1:E:111:LEU:HD21	1:E:127:VAL:HG11	1.99	0.44
1:E:668:LEU:HD23	1:E:668:LEU:H	1.82	0.44
1:F:702:LEU:HD22	1:F:827:ILE:HD12	1.99	0.44
1:A:150:THR:HG23	1:A:152:GLU:HG2	1.99	0.44
1:A:214:VAL:O	1:A:216:ALA:N	2.50	0.44
1:A:600:THR:O	1:A:603:LYS:HB2	2.18	0.44
1:A:915:ALA:HB2	1:A:1009:GLY:HA3	1.99	0.44
1:A:971:ARG:HA	1:A:974:PRO:HD2	1.99	0.44
1:B:362:PHE:CD2	1:B:366:LEU:HD21	2.52	0.44
1:B:873:ALA:N	1:B:874:PRO:HD2	2.32	0.44
1:C:397:GLY:O	1:C:400:LEU:HB3	2.17	0.44
1:C:597:TYR:CD2	1:C:655:PHE:HZ	2.34	0.44
1:C:673:GLU:H	1:C:673:GLU:HG2	1.35	0.44
1:C:1015:THR:OG1	1:C:1016:VAL:N	2.50	0.44
1:D:30:LEU:HD13	1:D:31:PRO:HD2	1.98	0.44
1:D:162:MET:O	1:D:164:ASP:N	2.50	0.44
1:D:362:PHE:O	1:D:365:THR:N	2.47	0.44
1:D:1016:VAL:O	1:D:1016:VAL:HG12	2.18	0.44
1:E:43:VAL:HG13	1:E:130:GLU:O	2.16	0.44
1:E:57:VAL:HG11	1:E:86:GLY:O	2.17	0.44
1:E:189:ASN:O	1:E:193:LEU:HB2	2.18	0.44
1:E:491:ALA:O	1:E:495:THR:OG1	2.28	0.44
1:F:53:ASP:N	1:F:53:ASP:OD1	2.49	0.44
1:F:61:VAL:HA	1:F:118:LEU:CD2	2.47	0.44
1:F:97:GLY:C	1:F:99:ASP:N	2.76	0.44
1:F:154:ILE:HG22	1:F:287:SER:HB2	2.00	0.44
1:F:193:LEU:HD22	1:F:265:VAL:HB	1.99	0.44
1:F:195:LYS:HG3	1:F:196:PHE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:344:LEU:HG	1:F:398:MET:HE1	1.98	0.44
1:F:393:LEU:HG	1:F:466:ILE:HA	1.99	0.44
1:A:84:SER:HB3	1:A:814:PRO:CA	2.46	0.44
1:A:102:ILE:HG21	1:C:101:ASP:OD2	2.17	0.44
1:A:480:LEU:HA	1:A:480:LEU:HD23	1.70	0.44
1:A:538:THR:O	1:A:542:LEU:HD13	2.17	0.44
1:A:1022:VAL:HG22	1:A:1023:PRO:HD3	1.99	0.44
1:C:647:ILE:HA	1:C:650:ARG:HG2	1.99	0.44
1:C:659:LYS:HD3	1:C:659:LYS:HA	1.85	0.44
1:C:667:ASN:ND2	1:C:668:LEU:O	2.51	0.44
1:D:742:SER:O	1:D:746:ILE:HG13	2.18	0.44
1:E:201:VAL:HG21	1:E:745:ASP:OD2	2.16	0.44
1:E:278:ILE:HG13	1:E:613:ASN:HB3	1.99	0.44
1:E:414:GLU:HG2	1:E:973:ARG:NH2	2.32	0.44
1:E:527:TYR:CD1	1:E:1020:PHE:HE2	2.35	0.44
1:E:563:PHE:O	1:E:564:LEU:HG	2.18	0.44
1:E:597:TYR:CD1	1:E:655:PHE:CZ	3.05	0.44
1:E:703:LEU:HG	1:E:716:VAL:CG1	2.45	0.44
1:E:921:LEU:HA	1:E:921:LEU:HD13	1.68	0.44
1:F:952:LEU:HB2	1:F:963:ALA:HB1	1.99	0.44
1:A:190:PRO:HB3	1:A:789:TRP:CH2	2.53	0.44
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.18	0.44
1:A:1018:ALA:C	1:A:1020:PHE:N	2.76	0.44
1:B:26:ALA:HB1	1:B:384:ALA:CB	2.48	0.44
1:B:408:ASP:O	1:B:411:VAL:HG12	2.18	0.44
1:B:1007:VAL:HG12	1:B:1008:MET:N	2.32	0.44
1:C:11:PHE:C	1:C:11:PHE:CD2	2.96	0.44
1:C:363:ARG:HB2	1:C:496:MET:SD	2.58	0.44
1:C:415:ASN:CG	1:C:438:ILE:HG21	2.43	0.44
1:E:68:ASN:HB2	1:E:114:ALA:HB2	1.99	0.44
1:E:184:MET:HB3	1:E:771:VAL:HG22	1.99	0.44
1:E:187:TRP:HE1	1:E:269:GLU:HG2	1.81	0.44
1:F:27:ILE:HG22	1:F:380:PHE:HB3	2.00	0.44
1:F:273:GLU:OE1	1:F:770:LYS:NZ	2.30	0.44
1:F:352:PHE:HD1	1:F:369:THR:HG21	1.83	0.44
1:F:573:MET:HG3	1:F:666:PHE:CE1	2.52	0.44
1:F:846:GLN:C	1:F:849:SER:HG	2.26	0.44
1:F:971:ARG:HB3	1:F:971:ARG:CZ	2.48	0.44
1:B:43:VAL:HG13	1:B:130:GLU:O	2.18	0.44
1:B:68:ASN:HD22	1:B:68:ASN:HA	1.67	0.44
1:B:347:ALA:O	1:B:351:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:ARG:HE	1:B:828:LEU:CB	2.27	0.44
1:C:990:VAL:HG12	1:C:1004:GLY:C	2.43	0.44
1:D:184:MET:HE2	1:D:268:ILE:HG23	1.99	0.44
1:D:224:PRO:CB	1:E:781:MET:HE1	2.48	0.44
1:D:398:MET:HE3	1:D:473:THR:HB	2.00	0.44
1:D:645:GLU:HA	1:D:645:GLU:OE2	2.18	0.44
1:D:898:PRO:O	1:D:901:VAL:HG12	2.18	0.44
1:D:987:MET:HB2	1:D:1008:MET:HE1	1.98	0.44
1:D:1008:MET:O	1:D:1009:GLY:C	2.60	0.44
1:E:104:GLN:NE2	1:F:109:ASN:HD22	2.16	0.44
1:E:139:VAL:H	1:E:327:TYR:HB3	1.82	0.44
1:E:367:ILE:HB	1:E:368:PRO:HD3	2.00	0.44
1:A:197:GLN:HA	1:A:798:MET:CE	2.47	0.44
1:A:391:ASN:O	1:A:395:MET:HG2	2.17	0.44
1:A:559:LEU:HD22	1:A:923:ASN:H	1.82	0.44
1:B:244:GLU:HG3	1:B:248:LYS:HD3	2.00	0.44
1:C:6:ILE:HD12	1:C:487:ILE:HG12	2.00	0.44
1:C:151:GLN:HE21	1:C:279:ALA:C	2.21	0.44
1:C:843:LEU:HD13	1:C:847:LEU:HD22	2.00	0.44
1:C:847:LEU:HD12	1:C:847:LEU:HA	1.69	0.44
1:D:198:LEU:N	1:D:798:MET:HE1	2.32	0.44
1:D:960:LEU:HD23	1:D:961:ILE:N	2.33	0.44
1:E:531:VAL:O	1:E:534:ILE:HG12	2.18	0.44
1:E:682:PHE:CE1	1:E:857:TYR:HB2	2.53	0.44
1:F:572:PHE:CE2	1:F:629:VAL:HB	2.53	0.44
2:F:2000:LMT:H121	2:F:2000:LMT:H91	1.86	0.44
1:A:267:LYS:HD2	1:A:268:ILE:H	1.83	0.44
1:A:666:PHE:CD1	1:A:666:PHE:C	2.96	0.44
1:A:683:GLU:HG2	1:A:819:TYR:CB	2.48	0.44
1:A:932:LEU:O	1:A:935:ILE:HG22	2.18	0.44
1:B:124:GLN:NE2	1:B:758:TYR:HD2	2.16	0.44
1:B:341:VAL:O	1:B:342:LYS:C	2.61	0.44
1:B:944:LEU:HB3	1:B:971:ARG:HH12	1.82	0.44
1:C:62:THR:HG21	1:C:818:ARG:HD3	2.00	0.44
1:C:247:GLY:C	1:C:249:ILE:H	2.26	0.44
1:C:350:LEU:HB3	1:C:984:LEU:HB3	2.00	0.44
1:C:447:MET:HB2	1:C:447:MET:HE3	1.60	0.44
1:C:504:ASP:O	1:C:506:GLY:N	2.51	0.44
1:D:294:ALA:HB3	1:D:297:ALA:CB	2.48	0.44
1:D:957:GLY:HA2	1:D:1040:ILE:HD11	1.99	0.44
1:E:3:ASN:HA	1:E:6:ILE:CD1	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:TYR:CE1	1:F:57:VAL:HG12	2.52	0.44
1:F:82:SER:HB2	1:F:816:LEU:HB2	1.99	0.44
1:F:143:ILE:HG22	1:F:286:ALA:HB2	2.00	0.44
1:F:594:VAL:HG22	1:F:655:PHE:CZ	2.52	0.44
1:A:240:LEU:HD12	1:A:246:PHE:CZ	2.53	0.43
1:A:435:MET:HB3	1:A:435:MET:HE3	1.65	0.43
1:A:567:GLU:OE1	1:A:996:GLY:HA2	2.18	0.43
1:A:728:LYS:C	1:A:729:ILE:HD12	2.42	0.43
1:A:978:THR:HG23	1:A:979:SER:N	2.33	0.43
1:B:136:PHE:CE1	1:B:292:LYS:HE2	2.53	0.43
1:B:250:LEU:HD12	1:B:251:LEU:N	2.33	0.43
1:B:750:LEU:O	1:B:753:ALA:HB3	2.18	0.43
1:B:982:PHE:O	1:B:983:ILE:C	2.61	0.43
1:C:566:ASP:CG	1:C:678:THR:HG23	2.43	0.43
1:D:250:LEU:HD12	1:D:251:LEU:H	1.83	0.43
1:E:484:VAL:O	1:E:488:LEU:HB3	2.17	0.43
1:E:703:LEU:O	1:E:703:LEU:HD23	2.18	0.43
1:F:159:ALA:HB2	1:F:177:LEU:CD1	2.46	0.43
1:F:413:VAL:HG22	1:F:489:THR:OG1	2.17	0.43
1:F:452:VAL:HG23	1:F:453:PHE:HD1	1.81	0.43
1:F:1022:VAL:N	1:F:1023:PRO:HD2	2.33	0.43
1:A:237:GLN:OE1	1:B:747:ASN:ND2	2.44	0.43
1:B:4:PHE:HE2	1:B:8:ARG:HD3	1.83	0.43
1:B:40:PRO:HA	1:B:41:PRO:HD3	1.74	0.43
1:B:219:LEU:HD23	1:C:754:TRP:CZ3	2.53	0.43
1:B:560:PRO:O	1:B:922:THR:OG1	2.34	0.43
1:C:34:GLN:HG2	1:C:35:TYR:CD1	2.53	0.43
1:C:77:TYR:CE1	1:C:93:THR:HG21	2.53	0.43
1:C:246:PHE:O	1:C:262:LEU:HD23	2.17	0.43
1:C:559:LEU:HA	1:C:560:PRO:HD2	1.84	0.43
1:C:740:GLY:C	1:C:793:ALA:HB1	2.43	0.43
1:C:776:GLU:HB2	1:C:779:TYR:HD1	1.83	0.43
1:D:891:LEU:HA	1:D:891:LEU:HD12	1.66	0.43
1:E:58:GLN:OE1	1:E:818:ARG:NH1	2.52	0.43
1:E:143:ILE:HG22	1:E:286:ALA:HB2	1.98	0.43
1:E:696:THR:HG23	1:E:699:ARG:NH1	2.32	0.43
1:F:119:PRO:O	1:F:123:GLN:HG3	2.18	0.43
1:F:572:PHE:CD2	1:F:631:LEU:HD11	2.51	0.43
1:F:574:THR:CG2	1:F:627:ALA:HB3	2.48	0.43
1:F:599:LEU:C	1:F:603:LYS:HG2	2.43	0.43
1:F:951:ASP:O	1:F:955:LYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ALA:HB1	1:B:725:PRO:O	2.18	0.43
1:A:435:MET:O	1:A:439:GLN:HB2	2.19	0.43
1:A:448:VAL:HG13	1:A:884:VAL:HG22	2.00	0.43
1:A:448:VAL:HG22	1:A:887:CYS:HB3	2.00	0.43
1:A:957:GLY:CA	1:A:1041:GLU:HA	2.48	0.43
1:B:545:TYR:HB2	1:B:1021:PHE:HE2	1.82	0.43
1:B:586:ARG:O	1:B:589:LYS:HB3	2.17	0.43
1:B:709:HIS:ND1	1:B:847:LEU:HD11	2.32	0.43
1:B:727:PHE:CB	1:B:809:TRP:HE1	2.31	0.43
1:C:46:SER:OG	1:C:89:GLN:HG2	2.18	0.43
1:C:188:MET:HA	1:C:266:ALA:HB2	2.01	0.43
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.19	0.43
1:D:331:PRO:O	1:D:334:LYS:HB2	2.18	0.43
1:D:347:ALA:HB3	1:D:402:ILE:HD12	2.00	0.43
1:D:352:PHE:CD2	1:D:352:PHE:C	2.95	0.43
1:D:987:MET:O	1:D:990:VAL:HG23	2.18	0.43
1:E:69:MET:CG	1:E:110:LYS:HB3	2.48	0.43
1:E:452:VAL:HG23	1:E:453:PHE:CD2	2.54	0.43
1:E:472:ILE:O	1:E:473:THR:C	2.61	0.43
1:E:602:GLU:OE2	1:E:650:ARG:NH1	2.42	0.43
1:E:641:GLU:HA	1:E:646:ALA:CB	2.48	0.43
1:E:900:SER:OG	1:E:1029:VAL:HG11	2.18	0.43
1:E:926:TYR:HE1	1:E:999:ALA:CB	2.31	0.43
1:E:987:MET:HB2	1:E:1008:MET:HE1	2.00	0.43
1:F:467:TYR:CE1	1:F:925:VAL:HG22	2.53	0.43
1:F:804:PHE:CD2	1:F:804:PHE:N	2.87	0.43
1:A:136:PHE:HE2	1:A:290:GLY:HA3	1.83	0.43
1:A:178:PHE:HB2	1:A:288:GLY:H	1.83	0.43
1:A:281:PHE:CE1	1:A:608:SER:HB2	2.54	0.43
1:A:712:MET:HE3	1:A:712:MET:O	2.18	0.43
1:B:356:TYR:C	1:B:358:PHE:N	2.76	0.43
1:B:909:VAL:O	1:B:911:GLY:N	2.51	0.43
1:C:16:ALA:O	1:C:19:ILE:N	2.51	0.43
1:C:31:PRO:HB2	1:C:389:SER:OG	2.18	0.43
1:C:293:LEU:HD13	1:C:294:ALA:N	2.33	0.43
1:C:723:ASP:HA	1:C:813:SER:HA	2.00	0.43
1:C:983:ILE:HD13	1:C:983:ILE:HA	1.77	0.43
1:D:32:VAL:HG22	1:D:390:ILE:HB	1.99	0.43
1:D:210:GLN:OE1	1:D:249:ILE:HG23	2.18	0.43
1:D:568:ASP:O	1:D:634:TRP:HZ3	2.01	0.43
1:D:680:PHE:HE1	1:D:844:MET:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:690:LEU:HG	1:D:694:LYS:HG2	2.00	0.43
1:D:919:ARG:NH1	1:D:990:VAL:HG12	2.32	0.43
1:E:191:ASN:O	1:E:194:ASN:HB3	2.18	0.43
1:E:609:VAL:HG13	1:E:629:VAL:CG2	2.44	0.43
1:F:147:GLY:O	1:F:149:MET:N	2.51	0.43
1:F:184:MET:HE2	1:F:268:ILE:HG23	2.01	0.43
1:F:242:SER:OG	1:F:243:THR:N	2.50	0.43
1:F:243:THR:O	1:F:246:PHE:HB2	2.19	0.43
1:F:694:LYS:CD	1:F:694:LYS:H	2.31	0.43
1:F:736:ALA:HB1	1:F:741:VAL:CG2	2.48	0.43
1:F:819:TYR:C	1:F:821:GLY:N	2.73	0.43
1:F:909:VAL:HG22	1:F:931:LEU:HD21	1.99	0.43
1:A:15:ILE:HD13	1:A:487:ILE:HD13	2.00	0.43
1:A:39:ALA:HA	1:A:40:PRO:HD2	1.68	0.43
1:A:46:SER:HB2	1:A:128:SER:HG	1.83	0.43
1:A:776:GLU:HB3	1:A:779:TYR:HE1	1.83	0.43
1:B:76:MET:HG2	1:B:864:TYR:CE2	2.51	0.43
1:C:69:MET:HE1	1:C:107:VAL:HG13	2.01	0.43
1:C:247:GLY:CA	1:C:263:ARG:HB2	2.48	0.43
1:C:873:ALA:N	1:C:874:PRO:HD2	2.33	0.43
1:D:184:MET:HG2	1:D:246:PHE:CE2	2.54	0.43
1:D:219:LEU:HA	1:E:754:TRP:HZ3	1.83	0.43
1:D:680:PHE:HB2	1:D:863:SER:OG	2.18	0.43
1:E:137:LEU:HD12	1:E:329:THR:HB	2.00	0.43
1:E:425:LEU:HD13	1:E:429:GLU:CG	2.47	0.43
1:E:682:PHE:HD2	1:E:827:ILE:HD12	1.84	0.43
1:E:931:LEU:HD23	1:E:931:LEU:HA	1.70	0.43
1:E:974:PRO:O	1:E:975:ILE:C	2.61	0.43
1:F:138:MET:HB2	1:F:138:MET:HE3	1.69	0.43
1:F:412:VAL:HG12	1:F:413:VAL:N	2.34	0.43
1:F:455:PRO:HG2	1:F:880:SER:CB	2.43	0.43
1:A:242:SER:O	1:A:246:PHE:CD1	2.71	0.43
1:A:554:TYR:CE1	1:A:558:ARG:HG3	2.53	0.43
1:A:674:LEU:HD13	1:A:675:GLY:O	2.19	0.43
1:A:692:HIS:HE2	1:A:813:SER:CB	2.31	0.43
1:A:941:ASN:OD1	1:A:941:ASN:N	2.50	0.43
1:B:291:ILE:HD13	1:B:306:ILE:HD13	2.01	0.43
1:B:576:VAL:HG13	1:B:663:VAL:HG22	2.00	0.43
1:B:688:ALA:HB3	1:B:690:LEU:CD2	2.48	0.43
1:B:903:LEU:HD23	1:B:903:LEU:HA	1.49	0.43
1:C:13:TRP:CE3	1:C:13:TRP:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:VAL:O	1:C:216:ALA:N	2.51	0.43
1:C:343:THR:HG21	1:C:989:LEU:CD2	2.42	0.43
1:D:53:ASP:OD1	1:D:56:THR:OG1	2.13	0.43
1:D:940:LYS:O	1:D:941:ASN:C	2.60	0.43
1:E:356:TYR:C	1:E:358:PHE:N	2.77	0.43
1:F:25:LEU:HD12	1:F:28:LEU:HD12	1.99	0.43
1:F:144:ASN:ND2	1:F:320:GLY:HA3	2.33	0.43
1:F:182:TYR:HD1	1:F:182:TYR:HA	1.69	0.43
1:F:184:MET:HB2	1:F:762:PHE:CD2	2.53	0.43
1:F:289:LEU:HD23	1:F:289:LEU:HA	1.82	0.43
1:F:344:LEU:C	1:F:344:LEU:HD13	2.44	0.43
1:F:375:VAL:HG11	1:F:405:LEU:HD22	2.00	0.43
1:F:507:GLU:HA	1:F:518:ARG:HG3	2.01	0.43
1:F:682:PHE:HA	1:F:859:TRP:CZ3	2.54	0.43
1:A:98:THR:O	1:A:99:ASP:C	2.61	0.43
1:A:394:THR:O	1:A:398:MET:HG2	2.18	0.43
1:A:474:ILE:O	1:A:478:MET:HB3	2.19	0.43
1:B:193:LEU:HD21	1:B:265:VAL:HG13	2.01	0.43
1:B:831:ALA:HB2	1:B:840:ALA:HB2	2.01	0.43
1:C:185:ARG:HA	1:C:185:ARG:HD3	1.78	0.43
1:C:418:ARG:O	1:C:422:GLU:HB2	2.19	0.43
1:C:550:VAL:O	1:C:553:ALA:HB3	2.19	0.43
1:C:682:PHE:CD1	1:C:682:PHE:C	2.97	0.43
1:C:934:THR:O	1:C:935:ILE:C	2.61	0.43
1:D:33:ALA:O	1:D:391:ASN:HB2	2.19	0.43
1:D:207:ILE:HG23	1:D:249:ILE:HD13	2.00	0.43
1:D:557:VAL:C	1:D:559:LEU:H	2.27	0.43
1:D:563:PHE:CE2	1:D:674:LEU:HD11	2.54	0.43
1:D:684:LEU:C	1:D:824:SER:HG	2.18	0.43
1:D:879:ILE:O	1:D:883:VAL:HG22	2.19	0.43
1:E:235:ILE:HD11	1:F:726:GLN:CD	2.44	0.43
1:E:250:LEU:HD12	1:E:251:LEU:N	2.33	0.43
1:E:713:LEU:HD21	1:E:843:LEU:HD12	2.01	0.43
1:F:135:SER:HB3	1:F:673:GLU:HA	2.01	0.43
1:F:401:ALA:O	1:F:402:ILE:C	2.60	0.43
1:F:425:LEU:HB3	1:F:429:GLU:OE1	2.19	0.43
1:F:446:ALA:CB	1:F:478:MET:HE2	2.49	0.43
1:F:478:MET:HE3	1:F:478:MET:C	2.44	0.43
1:A:527:TYR:CZ	1:A:531:VAL:HG21	2.53	0.43
1:A:570:GLY:O	1:A:631:LEU:HD23	2.19	0.43
1:A:693:GLU:CD	1:A:693:GLU:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:996:GLY:O	1:A:998:GLY:N	2.52	0.43
1:C:34:GLN:CG	1:C:333:VAL:HG22	2.48	0.43
1:C:751:GLY:O	1:C:753:ALA:N	2.52	0.43
1:C:931:LEU:HD23	1:C:931:LEU:HA	1.63	0.43
1:C:987:MET:HB3	1:C:987:MET:HE2	1.57	0.43
1:D:197:GLN:HA	1:D:798:MET:CE	2.49	0.43
1:D:886:LEU:HD23	1:F:18:ILE:CG1	2.49	0.43
1:E:195:LYS:HD2	1:E:196:PHE:CZ	2.53	0.43
1:E:270:LEU:HD13	1:E:270:LEU:HA	1.60	0.43
1:F:222:THR:HA	1:F:224:PRO:HD3	2.00	0.43
1:F:438:ILE:HG21	1:F:438:ILE:HD13	1.78	0.43
1:F:905:VAL:HB	1:F:906:PRO:HD3	2.01	0.43
1:A:4:PHE:HB3	1:A:8:ARG:NH1	2.33	0.43
1:A:350:LEU:HA	1:A:350:LEU:HD23	1.66	0.43
1:A:801:PHE:C	1:A:803:ALA:H	2.27	0.43
1:B:442:LEU:O	1:B:445:ILE:HG13	2.19	0.43
1:B:867:ARG:HH21	1:B:868:LEU:HA	1.84	0.43
1:B:971:ARG:HD2	1:B:974:PRO:HG3	2.01	0.43
1:C:137:LEU:HD12	1:C:329:THR:OG1	2.19	0.43
1:C:248:LYS:HD3	1:C:263:ARG:NH2	2.34	0.43
1:C:412:VAL:HG11	1:C:489:THR:HG21	2.00	0.43
1:C:870:GLY:C	1:C:872:GLN:N	2.76	0.43
1:C:906:PRO:O	1:C:910:ILE:HG22	2.19	0.43
1:D:2:PRO:O	1:D:5:PHE:HD1	2.02	0.43
1:D:193:LEU:HD22	1:D:265:VAL:HB	2.01	0.43
1:D:212:ALA:C	1:D:239:ARG:HG2	2.44	0.43
1:D:1015:THR:O	1:D:1017:LEU:N	2.52	0.43
1:E:214:VAL:CG2	1:E:236:ALA:HB3	2.47	0.43
1:E:390:ILE:O	1:E:390:ILE:HG13	2.18	0.43
1:E:652:THR:CG2	1:E:665:ALA:H	2.32	0.43
1:E:659:LYS:HE2	1:E:659:LYS:HA	2.01	0.43
1:E:682:PHE:CD2	1:E:827:ILE:HD12	2.53	0.43
1:E:1015:THR:O	1:E:1018:ALA:N	2.52	0.43
1:F:23:GLY:O	1:F:26:ALA:N	2.51	0.43
1:F:199:THR:CG2	1:F:792:ARG:H	2.32	0.43
1:F:457:ALA:CB	1:F:468:ARG:HA	2.48	0.43
1:F:575:MET:HB2	1:F:626:ILE:HD11	2.01	0.43
1:F:693:GLU:H	1:F:694:LYS:HZ3	1.66	0.43
1:A:101:ASP:OD1	1:A:101:ASP:N	2.51	0.43
1:A:376:LEU:O	1:A:379:THR:N	2.51	0.43
1:A:777:ALA:HB1	1:C:225:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:944:LEU:HA	1:A:944:LEU:HD23	1.66	0.43
1:A:971:ARG:CA	1:A:974:PRO:HD2	2.48	0.43
1:B:415:ASN:CG	1:B:418:ARG:HH22	2.26	0.43
1:C:11:PHE:O	1:C:15:ILE:HG13	2.18	0.43
1:C:11:PHE:HD2	1:C:11:PHE:C	2.27	0.43
1:C:189:ASN:HB3	1:C:192:GLU:HB2	2.01	0.43
1:C:450:SER:HB2	1:C:475:VAL:HG13	1.99	0.43
1:D:57:VAL:O	1:D:61:VAL:HG23	2.19	0.43
1:D:109:ASN:HD22	1:E:109:ASN:ND2	2.16	0.43
1:D:289:LEU:HD13	1:D:289:LEU:HA	1.73	0.43
1:D:602:GLU:CD	1:D:650:ARG:HD2	2.44	0.43
1:D:602:GLU:HB3	1:D:606:VAL:CG2	2.48	0.43
1:D:795:ASP:OD2	1:D:797:GLN:N	2.40	0.43
1:E:69:MET:HG2	1:E:110:LYS:CB	2.49	0.43
1:E:456:MET:SD	1:E:471:SER:OG	2.77	0.43
1:E:496:MET:HG2	1:E:496:MET:H	1.54	0.43
1:E:712:MET:HB3	1:E:713:LEU:HD22	2.00	0.43
1:E:922:THR:O	1:E:924:ASP:N	2.44	0.43
1:F:382:VAL:HG21	1:F:476:SER:HB2	2.00	0.43
1:F:412:VAL:HG22	1:F:435:MET:HE1	2.01	0.43
1:A:48:SER:O	1:A:122:VAL:HA	2.19	0.42
1:A:195:LYS:HG2	1:A:196:PHE:CE2	2.54	0.42
1:A:734:GLU:C	1:A:736:ALA:H	2.26	0.42
1:A:888:LEU:CD1	1:A:901:VAL:HB	2.49	0.42
1:A:893:GLU:CD	1:C:10:ILE:HB	2.43	0.42
1:B:56:THR:O	1:B:60:THR:OG1	2.34	0.42
1:B:901:VAL:O	1:B:904:VAL:HG23	2.19	0.42
1:C:435:MET:HE1	1:C:438:ILE:HD11	2.01	0.42
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.54	0.42
1:C:894:SER:O	1:C:895:TRP:HE3	2.02	0.42
1:C:944:LEU:HD12	1:C:975:ILE:HD13	2.01	0.42
1:D:250:LEU:HD13	1:D:261:LEU:HD23	2.00	0.42
1:D:376:LEU:O	1:D:378:GLY:N	2.51	0.42
1:D:593:GLU:OE1	1:D:659:LYS:HE3	2.19	0.42
1:D:753:ALA:C	1:D:754:TRP:HD1	2.27	0.42
1:E:371:ALA:O	1:E:375:VAL:HG23	2.19	0.42
1:E:555:LEU:CD1	1:E:914:LEU:HD12	2.49	0.42
1:E:705:GLU:OE2	1:E:847:LEU:HB3	2.19	0.42
1:F:177:LEU:HD23	1:F:178:PHE:N	2.34	0.42
1:F:588:GLN:N	1:F:613:ASN:ND2	2.67	0.42
1:F:591:LEU:HD13	1:F:611:ALA:HB1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1032:ARG:C	1:F:1032:ARG:HD2	2.42	0.42
1:A:423:GLU:O	1:A:502:LYS:HB3	2.19	0.42
1:A:764:ASP:C	1:A:766:GLY:N	2.77	0.42
1:B:851:LEU:HA	1:B:852:PRO:HD3	1.87	0.42
1:D:113:LEU:HG	1:F:127:VAL:O	2.19	0.42
1:D:413:VAL:O	1:D:416:VAL:HG13	2.20	0.42
1:D:451:ALA:HB3	1:D:884:VAL:HG22	2.01	0.42
1:D:602:GLU:HB3	1:D:606:VAL:HG23	2.01	0.42
1:D:885:PHE:CE1	1:D:899:PHE:HE2	2.37	0.42
1:D:960:LEU:O	1:D:963:ALA:N	2.52	0.42
1:E:303:ALA:O	1:E:307:ARG:HB2	2.19	0.42
1:E:355:MET:SD	1:E:368:PRO:HG2	2.59	0.42
1:E:764:ASP:O	1:E:766:GLY:N	2.51	0.42
1:E:905:VAL:HG13	1:E:935:ILE:CD1	2.49	0.42
1:F:634:TRP:CD1	1:F:634:TRP:N	2.86	0.42
1:F:717:ARG:HA	1:F:718:PRO:HD3	1.89	0.42
1:F:790:TYR:HE1	1:F:800:PRO:HA	1.82	0.42
1:A:149:MET:HE3	1:A:153:ASP:HB2	2.00	0.42
1:A:508:GLY:HA2	1:A:514:GLY:C	2.43	0.42
1:B:188:MET:HE1	1:B:200:PRO:HG3	2.00	0.42
1:B:731:ILE:HA	1:B:805:SER:HA	2.01	0.42
1:B:900:SER:HB2	1:B:1029:VAL:HG21	2.01	0.42
1:C:376:LEU:O	1:C:377:LEU:C	2.62	0.42
1:C:637:ARG:NH1	1:C:642:ASN:O	2.51	0.42
1:C:1018:ALA:C	1:C:1020:PHE:N	2.77	0.42
1:C:1027:VAL:O	1:C:1031:ARG:HG3	2.20	0.42
1:D:185:ARG:HD3	1:D:185:ARG:HA	1.91	0.42
1:D:404:LEU:HD11	1:D:449:LEU:CD2	2.49	0.42
1:D:699:ARG:NH2	1:D:722:GLU:OE2	2.51	0.42
1:E:440:GLY:O	1:E:891:LEU:HD11	2.19	0.42
1:E:531:VAL:HG21	1:E:968:VAL:HG11	2.01	0.42
1:E:926:TYR:HD1	1:E:1002:ALA:HB3	1.83	0.42
1:F:5:PHE:HE2	1:F:8:ARG:HH11	1.68	0.42
1:F:24:GLY:CA	1:F:377:LEU:HD22	2.49	0.42
1:F:31:PRO:HB2	1:F:389:SER:OG	2.18	0.42
1:F:55:LYS:HA	1:F:816:LEU:HD12	2.00	0.42
1:F:469:GLN:O	1:F:472:ILE:HG23	2.19	0.42
1:F:1035:ARG:C	1:F:1037:ASN:H	2.24	0.42
1:A:53:ASP:O	1:A:56:THR:HB	2.20	0.42
1:A:61:VAL:HG12	1:A:118:LEU:HD22	1.99	0.42
1:A:428:LYS:CD	1:A:428:LYS:N	2.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:CYS:O	1:A:497:LEU:HB3	2.19	0.42
1:C:153:ASP:O	1:C:156:ASP:HB3	2.19	0.42
1:C:396:PHE:O	1:C:400:LEU:HB2	2.19	0.42
1:D:294:ALA:HB3	1:D:297:ALA:HB2	2.01	0.42
1:D:527:TYR:HE1	1:D:972:LEU:HB2	1.84	0.42
1:D:552:MET:HG3	1:D:909:VAL:HG12	2.01	0.42
1:D:911:GLY:HA3	1:D:1013:THR:OG1	2.19	0.42
1:E:166:ILE:HG13	1:E:306:ILE:HG23	2.00	0.42
1:E:228:GLN:NE2	1:E:230:LEU:H	2.18	0.42
1:E:525:HIS:O	1:E:526:HIS:C	2.62	0.42
1:E:682:PHE:CE2	1:E:684:LEU:HB2	2.53	0.42
1:E:781:MET:HB2	1:E:782:LEU:HD22	2.00	0.42
1:E:953:MET:HE3	1:E:953:MET:HB2	1.70	0.42
1:E:994:GLY:O	1:E:997:SER:HB2	2.20	0.42
1:F:656:SER:HB3	1:F:664:PHE:CE1	2.54	0.42
1:F:733:GLN:HE22	1:F:743:ILE:CG2	2.32	0.42
1:F:888:LEU:HD23	1:F:888:LEU:HA	1.68	0.42
1:F:1015:THR:OG1	1:F:1016:VAL:N	2.50	0.42
1:A:262:LEU:O	1:A:265:VAL:HG22	2.19	0.42
1:A:508:GLY:HA2	1:A:514:GLY:CA	2.49	0.42
1:B:15:ILE:O	1:B:19:ILE:HG13	2.19	0.42
1:B:214:VAL:HG23	1:B:237:GLN:HB3	2.00	0.42
1:B:420:MET:HG2	1:B:430:ALA:CB	2.49	0.42
1:B:531:VAL:O	1:B:534:ILE:HG12	2.19	0.42
1:B:533:GLY:HA2	1:B:536:ARG:CZ	2.50	0.42
1:B:563:PHE:O	1:B:564:LEU:HD12	2.19	0.42
1:B:710:PRO:C	1:B:712:MET:N	2.77	0.42
1:C:291:ILE:HD13	1:C:306:ILE:HD13	2.02	0.42
1:C:390:ILE:O	1:C:390:ILE:HG22	2.19	0.42
1:C:544:LEU:O	1:C:548:ILE:HG13	2.19	0.42
1:C:577:GLN:HE22	1:C:721:LEU:HD11	1.85	0.42
1:C:733:GLN:OE1	1:C:743:ILE:HG23	2.20	0.42
1:D:68:ASN:HD22	1:D:68:ASN:HA	1.58	0.42
1:D:80:SER:HB2	1:D:818:ARG:HB2	2.01	0.42
1:D:224:PRO:HB3	1:E:781:MET:HE1	2.01	0.42
1:D:538:THR:O	1:D:541:TYR:N	2.44	0.42
1:D:549:VAL:O	1:D:552:MET:HB3	2.19	0.42
1:E:201:VAL:O	1:E:204:ILE:HB	2.19	0.42
1:E:727:PHE:HD1	1:E:809:TRP:NE1	2.18	0.42
1:E:904:VAL:HG13	1:E:938:SER:HB2	2.01	0.42
1:A:27:ILE:HD11	1:A:380:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LYS:HG3	1:A:759:VAL:HG13	2.01	0.42
1:A:220:GLY:HA2	1:B:781:MET:HG2	2.02	0.42
1:A:463:THR:HA	1:A:466:ILE:HG12	2.02	0.42
1:A:563:PHE:HB2	1:A:677:ALA:HB2	2.01	0.42
1:A:833:PRO:C	1:A:835:LYS:H	2.27	0.42
1:A:859:TRP:HB3	1:A:863:SER:HB3	2.02	0.42
1:B:562:SER:OG	1:B:563:PHE:N	2.51	0.42
1:B:907:LEU:HB3	1:B:1017:LEU:CD1	2.44	0.42
1:C:201:VAL:O	1:C:204:ILE:HB	2.20	0.42
1:C:602:GLU:OE2	1:C:650:ARG:NH1	2.53	0.42
1:C:1033:PHE:C	1:C:1035:ARG:N	2.77	0.42
1:D:541:TYR:N	1:D:541:TYR:CD2	2.88	0.42
1:D:552:MET:HB3	1:D:552:MET:HE2	1.91	0.42
1:D:658:ILE:O	1:D:659:LYS:NZ	2.47	0.42
1:D:781:MET:CE	1:F:225:VAL:HG22	2.41	0.42
1:E:239:ARG:HH12	1:E:761:ASP:C	2.22	0.42
1:E:843:LEU:HD13	1:E:847:LEU:HG	2.01	0.42
1:E:903:LEU:HD23	1:E:903:LEU:HA	1.85	0.42
1:F:368:PRO:O	1:F:371:ALA:HB3	2.19	0.42
1:F:457:ALA:HB2	1:F:471:SER:CB	2.50	0.42
1:F:556:PHE:HE1	1:F:923:ASN:ND2	2.17	0.42
1:F:1040:ILE:HG22	1:F:1041:GLU:HG3	2.00	0.42
1:A:130:GLU:CD	1:A:174:ASP:HB2	2.45	0.42
1:A:140:VAL:HG11	1:A:310:LEU:HD21	2.01	0.42
1:B:8:ARG:HB3	1:C:893:GLU:OE2	2.20	0.42
1:B:111:LEU:O	1:B:111:LEU:HD22	2.20	0.42
1:B:552:MET:HE2	1:B:552:MET:HB3	1.82	0.42
1:B:795:ASP:OD2	1:B:797:GLN:HG2	2.19	0.42
1:C:34:GLN:HE21	1:C:332:PHE:HD2	1.67	0.42
1:C:143:ILE:HG22	1:C:286:ALA:CB	2.47	0.42
1:C:185:ARG:NH2	1:C:772:TYR:HD1	2.18	0.42
1:C:535:LEU:HD22	1:C:1027:VAL:HG21	2.00	0.42
1:D:132:SER:OG	1:D:173:GLY:HA3	2.20	0.42
1:D:344:LEU:CD2	1:D:399:VAL:HA	2.46	0.42
1:D:544:LEU:O	1:D:548:ILE:HG13	2.20	0.42
1:D:638:PRO:HB2	1:D:639:GLY:H	1.61	0.42
1:D:764:ASP:C	1:D:766:GLY:N	2.77	0.42
1:E:43:VAL:HG22	1:E:131:LYS:HA	2.01	0.42
1:E:709:HIS:HB2	1:E:713:LEU:CD2	2.50	0.42
1:F:26:ALA:O	1:F:30:LEU:HB2	2.20	0.42
1:F:422:GLU:OE1	1:F:423:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:453:PHE:CE2	1:F:474:ILE:HD13	2.55	0.42
1:F:536:ARG:HD2	2:F:2000:LMT:H5B	2.01	0.42
1:F:619:GLY:HA2	1:F:815:ARG:HH12	1.85	0.42
1:F:674:LEU:HD23	1:F:674:LEU:HA	1.84	0.42
1:F:680:PHE:CD2	1:F:859:TRP:CZ3	3.07	0.42
1:F:762:PHE:HD2	1:F:771:VAL:HG22	1.85	0.42
1:F:885:PHE:CD2	1:F:885:PHE:C	2.97	0.42
1:A:330:THR:HB	1:A:331:PRO:HD3	2.01	0.42
1:A:680:PHE:C	1:A:680:PHE:CD2	2.97	0.42
1:A:728:LYS:HB2	1:A:810:GLU:OE2	2.20	0.42
1:A:743:ILE:HA	1:A:746:ILE:HG12	2.01	0.42
1:B:162:MET:O	1:B:164:ASP:N	2.53	0.42
1:B:189:ASN:O	1:B:193:LEU:HD23	2.20	0.42
1:B:587:THR:OG1	1:B:622:GLN:O	2.28	0.42
1:C:157:TYR:CD2	1:C:162:MET:HE2	2.55	0.42
1:C:566:ASP:OD2	1:C:678:THR:HG23	2.19	0.42
1:C:777:ALA:C	1:C:781:MET:HE2	2.44	0.42
1:C:989:LEU:HD23	1:C:989:LEU:HA	1.46	0.42
1:C:1035:ARG:HD2	1:C:1035:ARG:HA	1.61	0.42
1:D:352:PHE:HD2	1:D:353:LEU:HD23	1.85	0.42
1:E:154:ILE:HG22	1:E:287:SER:HB3	2.02	0.42
1:E:356:TYR:C	1:E:358:PHE:H	2.28	0.42
1:E:424:GLY:HA2	1:E:502:LYS:N	2.34	0.42
1:E:442:LEU:HD23	1:E:442:LEU:HA	1.64	0.42
1:E:601:LYS:HD2	1:E:601:LYS:H	1.85	0.42
1:E:946:VAL:HG22	1:E:1026:PHE:HD1	1.85	0.42
1:E:947:GLU:HG3	1:E:948:PHE:HD2	1.83	0.42
1:E:971:ARG:CZ	1:E:971:ARG:CB	2.97	0.42
1:A:170:SER:OG	1:B:74:ASN:HA	2.20	0.42
1:A:462:SER:O	1:A:465:ALA:HB3	2.19	0.42
1:A:982:PHE:HD2	1:A:1011:MET:HE2	1.84	0.42
1:B:578:LEU:CD1	1:B:586:ARG:HB2	2.50	0.42
1:B:727:PHE:HB2	1:B:809:TRP:NE1	2.32	0.42
1:D:217:GLY:O	1:D:234:ILE:HB	2.20	0.42
1:D:223:PRO:HG3	1:E:275:TYR:CD2	2.54	0.42
1:D:270:LEU:HD12	1:D:270:LEU:HA	1.68	0.42
1:D:275:TYR:HB2	1:F:223:PRO:HD3	2.01	0.42
1:D:370:ILE:O	1:D:373:PRO:HD2	2.19	0.42
1:D:372:VAL:HA	1:D:375:VAL:CG1	2.47	0.42
1:E:34:GLN:OE1	1:E:332:PHE:HE2	2.02	0.42
1:E:177:LEU:HG	1:E:289:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:PRO:O	1:E:194:ASN:HB2	2.20	0.42
1:E:444:GLY:O	1:E:447:MET:HB2	2.19	0.42
1:E:535:LEU:CD2	1:E:1027:VAL:HG11	2.49	0.42
1:F:39:ALA:HA	1:F:40:PRO:HD2	1.91	0.42
1:F:358:PHE:CB	1:F:977:MET:HE2	2.50	0.42
1:F:364:ALA:O	1:F:367:ILE:HD13	2.20	0.42
1:F:578:LEU:HD22	1:F:579:PRO:HD2	2.02	0.42
1:F:886:LEU:HD23	1:F:886:LEU:HA	1.87	0.42
1:F:959:GLY:CA	1:F:1041:GLU:H	2.25	0.42
1:A:13:TRP:NE1	1:A:492:LEU:HD21	2.33	0.42
1:A:112:GLN:OE1	1:A:115:MET:HG3	2.20	0.42
1:A:254:ASN:HB2	1:A:258:SER:O	2.20	0.42
1:A:559:LEU:HD22	1:A:923:ASN:HB2	2.02	0.42
1:B:21:LEU:HA	1:B:21:LEU:HD23	1.78	0.42
1:B:270:LEU:HD12	1:B:270:LEU:HA	1.75	0.42
1:B:417:GLU:HG2	1:B:497:LEU:HD21	2.02	0.42
1:B:907:LEU:HG	1:B:1017:LEU:CD2	2.45	0.42
1:B:993:THR:HA	1:B:997:SER:OG	2.20	0.42
1:C:26:ALA:O	1:C:30:LEU:HD13	2.18	0.42
1:C:276:ASP:OD2	1:C:276:ASP:N	2.50	0.42
1:C:364:ALA:HA	1:C:367:ILE:HG13	2.01	0.42
1:C:404:LEU:HB3	1:C:478:MET:SD	2.60	0.42
1:C:419:VAL:HG13	1:C:423:GLU:CD	2.45	0.42
1:C:563:PHE:HE2	1:C:671:ILE:HD11	1.84	0.42
1:D:277:ILE:C	1:D:278:ILE:HG13	2.44	0.42
1:D:404:LEU:HD12	1:D:937:LEU:CD2	2.50	0.42
1:D:734:GLU:C	1:D:736:ALA:N	2.78	0.42
1:E:189:ASN:HB3	1:E:192:GLU:HB2	2.02	0.42
1:E:352:PHE:CD2	1:E:353:LEU:HD23	2.45	0.42
1:F:397:GLY:CA	1:F:470:PHE:HD2	2.33	0.42
1:F:463:THR:O	1:F:466:ILE:HB	2.20	0.42
1:F:833:PRO:C	1:F:835:LYS:N	2.75	0.42
1:F:885:PHE:HB2	1:F:902:MET:CE	2.49	0.42
1:A:195:LYS:C	1:A:197:GLN:H	2.28	0.41
1:A:326:PRO:O	1:A:630:SER:HB2	2.20	0.41
1:A:583:THR:OG1	1:A:585:GLU:OE2	2.30	0.41
1:A:652:THR:HG23	1:A:664:PHE:CD1	2.56	0.41
1:B:19:ILE:HG22	1:B:378:GLY:HA3	2.01	0.41
1:B:28:LEU:HD23	1:B:28:LEU:HA	1.90	0.41
1:B:83:ASP:C	1:B:85:THR:H	2.28	0.41
1:B:736:ALA:HA	1:B:739:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:885:PHE:CD1	1:B:898:PRO:HB2	2.55	0.41
1:B:1028:VAL:HA	1:B:1031:ARG:HG2	2.02	0.41
1:C:189:ASN:O	1:C:193:LEU:N	2.52	0.41
1:C:273:GLU:CD	1:C:770:LYS:HD2	2.45	0.41
1:C:1018:ALA:O	1:C:1022:VAL:HG23	2.20	0.41
1:D:673:GLU:O	1:D:674:LEU:HB3	2.19	0.41
1:D:690:LEU:HG	1:D:694:LYS:CE	2.50	0.41
1:E:277:ILE:HG21	1:E:615:PHE:HB2	2.01	0.41
1:E:366:LEU:O	1:E:370:ILE:HG12	2.19	0.41
1:E:787:GLY:C	1:E:789:TRP:H	2.27	0.41
1:E:982:PHE:HE2	1:E:1007:VAL:HG13	1.85	0.41
1:E:1026:PHE:O	1:E:1030:ARG:HB2	2.20	0.41
1:F:399:VAL:HA	1:F:402:ILE:HG13	2.02	0.41
1:F:514:GLY:CA	1:F:517:ASN:HD21	2.32	0.41
1:F:723:ASP:OD1	1:F:813:SER:OG	2.35	0.41
1:A:194:ASN:ND2	1:A:798:MET:HG3	2.35	0.41
1:A:427:PRO:HD2	1:A:428:LYS:NZ	2.35	0.41
1:A:818:ARG:HH12	1:A:823:PRO:HG3	1.86	0.41
1:A:892:TYR:OH	1:A:943:ILE:HG12	2.20	0.41
1:A:901:VAL:O	1:A:904:VAL:HG23	2.19	0.41
1:B:370:ILE:C	1:B:373:PRO:HD2	2.46	0.41
1:B:740:GLY:O	1:B:794:ALA:N	2.53	0.41
1:B:778:LYS:HE3	1:B:779:TYR:OH	2.19	0.41
1:B:952:LEU:HB2	1:B:963:ALA:HB1	2.01	0.41
1:C:38:ILE:HD13	1:C:38:ILE:HG21	1.71	0.41
1:C:527:TYR:CE1	1:C:972:LEU:HD23	2.55	0.41
1:C:536:ARG:NH1	2:C:2000:LMT:O6B	2.53	0.41
1:C:783:PRO:O	1:C:786:ILE:HB	2.20	0.41
1:C:888:LEU:HD13	1:C:901:VAL:HG11	2.01	0.41
1:D:774:MET:HG2	1:D:775:SER:H	1.85	0.41
1:E:152:GLU:HB3	1:E:182:TYR:HE1	1.86	0.41
1:E:344:LEU:CD2	1:E:399:VAL:HA	2.47	0.41
1:E:559:LEU:HD12	1:E:559:LEU:HA	1.79	0.41
1:E:876:LEU:HD23	1:E:876:LEU:HA	1.86	0.41
1:F:3:ASN:HD22	1:F:435:MET:HG3	1.84	0.41
1:F:34:GLN:CG	1:F:333:VAL:HG22	2.50	0.41
1:F:184:MET:HE3	1:F:185:ARG:N	2.34	0.41
1:F:525:HIS:ND1	1:F:529:ASP:OD2	2.53	0.41
1:F:527:TYR:OH	1:F:1019:ILE:HB	2.21	0.41
1:F:659:LYS:HD3	1:F:659:LYS:HA	1.90	0.41
1:A:363:ARG:H	1:A:363:ARG:HG2	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:PRO:O	1:A:876:LEU:HD13	2.20	0.41
1:A:836:SER:OG	1:A:839:GLU:HG3	2.19	0.41
1:B:58:GLN:HG3	1:B:818:ARG:HD2	2.01	0.41
1:B:187:TRP:HB3	1:B:776:GLU:HA	2.03	0.41
1:B:400:LEU:HD12	1:B:400:LEU:O	2.20	0.41
1:B:617:PHE:N	1:B:626:ILE:HD12	2.36	0.41
1:B:641:GLU:HB2	1:B:650:ARG:HH22	1.85	0.41
1:B:987:MET:CB	1:B:1008:MET:HE1	2.51	0.41
1:C:555:LEU:HD22	1:C:555:LEU:HA	1.89	0.41
1:C:556:PHE:HE1	1:C:923:ASN:ND2	2.17	0.41
1:C:703:LEU:CD1	1:C:718:PRO:HD3	2.50	0.41
1:C:738:ALA:C	1:C:740:GLY:H	2.28	0.41
1:C:795:ASP:OD2	1:C:796:GLY:N	2.53	0.41
1:D:13:TRP:HE1	1:D:492:LEU:HD21	1.84	0.41
1:D:76:MET:HB2	1:D:93:THR:O	2.21	0.41
1:D:81:ASN:HB2	1:D:89:GLN:HB3	2.02	0.41
1:D:398:MET:O	1:D:401:ALA:N	2.53	0.41
1:D:754:TRP:CE2	1:D:780:ARG:CB	3.04	0.41
1:D:932:LEU:HA	1:D:935:ILE:HD12	2.01	0.41
1:E:555:LEU:HD23	1:E:555:LEU:HA	1.79	0.41
1:E:867:ARG:HH11	1:E:868:LEU:CA	2.30	0.41
1:E:985:GLY:O	1:E:988:PRO:HD2	2.19	0.41
1:E:1008:MET:HB2	1:E:1008:MET:HE3	1.66	0.41
1:F:65:ILE:HA	1:F:114:ALA:CB	2.50	0.41
1:F:111:LEU:C	1:F:113:LEU:N	2.78	0.41
1:F:136:PHE:HB2	1:F:327:TYR:HE2	1.86	0.41
1:F:228:GLN:HE21	1:F:230:LEU:H	1.66	0.41
1:F:699:ARG:NH2	1:F:718:PRO:HB2	2.34	0.41
1:F:712:MET:SD	1:F:843:LEU:HG	2.60	0.41
1:F:888:LEU:CD1	1:F:901:VAL:HG11	2.51	0.41
1:A:303:ALA:O	1:A:307:ARG:HB2	2.21	0.41
1:A:683:GLU:HG2	1:A:819:TYR:HB2	2.02	0.41
1:A:897:ILE:HD11	1:A:1030:ARG:NH2	2.32	0.41
1:B:727:PHE:CE2	1:B:729:ILE:HD11	2.55	0.41
1:B:1015:THR:C	1:B:1017:LEU:N	2.78	0.41
1:C:112:GLN:HA	1:C:115:MET:HB2	2.02	0.41
1:C:214:VAL:CG2	1:C:237:GLN:HB2	2.51	0.41
1:C:344:LEU:CA	1:C:399:VAL:HG22	2.50	0.41
1:C:534:ILE:C	1:C:536:ARG:N	2.78	0.41
1:C:539:GLY:O	1:C:542:LEU:HB2	2.19	0.41
1:C:583:THR:HG22	1:C:622:GLN:OE1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:588:GLN:O	1:C:592:ASN:CG	2.63	0.41
1:D:17:ILE:CG2	1:E:886:LEU:HG	2.51	0.41
1:D:262:LEU:O	1:D:265:VAL:HG22	2.20	0.41
1:D:342:LYS:O	1:D:345:VAL:HB	2.20	0.41
1:D:414:GLU:HG3	1:D:974:PRO:HG3	2.03	0.41
1:D:445:ILE:HG21	1:D:940:LYS:HD2	2.03	0.41
1:E:19:ILE:HA	1:E:22:ALA:HB3	2.02	0.41
1:E:144:ASN:HD22	1:E:149:MET:HG2	1.85	0.41
1:E:184:MET:HE2	1:E:268:ILE:HG23	2.02	0.41
1:E:203:VAL:HG12	1:E:207:ILE:HD11	2.03	0.41
1:E:293:LEU:HD11	1:E:297:ALA:O	2.20	0.41
1:F:27:ILE:HA	1:F:30:LEU:HD22	2.02	0.41
1:F:72:ILE:HD12	1:F:75:LEU:CD2	2.50	0.41
1:F:362:PHE:CE2	1:F:366:LEU:HD21	2.55	0.41
1:F:535:LEU:HD13	1:F:1027:VAL:HG21	2.02	0.41
1:F:674:LEU:HD22	1:F:861:GLY:HA2	2.03	0.41
1:A:26:ALA:O	1:A:30:LEU:HB2	2.20	0.41
1:A:151:GLN:O	1:A:155:SER:HB3	2.21	0.41
1:A:171:GLY:O	1:A:294:ALA:HB2	2.21	0.41
1:A:514:GLY:C	1:A:516:PHE:N	2.77	0.41
1:A:723:ASP:HA	1:A:813:SER:HA	2.02	0.41
1:A:1018:ALA:C	1:A:1020:PHE:H	2.28	0.41
1:B:350:LEU:HA	1:B:350:LEU:HD23	1.59	0.41
1:B:594:VAL:O	1:B:597:TYR:HB3	2.20	0.41
1:C:281:PHE:CD1	1:C:610:PHE:HD1	2.26	0.41
1:C:411:VAL:O	1:C:414:GLU:HB3	2.20	0.41
1:C:506:GLY:C	1:C:508:GLY:H	2.29	0.41
1:C:776:GLU:HB2	1:C:779:TYR:CE1	2.56	0.41
1:C:972:LEU:O	1:C:975:ILE:HB	2.20	0.41
1:C:1022:VAL:N	1:C:1023:PRO:HD2	2.36	0.41
1:D:49:TYR:HE1	1:D:60:THR:HG21	1.85	0.41
1:D:116:PRO:C	1:D:118:LEU:H	2.27	0.41
1:D:195:LYS:HB3	1:D:196:PHE:CE2	2.55	0.41
1:D:367:ILE:HG12	1:D:496:MET:HE3	2.02	0.41
1:D:412:VAL:O	1:D:416:VAL:HG12	2.20	0.41
1:D:739:LEU:HD23	1:D:799:VAL:HG11	2.02	0.41
1:D:750:LEU:O	1:D:753:ALA:HB3	2.20	0.41
1:D:801:PHE:C	1:D:803:ALA:H	2.27	0.41
1:E:76:MET:HE3	1:E:864:TYR:CE2	2.56	0.41
1:E:228:GLN:HE21	1:E:230:LEU:H	1.69	0.41
1:E:247:GLY:O	1:E:261:LEU:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:ILE:O	1:E:249:ILE:HG13	2.17	0.41
1:E:272:GLY:O	1:E:275:TYR:HE1	2.04	0.41
1:E:330:THR:HB	1:E:331:PRO:HD3	2.02	0.41
1:E:362:PHE:O	1:E:365:THR:OG1	2.27	0.41
1:E:738:ALA:O	1:E:740:GLY:N	2.53	0.41
1:E:932:LEU:HD23	1:E:932:LEU:HA	1.92	0.41
1:E:1015:THR:C	1:E:1017:LEU:N	2.77	0.41
1:F:24:GLY:HA2	1:F:27:ILE:HG23	2.02	0.41
1:F:446:ALA:HB2	1:F:478:MET:HE2	2.02	0.41
1:F:525:HIS:CE1	1:F:529:ASP:OD2	2.73	0.41
1:F:894:SER:O	1:F:895:TRP:HE3	2.03	0.41
1:F:896:SER:HB3	1:F:1029:VAL:HG12	2.02	0.41
1:A:68:ASN:HD22	1:A:68:ASN:HA	1.60	0.41
1:A:331:PRO:O	1:A:335:ILE:HG13	2.20	0.41
1:A:445:ILE:HD13	1:A:940:LYS:CE	2.51	0.41
1:A:535:LEU:HD23	1:A:535:LEU:HA	1.82	0.41
1:A:774:MET:HG2	1:A:775:SER:H	1.86	0.41
1:A:909:VAL:O	1:A:911:GLY:N	2.54	0.41
1:A:1026:PHE:O	1:A:1030:ARG:HB2	2.20	0.41
1:B:242:SER:O	1:B:246:PHE:HD1	2.03	0.41
1:B:506:GLY:O	1:B:509:LYS:HE2	2.20	0.41
1:B:507:GLU:O	1:B:508:GLY:C	2.64	0.41
1:B:847:LEU:C	1:B:849:SER:N	2.78	0.41
1:C:373:PRO:HB2	1:C:377:LEU:HD12	2.03	0.41
1:C:506:GLY:C	1:C:508:GLY:N	2.78	0.41
1:C:1024:VAL:HA	1:C:1027:VAL:CG2	2.50	0.41
1:D:14:VAL:HG11	1:E:890:ALA:HB2	2.02	0.41
1:D:201:VAL:HG11	1:D:745:ASP:OD2	2.21	0.41
1:D:352:PHE:CE1	1:D:365:THR:HG23	2.56	0.41
1:E:68:ASN:CB	1:E:114:ALA:HB2	2.50	0.41
1:E:319:SER:C	1:E:321:LEU:H	2.28	0.41
1:E:410:ILE:HD12	1:E:410:ILE:HA	1.85	0.41
1:E:641:GLU:HB2	1:E:650:ARG:NH2	2.35	0.41
1:F:8:ARG:HA	1:F:9:PRO:HD3	1.82	0.41
1:A:344:LEU:HG	1:A:399:VAL:HG22	2.03	0.41
1:A:682:PHE:C	1:A:682:PHE:CD2	2.99	0.41
1:B:250:LEU:HD23	1:C:737:GLN:OE1	2.21	0.41
1:B:559:LEU:HA	1:B:560:PRO:HD2	1.74	0.41
1:B:775:SER:OG	1:B:780:ARG:HG2	2.20	0.41
1:B:1016:VAL:HG22	2:B:2000:LMT:H82	2.02	0.41
1:C:279:ALA:HB3	1:C:286:ALA:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:514:GLY:C	1:C:516:PHE:N	2.72	0.41
1:C:721:LEU:HB3	1:C:814:PRO:HG2	2.02	0.41
1:D:21:LEU:HD23	1:D:21:LEU:HA	1.70	0.41
1:D:177:LEU:HD22	1:D:177:LEU:HA	1.74	0.41
1:D:961:ILE:HG22	1:D:965:LEU:HD12	2.02	0.41
1:E:30:LEU:HA	1:E:31:PRO:HD3	1.89	0.41
1:E:72:ILE:HG12	1:E:106:GLN:HB3	2.02	0.41
1:E:359:LEU:C	1:E:361:ASN:N	2.77	0.41
1:E:445:ILE:HD12	1:E:449:LEU:HD12	2.03	0.41
1:F:105:VAL:O	1:F:109:ASN:HB2	2.21	0.41
1:F:146:ASP:OD2	1:F:147:GLY:N	2.41	0.41
1:F:540:ARG:O	1:F:543:VAL:HB	2.21	0.41
1:F:859:TRP:O	1:F:864:TYR:HD1	2.03	0.41
1:A:108:GLN:HB2	1:A:129:VAL:HG11	2.02	0.41
1:A:368:PRO:HG3	1:A:413:VAL:HG21	2.02	0.41
1:A:413:VAL:HA	1:A:493:CYS:SG	2.61	0.41
1:A:427:PRO:O	1:A:430:ALA:HB3	2.20	0.41
1:A:468:ARG:CZ	1:A:468:ARG:HB2	2.50	0.41
1:A:488:LEU:O	1:A:488:LEU:HD22	2.21	0.41
1:A:552:MET:HG3	1:A:909:VAL:CG1	2.50	0.41
1:A:907:LEU:HD23	1:A:1017:LEU:HB3	2.02	0.41
1:A:1015:THR:OG1	1:A:1016:VAL:N	2.53	0.41
1:B:172:VAL:HG22	1:B:302:THR:HG23	2.01	0.41
1:B:427:PRO:O	1:B:428:LYS:C	2.62	0.41
1:B:549:VAL:HG13	1:B:550:VAL:N	2.35	0.41
1:C:249:ILE:HD12	1:C:262:LEU:HD23	2.03	0.41
1:C:608:SER:O	1:C:629:VAL:HA	2.21	0.41
1:D:232:ALA:HB1	1:E:725:PRO:O	2.21	0.41
1:D:424:GLY:HA3	1:D:502:LYS:HG2	2.02	0.41
1:D:516:PHE:O	1:D:519:MET:N	2.53	0.41
1:D:932:LEU:O	1:D:933:THR:C	2.64	0.41
1:D:937:LEU:HA	1:D:937:LEU:HD23	1.70	0.41
1:E:139:VAL:HG22	1:E:178:PHE:HE1	1.86	0.41
1:E:368:PRO:O	1:E:371:ALA:HB3	2.20	0.41
1:E:538:THR:O	1:E:541:TYR:N	2.50	0.41
1:E:764:ASP:C	1:E:766:GLY:N	2.79	0.41
1:E:845:GLU:O	1:E:849:SER:HB2	2.21	0.41
1:E:867:ARG:HD3	1:E:868:LEU:N	2.35	0.41
1:F:30:LEU:HA	1:F:31:PRO:HD3	1.72	0.41
1:F:352:PHE:HZ	1:F:362:PHE:CZ	2.39	0.41
1:F:531:VAL:O	1:F:534:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:863:SER:HA	1:F:866:GLU:OE2	2.21	0.41
1:A:131:LYS:HB2	1:A:295:THR:OG1	2.21	0.41
1:A:235:ILE:HD12	1:A:235:ILE:N	2.36	0.41
1:A:293:LEU:HD13	1:A:294:ALA:O	2.21	0.41
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.88	0.41
1:A:325:TYR:HA	1:A:326:PRO:HD2	1.94	0.41
1:A:452:VAL:HA	1:A:880:SER:HG	1.86	0.41
1:A:542:LEU:O	1:A:546:LEU:HD23	2.21	0.41
1:A:676:THR:HB	1:A:677:ALA:H	1.68	0.41
1:A:708:LYS:HE2	1:A:708:LYS:HB3	1.84	0.41
1:A:818:ARG:NH1	1:A:823:PRO:HG3	2.35	0.41
1:A:897:ILE:CD1	1:A:1030:ARG:HE	2.33	0.41
1:A:937:LEU:HA	1:A:937:LEU:HD23	1.65	0.41
1:B:111:LEU:C	1:B:113:LEU:N	2.79	0.41
1:B:182:TYR:HD2	1:B:765:ARG:HH22	1.69	0.41
1:B:302:THR:O	1:B:306:ILE:HB	2.21	0.41
1:B:362:PHE:O	1:B:366:LEU:HG	2.21	0.41
1:B:428:LYS:O	1:B:431:THR:HB	2.21	0.41
1:B:597:TYR:OH	1:B:651:ALA:HA	2.21	0.41
1:B:698:ALA:O	1:B:701:GLN:HB3	2.21	0.41
1:B:785:ASP:OD1	1:B:785:ASP:N	2.54	0.41
1:B:1018:ALA:C	1:B:1020:PHE:N	2.77	0.41
1:C:138:MET:HE3	1:C:138:MET:HB2	1.91	0.41
1:C:355:MET:SD	1:C:410:ILE:HD11	2.61	0.41
1:C:474:ILE:HG23	1:C:474:ILE:HD12	1.67	0.41
1:C:525:HIS:O	1:C:526:HIS:C	2.63	0.41
1:C:649:MET:HE2	1:C:653:ARG:HE	1.85	0.41
1:C:721:LEU:HA	1:C:721:LEU:HD12	1.87	0.41
1:C:738:ALA:C	1:C:740:GLY:N	2.78	0.41
1:C:751:GLY:O	1:C:754:TRP:N	2.53	0.41
1:D:23:GLY:HA2	1:D:377:LEU:O	2.21	0.41
1:D:383:LEU:HD21	1:D:473:THR:HA	2.03	0.41
1:D:536:ARG:HG3	2:D:2000:LMT:C3B	2.51	0.41
1:D:578:LEU:HD21	1:D:587:THR:HA	2.03	0.41
1:D:751:GLY:C	1:D:753:ALA:N	2.77	0.41
1:D:790:TYR:CE1	1:D:800:PRO:HB3	2.55	0.41
1:D:900:SER:CB	1:D:1029:VAL:HG21	2.51	0.41
1:D:941:ASN:HB3	1:D:975:ILE:HD12	2.03	0.41
1:E:45:ILE:HA	1:E:128:SER:O	2.21	0.41
1:E:207:ILE:O	1:E:211:ASN:HB3	2.21	0.41
1:E:344:LEU:CG	1:E:399:VAL:HG22	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:LEU:HD21	1:E:933:THR:OG1	2.20	0.41
1:E:401:ALA:O	1:E:402:ILE:C	2.64	0.41
1:E:573:MET:O	1:E:666:PHE:HD2	2.04	0.41
1:E:584:GLN:HB2	1:E:622:GLN:CG	2.51	0.41
1:E:644:VAL:HG12	1:E:645:GLU:N	2.36	0.41
1:E:709:HIS:HE1	1:E:847:LEU:HD21	1.85	0.41
1:E:758:TYR:CE1	1:E:770:LYS:HD3	2.55	0.41
1:E:898:PRO:O	1:E:902:MET:HG3	2.20	0.41
1:E:1027:VAL:HG13	1:E:1028:VAL:N	2.36	0.41
1:E:1031:ARG:O	1:E:1032:ARG:HG3	2.20	0.41
1:F:99:ASP:HB3	1:F:102:ILE:HB	2.03	0.41
1:F:195:LYS:HG3	1:F:196:PHE:CD1	2.55	0.41
1:F:352:PHE:HE1	1:F:366:LEU:CD2	2.33	0.41
1:F:559:LEU:HD22	1:F:559:LEU:HA	1.71	0.41
1:F:774:MET:HE2	1:F:774:MET:HB3	1.73	0.41
1:F:927:PHE:O	1:F:931:LEU:HB2	2.21	0.41
1:A:190:PRO:HB3	1:A:789:TRP:CE2	2.56	0.41
1:A:196:PHE:CD2	1:A:196:PHE:N	2.89	0.41
1:A:470:PHE:CD1	1:A:929:VAL:HG21	2.56	0.41
1:A:557:VAL:C	1:A:559:LEU:H	2.28	0.41
1:B:525:HIS:O	1:B:526:HIS:C	2.61	0.41
1:B:932:LEU:O	1:B:935:ILE:N	2.54	0.41
1:C:1027:VAL:HG23	1:C:1028:VAL:N	2.36	0.41
1:D:457:ALA:HB2	1:D:471:SER:CB	2.51	0.41
1:D:573:MET:HE2	1:D:666:PHE:CZ	2.56	0.41
1:D:886:LEU:HD21	1:F:17:ILE:CG2	2.49	0.41
1:D:972:LEU:HD13	1:D:972:LEU:C	2.46	0.41
1:D:1044:HIS:O	1:D:1045:THR:HB	2.20	0.41
1:E:355:MET:CE	1:E:410:ILE:HG13	2.41	0.41
1:E:364:ALA:HA	1:E:367:ILE:HD12	2.02	0.41
1:E:598:TYR:CD2	1:E:629:VAL:HG21	2.56	0.41
1:E:901:VAL:HG13	1:E:942:ALA:CB	2.51	0.41
1:F:139:VAL:HB	1:F:327:TYR:HB3	2.02	0.41
1:F:321:LEU:HD23	1:F:321:LEU:HA	1.88	0.41
1:F:361:ASN:O	1:F:364:ALA:HB3	2.21	0.41
1:F:987:MET:HG2	1:F:1008:MET:HE1	2.03	0.41
1:F:1018:ALA:C	1:F:1020:PHE:N	2.79	0.41
1:A:539:GLY:O	1:A:542:LEU:HB2	2.21	0.40
1:A:729:ILE:HD12	1:A:729:ILE:N	2.35	0.40
1:B:443:VAL:O	1:B:447:MET:HG2	2.21	0.40
1:C:888:LEU:HD11	1:C:943:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:ALA:HB2	1:D:299:ALA:H	1.86	0.40
1:D:122:VAL:O	1:D:125:GLN:N	2.52	0.40
1:D:496:MET:H	1:D:496:MET:HG2	1.75	0.40
1:D:545:TYR:O	1:D:548:ILE:N	2.54	0.40
1:D:907:LEU:HD21	1:D:1021:PHE:CB	2.51	0.40
1:D:948:PHE:O	1:D:949:ALA:C	2.61	0.40
1:E:536:ARG:CD	2:E:2000:LMT:H4B	2.51	0.40
1:E:692:HIS:HD2	1:E:816:LEU:HD22	1.86	0.40
1:E:867:ARG:C	1:E:867:ARG:HD3	2.46	0.40
1:F:175:VAL:HG12	1:F:289:LEU:HD22	2.02	0.40
1:F:498:LYS:HB2	1:F:498:LYS:HE3	1.83	0.40
1:F:703:LEU:HD23	1:F:716:VAL:HG13	2.04	0.40
1:F:843:LEU:HD22	1:F:846:GLN:HB3	2.03	0.40
1:A:82:SER:HB2	1:A:816:LEU:HB2	2.03	0.40
1:A:102:ILE:HA	1:A:102:ILE:HD13	1.84	0.40
1:A:194:ASN:HD21	1:A:798:MET:HG3	1.87	0.40
1:A:200:PRO:HA	1:A:203:VAL:HG23	2.03	0.40
1:A:247:GLY:C	1:A:249:ILE:H	2.29	0.40
1:A:952:LEU:O	1:A:956:GLU:HB2	2.21	0.40
1:B:149:MET:H	1:B:149:MET:HG2	1.54	0.40
1:B:348:ILE:O	1:B:351:VAL:HB	2.22	0.40
1:B:457:ALA:HB1	1:B:468:ARG:HG3	2.03	0.40
1:B:879:ILE:O	1:B:883:VAL:HG23	2.22	0.40
1:B:990:VAL:HG22	1:B:1004:GLY:HA3	2.04	0.40
1:C:190:PRO:HG3	1:C:779:TYR:CB	2.49	0.40
1:C:195:LYS:HB3	1:C:196:PHE:HD2	1.81	0.40
1:C:453:PHE:HB3	1:C:471:SER:HA	2.04	0.40
1:C:588:GLN:N	1:C:613:ASN:ND2	2.70	0.40
1:C:681:ASP:OD2	1:C:681:ASP:N	2.54	0.40
1:C:1027:VAL:HG23	1:C:1028:VAL:HG23	2.02	0.40
1:D:344:LEU:HD11	1:D:398:MET:CB	2.51	0.40
1:D:435:MET:HE1	1:D:485:ALA:O	2.20	0.40
1:D:527:TYR:CD1	1:D:972:LEU:HG	2.56	0.40
1:E:166:ILE:HD11	1:E:310:LEU:N	2.36	0.40
1:E:530:SER:O	1:E:534:ILE:HG23	2.21	0.40
1:E:695:LEU:HD23	1:E:695:LEU:HA	1.88	0.40
1:E:892:TYR:HE2	1:E:897:ILE:CG2	2.34	0.40
1:E:1011:MET:O	1:E:1015:THR:HG23	2.22	0.40
1:F:151:GLN:O	1:F:155:SER:HB3	2.22	0.40
1:F:175:VAL:HG11	1:F:289:LEU:HD22	2.03	0.40
1:F:568:ASP:OD1	1:F:644:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1016:VAL:HG23	1:F:1017:LEU:HD12	2.03	0.40
1:A:27:ILE:HD11	1:A:380:PHE:HD2	1.86	0.40
1:A:149:MET:HB2	1:A:153:ASP:HB2	2.02	0.40
1:A:396:PHE:O	1:A:400:LEU:HB2	2.20	0.40
1:A:437:GLN:OE1	1:A:438:ILE:HG22	2.21	0.40
1:A:556:PHE:HD1	1:A:913:LEU:HD21	1.85	0.40
1:A:910:ILE:O	1:A:910:ILE:HG13	2.19	0.40
1:B:62:THR:HG23	1:B:90:ILE:HD11	2.02	0.40
1:B:195:LYS:H	1:B:195:LYS:HG3	1.68	0.40
1:B:219:LEU:HD11	1:C:727:PHE:CD2	2.57	0.40
1:B:455:PRO:C	1:B:876:LEU:HD21	2.46	0.40
1:B:703:LEU:CD1	1:B:718:PRO:HD3	2.39	0.40
1:B:948:PHE:CD2	1:B:971:ARG:HG3	2.57	0.40
1:C:149:MET:HG3	1:C:154:ILE:CD1	2.50	0.40
1:C:426:PRO:HD2	1:C:429:GLU:HB3	2.03	0.40
1:C:578:LEU:HD22	1:C:579:PRO:HD2	2.02	0.40
1:C:597:TYR:CE1	1:C:601:LYS:HD2	2.56	0.40
1:D:101:ASP:HB3	1:E:102:ILE:HG21	2.03	0.40
1:D:163:LYS:HG2	1:D:163:LYS:O	2.21	0.40
1:D:393:LEU:O	1:D:470:PHE:HE1	2.05	0.40
1:D:437:GLN:HG3	1:D:948:PHE:CE1	2.56	0.40
1:D:545:TYR:O	1:D:546:LEU:C	2.64	0.40
1:E:124:GLN:NE2	1:E:758:TYR:HD2	2.20	0.40
1:E:444:GLY:HA2	1:E:447:MET:HB2	2.03	0.40
1:E:692:HIS:CD2	1:E:816:LEU:HD22	2.56	0.40
1:E:1005:THR:O	1:E:1006:GLY:C	2.63	0.40
1:F:457:ALA:HB2	1:F:471:SER:HB2	2.02	0.40
1:F:509:LYS:HA	1:F:509:LYS:HD2	1.71	0.40
1:F:590:VAL:O	1:F:593:GLU:N	2.54	0.40
1:A:211:ASN:HB2	1:A:240:LEU:HD11	2.04	0.40
1:A:886:LEU:HD22	1:C:14:VAL:HG22	2.03	0.40
1:A:941:ASN:HB3	1:A:975:ILE:HD12	2.03	0.40
1:A:960:LEU:HD23	1:A:1031:ARG:NH2	2.36	0.40
1:B:222:THR:HA	1:B:224:PRO:CD	2.50	0.40
1:B:530:SER:HG	1:B:531:VAL:N	2.20	0.40
1:C:343:THR:O	1:C:346:GLU:HB2	2.22	0.40
1:C:409:ALA:O	1:C:412:VAL:HB	2.20	0.40
1:C:527:TYR:C	1:C:530:SER:HG	2.24	0.40
1:D:235:ILE:O	1:E:728:LYS:HA	2.21	0.40
1:D:325:TYR:HA	1:D:326:PRO:HD2	2.00	0.40
1:D:343:THR:O	1:D:344:LEU:C	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:712:MET:HG3	1:D:713:LEU:HD13	2.03	0.40
1:D:713:LEU:HD21	1:D:843:LEU:HD12	2.03	0.40
1:D:979:SER:O	1:D:983:ILE:N	2.54	0.40
1:E:34:GLN:HE21	1:E:333:VAL:HG22	1.85	0.40
1:E:35:TYR:HD2	1:E:38:ILE:CD1	2.34	0.40
1:E:680:PHE:CD1	1:E:859:TRP:CZ3	3.10	0.40
1:E:945:ILE:HD13	1:E:945:ILE:HA	1.78	0.40
1:F:36:PRO:HG2	1:F:38:ILE:HD11	2.04	0.40
1:F:217:GLY:O	1:F:234:ILE:HD13	2.21	0.40
1:F:645:GLU:OE2	1:F:645:GLU:HA	2.21	0.40
1:F:742:SER:O	1:F:746:ILE:HG22	2.21	0.40
1:A:10:ILE:HG13	1:B:895:TRP:CZ2	2.56	0.40
1:A:721:LEU:HD23	1:A:721:LEU:HA	1.77	0.40
1:A:945:ILE:CG1	1:A:971:ARG:HH22	2.35	0.40
1:B:638:PRO:HB2	1:B:639:GLY:H	1.68	0.40
1:C:214:VAL:HG23	1:C:237:GLN:HB2	2.03	0.40
1:C:249:ILE:HD12	1:C:262:LEU:CD2	2.52	0.40
1:C:685:ILE:HD13	1:C:824:SER:HB3	2.03	0.40
1:C:692:HIS:ND1	1:C:692:HIS:C	2.79	0.40
1:C:1019:ILE:HG13	1:C:1020:PHE:CE1	2.56	0.40
1:D:255:GLN:CD	1:D:255:GLN:H	2.28	0.40
1:D:414:GLU:CG	1:D:974:PRO:HG3	2.51	0.40
1:D:445:ILE:HG21	1:D:940:LYS:HD3	2.04	0.40
1:D:531:VAL:HG11	1:D:968:VAL:HG21	2.03	0.40
1:D:1011:MET:O	1:D:1012:VAL:C	2.65	0.40
1:E:9:PRO:HD2	1:F:893:GLU:OE1	2.22	0.40
1:E:215:ALA:O	1:F:751:GLY:HA2	2.21	0.40
1:E:740:GLY:HA3	1:E:793:ALA:HB1	2.03	0.40
1:E:789:TRP:O	1:E:801:PHE:HD2	2.04	0.40
1:F:41:PRO:HD3	1:F:96:SER:HA	2.04	0.40
1:F:47:ALA:CB	1:F:122:VAL:HG13	2.48	0.40
1:F:371:ALA:HB1	1:F:484:VAL:HG11	2.02	0.40
1:F:675:GLY:HA3	1:F:862:MET:HG3	2.04	0.40
1:F:678:THR:O	1:F:680:PHE:HB3	2.21	0.40
1:F:910:ILE:O	1:F:914:LEU:HB2	2.22	0.40
1:F:1015:THR:C	1:F:1017:LEU:H	2.28	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	1042/1069 (98%)	880 (84%)	133 (13%)	29 (3%)	4	26
1	B	1040/1069 (97%)	894 (86%)	116 (11%)	30 (3%)	3	26
1	C	1042/1069 (98%)	901 (86%)	114 (11%)	27 (3%)	4	27
1	D	1042/1069 (98%)	888 (85%)	126 (12%)	28 (3%)	4	27
1	E	1040/1069 (97%)	895 (86%)	119 (11%)	26 (2%)	4	28
1	F	1042/1069 (98%)	884 (85%)	132 (13%)	26 (2%)	4	28
All	All	6248/6414 (97%)	5342 (86%)	740 (12%)	166 (3%)	4	27

All (166) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	GLN
1	A	508	GLY
1	A	638	PRO
1	A	833	PRO
1	A	871	ASN
1	B	216	ALA
1	B	360	GLN
1	B	377	LEU
1	B	507	GLU
1	B	509	LYS
1	B	516	PHE
1	B	638	PRO
1	B	673	GLU
1	B	893	GLU
1	B	1035	ARG
1	B	1040	ILE
1	C	216	ALA
1	C	360	GLN
1	C	836	SER
1	C	871	ASN

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Mol	Chain	Res	Type
1	C	1034	SER
1	D	133	SER
1	D	170	SER
1	D	216	ALA
1	D	360	GLN
1	D	638	PRO
1	D	674	LEU
1	D	820	ASN
1	D	1037	ASN
1	D	1042	HIS
1	E	360	GLN
1	E	516	PHE
1	E	638	PRO
1	E	820	ASN
1	E	893	GLU
1	E	1034	SER
1	F	216	ALA
1	F	360	GLN
1	F	439	GLN
1	F	871	ASN
1	F	1034	SER
1	F	1042	HIS
1	A	216	ALA
1	A	509	LYS
1	A	675	GLY
1	A	1036	LYS
1	A	1037	ASN
1	B	215	ALA
1	B	508	GLY
1	B	675	GLY
1	B	1038	GLU
1	C	6	ILE
1	C	511	GLY
1	C	835	LYS
1	D	390	ILE
1	D	508	GLY
1	D	677	ALA
1	D	871	ASN
1	D	1036	LYS
1	E	99	ASP
1	E	216	ALA
1	E	391	ASN

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Mol	Chain	Res	Type
1	E	673	GLU
1	E	1035	ARG
1	E	1040	ILE
1	E	1042	HIS
1	F	99	ASP
1	F	440	GLY
1	F	507	GLU
1	F	512	PHE
1	F	679	GLY
1	F	820	ASN
1	F	870	GLY
1	A	133	SER
1	A	215	ALA
1	A	674	LEU
1	A	1035	ARG
1	B	376	LEU
1	B	378	GLY
1	B	672	VAL
1	B	689	GLY
1	B	1034	SER
1	C	146	ASP
1	C	195	LYS
1	C	505	HIS
1	C	507	GLU
1	C	512	PHE
1	C	638	PRO
1	C	765	ARG
1	D	163	LYS
1	D	204	ILE
1	D	208	LYS
1	D	507	GLU
1	D	923	ASN
1	E	1038	GLU
1	F	376	LEU
1	F	638	PRO
1	F	923	ASN
1	A	208	LYS
1	A	226	LYS
1	A	506	GLY
1	A	568	ASP
1	A	775	SER
1	A	923	ASN

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Mol	Chain	Res	Type
1	B	163	LYS
1	C	204	ILE
1	C	215	ALA
1	C	568	ASP
1	C	1042	HIS
1	D	735	LYS
1	D	1043	SER
1	E	16	ALA
1	E	134	SER
1	F	163	LYS
1	F	765	ARG
1	F	833	PRO
1	F	1037	ASN
1	A	765	ARG
1	A	995	ALA
1	B	134	SER
1	B	735	LYS
1	B	736	ALA
1	B	995	ALA
1	B	1037	ASN
1	D	568	ASP
1	D	765	ARG
1	D	834	GLY
1	E	135	SER
1	E	163	LYS
1	E	208	LYS
1	E	376	LEU
1	E	923	ASN
1	E	995	ALA
1	E	1036	LYS
1	F	836	SER
1	F	995	ALA
1	A	99	ASP
1	A	376	LEU
1	A	439	GLN
1	A	639	GLY
1	B	321	LEU
1	B	807	SER
1	C	5	PHE
1	C	134	SER
1	C	226	LYS
1	D	376	LEU

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Mol	Chain	Res	Type
1	D	427	PRO
1	E	736	ALA
1	F	147	GLY
1	F	208	LYS
1	F	390	ILE
1	A	204	ILE
1	A	691	GLY
1	C	834	GLY
1	C	1016	VAL
1	E	672	VAL
1	D	221	GLY
1	E	204	ILE
1	B	204	ILE
1	B	427	PRO
1	C	390	ILE
1	C	639	GLY
1	A	834	GLY
1	C	675	GLY
1	D	506	GLY
1	F	511	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	849/871 (98%)	739 (87%)	110 (13%)	4	21
1	B	847/871 (97%)	746 (88%)	101 (12%)	5	24
1	C	849/871 (98%)	734 (86%)	115 (14%)	4	21
1	D	849/871 (98%)	728 (86%)	121 (14%)	3	18
1	E	847/871 (97%)	717 (85%)	130 (15%)	3	16
1	F	849/871 (98%)	727 (86%)	122 (14%)	3	18
All	All	5090/5226 (97%)	4391 (86%)	699 (14%)	3	20

All (699) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	10	ILE
1	A	44	THR
1	A	48	SER
1	A	57	VAL
1	A	61	VAL
1	A	65	ILE
1	A	67	GLN
1	A	76	MET
1	A	91	THR
1	A	104	GLN
1	A	107	VAL
1	A	111	LEU
1	A	150	THR
1	A	151	GLN
1	A	152	GLU
1	A	153	ASP
1	A	155	SER
1	A	166	ILE
1	A	177	LEU
1	A	193	LEU
1	A	195	LYS
1	A	203	VAL
1	A	205	THR
1	A	207	ILE
1	A	218	GLN
1	A	244	GLU
1	A	255	GLN
1	A	270	LEU
1	A	278	ILE
1	A	293	LEU
1	A	307	ARG
1	A	341	VAL
1	A	343	THR
1	A	353	LEU
1	A	360	GLN
1	A	362	PHE
1	A	365	THR
1	A	410	ILE
1	A	411	VAL
1	A	428	LYS
1	A	478	MET
1	A	492	LEU

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Mol	Chain	Res	Type
1	A	500	ILE
1	A	502	LYS
1	A	524	THR
1	A	538	THR
1	A	547	ILE
1	A	549	VAL
1	A	550	VAL
1	A	585	GLU
1	A	590	VAL
1	A	600	THR
1	A	602	GLU
1	A	623	ASN
1	A	626	ILE
1	A	629	VAL
1	A	633	ASP
1	A	644	VAL
1	A	658	ILE
1	A	659	LYS
1	A	662	MET
1	A	666	PHE
1	A	671	ILE
1	A	674	LEU
1	A	680	PHE
1	A	686	ASP
1	A	687	GLN
1	A	696	THR
1	A	703	LEU
1	A	711	ASP
1	A	713	LEU
1	A	716	VAL
1	A	723	ASP
1	A	741	VAL
1	A	748	THR
1	A	761	ASP
1	A	786	ILE
1	A	801	PHE
1	A	804	PHE
1	A	842	GLU
1	A	843	LEU
1	A	849	SER
1	A	850	LYS
1	A	864	TYR

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Mol	Chain	Res	Type
1	A	865	GLN
1	A	867	ARG
1	A	876	LEU
1	A	879	ILE
1	A	883	VAL
1	A	904	VAL
1	A	914	LEU
1	A	921	LEU
1	A	925	VAL
1	A	943	ILE
1	A	968	VAL
1	A	970	MET
1	A	971	ARG
1	A	976	LEU
1	A	980	LEU
1	A	984	LEU
1	A	990	VAL
1	A	991	ILE
1	A	1007	VAL
1	A	1015	THR
1	A	1024	VAL
1	A	1029	VAL
1	A	1030	ARG
1	A	1035	ARG
1	A	1038	GLU
1	B	10	ILE
1	B	13	TRP
1	B	25	LEU
1	B	27	ILE
1	B	57	VAL
1	B	60	THR
1	B	61	VAL
1	B	67	GLN
1	B	68	ASN
1	B	72	ILE
1	B	76	MET
1	B	83	ASP
1	B	88	VAL
1	B	111	LEU
1	B	153	ASP
1	B	166	ILE
1	B	177	LEU

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Mol	Chain	Res	Type
1	B	193	LEU
1	B	195	LYS
1	B	200	PRO
1	B	203	VAL
1	B	222	THR
1	B	255	GLN
1	B	259	ARG
1	B	265	VAL
1	B	270	LEU
1	B	277	ILE
1	B	278	ILE
1	B	307	ARG
1	B	314	GLU
1	B	327	TYR
1	B	334	LYS
1	B	341	VAL
1	B	343	THR
1	B	349	ILE
1	B	353	LEU
1	B	355	MET
1	B	363	ARG
1	B	365	THR
1	B	372	VAL
1	B	400	LEU
1	B	402	ILE
1	B	410	ILE
1	B	418	ARG
1	B	432	ARG
1	B	459	PHE
1	B	492	LEU
1	B	496	MET
1	B	523	SER
1	B	524	THR
1	B	542	LEU
1	B	563	PHE
1	B	564	LEU
1	B	569	GLN
1	B	590	VAL
1	B	592	ASN
1	B	617	PHE
1	B	626	ILE
1	B	630	SER

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Mol	Chain	Res	Type
1	B	634	TRP
1	B	652	THR
1	B	672	VAL
1	B	674	LEU
1	B	686	ASP
1	B	687	GLN
1	B	690	LEU
1	B	696	THR
1	B	721	LEU
1	B	723	ASP
1	B	730	ASP
1	B	743	ILE
1	B	764	ASP
1	B	792	ARG
1	B	804	PHE
1	B	827	ILE
1	B	842	GLU
1	B	843	LEU
1	B	849	SER
1	B	867	ARG
1	B	881	LEU
1	B	886	LEU
1	B	888	LEU
1	B	914	LEU
1	B	924	ASP
1	B	925	VAL
1	B	931	LEU
1	B	943	ILE
1	B	971	ARG
1	B	978	THR
1	B	980	LEU
1	B	984	LEU
1	B	990	VAL
1	B	991	ILE
1	B	993	THR
1	B	1007	VAL
1	B	1015	THR
1	B	1016	VAL
1	B	1017	LEU
1	B	1024	VAL
1	B	1030	ARG
1	B	1040	ILE

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Mol	Chain	Res	Type
1	C	6	ILE
1	C	7	ASP
1	C	13	TRP
1	C	27	ILE
1	C	59	ASP
1	C	61	VAL
1	C	62	THR
1	C	68	ASN
1	C	91	THR
1	C	93	THR
1	C	102	ILE
1	C	104	GLN
1	C	111	LEU
1	C	113	LEU
1	C	120	GLN
1	C	164	ASP
1	C	166	ILE
1	C	177	LEU
1	C	180	SER
1	C	199	THR
1	C	203	VAL
1	C	207	ILE
1	C	218	GLN
1	C	253	VAL
1	C	255	GLN
1	C	263	ARG
1	C	268	ILE
1	C	269	GLU
1	C	270	LEU
1	C	274	ASN
1	C	275	TYR
1	C	278	ILE
1	C	289	LEU
1	C	307	ARG
1	C	322	LYS
1	C	341	VAL
1	C	343	THR
1	C	349	ILE
1	C	350	LEU
1	C	353	LEU
1	C	355	MET
1	C	362	PHE

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Mol	Chain	Res	Type
1	C	363	ARG
1	C	443	VAL
1	C	447	MET
1	C	456	MET
1	C	463	THR
1	C	472	ILE
1	C	482	VAL
1	C	492	LEU
1	C	500	ILE
1	C	509	LYS
1	C	510	LYS
1	C	524	THR
1	C	526	HIS
1	C	546	LEU
1	C	550	VAL
1	C	555	LEU
1	C	559	LEU
1	C	564	LEU
1	C	590	VAL
1	C	593	GLU
1	C	600	THR
1	C	603	LYS
1	C	623	ASN
1	C	626	ILE
1	C	644	VAL
1	C	659	LYS
1	C	663	VAL
1	C	668	LEU
1	C	673	GLU
1	C	674	LEU
1	C	678	THR
1	C	686	ASP
1	C	687	GLN
1	C	695	LEU
1	C	696	THR
1	C	708	LYS
1	C	711	ASP
1	C	713	LEU
1	C	721	LEU
1	C	723	ASP
1	C	730	ASP
1	C	741	VAL

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Mol	Chain	Res	Type
1	C	749	THR
1	C	786	ILE
1	C	804	PHE
1	C	813	SER
1	C	843	LEU
1	C	847	LEU
1	C	850	LYS
1	C	860	THR
1	C	862	MET
1	C	865	GLN
1	C	880	SER
1	C	883	VAL
1	C	886	LEU
1	C	887	CYS
1	C	895	TRP
1	C	914	LEU
1	C	921	LEU
1	C	931	LEU
1	C	943	ILE
1	C	945	ILE
1	C	970	MET
1	C	971	ARG
1	C	980	LEU
1	C	984	LEU
1	C	990	VAL
1	C	1011	MET
1	C	1024	VAL
1	C	1030	ARG
1	C	1032	ARG
1	C	1035	ARG
1	C	1041	GLU
1	D	6	ILE
1	D	8	ARG
1	D	10	ILE
1	D	17	ILE
1	D	27	ILE
1	D	30	LEU
1	D	34	GLN
1	D	57	VAL
1	D	61	VAL
1	D	89	GLN
1	D	102	ILE

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Mol	Chain	Res	Type
1	D	105	VAL
1	D	107	VAL
1	D	109	ASN
1	D	111	LEU
1	D	138	MET
1	D	140	VAL
1	D	151	GLN
1	D	166	ILE
1	D	177	LEU
1	D	193	LEU
1	D	195	LYS
1	D	203	VAL
1	D	205	THR
1	D	207	ILE
1	D	214	VAL
1	D	218	GLN
1	D	222	THR
1	D	238	THR
1	D	244	GLU
1	D	253	VAL
1	D	255	GLN
1	D	263	ARG
1	D	270	LEU
1	D	293	LEU
1	D	330	THR
1	D	337	ILE
1	D	341	VAL
1	D	343	THR
1	D	350	LEU
1	D	353	LEU
1	D	357	LEU
1	D	358	PHE
1	D	360	GLN
1	D	365	THR
1	D	372	VAL
1	D	391	ASN
1	D	395	MET
1	D	402	ILE
1	D	416	VAL
1	D	429	GLU
1	D	448	VAL
1	D	478	MET

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Mol	Chain	Res	Type
1	D	492	LEU
1	D	500	ILE
1	D	502	LYS
1	D	509	LYS
1	D	524	THR
1	D	538	THR
1	D	550	VAL
1	D	559	LEU
1	D	564	LEU
1	D	578	LEU
1	D	589	LYS
1	D	590	VAL
1	D	599	LEU
1	D	602	GLU
1	D	603	LYS
1	D	623	ASN
1	D	629	VAL
1	D	633	ASP
1	D	634	TRP
1	D	644	VAL
1	D	658	ILE
1	D	659	LYS
1	D	662	MET
1	D	672	VAL
1	D	674	LEU
1	D	680	PHE
1	D	687	GLN
1	D	694	LYS
1	D	696	THR
1	D	713	LEU
1	D	716	VAL
1	D	721	LEU
1	D	723	ASP
1	D	786	ILE
1	D	791	VAL
1	D	804	PHE
1	D	842	GLU
1	D	843	LEU
1	D	864	TYR
1	D	867	ARG
1	D	876	LEU
1	D	886	LEU

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Mol	Chain	Res	Type
1	D	888	LEU
1	D	900	SER
1	D	907	LEU
1	D	913	LEU
1	D	914	LEU
1	D	932	LEU
1	D	933	THR
1	D	940	LYS
1	D	943	ILE
1	D	950	LYS
1	D	951	ASP
1	D	971	ARG
1	D	973	ARG
1	D	980	LEU
1	D	990	VAL
1	D	993	THR
1	D	1007	VAL
1	D	1011	MET
1	D	1015	THR
1	D	1016	VAL
1	D	1024	VAL
1	D	1035	ARG
1	D	1038	GLU
1	D	1040	ILE
1	D	1044	HIS
1	D	1045	THR
1	E	6	ILE
1	E	10	ILE
1	E	14	VAL
1	E	20	MET
1	E	27	ILE
1	E	32	VAL
1	E	57	VAL
1	E	60	THR
1	E	65	ILE
1	E	68	ASN
1	E	69	MET
1	E	76	MET
1	E	90	ILE
1	E	91	THR
1	E	105	VAL
1	E	111	LEU

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Mol	Chain	Res	Type
1	E	118	LEU
1	E	150	THR
1	E	151	GLN
1	E	153	ASP
1	E	166	ILE
1	E	177	LEU
1	E	182	TYR
1	E	189	ASN
1	E	193	LEU
1	E	195	LYS
1	E	203	VAL
1	E	207	ILE
1	E	214	VAL
1	E	218	GLN
1	E	235	ILE
1	E	239	ARG
1	E	249	ILE
1	E	253	VAL
1	E	255	GLN
1	E	259	ARG
1	E	270	LEU
1	E	277	ILE
1	E	278	ILE
1	E	293	LEU
1	E	307	ARG
1	E	313	MET
1	E	314	GLU
1	E	324	VAL
1	E	329	THR
1	E	336	SER
1	E	341	VAL
1	E	343	THR
1	E	345	VAL
1	E	353	LEU
1	E	355	MET
1	E	357	LEU
1	E	363	ARG
1	E	372	VAL
1	E	382	VAL
1	E	389	SER
1	E	393	LEU
1	E	395	MET

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Mol	Chain	Res	Type
1	E	410	ILE
1	E	418	ARG
1	E	433	LYS
1	E	456	MET
1	E	472	ILE
1	E	484	VAL
1	E	492	LEU
1	E	496	MET
1	E	519	MET
1	E	536	ARG
1	E	546	LEU
1	E	547	ILE
1	E	550	VAL
1	E	555	LEU
1	E	558	ARG
1	E	563	PHE
1	E	564	LEU
1	E	569	GLN
1	E	571	VAL
1	E	583	THR
1	E	590	VAL
1	E	600	THR
1	E	601	LYS
1	E	626	ILE
1	E	630	SER
1	E	633	ASP
1	E	634	TRP
1	E	640	GLU
1	E	644	VAL
1	E	659	LYS
1	E	662	MET
1	E	666	PHE
1	E	668	LEU
1	E	672	VAL
1	E	680	PHE
1	E	694	LYS
1	E	696	THR
1	E	711	ASP
1	E	713	LEU
1	E	721	LEU
1	E	730	ASP
1	E	743	ILE

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Mol	Chain	Res	Type
1	E	782	LEU
1	E	786	ILE
1	E	804	PHE
1	E	815	ARG
1	E	842	GLU
1	E	843	LEU
1	E	850	LYS
1	E	871	ASN
1	E	876	LEU
1	E	879	ILE
1	E	886	LEU
1	E	887	CYS
1	E	900	SER
1	E	905	VAL
1	E	910	ILE
1	E	914	LEU
1	E	921	LEU
1	E	925	VAL
1	E	935	ILE
1	E	943	ILE
1	E	947	GLU
1	E	968	VAL
1	E	973	ARG
1	E	980	LEU
1	E	991	ILE
1	E	1007	VAL
1	E	1024	VAL
1	E	1027	VAL
1	E	1035	ARG
1	E	1037	ASN
1	F	3	ASN
1	F	6	ILE
1	F	10	ILE
1	F	17	ILE
1	F	27	ILE
1	F	37	THR
1	F	44	THR
1	F	45	ILE
1	F	57	VAL
1	F	59	ASP
1	F	60	THR
1	F	62	THR

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Mol	Chain	Res	Type
1	F	70	ASN
1	F	76	MET
1	F	90	ILE
1	F	91	THR
1	F	92	LEU
1	F	94	PHE
1	F	99	ASP
1	F	101	ASP
1	F	125	GLN
1	F	132	SER
1	F	166	ILE
1	F	177	LEU
1	F	193	LEU
1	F	203	VAL
1	F	205	THR
1	F	235	ILE
1	F	253	VAL
1	F	270	LEU
1	F	278	ILE
1	F	300	LEU
1	F	307	ARG
1	F	312	LYS
1	F	337	ILE
1	F	339	GLU
1	F	341	VAL
1	F	343	THR
1	F	350	LEU
1	F	353	LEU
1	F	358	PHE
1	F	393	LEU
1	F	402	ILE
1	F	412	VAL
1	F	419	VAL
1	F	429	GLU
1	F	431	THR
1	F	456	MET
1	F	472	ILE
1	F	478	MET
1	F	482	VAL
1	F	489	THR
1	F	492	LEU
1	F	502	LYS

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Mol	Chain	Res	Type
1	F	509	LYS
1	F	510	LYS
1	F	517	ASN
1	F	519	MET
1	F	524	THR
1	F	526	HIS
1	F	538	THR
1	F	540	ARG
1	F	544	LEU
1	F	559	LEU
1	F	571	VAL
1	F	585	GLU
1	F	586	ARG
1	F	590	VAL
1	F	600	THR
1	F	617	PHE
1	F	623	ASN
1	F	626	ILE
1	F	629	VAL
1	F	630	SER
1	F	633	ASP
1	F	644	VAL
1	F	659	LYS
1	F	668	LEU
1	F	672	VAL
1	F	680	PHE
1	F	686	ASP
1	F	694	LYS
1	F	696	THR
1	F	713	LEU
1	F	716	VAL
1	F	723	ASP
1	F	731	ILE
1	F	743	ILE
1	F	746	ILE
1	F	749	THR
1	F	767	ARG
1	F	768	VAL
1	F	804	PHE
1	F	827	ILE
1	F	843	LEU
1	F	847	LEU

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Mol	Chain	Res	Type
1	F	862	MET
1	F	863	SER
1	F	865	GLN
1	F	866	GLU
1	F	883	VAL
1	F	884	VAL
1	F	895	TRP
1	F	910	ILE
1	F	914	LEU
1	F	921	LEU
1	F	925	VAL
1	F	931	LEU
1	F	935	ILE
1	F	940	LYS
1	F	950	LYS
1	F	961	ILE
1	F	968	VAL
1	F	971	ARG
1	F	980	LEU
1	F	984	LEU
1	F	990	VAL
1	F	991	ILE
1	F	1007	VAL
1	F	1011	MET
1	F	1024	VAL
1	F	1032	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	63	GLN
1	A	125	GLN
1	A	151	GLN
1	A	161	ASN
1	A	194	ASN
1	A	211	ASN
1	A	218	GLN
1	A	525	HIS
1	A	592	ASN
1	A	622	GLN
1	A	642	ASN

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Mol	Chain	Res	Type
1	A	719	ASN
1	A	865	GLN
1	B	125	GLN
1	B	189	ASN
1	B	191	ASN
1	B	210	GLN
1	B	360	GLN
1	B	525	HIS
1	B	642	ASN
1	B	1000	GLN
1	B	1037	ASN
1	C	112	GLN
1	C	211	ASN
1	C	231	ASN
1	C	577	GLN
1	C	588	GLN
1	C	592	ASN
1	C	733	GLN
1	C	928	GLN
1	D	74	ASN
1	D	108	GLN
1	D	109	ASN
1	D	123	GLN
1	D	231	ASN
1	D	517	ASN
1	D	526	HIS
1	D	577	GLN
1	D	584	GLN
1	D	588	GLN
1	D	605	ASN
1	D	642	ASN
1	D	719	ASN
1	D	744	ASN
1	D	865	GLN
1	E	34	GLN
1	E	104	GLN
1	E	106	GLN
1	E	108	GLN
1	E	112	GLN
1	E	125	GLN
1	E	211	ASN
1	E	213	GLN

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Mol	Chain	Res	Type
1	E	255	GLN
1	E	338	HIS
1	E	604	ASN
1	E	667	ASN
1	E	744	ASN
1	E	846	GLN
1	E	865	GLN
1	F	70	ASN
1	F	437	GLN
1	F	517	ASN
1	F	588	GLN
1	F	592	ASN
1	F	719	ASN
1	F	760	ASN
1	F	820	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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
2	LMT	E	2000	-	36,36,36	1.85	9 (25%)	47,47,47	1.40	8 (17%)
2	LMT	F	2000	-	36,36,36	1.90	10 (27%)	47,47,47	1.53	9 (19%)
2	LMT	B	2000	-	36,36,36	1.94	10 (27%)	47,47,47	1.29	7 (14%)
2	LMT	C	2000	-	36,36,36	1.80	9 (25%)	47,47,47	1.76	10 (21%)
2	LMT	A	2000	-	36,36,36	2.01	10 (27%)	47,47,47	1.57	11 (23%)
2	LMT	D	2000	-	36,36,36	2.01	9 (25%)	47,47,47	1.35	6 (12%)

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
2	LMT	E	2000	-	2/2/10/10	10/21/61/61	0/2/2/2
2	LMT	F	2000	-	3/3/10/10	12/21/61/61	0/2/2/2
2	LMT	B	2000	-	1/1/10/10	13/21/61/61	0/2/2/2
2	LMT	C	2000	-	3/3/10/10	6/21/61/61	0/2/2/2
2	LMT	A	2000	-	2/2/10/10	14/21/61/61	0/2/2/2
2	LMT	D	2000	-	2/2/10/10	11/21/61/61	0/2/2/2

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2000	LMT	O5'-C5'	4.95	1.56	1.44
2	D	2000	LMT	O1'-C1'	4.76	1.48	1.40
2	B	2000	LMT	O1'-C1'	4.70	1.48	1.40
2	A	2000	LMT	O1'-C1'	4.53	1.47	1.40
2	E	2000	LMT	O5'-C5'	4.43	1.55	1.44
2	D	2000	LMT	O5'-C5'	4.35	1.55	1.44
2	E	2000	LMT	O1'-C1'	4.15	1.47	1.40
2	F	2000	LMT	O5B-C1B	4.15	1.52	1.41
2	F	2000	LMT	O1'-C1'	4.09	1.47	1.40
2	C	2000	LMT	O1'-C1'	4.08	1.47	1.40
2	B	2000	LMT	O5B-C1B	4.03	1.52	1.41
2	F	2000	LMT	O5'-C5'	4.02	1.54	1.44
2	D	2000	LMT	O5'-C1'	3.97	1.52	1.41
2	A	2000	LMT	O5'-C1'	3.94	1.52	1.41
2	C	2000	LMT	C6'-C5'	-3.93	1.38	1.51
2	A	2000	LMT	O5B-C1B	3.91	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2000	LMT	O5B-C1B	3.72	1.51	1.41
2	B	2000	LMT	O5'-C5'	3.67	1.53	1.44
2	E	2000	LMT	O5'-C1'	3.66	1.51	1.41
2	D	2000	LMT	C6'-C5'	-3.60	1.39	1.51
2	C	2000	LMT	O5B-C1B	3.54	1.51	1.41
2	B	2000	LMT	O3B-C3B	3.36	1.51	1.43
2	B	2000	LMT	C6'-C5'	-3.34	1.40	1.51
2	F	2000	LMT	C6'-C5'	-3.32	1.40	1.51
2	A	2000	LMT	C6'-C5'	-3.31	1.40	1.51
2	F	2000	LMT	O5'-C1'	3.30	1.50	1.41
2	E	2000	LMT	O5B-C1B	3.28	1.50	1.41
2	C	2000	LMT	O5'-C5'	3.27	1.52	1.44
2	E	2000	LMT	C6'-C5'	-3.19	1.41	1.51
2	C	2000	LMT	O2'-C2'	2.98	1.50	1.43
2	B	2000	LMT	O5'-C1'	2.97	1.49	1.41
2	D	2000	LMT	O3B-C3B	2.92	1.50	1.43
2	C	2000	LMT	O3B-C3B	2.82	1.49	1.43
2	E	2000	LMT	O3B-C3B	2.81	1.49	1.43
2	F	2000	LMT	C3B-C2B	-2.79	1.45	1.52
2	F	2000	LMT	O3B-C3B	2.74	1.49	1.43
2	D	2000	LMT	O2'-C2'	2.73	1.49	1.43
2	C	2000	LMT	O5'-C1'	2.66	1.48	1.41
2	E	2000	LMT	C3'-C2'	-2.63	1.45	1.52
2	A	2000	LMT	O3B-C3B	2.36	1.48	1.43
2	A	2000	LMT	C5-C4	2.35	1.63	1.51
2	F	2000	LMT	O2'-C2'	2.34	1.48	1.43
2	F	2000	LMT	C3'-C2'	-2.31	1.46	1.52
2	B	2000	LMT	C3B-C2B	-2.25	1.46	1.52
2	A	2000	LMT	O2'-C2'	2.25	1.48	1.43
2	C	2000	LMT	C3B-C2B	-2.25	1.46	1.52
2	D	2000	LMT	C3'-C2'	-2.25	1.46	1.52
2	E	2000	LMT	O2'-C2'	2.25	1.48	1.43
2	A	2000	LMT	C3'-C2'	-2.22	1.46	1.52
2	F	2000	LMT	C5-C4	2.21	1.62	1.51
2	D	2000	LMT	C5-C4	2.18	1.62	1.51
2	B	2000	LMT	C5-C4	2.18	1.62	1.51
2	C	2000	LMT	C5-C4	2.13	1.62	1.51
2	E	2000	LMT	C5-C4	2.11	1.62	1.51
2	B	2000	LMT	O2'-C2'	2.09	1.48	1.43
2	A	2000	LMT	C8-C7	2.08	1.62	1.51
2	B	2000	LMT	C2-C1	2.02	1.59	1.51

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2000	LMT	C2'-C3'-C4'	5.24	121.58	109.68
2	F	2000	LMT	O1'-C1'-C2'	4.92	115.75	108.27
2	C	2000	LMT	O1'-C1'-C2'	4.17	114.61	108.27
2	D	2000	LMT	C1'-O5'-C5'	3.87	121.28	113.72
2	E	2000	LMT	C1B-O1B-C4'	-3.78	109.02	117.98
2	C	2000	LMT	O1B-C1B-C2B	3.72	117.24	108.09
2	B	2000	LMT	O1'-C1'-C2'	3.66	113.83	108.27
2	A	2000	LMT	O5B-C5B-C4B	3.50	116.01	109.70
2	F	2000	LMT	O5B-C5B-C4B	3.41	115.85	109.70
2	C	2000	LMT	C1'-C2'-C3'	3.40	117.17	110.01
2	F	2000	LMT	C1B-O5B-C5B	3.19	119.95	113.72
2	A	2000	LMT	O1B-C1B-C2B	3.15	115.83	108.09
2	A	2000	LMT	C3B-C4B-C5B	3.05	115.77	110.23
2	A	2000	LMT	O1B-C4'-C3'	3.02	114.91	107.23
2	A	2000	LMT	O5'-C5'-C6'	2.98	113.83	106.44
2	D	2000	LMT	O5'-C5'-C4'	2.94	115.80	109.72
2	C	2000	LMT	O6'-C6'-C5'	-2.93	101.35	111.33
2	C	2000	LMT	C6B-C5B-C4B	-2.88	105.94	113.02
2	B	2000	LMT	C4B-C3B-C2B	-2.84	105.84	110.83
2	F	2000	LMT	C1B-O1B-C4'	-2.84	111.26	117.98
2	A	2000	LMT	C6'-C5'-C4'	-2.81	105.47	113.38
2	F	2000	LMT	O1B-C1B-C2B	2.70	114.72	108.09
2	F	2000	LMT	C4B-C3B-C2B	-2.69	106.10	110.83
2	D	2000	LMT	O5B-C5B-C4B	2.68	114.52	109.70
2	F	2000	LMT	O2B-C2B-C3B	-2.63	104.18	110.38
2	E	2000	LMT	O1B-C4'-C3'	2.62	113.88	107.23
2	D	2000	LMT	O4'-C4B-C5B	2.55	115.61	109.32
2	E	2000	LMT	O5'-C5'-C6'	2.53	112.72	106.44
2	A	2000	LMT	O5'-C1'-O1'	2.53	116.02	110.04
2	C	2000	LMT	C1B-O5B-C5B	-2.49	108.86	113.72
2	B	2000	LMT	C1'-C2'-C3'	2.49	115.24	110.01
2	B	2000	LMT	C2'-C3'-C4'	2.42	115.16	109.68
2	A	2000	LMT	C4B-C3B-C2B	2.37	114.99	110.83
2	E	2000	LMT	C1B-O5B-C5B	-2.33	109.18	113.72
2	E	2000	LMT	O5B-C5B-C6B	2.31	112.17	106.44
2	C	2000	LMT	C1'-O5'-C5'	-2.31	109.21	113.72
2	B	2000	LMT	O5B-C1B-C2B	2.30	115.09	110.37
2	C	2000	LMT	O1B-C4'-C5'	-2.28	103.49	109.48
2	A	2000	LMT	O3B-C3B-C4B	-2.28	105.00	110.38
2	A	2000	LMT	C1B-O1B-C4'	-2.26	112.62	117.98
2	A	2000	LMT	C1-O1'-C1'	2.16	117.37	113.68
2	F	2000	LMT	O2B-C2B-C1B	2.14	115.18	110.08
2	E	2000	LMT	C6'-C5'-C4'	-2.14	107.37	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2000	LMT	O3B-C3B-C2B	2.11	115.35	110.38
2	D	2000	LMT	C6'-C5'-C4'	-2.10	107.48	113.38
2	C	2000	LMT	O2'-C2'-C3'	-2.10	105.43	110.38
2	D	2000	LMT	O1B-C1B-C2B	2.08	113.21	108.09
2	F	2000	LMT	O5B-C1B-C2B	2.07	114.63	110.37
2	B	2000	LMT	O5B-C5B-C6B	2.06	111.54	106.44
2	E	2000	LMT	O5B-C5B-C4B	2.04	113.38	109.70
2	E	2000	LMT	C2'-C3'-C4'	2.03	114.29	109.68

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2000	LMT	C3'
2	A	2000	LMT	C4B
2	B	2000	LMT	C3'
2	C	2000	LMT	C1B
2	C	2000	LMT	C2B
2	C	2000	LMT	C4B
2	D	2000	LMT	C3'
2	D	2000	LMT	C4B
2	E	2000	LMT	C3'
2	E	2000	LMT	C4B
2	F	2000	LMT	C2'
2	F	2000	LMT	C4B
2	F	2000	LMT	C3'

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2000	LMT	C2'-C1'-O1'-C1
2	A	2000	LMT	O5'-C1'-O1'-C1
2	D	2000	LMT	O5'-C1'-O1'-C1
2	E	2000	LMT	O5'-C1'-O1'-C1
2	B	2000	LMT	O5B-C1B-O1B-C4'
2	C	2000	LMT	C2B-C1B-O1B-C4'
2	A	2000	LMT	O5B-C5B-C6B-O6B
2	A	2000	LMT	O5'-C5'-C6'-O6'
2	C	2000	LMT	O5'-C5'-C6'-O6'
2	A	2000	LMT	C4B-C5B-C6B-O6B
2	C	2000	LMT	C4'-C5'-C6'-O6'
2	F	2000	LMT	O5'-C1'-O1'-C1
2	D	2000	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
2	B	2000	LMT	O5B-C5B-C6B-O6B
2	B	2000	LMT	O5'-C5'-C6'-O6'
2	B	2000	LMT	C4'-C5'-C6'-O6'
2	E	2000	LMT	C2'-C1'-O1'-C1
2	F	2000	LMT	C2'-C1'-O1'-C1
2	F	2000	LMT	O5'-C5'-C6'-O6'
2	D	2000	LMT	C4'-C5'-C6'-O6'
2	A	2000	LMT	C4'-C5'-C6'-O6'
2	B	2000	LMT	C4B-C5B-C6B-O6B
2	D	2000	LMT	C7-C8-C9-C10
2	F	2000	LMT	C4'-C5'-C6'-O6'
2	C	2000	LMT	O5'-C1'-O1'-C1
2	B	2000	LMT	C3-C4-C5-C6
2	E	2000	LMT	O5B-C5B-C6B-O6B
2	E	2000	LMT	C2-C1-O1'-C1'
2	F	2000	LMT	C2-C1-O1'-C1'
2	F	2000	LMT	C11-C10-C9-C8
2	F	2000	LMT	C6-C7-C8-C9
2	B	2000	LMT	C6-C7-C8-C9
2	A	2000	LMT	C4-C5-C6-C7
2	A	2000	LMT	C11-C10-C9-C8
2	F	2000	LMT	O5B-C5B-C6B-O6B
2	F	2000	LMT	C9-C10-C11-C12
2	E	2000	LMT	C1-C2-C3-C4
2	E	2000	LMT	C4-C5-C6-C7
2	D	2000	LMT	C2'-C1'-O1'-C1
2	B	2000	LMT	C5-C6-C7-C8
2	B	2000	LMT	C1-C2-C3-C4
2	D	2000	LMT	C6-C7-C8-C9
2	F	2000	LMT	C1-C2-C3-C4
2	B	2000	LMT	C2B-C1B-O1B-C4'
2	D	2000	LMT	C2-C1-O1'-C1'
2	E	2000	LMT	C6-C7-C8-C9
2	F	2000	LMT	O1'-C1-C2-C3
2	A	2000	LMT	C1-C2-C3-C4
2	A	2000	LMT	C5-C6-C7-C8
2	E	2000	LMT	O1'-C1-C2-C3
2	A	2000	LMT	O5B-C1B-O1B-C4'
2	D	2000	LMT	O1'-C1-C2-C3
2	C	2000	LMT	C1-C2-C3-C4
2	B	2000	LMT	C7-C8-C9-C10
2	A	2000	LMT	C7-C8-C9-C10

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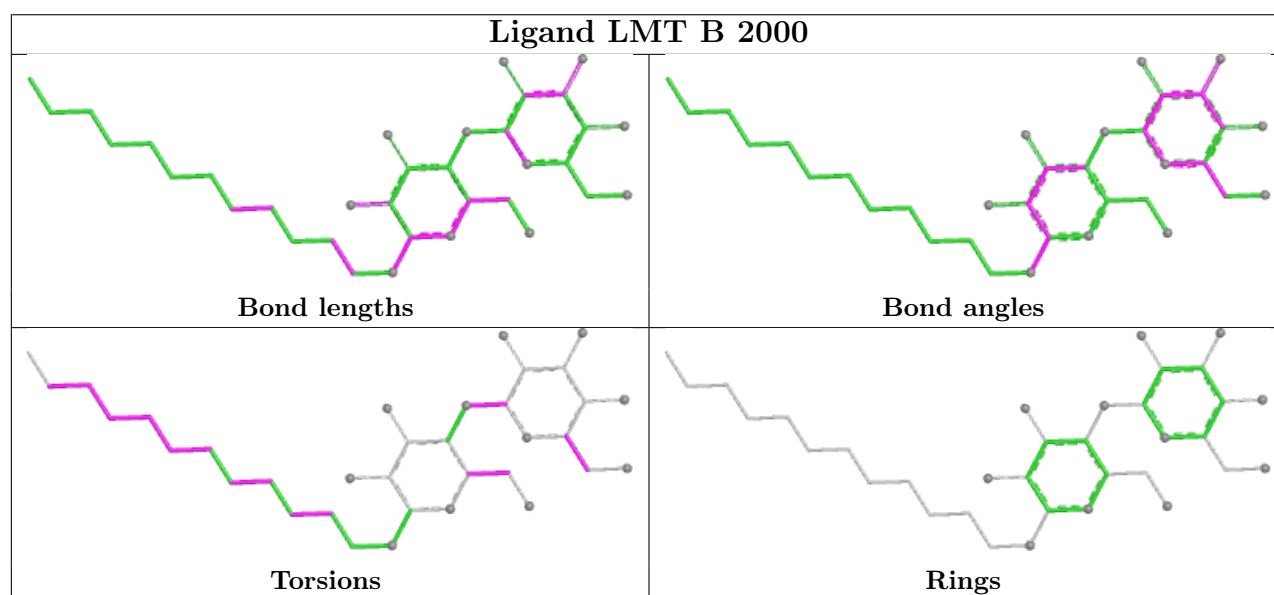
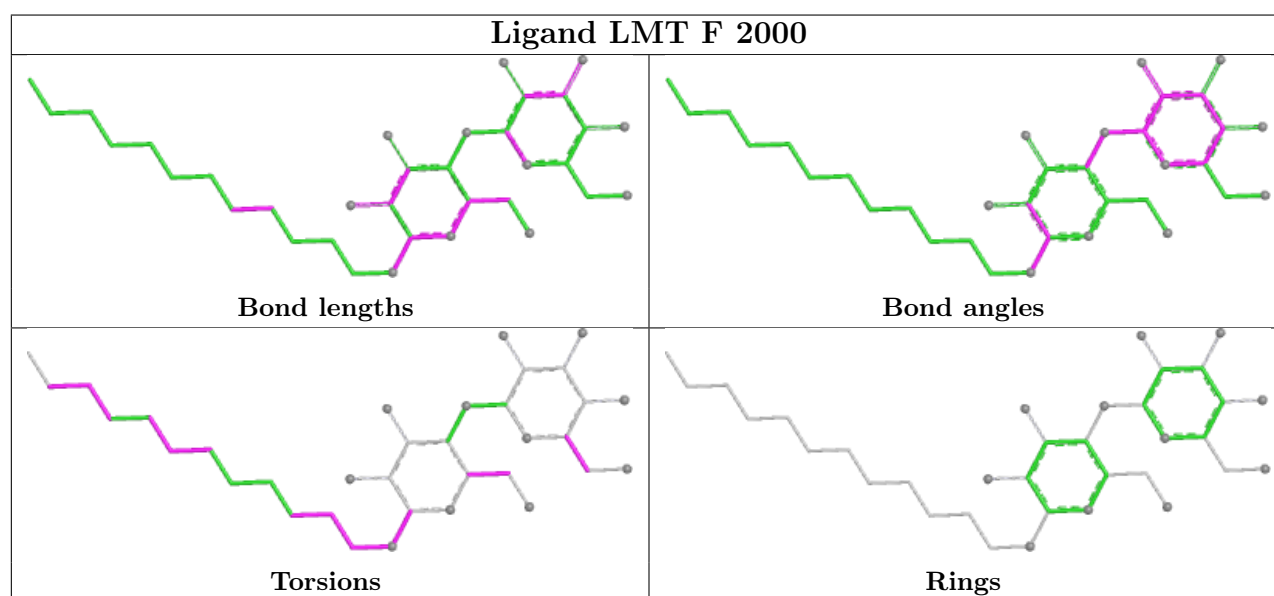
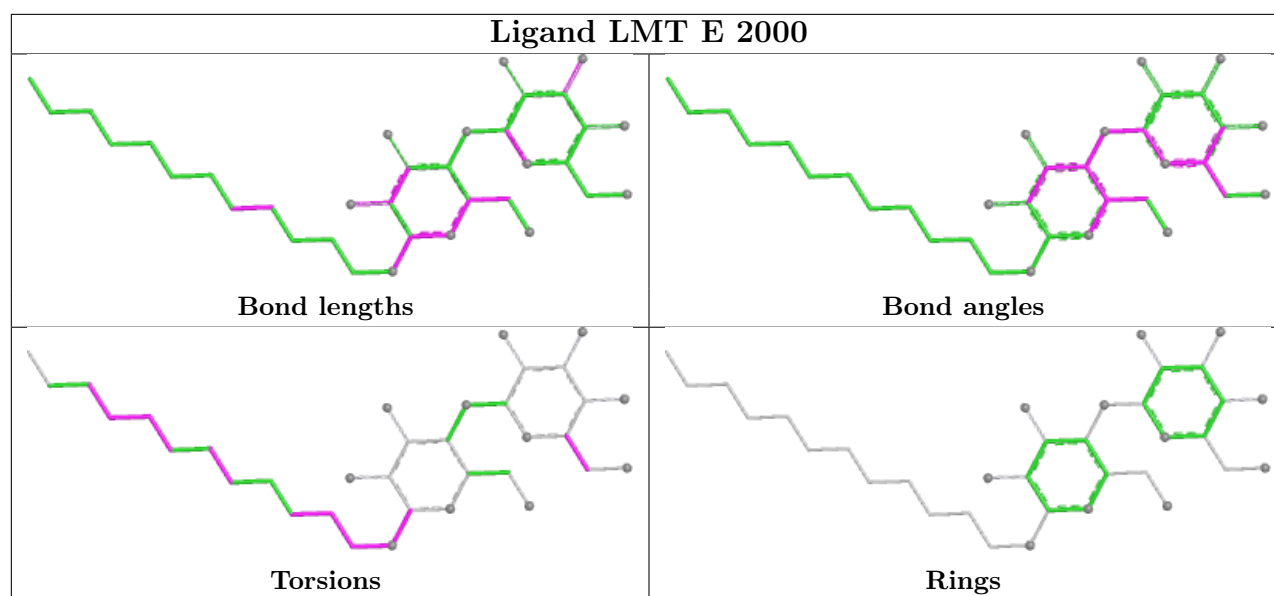
Mol	Chain	Res	Type	Atoms
2	B	2000	LMT	C11-C10-C9-C8
2	B	2000	LMT	C9-C10-C11-C12
2	F	2000	LMT	C5-C6-C7-C8
2	E	2000	LMT	C7-C8-C9-C10
2	D	2000	LMT	O5B-C5B-C6B-O6B
2	A	2000	LMT	O1'-C1-C2-C3
2	E	2000	LMT	C11-C10-C9-C8
2	D	2000	LMT	C3'-C4'-O1B-C1B
2	A	2000	LMT	C3-C4-C5-C6
2	D	2000	LMT	C5'-C4'-O1B-C1B
2	C	2000	LMT	C5-C6-C7-C8

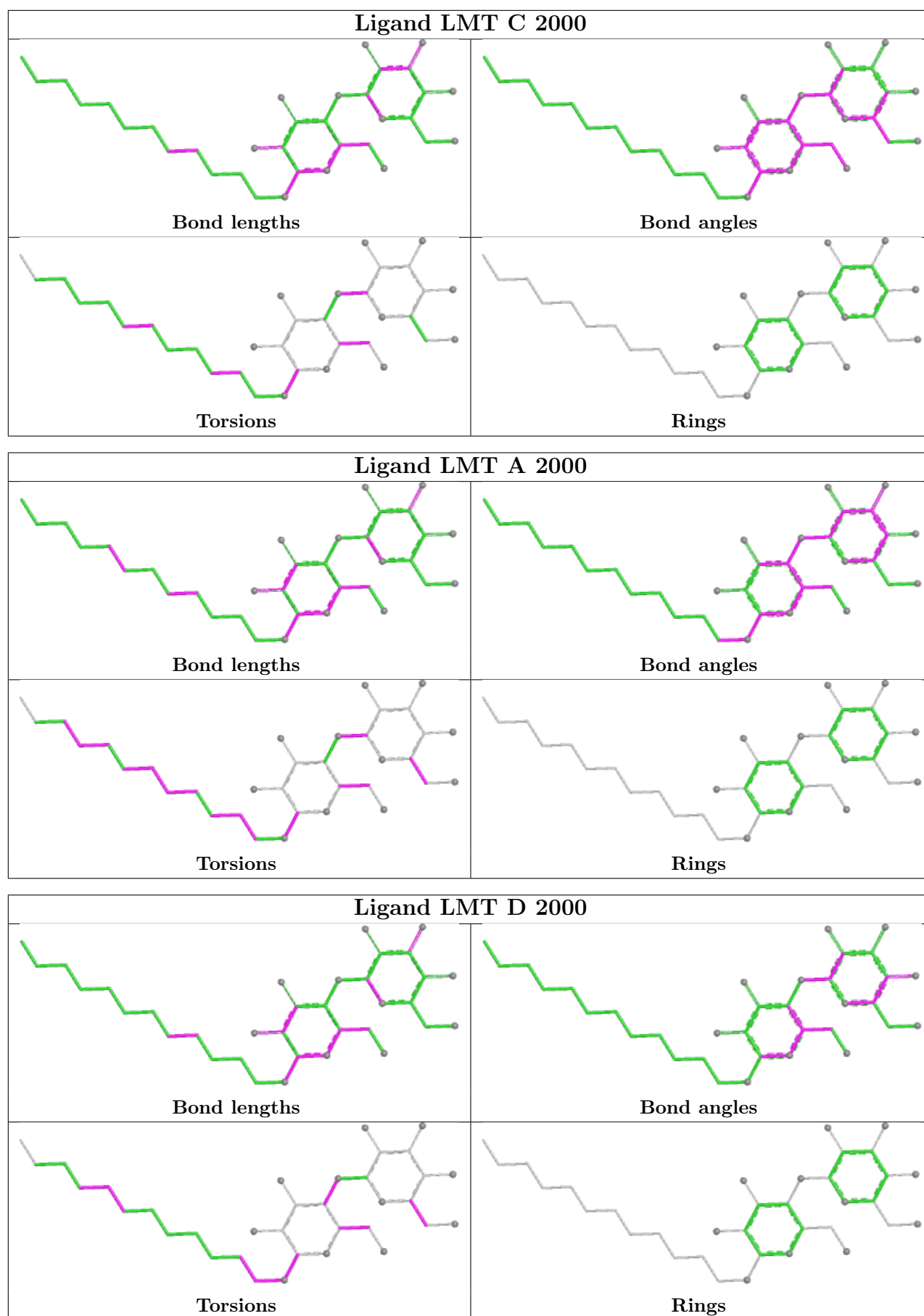
There are no ring outliers.

6 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2000	LMT	6	0
2	F	2000	LMT	2	0
2	B	2000	LMT	12	0
2	C	2000	LMT	5	0
2	A	2000	LMT	1	0
2	D	2000	LMT	3	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	1044/1069 (97%)	-0.28	6 (0%)	85 63	5, 35, 83, 118	0
1	B	1042/1069 (97%)	-0.48	1 (0%)	92 85	3, 27, 62, 108	0
1	C	1044/1069 (97%)	-0.40	1 (0%)	92 85	4, 29, 60, 88	0
1	D	1044/1069 (97%)	-0.18	8 (0%)	82 58	10, 49, 88, 114	0
1	E	1042/1069 (97%)	-0.15	12 (1%)	76 49	5, 46, 100, 129	0
1	F	1044/1069 (97%)	-0.04	29 (2%)	55 30	5, 54, 104, 142	0
All	All	6260/6414 (97%)	-0.26	57 (0%)	81 56	3, 39, 90, 142	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	706	ALA	5.8
1	D	295	THR	4.3
1	F	116	PRO	4.3
1	F	856	GLY	3.8
1	F	848	ALA	3.7
1	D	306	ILE	3.7
1	A	606	VAL	3.6
1	F	494	ALA	3.3
1	E	293	LEU	3.3
1	F	849	SER	3.3
1	E	175	VAL	3.0
1	E	164	ASP	3.0
1	D	706	ALA	3.0
1	A	714	THR	3.0
1	F	49	TYR	2.9
1	F	61	VAL	2.9
1	F	122	VAL	2.9
1	F	310	LEU	2.7
1	A	679	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	840	ALA	2.7
1	F	827	ILE	2.6
1	E	405	LEU	2.6
1	F	118	LEU	2.6
1	E	291	ILE	2.6
1	F	103	ALA	2.5
1	E	292	LYS	2.5
1	D	465	ALA	2.4
1	F	720	GLY	2.4
1	D	678	THR	2.4
1	F	75	LEU	2.4
1	D	310	LEU	2.3
1	E	715	SER	2.3
1	F	698	ALA	2.3
1	F	390	ILE	2.3
1	F	79	SER	2.3
1	A	473	THR	2.3
1	D	33	ALA	2.3
1	F	493	CYS	2.3
1	E	171	GLY	2.3
1	F	65	ILE	2.2
1	F	857	TYR	2.2
1	F	702	LEU	2.2
1	B	514	GLY	2.2
1	F	823	PRO	2.2
1	F	858	ASP	2.1
1	E	72	ILE	2.1
1	F	115	MET	2.1
1	D	64	VAL	2.1
1	A	467	TYR	2.1
1	F	821	GLY	2.1
1	C	402	ILE	2.1
1	E	78	MET	2.1
1	F	173	GLY	2.0
1	E	427	PRO	2.0
1	F	789	TRP	2.0
1	A	825	MET	2.0
1	F	854	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

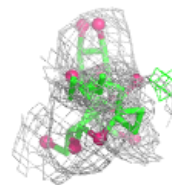
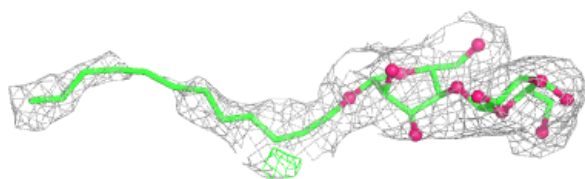
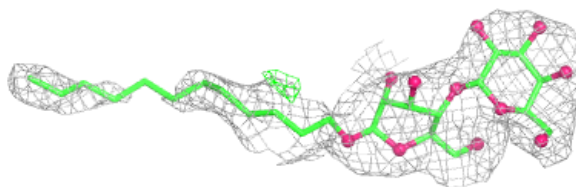
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LMT	A	2000	35/35	0.75	0.11	2,31,49,54	0
2	LMT	B	2000	35/35	0.77	0.10	6,32,47,61	0
2	LMT	E	2000	35/35	0.78	0.11	3,34,48,49	0
2	LMT	D	2000	35/35	0.84	0.09	1,25,38,40	0
2	LMT	C	2000	35/35	0.88	0.08	5,22,46,50	0
2	LMT	F	2000	35/35	0.89	0.08	13,38,54,58	0

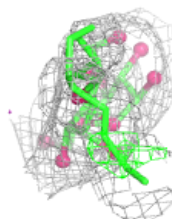
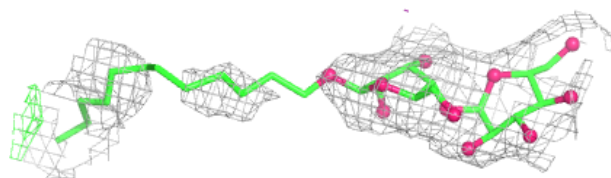
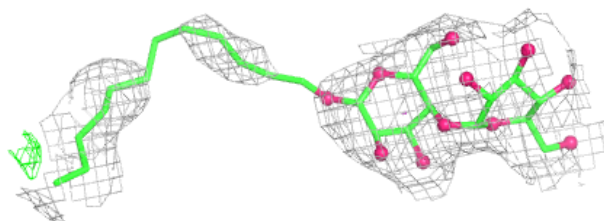
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT A 2000:

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

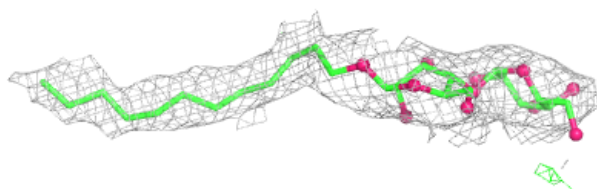
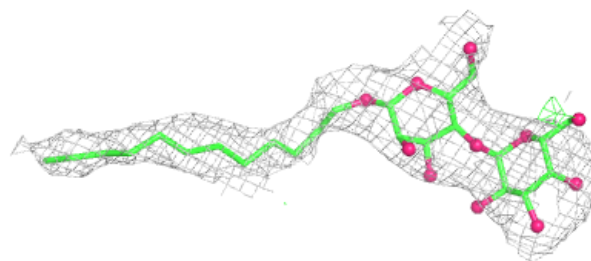
**Electron density around LMT B 2000:**

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

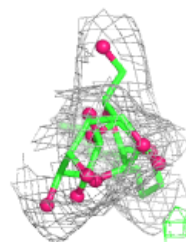
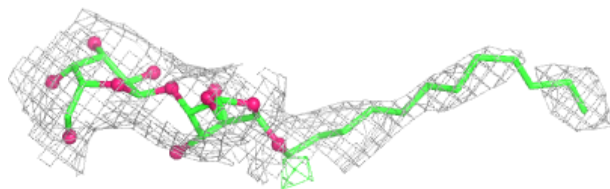
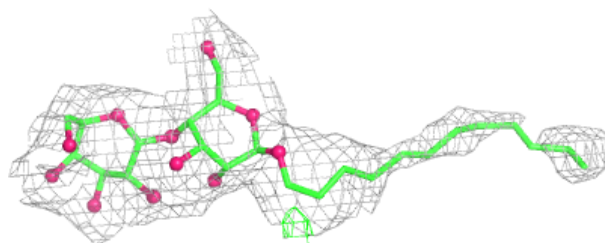


Electron density around LMT E 2000:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

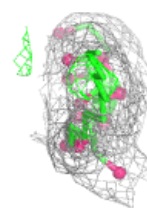
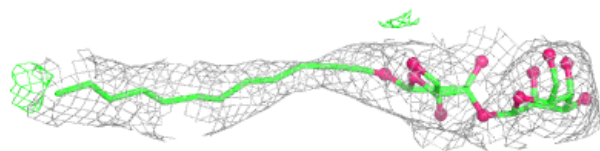
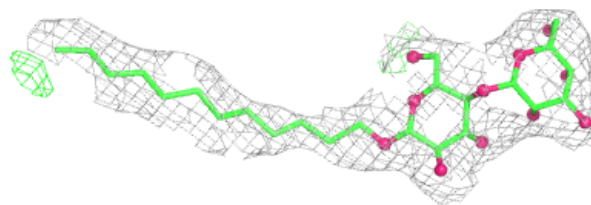
**Electron density around LMT D 2000:**

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

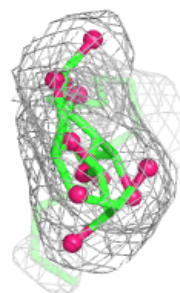
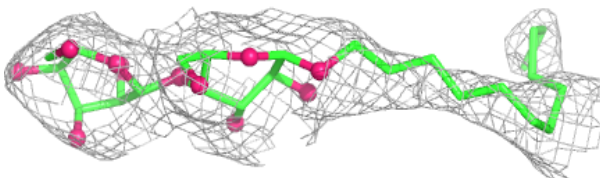


Electron density around LMT C 2000:

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

**Electron density around LMT F 2000:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.