



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:59 PM UTC

PDB ID : 3G60 / pdb_00003g60
Title : Structure of P-glycoprotein Reveals a Molecular Basis for Poly-Specific Drug Binding
Authors : Aller, S.G.; Yu, J.; Ward, A.; Weng, Y.; Chittaboina, S.; Zhuo, R.; Harrell, P.M.; Trinh, Y.T.; Zhang, Q.; Urbatsch, I.L.; Chang, G.
Deposited on : 2009-02-05
Resolution : 4.40 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

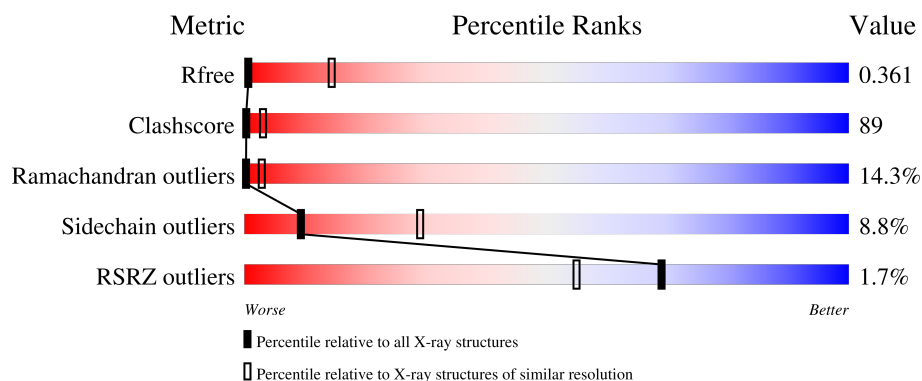
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

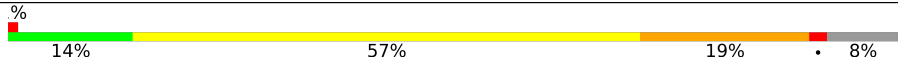
The reported resolution of this entry is 4.40 Å.

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	1088 (4.90-3.90)
Clashscore	190562	1135 (4.90-3.90)
Ramachandran outliers	187476	1026 (4.90-3.90)
Sidechain outliers	187428	1010 (4.90-3.90)
RSRZ outliers	180081	1084 (4.90-3.90)

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	1284	
1	B	1284	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18414 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.

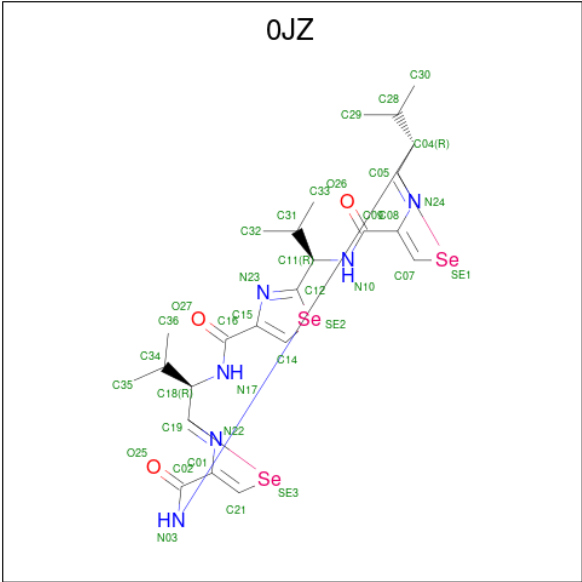
- Molecule 1 is a protein called Multidrug resistance protein 1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1182	Total	C	N	O	S	0	0	0
			9171	5895	1552	1686	38			
1	B	1182	Total	C	N	O	S	0	0	0
			9171	5895	1552	1686	38			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1277	TYR	-	expression tag	UNP Q5I1Y5
A	1278	VAL	-	expression tag	UNP Q5I1Y5
A	1279	HIS	-	expression tag	UNP Q5I1Y5
A	1280	HIS	-	expression tag	UNP Q5I1Y5
A	1281	HIS	-	expression tag	UNP Q5I1Y5
A	1282	HIS	-	expression tag	UNP Q5I1Y5
A	1283	HIS	-	expression tag	UNP Q5I1Y5
A	1284	HIS	-	expression tag	UNP Q5I1Y5
B	1277	TYR	-	expression tag	UNP Q5I1Y5
B	1278	VAL	-	expression tag	UNP Q5I1Y5
B	1279	HIS	-	expression tag	UNP Q5I1Y5
B	1280	HIS	-	expression tag	UNP Q5I1Y5
B	1281	HIS	-	expression tag	UNP Q5I1Y5
B	1282	HIS	-	expression tag	UNP Q5I1Y5
B	1283	HIS	-	expression tag	UNP Q5I1Y5
B	1284	HIS	-	expression tag	UNP Q5I1Y5

- Molecule 2 is (4R,11R,18R)-4,11,18-tri(propan-2-yl)-6,13,20-triseleno-3,10,17,22,23,24-hexaazatetracyclo[17.2.1.1.5,8.1.12,15]tetracos-1(21),5(24),7,12(23),14,19(22)-hexaene-2,9,16-tri-one (CCD ID: 0JZ) (formula: C₂₄H₃₀N₆O₃Se₃).

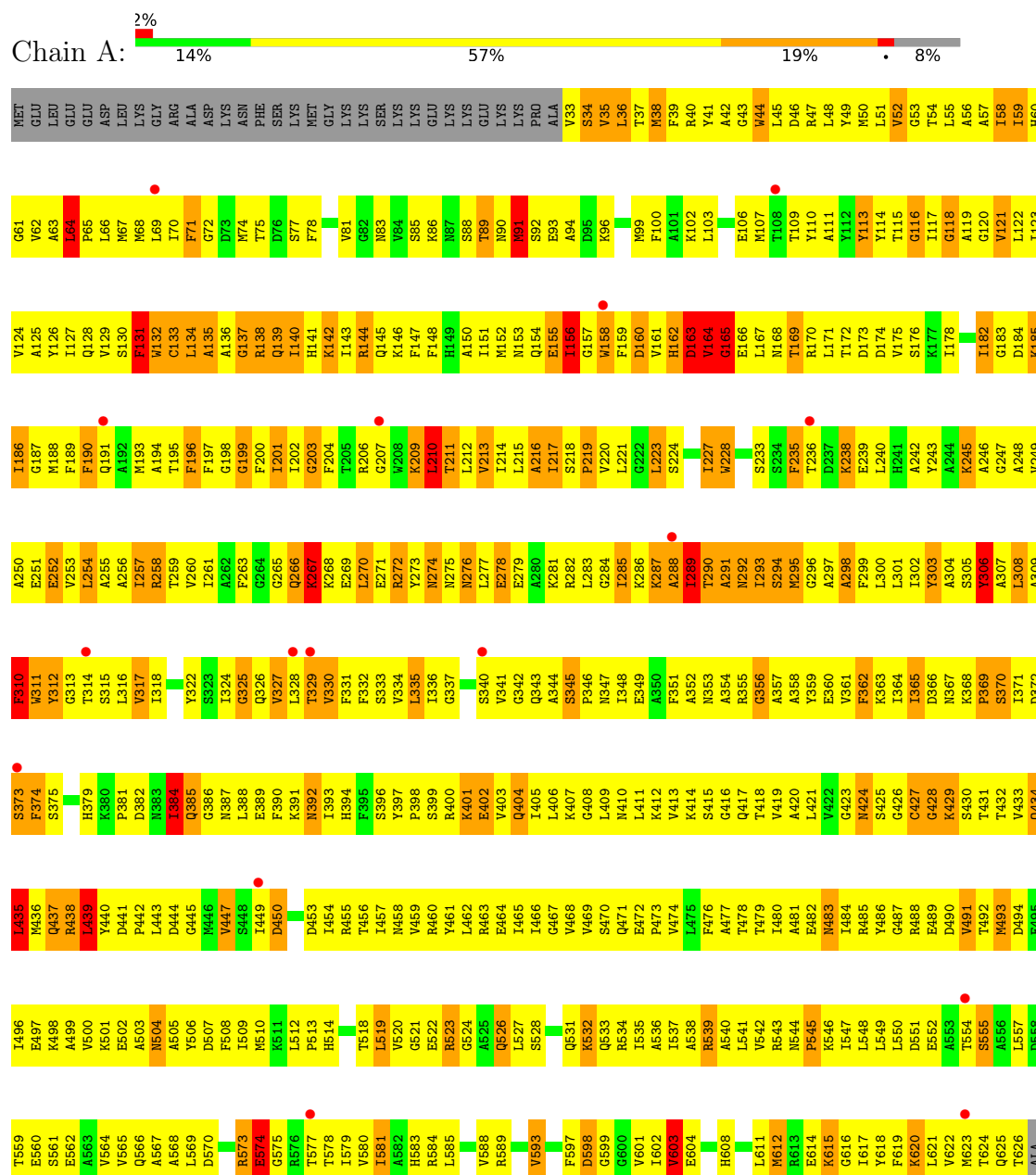


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	Se	0	0
			36	24	6	3	3		
2	B	1	Total	C	N	O	Se	0	0
			36	24	6	3	3		

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: Multidrug resistance protein 1a



S1122	G1059	A995	N928	I863	P803	T743	ALA	M623	T554	M493	T432	P372	H311	E251	G187
I1123	Q1060	K996	K929	I864	K804	Q744	L684	T624	S855	D494	V433	S373	Y312	E252	M188
A1124	T1051	A997	A930	A865	T805	Q745	D685	Q625	E935	E935	Q434	F374	T314	E253	F189
E1125	L1062	T998	A931	I866	T806	Q746	E686	T626	L557	L496	L435	S375	T314	L254	F190
N1126	A1063	V999	H932	A867	T807	N747	D687	ALA	D558	E497	Q435	K376	L316	A255	Q191
T1127	L1064	G988	G808	G868	G808	N748	N748	GLY	T559	K498	Q437	S377	L316	A256	A192
A1128	V1065	A1001	A809	G869	A809	N749	P689	ASN	E560	A499	R438	G378	V317	L257	M193
Y1129	G1066	G935	L810	E871	L810	L750	P690	GLU	S661	V500	L439	H379	I318	R258	A194
G1130	H1003	I936	T811	M872	T811	F751	A691	ILE	S662	K501	Y440	K380	T259	T195	F196
D1131	S1068	T937	T812	K873	T812	S752	S692	LEU	A563	E502	P442	P381	K320	V260	F197
N1132	G1069	F938	L753	M874	L753	L753	F693	LEU	V564	A503	P442	E321	E321	L261	F197
S1133	L1070	L875	L814	L875	L814	W694	W694	ASN	V665	N504	L443	N383	Y322	A262	G198
L1134	G1071	G878	A815	G878	A815	F755	L696	ASN	Q566	A505	D444	L384	S323	G199	G199
V1135	K1072	A879	N816	Q878	N816	L756	I696	GLU	A567	Y506	G445	Q385	I324	F200	F200
T1136	S1073	A879	D817	A879	D817	L757	L697	ALA	A568	D507	M446	G386	G325	G285	I201
S1137	T1074	L758	L758	L758	L758	F759	K698	CYS	L569	F508	V447	N387	Q326	Q266	I202
Y1138	V1075	K881	A820	K881	A820	I760	L699	LYS	L569	M510	I449	L388	Q328	K267	G203
E1139	P1076	D882	Q820	D882	Q820	N700	N700	SER	D570	K511	I449	L388	L328	K268	F204
E1140	Q1077	K883	W821	K883	W821	I761	S701	LYS	D570	K511	D450	F390	T329	E269	T205
I1141	L1078	K884	K822	K884	K822	F762	T702	ASP	E574	L512	D450	F390	V330	R206	R206
S948	L1079	E885	G823	E885	G823	F763	E703	GLU	G575	P513	D453	N392	F331	L270	G207
I1142	D1015	L886	A824	L886	A824	I764	W704	ILE	T577	H514	I454	N393	F332	R272	K208
A1143	S1016	E887	T825	E887	T825	T765	P705	ASP	T577	Q515	R455	K394	F333	Y273	K209
A1144	A1087	Q888	Q826	Q888	Q826	F766	W706	ASN	T578	T518	T456	F395	V334	N274	L215
A1145	F1082	S889	S827	S889	S827	F767	F707	LEU	I579	T518	I457	S396	V336	N275	T211
E1146	Y1083	A896	R828	A896	R828	L768	W708	ASP	V580	L519	M458	N397	I336	N276	L212
E1147	D1084	I897	L829	I897	L829	Q769	W709	MET	L581	V520	V459	F398	G337	L277	V213
M1086	P1086	A893	A830	A893	A830	Q770	G710	SER	A582	G521	R460	F399	F332	E278	T214
A1087	A1087	T894	W831	T894	W831	F771	I711	SER	H583	E522	Y461	R400	S333	E279	L215
M1026	Y958	E895	R832	E895	R832	T772	F712	LYS	R584	R523	L462	R401	V341	E279	L215
L1027	L959	A896	R833	A896	R833	F773	G713	ASP	L585	G524	R463	E402	G342	A280	A216
V1090	F1091	I897	Q834	I897	Q834	G774	A714	SER	A525	E464	E464	N403	Q343	K281	T217
D1155	L1092	E896	R835	E896	R835	K775	I715	GLY	V588	Q526	I465	Q404	Q343	R282	S218
S1156	D1093	N899	I836	N899	I836	A776	I716	SER	R589	L527	I466	L405	A344	L283	P219
L1157	G1094	Q963	A837	Q963	A837	Q777	N717	SER	V593	S528	G467	L406	S345	G284	V220
P1158	K1095	L964	N838	L964	N838	E778	G718	LEU	V593	G529	V468	K407	P346	I285	L221
D1159	E1096	T902	L839	T902	L839	I779	G719	ILE	F597	G530	V469	G408	N347	K286	G222
K1160	I1097	V903	G840	V903	G840	L780	L720	ARG	F597	Q531	S470	L409	E349	K287	L223
Y1161	K1098	V904	T841	V904	T841	T781	Q721	ARG	D598	K532	Q471	N410	A350	A288	S224
M1162	Q1099	S905	G842	S905	G842	K782	P722	ARG	G599	Q533	Q471	N410	F351	T289	T227
T1163	L1100	N969	I843	N969	I843	R783	A723	SER	G600	R534	P473	K412	A352	A291	W228
R1164	N1101	V970	I844	V970	I844	L784	F724	THR	V601	I535	V474	V413	N353	N292	G233
V1165	V1102	L971	I845	L971	I845	R785	S725	ARG	I602	A536	L475	K414	A354	I293	S234
G1166	Q1103	E909	S846	E909	S846	Y786	W726	LYS	F603	I537	F477	S415	R355	S294	G235
D1167	T1042	Q910	L847	Q910	L847	M787	I727	SER	E604	A538	A477	Q417	G356	N295	F236
G1168	S1045	F974	I848	F974	I848	V788	F728	ILE	H608	R539	T478	Q417	A357	G296	T236
A1107	I1046	E913	Y849	E913	Y849	F789	S729	CYS	L540	A540	T479	T418	A358	A297	D237
Q1108	P1047	T914	K851	T914	K851	K790	W730	GLY	L541	V542	I480	V419	Y359	A298	K238
L1109	V978	N915	Q852	N915	Q852	M792	V732	HIS	L611	R543	E482	L421	V361	E239	E239
S1113	Q1050	A916	L853	A916	L853	L793	G733	ASP	M612	N544	M483	V422	F362	L300	L240
Q1114	G1051	Q918	T854	Q918	T854	V734	W734	GLN	E614	P545	I484	G423	K363	L301	H241
E1115	S919	Q918	L855	Q918	L855	Q795	F735	ASP	K615	K546	R485	N424	Y303	I302	A242
P1116	L1052	N982	L856	N982	L856	T796	T736	ARG	G616	I547	Y486	S425	I365	Y243	Y243
L1180	S1053	L920	L857	L920	L857	Y797	W737	LYS	I617	L548	G487	G426	G365	A304	A244
A1181	Q1117	O921	L858	Q1117	L858	S798	G738	LEU	Y618	L549	R488	C427	N367	S305	K245
T1182	E1055	I922	A859	T1182	A859	W799	G739	SER	F619	L550	E489	G428	K388	A246	A246
A1183	P1119	F923	I860	P1119	I860	P800	P740	THR	K620	D551	D490	K429	P369	A307	G247
R1184	K1057	G923	V861	K1057	V861	D801	L621	LYS	L621	E552	S430	S430	L308	L308	A248
A1185	C1121	Y994	P862	A1185	P862	D802	E742	GLU	V622	A553	T492	T431	I371	F310	A250

L1186	V1247
V1187	K1248
R1188	E1249
Q1189	H1250
P1190	G1251
H1191	T1252
I1192	H1253
L1193	Q1254
L1194	Q1255
L1195	L1256
D1196	L1257
E1197	A1258
A1198	Q1259
T1199	K1260
S1200	G1261
A1201	
L1202	F1264
D1203	S1265
T1204	M1266
E1205	V1267
S1206	S1268
E1207	V1269
K1208	Q1270
V1209	A1271
V1210	GLY
Q1211	ALA
E1212	LYS
A1213	ARG
L1214	SER
D1215	TYR
K1216	VAL
A1217	HIS
R1218	HIS
E1219	HIS
G1220	HIS
R1221	HIS
T1222	HIS
C1223	
I1224	
V1225	
I1226	
A1227	
H1228	
R1229	
L1230	
S1231	
Q1234	
N1235	
A1236	
D1237	
L1238	
I1239	
V1240	
V1241	
I1242	
Q1243	
N1244	
G1245	
K1246	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.63Å 115.09Å 374.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 4.40 19.99 – 4.40	Depositor EDS
% Data completeness (in resolution range)	94.7 (19.99-4.40) 93.5 (19.99-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.10 (at 4.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.314 , 0.365 0.316 , 0.361	Depositor DCC
R_{free} test set	2835 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	201.9	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 119.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18414	wwPDB-VP
Average B, all atoms (Å ²)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 0JZ

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	0.58	0/9339	1.10	90/12626 (0.7%)
1	B	0.58	2/9339 (0.0%)	1.09	90/12626 (0.7%)
All	All	0.58	2/18678 (0.0%)	1.09	180/25252 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	VAL	C-O	-8.32	1.14	1.24
1	B	689	PRO	CA-C	5.39	1.57	1.52

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	427	CYS	N-CA-C	20.17	136.24	111.02
1	B	852	GLN	N-CA-C	-13.36	94.92	112.68
1	B	64	LEU	CA-C-N	-11.95	106.54	118.97
1	B	64	LEU	C-N-CA	-11.95	106.54	118.97
1	A	64	LEU	CA-C-N	-11.37	106.43	119.05
1	A	64	LEU	C-N-CA	-11.37	106.43	119.05
1	A	159	PHE	N-CA-C	-11.12	99.42	113.43
1	B	159	PHE	N-CA-C	-10.91	99.69	113.43
1	B	804	LYS	N-CA-C	-9.94	98.39	111.71
1	A	603	VAL	N-CA-C	9.89	129.92	109.34
1	A	1098	LYS	N-CA-C	-9.79	89.94	110.80
1	A	164	VAL	N-CA-C	-9.31	89.98	109.34
1	A	267	LYS	N-CA-C	9.26	130.52	110.80
1	A	450	ASP	N-CA-C	-9.24	92.46	108.08
1	B	213	VAL	N-CA-C	-8.87	101.57	110.62
1	A	708	VAL	N-CA-C	-8.83	101.95	110.42
1	B	289	ILE	N-CA-C	-8.77	102.32	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	688	VAL	N-CA-C	8.72	116.93	107.60
1	B	345	SER	CA-C-N	-8.70	109.39	119.05
1	B	345	SER	C-N-CA	-8.70	109.39	119.05
1	A	289	ILE	N-CA-C	-8.70	102.39	110.82
1	A	861	VAL	CA-C-N	-8.63	109.78	119.28
1	A	861	VAL	C-N-CA	-8.63	109.78	119.28
1	B	450	ASP	N-CA-C	-8.62	93.51	108.08
1	A	345	SER	CA-C-N	-8.52	109.60	119.05
1	A	345	SER	C-N-CA	-8.52	109.60	119.05
1	B	708	VAL	N-CA-C	-8.50	102.26	110.42
1	B	861	VAL	CA-C-N	-8.40	110.05	119.28
1	B	861	VAL	C-N-CA	-8.40	110.05	119.28
1	B	267	LYS	N-CA-C	8.39	128.68	110.80
1	A	213	VAL	N-CA-C	-8.31	102.14	110.62
1	B	211	THR	N-CA-C	-8.14	102.38	111.82
1	A	721	GLN	CA-C-N	-8.08	110.10	119.47
1	A	721	GLN	C-N-CA	-8.08	110.10	119.47
1	B	721	GLN	CA-C-N	-8.06	110.12	119.47
1	B	721	GLN	C-N-CA	-8.06	110.12	119.47
1	A	804	LYS	N-CA-C	-8.03	100.42	112.54
1	A	211	THR	N-CA-C	-7.97	102.57	111.82
1	B	917	ALA	N-CA-C	-7.94	102.70	111.36
1	A	852	GLN	N-CA-C	-7.91	102.16	112.68
1	B	372	ASP	N-CA-C	-7.77	102.89	113.30
1	A	917	ALA	N-CA-C	-7.77	102.81	111.28
1	A	1191	HIS	N-CA-C	-7.70	101.54	113.02
1	A	165	GLY	N-CA-C	-7.58	95.21	113.18
1	A	293	ILE	N-CA-C	-7.57	101.97	112.50
1	B	818	ALA	N-CA-C	-7.57	102.97	111.07
1	B	296	GLY	N-CA-C	-7.53	104.35	113.99
1	A	1206	SER	N-CA-C	-7.51	100.07	111.56
1	B	293	ILE	N-CA-C	-7.50	102.08	112.50
1	B	1191	HIS	N-CA-C	-7.44	101.94	113.02
1	A	296	GLY	N-CA-C	-7.43	104.47	113.99
1	A	42	ALA	N-CA-C	7.25	126.24	110.80
1	A	574	GLU	N-CA-C	7.24	126.21	110.80
1	B	797	VAL	N-CA-C	7.22	124.35	109.34
1	A	818	ALA	N-CA-C	-7.21	103.36	111.07
1	B	290	THR	N-CA-C	-7.16	103.51	111.82
1	B	685	ASP	N-CA-C	7.04	114.55	108.78
1	B	377	SER	N-CA-C	7.02	125.76	110.80
1	A	699	LEU	N-CA-C	-6.99	104.62	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	LEU	N-CA-C	-6.98	103.10	111.69
1	A	688	VAL	N-CA-C	6.96	115.67	107.73
1	A	163	ASP	N-CA-C	-6.95	104.46	114.12
1	A	860	ILE	N-CA-C	6.86	117.61	110.62
1	A	77	SER	N-CA-C	-6.80	103.87	111.28
1	B	362	PHE	N-CA-C	-6.77	103.98	111.36
1	B	36	LEU	N-CA-C	6.76	118.44	111.14
1	A	290	THR	N-CA-C	-6.73	104.01	111.82
1	A	287	LYS	N-CA-C	-6.72	103.76	112.23
1	A	362	PHE	N-CA-C	-6.69	104.07	111.36
1	B	268	LYS	N-CA-C	-6.69	100.85	111.02
1	B	1020	GLN	N-CA-C	6.67	125.00	110.80
1	A	851	TRP	N-CA-C	6.66	124.99	110.80
1	A	1160	LYS	N-CA-C	-6.62	97.15	109.32
1	A	1142	VAL	N-CA-C	-6.58	103.90	110.62
1	B	287	LYS	N-CA-C	-6.54	103.98	112.23
1	B	77	SER	N-CA-C	-6.51	104.18	111.28
1	B	1142	VAL	N-CA-C	-6.49	104.00	110.62
1	A	292	ASN	N-CA-C	-6.48	104.30	111.82
1	A	36	LEU	N-CA-C	6.47	118.13	111.14
1	B	292	ASN	N-CA-C	-6.45	104.34	111.82
1	B	689	PRO	CA-C-N	6.36	125.86	119.24
1	B	689	PRO	C-N-CA	6.36	125.86	119.24
1	A	372	ASP	N-CA-C	-6.34	105.41	113.02
1	A	384	ILE	N-CA-C	-6.34	96.15	109.34
1	A	1026	MET	N-CA-C	-6.33	105.32	114.12
1	A	327	VAL	N-CA-C	-6.33	103.18	112.04
1	B	42	ALA	N-CA-C	6.28	124.17	110.80
1	B	860	ILE	N-CA-C	6.28	117.02	110.62
1	B	603	VAL	N-CA-C	6.20	122.23	109.34
1	B	739	GLY	CA-C-N	6.17	126.74	120.38
1	B	739	GLY	C-N-CA	6.17	126.74	120.38
1	A	437	GLN	N-CA-C	-6.15	104.42	112.41
1	A	817	ASP	N-CA-C	6.08	117.91	111.28
1	B	977	ILE	N-CA-C	-6.08	104.58	110.72
1	A	182	ILE	N-CA-C	6.08	116.26	110.42
1	B	699	LEU	N-CA-C	-5.97	105.25	112.54
1	A	905	SER	N-CA-C	-5.91	106.20	113.41
1	A	798	SER	N-CA-C	-5.88	106.06	113.18
1	B	1097	ILE	N-CA-C	-5.87	101.97	109.30
1	B	327	VAL	N-CA-C	-5.84	103.80	111.09
1	B	165	GLY	N-CA-C	-5.82	99.38	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	796	ASP	N-CA-C	5.82	123.21	110.80
1	A	739	GLY	CA-C-N	5.82	126.37	120.38
1	A	739	GLY	C-N-CA	5.82	126.37	120.38
1	A	796	ASP	N-CA-C	5.75	123.06	110.80
1	A	922	ILE	CA-C-N	-5.75	112.65	119.84
1	A	922	ILE	C-N-CA	-5.75	112.65	119.84
1	B	905	SER	N-CA-C	-5.75	106.40	113.41
1	B	922	ILE	CA-C-N	-5.74	112.67	119.84
1	B	922	ILE	C-N-CA	-5.74	112.67	119.84
1	B	689	PRO	N-CA-C	5.71	117.66	110.70
1	B	288	ALA	N-CA-C	-5.68	106.18	113.23
1	B	798	SER	N-CA-C	-5.67	106.31	113.18
1	A	1269	VAL	N-CA-C	-5.64	104.04	111.09
1	B	612	MET	N-CA-C	-5.64	105.21	111.36
1	A	1097	ILE	N-CA-C	-5.63	101.40	108.84
1	A	303	TYR	N-CA-C	-5.58	98.91	110.80
1	B	383	ASN	N-CA-C	5.57	119.70	113.01
1	A	217	ILE	N-CA-C	5.56	116.20	110.36
1	A	210	LEU	N-CA-C	-5.56	104.86	111.69
1	B	1107	ALA	N-CA-C	-5.55	104.63	111.40
1	B	182	ILE	N-CA-C	5.50	115.70	110.42
1	B	817	ASP	N-CA-C	5.47	117.24	111.28
1	A	1018	SER	N-CA-C	-5.45	99.19	110.80
1	B	743	THR	N-CA-C	-5.45	105.34	111.28
1	B	580	VAL	N-CA-C	5.45	115.90	107.78
1	A	714	ALA	N-CA-C	-5.42	105.07	110.97
1	A	943	ALA	N-CA-C	-5.41	104.41	111.02
1	A	294	SER	N-CA-C	-5.40	106.19	112.89
1	B	851	TRP	N-CA-C	5.38	122.26	110.80
1	A	1258	ALA	N-CA-C	-5.37	105.99	112.54
1	A	977	ILE	N-CA-C	-5.37	105.30	110.72
1	B	740	PRO	N-CA-C	5.36	117.24	110.70
1	B	1258	ALA	N-CA-C	-5.36	106.00	112.54
1	B	714	ALA	N-CA-C	-5.36	105.13	110.97
1	A	847	LEU	N-CA-C	-5.33	105.14	111.69
1	B	294	SER	N-CA-C	-5.32	106.29	112.89
1	B	163	ASP	N-CA-C	-5.32	106.17	113.30
1	B	437	GLN	N-CA-C	-5.32	106.11	112.59
1	B	1269	VAL	N-CA-C	-5.30	104.47	111.09
1	B	384	ILE	N-CA-C	-5.29	98.33	109.34
1	B	1157	LEU	CA-C-N	5.28	126.44	119.84
1	B	1157	LEU	C-N-CA	5.28	126.44	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	702	THR	N-CA-C	-5.27	104.59	111.02
1	A	752	SER	N-CA-C	-5.26	105.44	111.07
1	B	1040	TYR	CA-C-N	5.25	126.40	119.84
1	B	1040	TYR	C-N-CA	5.25	126.40	119.84
1	B	303	TYR	N-CA-C	-5.25	99.62	110.80
1	B	1164	ARG	N-CA-C	-5.24	103.11	110.50
1	B	164	VAL	O-C-N	-5.24	116.02	122.57
1	B	685	ASP	CB-CA-C	-5.23	109.54	117.07
1	B	752	SER	N-CA-C	-5.23	105.47	111.07
1	B	208	TRP	CB-CA-C	-5.22	100.02	110.42
1	A	450	ASP	CB-CA-C	-5.22	110.58	116.63
1	A	612	MET	N-CA-C	-5.18	105.71	111.36
1	A	235	PHE	N-CA-C	-5.16	105.77	111.71
1	B	250	ALA	N-CA-C	-5.15	106.24	112.88
1	A	702	THR	N-CA-C	-5.14	104.74	111.02
1	A	603	VAL	CB-CA-C	-5.12	102.89	111.29
1	A	288	ALA	N-CA-C	-5.12	106.88	113.23
1	A	306	TYR	N-CA-C	-5.12	102.98	111.37
1	B	1020	GLN	N-CA-CB	-5.11	101.86	110.49
1	B	1216	LYS	N-CA-C	-5.10	106.91	113.23
1	A	1045	SER	N-CA-C	-5.09	107.23	112.93
1	A	1019	THR	N-CA-C	5.09	118.75	112.24
1	A	298	ALA	N-CA-C	-5.08	105.66	111.14
1	A	1157	LEU	CA-C-N	5.08	126.19	119.84
1	A	1157	LEU	C-N-CA	5.08	126.19	119.84
1	A	1096	GLU	N-CA-C	5.08	116.58	108.41
1	B	335	LEU	N-CA-C	-5.06	105.04	111.11
1	A	291	ALA	N-CA-C	-5.06	105.85	112.23
1	A	335	LEU	N-CA-C	-5.06	105.04	111.11
1	A	740	PRO	N-CA-C	5.06	116.87	110.70
1	A	1164	ARG	N-CA-C	-5.05	103.38	110.50
1	B	291	ALA	N-CA-C	-5.04	105.97	111.82
1	A	142	LYS	N-CA-C	-5.02	105.50	110.97
1	A	1040	TYR	CA-C-N	5.02	126.12	119.84
1	A	1040	TYR	C-N-CA	5.02	126.12	119.84
1	B	1213	ALA	N-CA-C	-5.01	105.90	111.36
1	B	1096	GLU	N-CA-C	5.00	116.46	108.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9171	0	9344	1665	0
1	B	9171	0	9344	1636	0
2	A	36	0	27	12	0
2	B	36	0	27	10	0
All	All	18414	0	18742	3298	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 89.

All (3298) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:797:VAL:O	1:B:801:ASP:HB2	1.45	1.15
1:A:523:ARG:HD3	1:A:524:GLY:H	0.99	1.13
1:B:523:ARG:HD3	1:B:524:GLY:H	0.98	1.12
1:B:858:LEU:O	1:B:862:PRO:HD2	1.51	1.11
1:B:1204:THR:O	1:B:1206:SER:N	1.83	1.10
1:B:61:GLY:O	1:B:65:PRO:HD2	1.53	1.07
1:B:314:THR:HG23	1:B:327:VAL:HG21	1.30	1.07
1:A:979:PHE:O	1:A:982:MET:HG2	1.56	1.05
1:A:61:GLY:O	1:A:65:PRO:HD2	1.55	1.05
1:B:1020:GLN:HG2	1:B:1021:GLY:H	1.16	1.05
1:A:270:LEU:HD23	1:A:270:LEU:H	1.19	1.04
1:A:858:LEU:O	1:A:862:PRO:HD2	1.55	1.04
1:A:35:VAL:HG23	1:A:36:LEU:H	1.19	1.03
1:B:35:VAL:HG23	1:B:36:LEU:H	1.20	1.03
1:B:318:ILE:HD13	1:B:327:VAL:HG13	1.39	1.02
1:B:286:LYS:HA	1:B:289:ILE:HB	1.41	1.02
1:A:293:ILE:HG22	1:A:766:PHE:HB3	1.43	1.01
1:A:267:LYS:N	1:A:270:LEU:HD21	1.76	1.00
1:B:270:LEU:HD23	1:B:270:LEU:H	1.18	1.00
1:B:1114:GLN:HE22	1:B:1200:SER:HB3	1.25	1.00
1:A:286:LYS:HA	1:A:289:ILE:HB	1.43	1.00
1:B:795:GLN:HA	1:B:1012:PRO:HG3	1.39	1.00
1:B:416:GLY:H	1:B:577:THR:HG22	1.26	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:979:PHE:O	1:B:982:MET:HG2	1.62	0.99
1:A:164:VAL:HG23	1:A:164:VAL:O	1.58	0.99
1:A:336:ILE:HG12	2:A:6001:OJZ:SE1	2.12	0.99
1:B:267:LYS:N	1:B:270:LEU:HD21	1.77	0.98
1:A:686:GLU:HG2	1:A:813:ARG:HH22	1.29	0.97
1:A:1114:GLN:HE22	1:A:1200:SER:HB3	1.27	0.97
1:A:1063:ALA:HB3	1:A:1239:ILE:HA	1.45	0.97
1:B:797:VAL:O	1:B:801:ASP:CB	2.12	0.97
1:A:246:ALA:HB1	1:A:277:LEU:HB3	1.46	0.96
1:B:246:ALA:HB1	1:B:277:LEU:HB3	1.45	0.96
1:B:1063:ALA:HB3	1:B:1239:ILE:HA	1.46	0.95
1:A:919:SER:O	1:A:923:PRO:HD2	1.66	0.95
1:B:718:GLY:O	1:B:722:PRO:HD2	1.66	0.95
1:A:797:VAL:O	1:A:801:ASP:HB2	1.66	0.95
1:B:919:SER:O	1:B:923:PRO:HD2	1.66	0.94
1:A:416:GLY:H	1:A:577:THR:HG22	1.30	0.94
1:A:288:ALA:HA	1:A:291:ALA:HB3	1.48	0.94
1:A:853:LEU:HG	1:A:973:VAL:HG21	1.48	0.94
1:B:58:ILE:HG13	1:B:193:MET:HG3	1.49	0.94
1:B:288:ALA:HA	1:B:291:ALA:HB3	1.48	0.94
1:A:718:GLY:O	1:A:722:PRO:HD2	1.68	0.93
1:A:58:ILE:HG13	1:A:193:MET:HG3	1.50	0.93
1:A:155:GLU:HB3	1:A:156:ILE:HD12	1.48	0.93
1:A:1014:ILE:HD12	1:A:1106:ARG:HH12	1.34	0.93
1:B:978:VAL:HG13	2:B:6002:OJZ:H35B	1.51	0.93
1:A:1144:ALA:HA	1:A:1186:LEU:HD11	1.51	0.93
1:B:523:ARG:HD3	1:B:524:GLY:N	1.83	0.93
1:B:1036:VAL:HB	1:B:1052:LEU:HB3	1.52	0.92
1:B:1144:ALA:HA	1:B:1186:LEU:HD11	1.50	0.92
1:A:523:ARG:HD3	1:A:524:GLY:N	1.84	0.92
1:A:361:VAL:O	1:A:365:ILE:HG13	1.71	0.91
1:A:1090:VAL:HG13	1:A:1097:ILE:HB	1.51	0.91
1:B:1122:SER:HA	1:B:1164:ARG:HA	1.52	0.90
1:B:1090:VAL:HG13	1:B:1097:ILE:HB	1.50	0.90
1:B:361:VAL:O	1:B:365:ILE:HG13	1.72	0.90
1:A:1036:VAL:HB	1:A:1052:LEU:HB3	1.52	0.90
1:A:1032:GLN:HB2	1:A:1091:PHE:HB2	1.54	0.89
1:A:278:GLU:O	1:A:282:ARG:HG2	1.71	0.89
1:B:956:GLY:O	1:B:966:THR:HB	1.72	0.89
1:B:519:LEU:HD13	1:B:519:LEU:H	1.36	0.89
1:B:573:ARG:HD2	1:B:578:THR:HG21	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:996:LYS:H	1:B:996:LYS:HD3	1.37	0.89
1:A:267:LYS:HB3	1:A:790:LYS:HE2	1.54	0.89
1:B:387:ASN:HD22	1:B:414:LYS:HA	1.36	0.89
1:A:927:ALA:HA	1:A:930:LYS:HE3	1.54	0.89
1:B:693:PHE:O	1:B:696:ILE:HG12	1.72	0.89
1:A:992:PRO:HB2	1:A:996:LYS:HZ1	1.38	0.88
1:A:1197:GLU:HG2	1:A:1227:ALA:HA	1.55	0.88
1:A:849:TYR:OH	1:A:976:ALA:HB2	1.73	0.88
1:B:1032:GLN:HB2	1:B:1091:PHE:HB2	1.52	0.88
1:B:1216:LYS:HA	1:B:1216:LYS:HE2	1.53	0.88
1:A:1216:LYS:HE2	1:A:1216:LYS:HA	1.53	0.88
1:B:278:GLU:O	1:B:282:ARG:HG2	1.73	0.88
1:A:136:ALA:HB2	1:A:182:ILE:HB	1.56	0.88
1:A:158:TRP:HE1	1:A:900:PHE:HB3	1.36	0.88
1:A:573:ARG:HD2	1:A:578:THR:HG21	1.54	0.87
1:B:690:PRO:HG2	1:B:1006:ARG:NH2	1.90	0.87
1:B:849:TYR:OH	1:B:976:ALA:HB2	1.74	0.87
1:A:519:LEU:H	1:A:519:LEU:HD13	1.36	0.87
1:B:136:ALA:HB2	1:B:182:ILE:HB	1.57	0.87
1:B:1193:LEU:HB2	1:B:1223:CYS:HB3	1.57	0.87
1:B:1197:GLU:HG2	1:B:1227:ALA:HA	1.56	0.87
1:A:478:THR:HG22	1:A:479:THR:H	1.40	0.86
1:A:996:LYS:H	1:A:996:LYS:HD3	1.39	0.86
1:B:523:ARG:CD	1:B:524:GLY:H	1.84	0.86
1:B:927:ALA:HA	1:B:930:LYS:HE3	1.55	0.86
1:A:1122:SER:HA	1:A:1164:ARG:HA	1.57	0.86
1:A:1193:LEU:HB2	1:A:1223:CYS:HB3	1.56	0.86
1:B:786:TYR:HE2	1:B:790:LYS:HZ2	1.24	0.86
1:A:163:ASP:O	1:A:164:VAL:C	2.19	0.86
1:B:379:HIS:HB3	1:B:457:ILE:HA	1.58	0.86
1:A:387:ASN:HD22	1:A:414:LYS:HA	1.38	0.86
1:A:964:LEU:HD13	1:A:965:MET:N	1.91	0.86
1:A:172:THR:O	1:A:175:VAL:HG12	1.76	0.85
1:B:314:THR:CG2	1:B:327:VAL:HG21	2.05	0.85
1:B:857:LEU:HD11	1:B:976:ALA:HB3	1.56	0.85
1:A:1079:LEU:HD23	1:A:1194:LEU:HD21	1.59	0.85
1:B:202:ILE:HD12	1:B:203:GLY:N	1.90	0.85
1:A:72:GLY:HA2	1:A:326:GLN:NE2	1.92	0.85
1:B:1039:ASN:HB2	1:B:1047:PRO:HA	1.58	0.85
1:A:964:LEU:HD13	1:A:965:MET:H	1.41	0.85
1:B:976:ALA:HA	1:B:979:PHE:CD2	2.11	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1091:PHE:HE1	1:B:1096:GLU:HG2	1.41	0.85
1:B:802:ASP:CG	1:B:1041:PRO:HB2	2.01	0.85
1:A:163:ASP:HB2	1:A:166:GLU:HB3	1.58	0.84
1:A:523:ARG:CD	1:A:524:GLY:H	1.86	0.84
1:A:976:ALA:HA	1:A:979:PHE:CD2	2.12	0.84
1:A:1037:VAL:HG12	1:A:1051:GLY:H	1.42	0.84
1:B:401:LYS:H	1:B:401:LYS:HD2	1.42	0.84
1:B:1014:ILE:HA	1:B:1102:VAL:HG11	1.59	0.84
1:B:172:THR:O	1:B:175:VAL:HG12	1.77	0.84
1:A:694:TRP:O	1:A:697:LEU:HG	1.77	0.84
1:B:118:GLY:O	1:B:121:VAL:HG22	1.77	0.83
1:B:379:HIS:O	1:B:381:PRO:HD3	1.77	0.83
1:A:278:GLU:C	1:A:282:ARG:HG2	2.03	0.83
1:A:725:SER:HA	2:A:6001:OJZ:H36	1.59	0.83
1:A:1091:PHE:HE1	1:A:1096:GLU:HG2	1.41	0.83
1:B:1079:LEU:HD23	1:B:1194:LEU:HD21	1.60	0.83
1:A:429:LYS:HD3	1:A:429:LYS:H	1.39	0.83
1:B:1037:VAL:HG12	1:B:1051:GLY:H	1.42	0.83
1:A:1039:ASN:HB2	1:A:1047:PRO:HA	1.60	0.83
1:B:379:HIS:HB2	1:B:456:THR:O	1.79	0.83
1:B:478:THR:HG22	1:B:479:THR:H	1.43	0.83
1:A:118:GLY:O	1:A:121:VAL:HG22	1.78	0.83
1:B:72:GLY:HA2	1:B:326:GLN:NE2	1.93	0.83
1:B:59:ILE:HD11	1:B:124:VAL:HG11	1.61	0.83
1:A:202:ILE:HD12	1:A:203:GLY:N	1.93	0.82
1:A:564:VAL:O	1:A:567:ALA:HB3	1.79	0.82
1:A:853:LEU:HB3	1:A:973:VAL:CG1	2.08	0.82
1:A:1179:ARG:NH2	1:A:1209:VAL:HG11	1.94	0.82
1:B:155:GLU:HB3	1:B:156:ILE:HD12	1.59	0.82
1:B:318:ILE:HD11	1:B:325:GLY:N	1.93	0.82
1:B:964:LEU:HD13	1:B:965:MET:N	1.93	0.82
1:A:918:GLN:O	1:A:921:GLN:HB3	1.80	0.82
1:B:392:ASN:O	1:B:445:GLY:HA3	1.80	0.82
1:B:905:SER:C	1:B:907:THR:H	1.88	0.82
1:B:773:PHE:O	1:B:776:ALA:HB3	1.80	0.82
1:A:358:ALA:O	1:A:362:PHE:HB2	1.79	0.82
1:A:1218:ARG:HH22	1:A:1235:ASN:HD22	1.28	0.82
1:B:797:VAL:O	1:B:801:ASP:CG	2.23	0.82
1:B:694:TRP:O	1:B:697:LEU:HG	1.80	0.82
1:B:918:GLN:O	1:B:921:GLN:HB3	1.79	0.82
1:B:1179:ARG:NH2	1:B:1209:VAL:HG11	1.95	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1092:LEU:HB3	1:B:1097:ILE:HD11	1.61	0.81
1:B:187:GLY:O	1:B:190:PHE:HB3	1.81	0.81
1:B:1020:GLN:CG	1:B:1021:GLY:H	1.89	0.81
1:B:163:ASP:HB2	1:B:166:GLU:HB3	1.61	0.81
1:B:856:LEU:HD22	1:B:955:PHE:HD1	1.46	0.81
1:A:905:SER:C	1:A:907:THR:H	1.86	0.81
1:A:1121:CYS:HB2	1:A:1126:ASN:HD21	1.46	0.81
1:B:318:ILE:HD11	1:B:324:ILE:HD12	1.62	0.81
1:B:1121:CYS:HB2	1:B:1126:ASN:HD21	1.44	0.81
1:B:1142:VAL:O	1:B:1146:LYS:HG2	1.81	0.81
1:B:358:ALA:O	1:B:362:PHE:HB2	1.80	0.80
1:B:457:ILE:HD11	1:B:462:LEU:HD13	1.63	0.80
1:A:401:LYS:H	1:A:401:LYS:HD2	1.44	0.80
1:B:278:GLU:C	1:B:282:ARG:HG2	2.05	0.80
1:A:574:GLU:HG3	1:A:574:GLU:O	1.79	0.80
1:A:715:ILE:HG12	1:A:836:ILE:HD12	1.64	0.80
1:A:457:ILE:HD11	1:A:462:LEU:HD13	1.63	0.80
1:B:564:VAL:O	1:B:567:ALA:HB3	1.80	0.80
1:B:715:ILE:HG12	1:B:836:ILE:HD12	1.64	0.80
1:A:388:LEU:HB2	1:A:413:VAL:CG1	2.12	0.80
1:B:795:GLN:O	1:B:796:ASP:HB3	1.80	0.80
1:A:158:TRP:O	1:A:164:VAL:CG1	2.30	0.80
1:A:811:THR:O	1:A:814:LEU:HB2	1.82	0.80
1:B:1218:ARG:HH22	1:B:1235:ASN:HD22	1.27	0.80
1:A:379:HIS:HB3	1:A:457:ILE:HA	1.64	0.79
1:B:508:PHE:HE2	1:B:534:ARG:HD2	1.47	0.79
1:A:158:TRP:HE1	1:A:900:PHE:CB	1.95	0.79
1:A:210:LEU:O	1:A:214:ILE:HG13	1.82	0.79
1:B:388:LEU:HB2	1:B:413:VAL:CG1	2.12	0.79
1:A:856:LEU:HD22	1:A:955:PHE:HD1	1.46	0.79
1:B:785:ARG:HH21	1:B:815:ALA:HA	1.46	0.79
1:A:59:ILE:HD11	1:A:124:VAL:HG11	1.62	0.79
1:A:1142:VAL:O	1:A:1146:LYS:HG2	1.82	0.79
1:A:508:PHE:HE2	1:A:534:ARG:HD2	1.47	0.79
1:A:90:ASN:HB2	1:A:91:MET:HE2	1.63	0.79
1:A:286:LYS:O	1:A:290:THR:HG23	1.83	0.79
1:A:35:VAL:HG23	1:A:36:LEU:N	1.97	0.78
1:B:90:ASN:HB2	1:B:91:MET:HE2	1.64	0.78
1:B:811:THR:O	1:B:814:LEU:HB2	1.81	0.78
1:B:964:LEU:HD13	1:B:965:MET:H	1.45	0.78
1:A:689:PRO:HB2	1:A:690:PRO:HD3	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:LEU:HD12	1:A:1224:ILE:HG23	1.65	0.78
1:A:392:ASN:O	1:A:445:GLY:HA3	1.84	0.78
1:A:504:ASN:O	1:A:534:ARG:HD3	1.83	0.78
1:B:35:VAL:HG23	1:B:36:LEU:N	1.98	0.78
1:A:1092:LEU:HB3	1:A:1097:ILE:HD11	1.63	0.78
1:B:1023:LYS:HB3	1:B:1026:MET:HG2	1.65	0.78
1:A:799:TRP:O	1:A:803:PRO:HB3	1.84	0.78
1:B:210:LEU:O	1:B:214:ILE:HG13	1.82	0.78
1:B:696:ILE:O	1:B:700:ASN:HB2	1.82	0.78
1:B:1113:SER:HA	1:B:1196:ASP:HB3	1.66	0.78
1:A:797:VAL:O	1:A:801:ASP:CB	2.32	0.78
1:A:864:ILE:HD12	1:A:865:ALA:N	1.99	0.78
1:A:1260:LYS:H	1:A:1260:LYS:HD2	1.48	0.78
1:B:1092:LEU:HD22	1:B:1097:ILE:HD11	1.66	0.78
1:A:959:LEU:HD22	1:A:964:LEU:HG	1.66	0.77
1:B:897:ILE:HD12	1:B:898:GLU:N	1.99	0.77
1:B:864:ILE:HD12	1:B:865:ALA:N	1.99	0.77
1:B:163:ASP:O	1:B:165:GLY:N	2.17	0.77
1:A:308:LEU:HD12	1:A:751:PHE:CE2	2.20	0.77
1:B:286:LYS:O	1:B:290:THR:HG23	1.84	0.77
1:B:379:HIS:CB	1:B:457:ILE:HA	2.15	0.77
1:B:1181:ALA:O	1:B:1184:ARG:HB3	1.84	0.77
1:A:91:MET:HB2	1:A:94:ALA:HB3	1.67	0.77
1:A:314:THR:HG23	1:A:327:VAL:HG21	1.65	0.77
1:A:550:LEU:HB2	1:A:580:VAL:HG23	1.67	0.77
1:A:857:LEU:CD1	1:A:976:ALA:HB3	2.15	0.77
1:B:128:GLN:O	1:B:131:PHE:HB3	1.85	0.77
1:A:785:ARG:HH21	1:A:815:ALA:HA	1.50	0.77
1:B:756:LEU:HD12	1:B:757:ILE:N	2.00	0.77
1:A:1092:LEU:HD22	1:A:1097:ILE:HD11	1.66	0.77
1:A:795:GLN:O	1:A:796:ASP:HB3	1.84	0.77
1:B:1038:PHE:HB2	1:B:1085:PRO:HA	1.66	0.77
1:A:756:LEU:HD12	1:A:757:ILE:N	1.99	0.76
1:A:800:PHE:O	1:A:803:PRO:HD3	1.85	0.76
1:A:843:ILE:HA	1:A:846:SER:HB3	1.67	0.76
1:A:1014:ILE:HB	1:A:1102:VAL:HG21	1.66	0.76
1:B:285:ILE:O	1:B:289:ILE:HG12	1.84	0.76
1:B:550:LEU:HB2	1:B:580:VAL:HG23	1.65	0.76
1:A:773:PHE:O	1:A:776:ALA:HB3	1.85	0.76
1:B:215:LEU:O	1:B:219:PRO:HD2	1.86	0.76
1:B:306:TYR:O	1:B:310:PHE:HB2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:753:LEU:HD12	1:B:756:LEU:HD11	1.68	0.76
1:A:1038:PHE:HB2	1:A:1085:PRO:HA	1.67	0.76
1:B:91:MET:HB2	1:B:94:ALA:HB3	1.68	0.76
1:B:1260:LYS:HD2	1:B:1260:LYS:H	1.50	0.76
1:A:1113:SER:HA	1:A:1196:ASP:HB3	1.67	0.76
1:B:314:THR:HG23	1:B:327:VAL:CG2	2.11	0.76
1:A:285:ILE:O	1:A:289:ILE:HG12	1.86	0.76
1:B:286:LYS:HG2	1:B:778:GLU:CG	2.15	0.76
1:B:324:ILE:HD12	1:B:326:GLN:H	1.51	0.76
1:B:504:ASN:O	1:B:534:ARG:HD3	1.85	0.76
1:B:1062:LEU:HD12	1:B:1224:ILE:HG23	1.66	0.76
1:A:722:PRO:HB2	1:A:841:THR:HG21	1.68	0.76
1:A:753:LEU:HD12	1:A:756:LEU:HD11	1.68	0.76
1:B:394:HIS:HB2	1:B:444:ASP:HB3	1.67	0.76
1:B:800:PHE:O	1:B:803:PRO:HD3	1.85	0.76
1:B:1056:VAL:HG23	1:B:1060:GLN:HE22	1.50	0.76
1:A:740:PRO:HG2	1:A:741:PRO:HD3	1.68	0.76
1:A:1181:ALA:O	1:A:1184:ARG:HB3	1.85	0.76
1:A:1020:GLN:HG3	1:A:1101:ASN:HB2	1.68	0.75
1:B:512:LEU:HD12	1:B:513:PRO:HD2	1.68	0.75
1:B:608:HIS:HD1	1:B:618:TYR:HE2	1.33	0.75
1:B:799:TRP:O	1:B:803:PRO:HB3	1.86	0.75
1:A:396:SER:HA	1:A:404:GLN:HA	1.67	0.75
1:A:897:ILE:HD12	1:A:898:GLU:N	2.01	0.75
1:A:608:HIS:HD1	1:A:618:TYR:HE2	1.33	0.75
1:A:853:LEU:HD22	1:A:853:LEU:H	1.51	0.75
1:B:35:VAL:HG12	1:B:359:TYR:CE2	2.22	0.75
1:B:270:LEU:HD23	1:B:270:LEU:N	1.98	0.75
1:B:740:PRO:HG2	1:B:741:PRO:HD3	1.68	0.75
1:B:819:ALA:O	1:B:822:LYS:HB3	1.86	0.75
1:B:843:ILE:HA	1:B:846:SER:HB3	1.68	0.75
1:B:1033:PHE:HB3	1:B:1036:VAL:HG21	1.68	0.75
1:A:270:LEU:HD23	1:A:270:LEU:N	1.99	0.75
1:B:992:PRO:HB2	1:B:996:LYS:HZ1	1.52	0.75
1:A:282:ARG:O	1:A:286:LYS:HB2	1.86	0.75
1:A:819:ALA:O	1:A:822:LYS:HB3	1.87	0.75
1:B:1109:LEU:HD21	1:B:1188:ARG:HH11	1.51	0.75
1:A:218:SER:HB2	1:A:219:PRO:HD3	1.69	0.75
1:A:434:GLN:HE21	1:A:439:LEU:HG	1.51	0.75
1:B:332:PHE:O	1:B:335:LEU:HB3	1.85	0.75
1:B:407:LYS:NZ	1:B:601:VAL:HA	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:949:TYR:OH	2:B:6002:OJZ:H32	1.87	0.75
1:A:512:LEU:HD12	1:A:513:PRO:HD2	1.68	0.75
1:B:797:VAL:HG12	1:B:798:SER:N	2.01	0.75
1:A:265:GLY:HA2	1:A:793:LEU:HD21	1.68	0.75
1:B:543:ARG:NH2	1:B:905:SER:O	2.20	0.75
1:A:1033:PHE:HB3	1:A:1036:VAL:HG21	1.68	0.74
1:A:1109:LEU:HD21	1:A:1188:ARG:HH11	1.51	0.74
1:B:401:LYS:NZ	1:B:401:LYS:HB3	2.02	0.74
1:B:1199:THR:HG23	1:B:1210:VAL:HG11	1.67	0.74
1:A:686:GLU:HG2	1:A:813:ARG:NH2	2.02	0.74
1:A:1056:VAL:HG23	1:A:1060:GLN:HE22	1.50	0.74
1:A:254:LEU:HD23	1:A:811:THR:HG22	1.69	0.74
1:B:1138:TYR:O	1:B:1142:VAL:HG23	1.86	0.74
1:A:35:VAL:HG12	1:A:359:TYR:CE2	2.22	0.74
1:A:360:GLU:HA	1:A:363:LYS:HE2	1.70	0.74
1:A:482:GLU:O	1:A:483:ASN:C	2.29	0.74
1:A:306:TYR:O	1:A:310:PHE:HB2	1.87	0.74
1:A:407:LYS:NZ	1:A:601:VAL:HA	2.01	0.74
1:B:396:SER:HA	1:B:404:GLN:HA	1.70	0.74
1:B:722:PRO:HB2	1:B:841:THR:HG21	1.69	0.74
1:A:206:ARG:O	1:A:211:THR:HB	1.86	0.74
1:A:713:CYS:SG	1:A:769:GLN:HB3	2.27	0.74
1:A:696:ILE:O	1:A:700:ASN:HB2	1.86	0.74
1:B:892:ILE:HB	1:B:916:TYR:CE1	2.23	0.74
1:A:215:LEU:O	1:A:219:PRO:HD2	1.88	0.74
1:B:482:GLU:O	1:B:483:ASN:C	2.31	0.74
1:A:1063:ALA:HB2	1:A:1236:ALA:HB1	1.70	0.74
1:B:278:GLU:HB3	1:B:782:LYS:HG2	1.67	0.74
1:B:298:ALA:O	1:B:302:ILE:HG12	1.87	0.74
1:B:857:LEU:HD12	1:B:973:VAL:HG12	1.70	0.74
1:A:128:GLN:O	1:A:131:PHE:HB3	1.88	0.74
1:A:1138:TYR:O	1:A:1142:VAL:HG23	1.88	0.74
1:A:1199:THR:HG23	1:A:1210:VAL:HG11	1.69	0.74
1:B:557:LEU:HG	1:B:561:SER:OG	1.87	0.74
1:B:690:PRO:HG2	1:B:1006:ARG:HH22	1.52	0.74
1:B:202:ILE:HD12	1:B:203:GLY:H	1.52	0.73
1:B:703:GLU:HB3	1:B:780:LEU:HD23	1.70	0.73
1:A:892:ILE:HB	1:A:916:TYR:CE1	2.23	0.73
1:B:218:SER:HB2	1:B:219:PRO:HD3	1.69	0.73
1:B:851:TRP:HA	1:B:854:THR:HB	1.70	0.73
1:B:928:MET:O	1:B:931:ALA:HB3	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:MET:HG3	1:A:131:PHE:CZ	2.23	0.73
1:A:103:LEU:HB2	1:A:960:VAL:CG2	2.17	0.73
1:A:210:LEU:HD23	1:A:317:VAL:HG11	1.70	0.73
1:A:318:ILE:HD13	1:A:327:VAL:HG13	1.71	0.73
1:B:36:LEU:HD12	1:B:37:THR:N	2.03	0.73
1:B:725:SER:HB3	1:B:975:SER:HB3	1.71	0.73
1:B:1100:LEU:HG	1:B:1101:ASN:H	1.53	0.73
1:A:36:LEU:HD12	1:A:37:THR:N	2.02	0.73
1:A:557:LEU:HG	1:A:561:SER:OG	1.88	0.73
1:A:703:GLU:HB3	1:A:780:LEU:HD23	1.71	0.73
1:A:801:ASP:HB3	1:A:1083:TYR:OH	1.87	0.73
1:B:282:ARG:O	1:B:286:LYS:HB2	1.87	0.73
1:B:722:PRO:HD3	1:B:982:MET:HE1	1.70	0.73
1:B:1027:LEU:H	1:B:1027:LEU:HD23	1.53	0.73
1:A:394:HIS:HB2	1:A:444:ASP:HB3	1.69	0.73
1:A:722:PRO:O	1:A:725:SER:HB2	1.89	0.73
1:B:543:ARG:HH12	1:B:905:SER:HA	1.53	0.73
1:A:722:PRO:HD3	1:A:982:MET:HE1	1.71	0.73
1:B:722:PRO:O	1:B:725:SER:HB2	1.87	0.73
1:B:1063:ALA:HB2	1:B:1236:ALA:HB1	1.69	0.73
1:A:972:LEU:HD12	1:A:972:LEU:H	1.52	0.73
1:A:1242:ILE:HA	1:A:1247:VAL:HA	1.70	0.73
1:B:407:LYS:HZ1	1:B:601:VAL:HA	1.54	0.73
1:A:332:PHE:O	1:A:335:LEU:HB3	1.88	0.73
1:A:1013:GLU:O	1:A:1014:ILE:HG23	1.89	0.73
1:B:922:ILE:HB	1:B:923:PRO:HD3	1.70	0.73
1:A:138:ARG:NH2	1:B:515:GLN:HE21	1.86	0.73
1:A:928:MET:O	1:A:931:ALA:HB3	1.89	0.73
1:A:969:ASN:HD22	1:A:970:VAL:H	1.36	0.73
1:B:930:LYS:O	1:B:933:VAL:HB	1.88	0.73
1:B:972:LEU:H	1:B:972:LEU:HD12	1.52	0.73
1:B:1242:ILE:HA	1:B:1247:VAL:HA	1.69	0.73
1:A:992:PRO:HB2	1:A:996:LYS:NZ	2.04	0.72
1:B:1218:ARG:HH22	1:B:1235:ASN:ND2	1.87	0.72
1:A:922:ILE:HB	1:A:923:PRO:HD3	1.69	0.72
1:B:713:CYS:SG	1:B:769:GLN:HB3	2.29	0.72
1:A:204:PHE:HA	1:A:211:THR:HG21	1.71	0.72
1:A:257:ILE:HD13	1:A:257:ILE:C	2.14	0.72
1:B:158:TRP:O	1:B:164:VAL:CG1	2.37	0.72
1:B:825:THR:O	1:B:829:LEU:HG	1.89	0.72
1:A:1014:ILE:HD12	1:A:1106:ARG:NH1	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:GLY:N	1:B:577:THR:HG22	2.02	0.72
1:B:715:ILE:HG23	1:B:836:ILE:HG21	1.71	0.72
1:B:721:GLN:HB3	1:B:722:PRO:HD3	1.71	0.72
1:A:942:GLN:O	1:A:945:MET:HB3	1.90	0.72
1:B:133:CYS:SG	1:B:931:ALA:HA	2.30	0.72
1:B:50:MET:HG3	1:B:131:PHE:CZ	2.23	0.72
1:B:207:GLY:HA3	1:B:211:THR:HB	1.72	0.72
1:B:289:ILE:O	1:B:293:ILE:HG12	1.90	0.72
1:A:214:ILE:CD1	1:A:330:VAL:HB	2.20	0.72
1:A:303:TYR:O	1:A:306:TYR:N	2.23	0.72
1:B:132:TRP:HB2	1:B:186:ILE:HD13	1.71	0.72
1:B:360:GLU:HA	1:B:363:LYS:HE2	1.72	0.72
1:A:158:TRP:HA	1:A:162:HIS:HD2	1.55	0.72
1:A:168:ASN:O	1:A:171:LEU:HB3	1.90	0.72
1:A:401:LYS:HB3	1:A:401:LYS:NZ	2.04	0.72
1:A:715:ILE:HG23	1:A:836:ILE:HG21	1.71	0.72
1:B:133:CYS:O	1:B:134:LEU:C	2.31	0.72
1:B:992:PRO:HB2	1:B:996:LYS:NZ	2.05	0.72
1:A:504:ASN:OD1	1:A:568:ALA:HB2	1.90	0.72
1:B:502:GLU:C	1:B:504:ASN:H	1.97	0.72
1:A:1218:ARG:HH22	1:A:1235:ASN:ND2	1.87	0.71
1:B:71:PHE:HA	1:B:74:MET:HE3	1.72	0.71
1:B:210:LEU:HD23	1:B:317:VAL:HG11	1.70	0.71
1:B:504:ASN:OD1	1:B:568:ALA:HB2	1.89	0.71
1:B:959:LEU:HD22	1:B:964:LEU:HB2	1.71	0.71
1:B:1121:CYS:HB2	1:B:1126:ASN:ND2	2.05	0.71
1:A:267:LYS:HA	1:A:270:LEU:HD11	1.72	0.71
1:A:721:GLN:HB3	1:A:722:PRO:HD3	1.71	0.71
1:B:795:GLN:HE21	1:B:796:ASP:H	1.38	0.71
1:B:1150:ILE:HB	1:B:1179:ARG:HB3	1.72	0.71
1:A:211:THR:O	1:A:215:LEU:HG	1.88	0.71
1:A:399:SER:O	1:A:402:GLU:HB2	1.90	0.71
1:B:59:ILE:CD1	1:B:124:VAL:HG11	2.20	0.71
1:B:246:ALA:HB2	1:B:281:LYS:HZ2	1.54	0.71
1:A:725:SER:HB3	1:A:975:SER:HB3	1.71	0.71
1:B:390:PHE:HE1	1:B:432:THR:HB	1.55	0.71
1:B:849:TYR:HB2	1:B:854:THR:OG1	1.90	0.71
1:B:993:ASP:N	1:B:996:LYS:HZ1	1.88	0.71
1:A:187:GLY:O	1:A:190:PHE:HB3	1.89	0.71
1:A:1100:LEU:HG	1:A:1101:ASN:H	1.56	0.71
1:B:288:ALA:HA	1:B:291:ALA:CB	2.18	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ILE:HG13	1:A:187:GLY:N	2.05	0.71
1:A:289:ILE:O	1:A:293:ILE:HG12	1.89	0.71
1:B:942:GLN:O	1:B:945:MET:HB3	1.90	0.71
1:A:407:LYS:HZ1	1:A:601:VAL:HA	1.56	0.71
1:B:291:ALA:O	1:B:294:SER:HB2	1.90	0.71
1:B:399:SER:O	1:B:402:GLU:HB2	1.90	0.71
1:A:122:LEU:HD12	1:A:939:SER:HB2	1.72	0.71
1:A:207:GLY:HA3	1:A:211:THR:H	1.55	0.71
1:A:239:GLU:HB3	1:A:285:ILE:HG12	1.72	0.71
1:A:384:ILE:HG22	1:A:385:GLN:H	1.56	0.71
1:A:797:VAL:HG12	1:A:798:SER:N	2.04	0.71
1:B:168:ASN:O	1:B:171:LEU:HB3	1.91	0.71
1:B:1114:GLN:NE2	1:B:1200:SER:HB3	2.03	0.71
1:A:471:GLN:O	1:A:473:PRO:HD3	1.91	0.70
1:A:688:VAL:HB	1:A:1006:ARG:HH12	1.56	0.70
1:B:211:THR:O	1:B:215:LEU:HG	1.91	0.70
1:A:59:ILE:CD1	1:A:124:VAL:HG11	2.21	0.70
1:A:133:CYS:O	1:A:134:LEU:C	2.34	0.70
1:A:1150:ILE:HB	1:A:1179:ARG:HB3	1.72	0.70
1:A:1248:LYS:HA	1:A:1248:LYS:HE3	1.72	0.70
1:B:239:GLU:HB3	1:B:285:ILE:HG12	1.73	0.70
1:A:71:PHE:HA	1:A:74:MET:HE3	1.74	0.70
1:A:157:GLY:HA2	1:A:160:ASP:HB2	1.72	0.70
1:A:288:ALA:HA	1:A:291:ALA:CB	2.19	0.70
1:A:291:ALA:O	1:A:294:SER:HB2	1.91	0.70
1:B:290:THR:HG22	1:B:770:GLY:C	2.17	0.70
1:B:1098:LYS:HG2	1:B:1098:LYS:O	1.90	0.70
1:A:132:TRP:HB2	1:A:186:ILE:HD13	1.71	0.70
1:B:109:THR:O	1:B:113:TYR:HB3	1.92	0.70
1:A:298:ALA:O	1:A:302:ILE:HG12	1.92	0.70
1:A:801:ASP:HB3	1:A:1083:TYR:CZ	2.26	0.70
1:B:35:VAL:CG2	1:B:36:LEU:H	2.03	0.70
1:A:1019:THR:HB	1:A:1099:GLN:O	1.91	0.70
1:B:158:TRP:HA	1:B:162:HIS:HD2	1.56	0.70
1:B:482:GLU:O	1:B:485:ARG:N	2.25	0.70
1:A:1121:CYS:HB2	1:A:1126:ASN:ND2	2.06	0.70
1:B:186:ILE:HG13	1:B:187:GLY:N	2.05	0.70
1:B:257:ILE:C	1:B:257:ILE:HD13	2.17	0.70
1:A:1218:ARG:NH2	1:A:1235:ASN:HD22	1.88	0.70
1:A:416:GLY:N	1:A:577:THR:HG22	2.05	0.70
1:A:482:GLU:O	1:A:485:ARG:N	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ALA:CB	1:B:277:LEU:HB3	2.22	0.70
1:B:471:GLN:O	1:B:473:PRO:HD3	1.92	0.70
1:B:1218:ARG:NH2	1:B:1235:ASN:HD22	1.88	0.70
1:A:386:GLY:HA3	1:A:450:ASP:HA	1.73	0.69
1:B:465:ILE:C	1:B:466:ILE:HD12	2.17	0.69
1:B:969:ASN:HD22	1:B:970:VAL:H	1.38	0.69
1:A:211:THR:HA	1:A:214:ILE:HD12	1.73	0.69
1:A:791:SER:HA	1:A:1010:LYS:HE3	1.74	0.69
1:A:1026:MET:HE3	1:A:1095:LYS:HD3	1.73	0.69
1:B:1031:VAL:HB	1:B:1056:VAL:HG12	1.75	0.69
1:A:158:TRP:O	1:A:164:VAL:HG11	1.91	0.69
1:A:1193:LEU:HD11	1:A:1217:ALA:O	1.93	0.69
1:B:35:VAL:O	1:B:39:PHE:HB2	1.92	0.69
1:B:689:PRO:N	1:B:690:PRO:HD2	2.08	0.69
1:B:781:THR:HG23	1:B:818:ALA:HB1	1.74	0.69
1:A:133:CYS:SG	1:A:931:ALA:HA	2.32	0.69
1:A:905:SER:O	1:A:907:THR:N	2.26	0.69
1:B:254:LEU:HD12	1:B:789:PHE:HZ	1.58	0.69
1:B:285:ILE:O	1:B:285:ILE:HD13	1.92	0.69
1:B:384:ILE:O	1:B:385:GLN:O	2.11	0.69
1:A:554:THR:OG1	1:A:562:GLU:HG3	1.93	0.69
1:A:697:LEU:HA	1:A:700:ASN:HB2	1.75	0.69
1:A:1001:ALA:O	1:A:1005:ILE:HG12	1.92	0.69
1:B:310:PHE:CZ	1:B:331:PHE:HB3	2.27	0.69
1:B:447:VAL:HG13	1:B:454:ILE:HG21	1.75	0.69
1:B:697:LEU:HA	1:B:700:ASN:HB2	1.73	0.69
1:B:1248:LYS:HE3	1:B:1248:LYS:HA	1.73	0.69
1:A:930:LYS:O	1:A:933:VAL:HB	1.92	0.69
1:B:554:THR:OG1	1:B:562:GLU:HG3	1.92	0.69
1:B:784:LEU:O	1:B:788:VAL:HG23	1.93	0.69
1:B:856:LEU:HD22	1:B:955:PHE:CD1	2.28	0.69
1:A:795:GLN:HE21	1:A:796:ASP:H	1.40	0.69
1:A:826:GLY:HA2	1:A:829:LEU:HD12	1.73	0.69
1:A:1138:TYR:O	1:A:1141:ILE:HG12	1.92	0.69
1:B:552:GLU:HB3	1:B:555:SER:OG	1.92	0.69
1:B:1106:ARG:HA	1:B:1109:LEU:HD13	1.75	0.69
1:B:1127:ILE:HD13	1:B:1180:ILE:HG23	1.75	0.69
1:B:705:PRO:HG2	1:B:706:TYR:H	1.58	0.69
1:B:1011:THR:N	1:B:1012:PRO:CD	2.56	0.69
1:B:1014:ILE:O	1:B:1015:ASP:HB2	1.92	0.69
1:A:195:THR:HG23	1:A:196:PHE:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ILE:HD12	1:A:326:GLN:H	1.56	0.69
1:A:779:ILE:HG13	1:A:780:LEU:N	2.08	0.69
1:A:1020:GLN:HG3	1:A:1101:ASN:CB	2.23	0.69
1:A:257:ILE:HG21	1:A:800:PHE:HB3	1.75	0.68
1:A:919:SER:O	1:A:923:PRO:CD	2.41	0.68
1:B:1137:SER:OG	1:B:1140:GLU:HB2	1.94	0.68
1:A:502:GLU:C	1:A:504:ASN:H	2.01	0.68
1:A:1127:ILE:HD13	1:A:1180:ILE:HG23	1.74	0.68
1:A:60:HIS:O	1:A:63:ALA:HB3	1.93	0.68
1:A:109:THR:O	1:A:113:TYR:HB3	1.93	0.68
1:A:394:HIS:HA	1:A:406:LEU:O	1.93	0.68
1:A:762:SER:HA	1:A:765:THR:HG22	1.74	0.68
1:A:1031:VAL:HB	1:A:1056:VAL:HG12	1.75	0.68
1:A:39:PHE:HE2	1:A:358:ALA:HB3	1.58	0.68
1:A:99:MET:HB3	1:A:960:VAL:O	1.93	0.68
1:A:559:THR:O	1:A:562:GLU:HB3	1.94	0.68
1:A:853:LEU:HB3	1:A:973:VAL:HG11	1.75	0.68
1:B:826:GLY:HA2	1:B:829:LEU:HD12	1.75	0.68
1:B:210:LEU:HG	1:B:322:TYR:CD2	2.28	0.68
1:B:919:SER:O	1:B:923:PRO:CD	2.41	0.68
1:A:390:PHE:HE1	1:A:432:THR:HB	1.59	0.68
1:A:1054:LEU:HD11	1:A:1240:VAL:HG11	1.75	0.68
1:B:267:LYS:H	1:B:270:LEU:HD21	1.57	0.68
1:B:861:VAL:HB	1:B:862:PRO:HD3	1.76	0.68
1:B:1048:VAL:O	1:B:1049:LEU:HD22	1.94	0.68
1:A:138:ARG:HH22	1:B:515:GLN:HE21	1.40	0.68
1:A:388:LEU:HB2	1:A:413:VAL:HG12	1.76	0.68
1:A:1106:ARG:HA	1:A:1109:LEU:HD13	1.76	0.68
1:B:802:ASP:CB	1:B:1041:PRO:HB2	2.22	0.68
1:A:164:VAL:O	1:A:164:VAL:CG2	2.32	0.68
1:B:157:GLY:HA2	1:B:160:ASP:HB2	1.74	0.68
1:A:705:PRO:HG2	1:A:706:TYR:H	1.59	0.68
1:B:559:THR:O	1:B:562:GLU:HB3	1.93	0.68
1:A:465:ILE:C	1:A:466:ILE:HD12	2.19	0.68
1:A:781:THR:HG23	1:A:818:ALA:HB1	1.75	0.68
1:A:267:LYS:CB	1:A:790:LYS:HE2	2.23	0.67
1:A:1266:MET:O	1:A:1269:VAL:HG12	1.93	0.67
1:A:35:VAL:O	1:A:39:PHE:HB2	1.95	0.67
1:A:178:ILE:HG12	1:A:358:ALA:HB2	1.76	0.67
1:A:251:GLU:OE1	1:A:811:THR:HB	1.94	0.67
1:A:285:ILE:O	1:A:285:ILE:HD13	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ILE:CG2	1:A:428:GLY:HA2	2.25	0.67
1:B:779:ILE:HG13	1:B:780:LEU:N	2.08	0.67
1:B:1054:LEU:HD11	1:B:1240:VAL:HG11	1.75	0.67
1:A:857:LEU:HD13	1:A:976:ALA:HB3	1.76	0.67
1:A:861:VAL:HB	1:A:862:PRO:HD3	1.74	0.67
1:A:1039:ASN:ND2	1:A:1047:PRO:HA	2.09	0.67
1:B:766:PHE:HA	1:B:769:GLN:HE21	1.59	0.67
1:B:1039:ASN:CB	1:B:1047:PRO:HA	2.24	0.67
1:B:1063:ALA:HB2	1:B:1236:ALA:CB	2.24	0.67
1:A:202:ILE:HD12	1:A:203:GLY:H	1.56	0.67
1:A:467:GLY:HA3	1:A:545:PRO:HG3	1.77	0.67
1:A:1039:ASN:CB	1:A:1047:PRO:HA	2.24	0.67
1:B:303:TYR:O	1:B:306:TYR:N	2.27	0.67
1:B:375:SER:C	1:B:376:LYS:HD2	2.19	0.67
1:A:283:LEU:HD12	1:A:284:GLY:N	2.08	0.67
1:A:552:GLU:HB3	1:A:555:SER:OG	1.95	0.67
1:A:569:LEU:O	1:A:573:ARG:HG3	1.93	0.67
1:B:484:ILE:HG21	1:B:496:ILE:HG23	1.74	0.67
1:B:784:LEU:HD12	1:B:1004:ILE:HD11	1.76	0.67
1:A:1114:GLN:NE2	1:A:1200:SER:HB3	2.05	0.67
1:B:254:LEU:HD12	1:B:789:PHE:CZ	2.30	0.67
1:A:856:LEU:HD22	1:A:955:PHE:CD1	2.28	0.67
1:A:1063:ALA:HB2	1:A:1236:ALA:CB	2.25	0.67
1:A:1202:LEU:HD21	1:A:1206:SER:HB3	1.76	0.67
1:B:257:ILE:O	1:B:260:VAL:HB	1.95	0.67
1:B:792:MET:HA	1:B:795:GLN:HB2	1.77	0.67
1:B:1266:MET:O	1:B:1269:VAL:HG12	1.94	0.67
1:A:484:ILE:HG21	1:A:496:ILE:HG23	1.75	0.67
1:B:195:THR:HG23	1:B:196:PHE:H	1.60	0.67
1:B:211:THR:HA	1:B:214:ILE:HD12	1.76	0.67
1:B:1066:GLY:H	1:B:1072:LYS:HE2	1.60	0.67
1:B:60:HIS:O	1:B:63:ALA:HB3	1.94	0.66
1:B:1001:ALA:O	1:B:1005:ILE:HG12	1.94	0.66
1:B:1118:LEU:HB3	1:B:1129:TYR:OH	1.95	0.66
1:A:178:ILE:HG12	1:A:358:ALA:CB	2.25	0.66
1:A:1218:ARG:HH12	1:A:1235:ASN:ND2	1.93	0.66
1:B:467:GLY:HA3	1:B:545:PRO:HG3	1.77	0.66
1:A:825:THR:O	1:A:829:LEU:HG	1.94	0.66
1:A:906:LEU:O	1:A:906:LEU:HD23	1.96	0.66
1:B:447:VAL:HG13	1:B:454:ILE:CG2	2.25	0.66
1:B:858:LEU:HD12	1:B:859:ALA:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1193:LEU:HD11	1:B:1217:ALA:O	1.95	0.66
1:B:1243:GLN:O	1:B:1246:LYS:HD2	1.96	0.66
1:A:209:LYS:O	1:A:212:LEU:HB3	1.95	0.66
1:A:846:SER:OG	1:A:854:THR:HG23	1.94	0.66
1:B:59:ILE:HD11	1:B:124:VAL:HG21	1.78	0.66
1:B:283:LEU:HD12	1:B:284:GLY:N	2.10	0.66
1:A:96:LYS:HG2	1:A:962:GLN:HB2	1.75	0.66
1:A:447:VAL:HG13	1:A:454:ILE:HG21	1.77	0.66
1:A:1189:GLN:N	1:A:1190:PRO:HD3	2.09	0.66
1:B:388:LEU:HB2	1:B:413:VAL:HG12	1.76	0.66
1:B:692:SER:HB2	1:B:695:ARG:HB3	1.77	0.66
1:A:267:LYS:H	1:A:270:LEU:HD21	1.61	0.66
1:A:978:VAL:HG21	2:A:6001:OJZ:H35A	1.78	0.66
1:B:508:PHE:CE2	1:B:534:ARG:HD2	2.30	0.66
1:B:902:THR:HG23	1:B:903:VAL:H	1.60	0.66
1:A:257:ILE:O	1:A:260:VAL:HB	1.96	0.66
1:A:506:TYR:O	1:A:510:MET:HG2	1.93	0.66
1:A:784:LEU:HD12	1:A:1004:ILE:HD11	1.77	0.66
1:A:1150:ILE:O	1:A:1154:ILE:HD13	1.95	0.66
1:B:218:SER:HB2	1:B:219:PRO:CD	2.26	0.66
1:B:321:GLU:O	1:B:322:TYR:C	2.38	0.66
1:B:603:VAL:HG23	1:B:604:GLU:H	1.61	0.66
1:B:1185:ALA:O	1:B:1190:PRO:HD3	1.96	0.66
1:B:1218:ARG:HH12	1:B:1235:ASN:ND2	1.93	0.66
1:A:905:SER:C	1:A:907:THR:N	2.54	0.66
1:B:735:PHE:HD2	1:B:747:ASN:HD21	1.44	0.66
1:B:762:SER:HA	1:B:765:THR:HG22	1.76	0.66
1:A:508:PHE:CE2	1:A:534:ARG:HD2	2.30	0.66
1:B:56:ALA:O	1:B:59:ILE:HG13	1.96	0.66
1:B:883:LYS:O	1:B:887:GLU:HB2	1.95	0.66
1:B:1075:VAL:O	1:B:1076:VAL:C	2.39	0.66
1:B:1150:ILE:O	1:B:1154:ILE:HD13	1.94	0.66
1:B:1189:GLN:N	1:B:1190:PRO:HD3	2.11	0.66
1:A:175:VAL:HG13	1:A:176:SER:N	2.11	0.66
1:B:183:GLY:O	1:B:186:ILE:HG12	1.96	0.66
1:B:820:GLN:HG3	1:B:1000:SER:CB	2.26	0.66
1:A:331:PHE:O	1:A:334:VAL:HG12	1.96	0.65
1:B:39:PHE:HE2	1:B:358:ALA:HB3	1.60	0.65
1:B:384:ILE:HG22	1:B:385:GLN:H	1.60	0.65
1:B:458:ASN:HD22	1:B:459:VAL:N	1.95	0.65
1:B:506:TYR:O	1:B:510:MET:HG2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ILE:O	1:A:326:GLN:N	2.30	0.65
1:A:1039:ASN:HD22	1:A:1047:PRO:HA	1.62	0.65
1:B:178:ILE:HG12	1:B:358:ALA:CB	2.26	0.65
1:B:1202:LEU:HD21	1:B:1206:SER:HB3	1.77	0.65
1:A:246:ALA:CB	1:A:277:LEU:HB3	2.23	0.65
1:A:792:MET:HA	1:A:795:GLN:HB2	1.77	0.65
1:B:386:GLY:HA3	1:B:450:ASP:HA	1.76	0.65
1:A:363:LYS:O	1:A:367:ASN:HB3	1.97	0.65
1:B:178:ILE:HG12	1:B:358:ALA:HB2	1.77	0.65
1:A:447:VAL:HG13	1:A:454:ILE:CG2	2.26	0.65
1:A:858:LEU:HD12	1:A:859:ALA:N	2.11	0.65
1:A:1119:PHE:HD2	1:A:1121:CYS:HG	1.45	0.65
1:A:1137:SER:OG	1:A:1140:GLU:HB2	1.96	0.65
1:B:324:ILE:O	1:B:326:GLN:N	2.29	0.65
1:B:1195:LEU:HD23	1:B:1214:LEU:HD11	1.78	0.65
1:A:154:GLN:NE2	1:A:162:HIS:NE2	2.42	0.65
1:A:185:LYS:NZ	1:A:185:LYS:HB3	2.11	0.65
1:A:538:ALA:O	1:A:541:LEU:HB3	1.97	0.65
1:B:311:TRP:HA	1:B:311:TRP:HE3	1.61	0.65
1:B:1138:TYR:O	1:B:1141:ILE:HG12	1.97	0.65
1:A:163:ASP:O	1:A:164:VAL:O	2.15	0.65
1:A:424:ASN:HB3	1:A:598:ASP:OD1	1.97	0.65
1:A:426:GLY:O	1:A:599:GLY:HA2	1.96	0.65
1:A:1075:VAL:O	1:A:1076:VAL:C	2.40	0.65
1:A:1118:LEU:HB3	1:A:1129:TYR:OH	1.95	0.65
1:A:1243:GLN:O	1:A:1246:LYS:HD2	1.96	0.65
1:A:902:THR:HG23	1:A:903:VAL:H	1.62	0.65
1:A:1185:ALA:O	1:A:1190:PRO:HD3	1.97	0.65
1:B:424:ASN:HB3	1:B:598:ASP:OD1	1.97	0.65
1:B:857:LEU:C	1:B:857:LEU:HD23	2.22	0.65
1:A:458:ASN:HD22	1:A:459:VAL:N	1.94	0.65
1:A:1048:VAL:O	1:A:1049:LEU:HD22	1.97	0.65
1:B:478:THR:HG21	1:B:482:GLU:HG3	1.78	0.65
1:B:1058:LYS:O	1:B:1060:GLN:HG3	1.96	0.65
1:B:88:SER:O	1:B:90:ASN:N	2.30	0.65
1:B:421:LEU:HB3	1:B:429:LYS:HB3	1.78	0.65
1:B:1011:THR:H	1:B:1012:PRO:CD	2.10	0.65
1:B:1214:LEU:HA	1:B:1217:ALA:HB3	1.79	0.65
1:A:35:VAL:CG2	1:A:36:LEU:H	2.02	0.64
1:A:1066:GLY:H	1:A:1072:LYS:HE2	1.61	0.64
1:A:1195:LEU:HD23	1:A:1214:LEU:HD11	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:TYR:CE2	1:B:134:LEU:HD12	2.32	0.64
1:B:121:VAL:HG23	1:B:122:LEU:N	2.12	0.64
1:B:163:ASP:C	1:B:165:GLY:H	2.05	0.64
1:B:311:TRP:HA	1:B:311:TRP:CE3	2.32	0.64
1:A:270:LEU:H	1:A:270:LEU:CD2	2.02	0.64
1:A:509:ILE:HD12	1:A:510:MET:N	2.13	0.64
1:A:735:PHE:HD2	1:A:747:ASN:HD21	1.44	0.64
1:A:1023:LYS:C	1:A:1025:ASN:H	2.06	0.64
1:B:270:LEU:H	1:B:270:LEU:CD2	2.01	0.64
1:B:1020:GLN:CD	1:B:1020:GLN:N	2.56	0.64
1:A:59:ILE:HD11	1:A:124:VAL:HG21	1.78	0.64
1:A:857:LEU:HD11	1:A:976:ALA:HB3	1.79	0.64
1:A:972:LEU:O	1:A:975:SER:HB2	1.97	0.64
1:B:423:GLY:HA2	1:B:597:PHE:O	1.97	0.64
1:A:65:PRO:O	1:A:68:MET:N	2.31	0.64
1:A:103:LEU:HD22	1:A:960:VAL:H	1.62	0.64
1:A:1009:GLU:C	1:A:1010:LYS:HG3	2.22	0.64
1:A:1234:GLN:HA	1:A:1253:HIS:HD2	1.62	0.64
1:B:158:TRP:CZ2	1:B:900:PHE:HB2	2.33	0.64
1:B:363:LYS:O	1:B:367:ASN:HB3	1.97	0.64
1:B:458:ASN:HD22	1:B:459:VAL:H	1.44	0.64
1:B:1203:ASP:O	1:B:1204:THR:O	2.15	0.64
1:A:703:GLU:HG2	1:A:784:LEU:HD21	1.79	0.64
1:B:799:TRP:HA	1:B:799:TRP:CE3	2.33	0.64
1:A:154:GLN:HE22	1:A:162:HIS:CD2	2.16	0.64
1:A:218:SER:HB2	1:A:219:PRO:CD	2.26	0.64
1:A:883:LYS:O	1:A:887:GLU:HB2	1.98	0.64
1:A:1080:GLU:OE2	1:A:1109:LEU:HD12	1.97	0.64
1:B:881:LYS:HB2	1:B:881:LYS:NZ	2.12	0.64
1:B:1014:ILE:HD12	1:B:1106:ARG:HH11	1.62	0.64
1:B:1080:GLU:OE2	1:B:1109:LEU:HD12	1.97	0.64
1:A:121:VAL:HG23	1:A:122:LEU:N	2.12	0.64
1:A:405:ILE:HG21	1:A:428:GLY:HA2	1.79	0.64
1:B:318:ILE:CD1	1:B:324:ILE:HD12	2.27	0.64
1:B:879:ALA:O	1:B:883:LYS:HG2	1.97	0.64
1:B:933:VAL:O	1:B:934:PHE:C	2.40	0.64
1:A:766:PHE:HA	1:A:769:GLN:HE21	1.62	0.64
1:B:185:LYS:NZ	1:B:185:LYS:HB3	2.11	0.64
1:B:207:GLY:HA3	1:B:211:THR:N	2.12	0.64
1:B:207:GLY:HA2	1:B:210:LEU:HB3	1.80	0.64
1:B:293:ILE:HG22	1:B:766:PHE:HB3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:PHE:O	1:B:334:VAL:HG12	1.97	0.64
1:B:1039:ASN:HD22	1:B:1047:PRO:HA	1.63	0.64
1:A:49:TYR:CE2	1:A:134:LEU:HD12	2.33	0.64
1:A:458:ASN:HD22	1:A:459:VAL:H	1.45	0.64
1:B:972:LEU:O	1:B:975:SER:HB2	1.98	0.64
1:A:183:GLY:O	1:A:186:ILE:HG12	1.97	0.63
1:A:311:TRP:HA	1:A:311:TRP:HE3	1.63	0.63
1:A:478:THR:HG21	1:A:482:GLU:HG3	1.78	0.63
1:A:799:TRP:HA	1:A:799:TRP:HE3	1.63	0.63
1:B:703:GLU:HG2	1:B:784:LEU:HD21	1.78	0.63
1:B:780:LEU:O	1:B:784:LEU:HD23	1.98	0.63
1:A:148:PHE:HB3	1:A:913:GLU:CD	2.24	0.63
1:A:185:LYS:HB3	1:A:185:LYS:HZ2	1.63	0.63
1:A:221:LEU:HD11	1:A:309:ALA:HB3	1.80	0.63
1:A:718:GLY:HA3	1:A:837:ALA:HB2	1.80	0.63
1:A:846:SER:HA	1:A:849:TYR:CD1	2.34	0.63
1:A:857:LEU:HD23	1:A:857:LEU:C	2.22	0.63
1:A:881:LYS:HB2	1:A:881:LYS:NZ	2.13	0.63
1:B:394:HIS:HA	1:B:406:LEU:O	1.97	0.63
1:A:256:ALA:O	1:A:260:VAL:HG23	1.98	0.63
1:A:357:ALA:O	1:A:361:VAL:HG22	1.98	0.63
1:A:797:VAL:O	1:A:801:ASP:CG	2.40	0.63
1:A:846:SER:HG	1:A:854:THR:HG23	1.63	0.63
1:A:879:ALA:O	1:A:883:LYS:HG2	1.99	0.63
1:B:569:LEU:O	1:B:573:ARG:HG3	1.98	0.63
1:B:766:PHE:O	1:B:767:PHE:C	2.41	0.63
1:B:1039:ASN:ND2	1:B:1047:PRO:HA	2.12	0.63
1:A:611:LEU:HD23	1:A:618:TYR:HB2	1.80	0.63
1:B:175:VAL:HG13	1:B:176:SER:N	2.13	0.63
1:B:1214:LEU:O	1:B:1214:LEU:HD23	1.98	0.63
1:A:1058:LYS:O	1:A:1060:GLN:HG3	1.98	0.63
1:A:1079:LEU:CD2	1:A:1194:LEU:HD21	2.28	0.63
1:A:1038:PHE:CG	1:A:1039:ASN:N	2.66	0.63
1:A:1221:ARG:H	1:A:1221:ARG:HD2	1.64	0.63
1:A:1267:VAL:O	1:A:1270:GLN:HB3	1.99	0.63
1:B:981:ALA:HB3	2:B:6002:OJZ:H35	1.78	0.63
1:B:1179:ARG:HH21	1:B:1209:VAL:HG11	1.61	0.63
1:B:1234:GLN:HA	1:B:1253:HIS:HD2	1.63	0.63
1:A:288:ALA:CA	1:A:291:ALA:HB3	2.26	0.63
1:B:45:LEU:HD22	1:B:45:LEU:H	1.63	0.63
1:B:711:ILE:O	1:B:714:ALA:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:TRP:HA	1:A:311:TRP:CE3	2.33	0.63
1:A:535:ILE:O	1:A:538:ALA:HB3	1.99	0.63
1:A:1095:LYS:H	1:A:1095:LYS:HD2	1.62	0.63
1:B:221:LEU:HD11	1:B:309:ALA:HB3	1.81	0.63
1:A:50:MET:HG3	1:A:131:PHE:CE2	2.33	0.63
1:A:56:ALA:O	1:A:59:ILE:HG13	1.99	0.63
1:A:423:GLY:HA2	1:A:597:PHE:O	1.99	0.63
1:A:780:LEU:O	1:A:784:LEU:HD23	1.98	0.63
1:B:144:ARG:NH1	1:B:175:VAL:HG11	2.14	0.63
1:B:245:LYS:HZ1	1:B:245:LYS:HA	1.64	0.63
1:A:45:LEU:HD22	1:A:45:LEU:H	1.63	0.62
1:A:784:LEU:O	1:A:788:VAL:HG23	1.98	0.62
1:A:853:LEU:HB3	1:A:973:VAL:HG13	1.78	0.62
1:A:916:TYR:O	1:A:920:LEU:HD23	1.99	0.62
1:A:969:ASN:HD22	1:A:970:VAL:N	1.96	0.62
1:B:365:ILE:HG22	1:B:366:ASP:N	2.14	0.62
1:B:385:GLN:NE2	1:B:386:GLY:H	1.96	0.62
1:B:779:ILE:HG13	1:B:780:LEU:H	1.64	0.62
1:A:471:GLN:HG2	1:A:472:GLU:N	2.14	0.62
1:A:993:ASP:C	1:A:995:ALA:H	2.07	0.62
1:B:198:GLY:O	1:B:202:ILE:HG13	1.98	0.62
1:B:208:TRP:O	1:B:209:LYS:HG2	1.99	0.62
1:B:318:ILE:HD12	1:B:324:ILE:H	1.64	0.62
1:B:459:VAL:O	1:B:462:LEU:HB3	1.99	0.62
1:B:471:GLN:HG2	1:B:472:GLU:N	2.13	0.62
1:B:843:ILE:O	1:B:846:SER:HB3	1.99	0.62
1:A:428:GLY:O	1:A:431:THR:HB	1.99	0.62
1:A:766:PHE:O	1:A:767:PHE:C	2.40	0.62
1:A:1214:LEU:HA	1:A:1217:ALA:HB3	1.81	0.62
1:B:696:ILE:HD13	1:B:998:THR:HG23	1.79	0.62
1:A:39:PHE:CE2	1:A:355:ARG:HA	2.34	0.62
1:A:253:VAL:HB	1:A:1119:PHE:HE1	1.63	0.62
1:A:1042:THR:C	1:A:1044:PRO:HD2	2.24	0.62
1:B:807:THR:O	1:B:811:THR:HG23	2.00	0.62
1:B:1048:VAL:HG23	1:B:1049:LEU:CD2	2.30	0.62
1:A:388:LEU:N	1:A:388:LEU:HD12	2.14	0.62
1:A:799:TRP:HA	1:A:799:TRP:CE3	2.32	0.62
1:A:1019:THR:OG1	1:A:1101:ASN:HA	1.99	0.62
1:B:267:LYS:HA	1:B:270:LEU:HD11	1.81	0.62
1:B:509:ILE:HD12	1:B:510:MET:N	2.15	0.62
1:B:799:TRP:HA	1:B:799:TRP:HE3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:857:LEU:HD12	1:B:973:VAL:CG1	2.29	0.62
1:B:1063:ALA:HB3	1:B:1239:ILE:CA	2.28	0.62
1:B:1100:LEU:HG	1:B:1101:ASN:N	2.14	0.62
1:B:1221:ARG:H	1:B:1221:ARG:HD2	1.64	0.62
1:A:195:THR:HB	1:A:340:SER:OG	1.99	0.62
1:A:246:ALA:HB2	1:A:281:LYS:HZ2	1.64	0.62
1:A:308:LEU:HD12	1:A:751:PHE:HE2	1.62	0.62
1:B:257:ILE:HG23	1:B:258:ARG:N	2.15	0.62
1:B:388:LEU:HD12	1:B:388:LEU:N	2.14	0.62
1:B:608:HIS:ND1	1:B:618:TYR:HE2	1.97	0.62
1:B:908:ARG:O	1:B:909:GLU:C	2.41	0.62
1:A:696:ILE:HD13	1:A:998:THR:HG23	1.80	0.62
1:A:1137:SER:O	1:A:1141:ILE:HG23	2.00	0.62
1:A:1196:ASP:HA	1:A:1226:ILE:CG1	2.29	0.62
1:B:65:PRO:O	1:B:68:MET:N	2.33	0.62
1:B:195:THR:HB	1:B:340:SER:OG	1.99	0.62
1:B:207:GLY:HA3	1:B:211:THR:H	1.63	0.62
1:B:211:THR:O	1:B:214:ILE:HB	1.99	0.62
1:B:287:LYS:O	1:B:291:ALA:HB2	2.00	0.62
1:B:1158:PRO:O	1:B:1159:ASP:HB2	2.00	0.62
1:A:144:ARG:NH1	1:A:175:VAL:HG11	2.15	0.62
1:A:385:GLN:NE2	1:A:386:GLY:H	1.98	0.62
1:A:820:GLN:HG3	1:A:1000:SER:CB	2.30	0.62
1:A:1048:VAL:HG23	1:A:1049:LEU:CD2	2.29	0.62
1:A:711:ILE:O	1:A:714:ALA:HB3	2.00	0.62
1:A:742:GLU:O	1:A:746:GLN:HG2	2.00	0.62
1:A:933:VAL:O	1:A:934:PHE:C	2.43	0.62
1:A:1179:ARG:HH21	1:A:1209:VAL:HG11	1.60	0.62
1:B:158:TRP:HE1	1:B:900:PHE:HB3	1.65	0.62
1:B:846:SER:HA	1:B:849:TYR:CD1	2.35	0.62
1:B:1037:VAL:HG12	1:B:1051:GLY:N	2.14	0.62
1:A:107:MET:HA	1:A:110:TYR:HD2	1.63	0.62
1:B:324:ILE:O	1:B:325:GLY:C	2.43	0.62
1:B:905:SER:O	1:B:907:THR:N	2.33	0.62
1:B:1216:LYS:HA	1:B:1216:LYS:CE	2.30	0.62
1:A:537:ILE:O	1:A:541:LEU:HB2	1.99	0.61
1:B:39:PHE:CE2	1:B:355:ARG:HA	2.35	0.61
1:B:217:ILE:HD11	1:B:331:PHE:HE2	1.64	0.61
1:B:379:HIS:C	1:B:381:PRO:HD3	2.24	0.61
1:B:916:TYR:O	1:B:920:LEU:HD23	1.99	0.61
1:B:50:MET:HG3	1:B:131:PHE:CE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:GLU:O	1:B:157:GLY:N	2.33	0.61
1:B:215:LEU:C	1:B:219:PRO:HD2	2.25	0.61
1:B:538:ALA:O	1:B:541:LEU:HB3	1.99	0.61
1:B:574:GLU:O	1:B:574:GLU:HG3	1.98	0.61
1:B:956:GLY:O	1:B:966:THR:CB	2.46	0.61
1:B:1196:ASP:HA	1:B:1226:ILE:CG1	2.30	0.61
1:A:806:THR:O	1:A:810:LEU:HG	2.00	0.61
1:A:1037:VAL:HG12	1:A:1051:GLY:N	2.14	0.61
1:B:107:MET:HA	1:B:110:TYR:HD2	1.63	0.61
1:B:209:LYS:O	1:B:212:LEU:HB3	2.01	0.61
1:B:238:LYS:NZ	1:B:242:ALA:HB2	2.15	0.61
1:B:324:ILE:HD13	1:B:326:GLN:HB3	1.83	0.61
1:B:910:GLN:O	1:B:911:LYS:C	2.43	0.61
1:B:1095:LYS:H	1:B:1095:LYS:HD2	1.64	0.61
1:A:282:ARG:O	1:A:286:LYS:HD3	2.00	0.61
1:A:913:GLU:OE2	1:A:913:GLU:HA	2.00	0.61
1:B:67:MET:SD	1:B:113:TYR:HE1	2.23	0.61
1:B:286:LYS:CA	1:B:289:ILE:HB	2.24	0.61
1:B:718:GLY:HA3	1:B:837:ALA:HB2	1.81	0.61
1:B:1184:ARG:O	1:B:1187:VAL:HB	2.00	0.61
1:A:67:MET:SD	1:A:113:TYR:HE1	2.24	0.61
1:A:204:PHE:CA	1:A:211:THR:HG21	2.30	0.61
1:A:303:TYR:O	1:A:304:ALA:C	2.43	0.61
1:A:324:ILE:O	1:A:325:GLY:C	2.43	0.61
1:B:158:TRP:O	1:B:164:VAL:HG11	2.00	0.61
1:B:282:ARG:O	1:B:286:LYS:HD3	2.00	0.61
1:A:131:PHE:O	1:A:132:TRP:C	2.44	0.61
1:A:217:ILE:HD11	1:A:331:PHE:HE2	1.65	0.61
1:A:267:LYS:CA	1:A:270:LEU:HD21	2.30	0.61
1:A:286:LYS:CA	1:A:289:ILE:HB	2.26	0.61
1:A:318:ILE:HD12	1:A:322:TYR:O	2.00	0.61
1:A:1216:LYS:HA	1:A:1216:LYS:CE	2.30	0.61
1:B:154:GLN:NE2	1:B:162:HIS:NE2	2.42	0.61
1:B:969:ASN:HD22	1:B:970:VAL:N	1.98	0.61
1:B:1196:ASP:CG	1:B:1226:ILE:HD11	2.26	0.61
1:A:133:CYS:O	1:A:135:ALA:N	2.34	0.61
1:A:257:ILE:HG23	1:A:258:ARG:N	2.15	0.61
1:A:908:ARG:O	1:A:909:GLU:C	2.42	0.61
1:B:611:LEU:HD23	1:B:618:TYR:HB2	1.81	0.61
1:A:603:VAL:HG23	1:A:604:GLU:H	1.66	0.61
1:B:118:GLY:O	1:B:119:ALA:C	2.44	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:766:PHE:O	1:B:769:GLN:HG2	2.00	0.61
1:B:806:THR:O	1:B:810:LEU:HG	2.01	0.61
1:B:1038:PHE:CG	1:B:1039:ASN:N	2.68	0.61
1:A:492:THR:HG22	1:A:494:ASP:H	1.66	0.61
1:A:1158:PRO:O	1:A:1159:ASP:HB2	2.01	0.61
1:B:37:THR:O	1:B:38:MET:C	2.43	0.61
1:B:268:LYS:HZ2	1:B:272:ARG:HD3	1.66	0.61
1:B:968:GLU:O	1:B:971:LEU:HD23	2.01	0.61
1:A:185:LYS:HZ3	1:A:186:ILE:N	1.99	0.61
1:A:287:LYS:O	1:A:291:ALA:HB2	2.01	0.61
1:A:438:ARG:O	1:A:439:LEU:C	2.41	0.61
1:A:843:ILE:O	1:A:846:SER:HB3	2.00	0.61
1:B:154:GLN:HE22	1:B:162:HIS:CD2	2.19	0.61
1:B:163:ASP:C	1:B:165:GLY:N	2.59	0.61
1:B:1148:ALA:HB1	1:B:1179:ARG:O	2.01	0.61
1:A:53:GLY:O	1:A:54:THR:C	2.42	0.60
1:A:238:LYS:NZ	1:A:242:ALA:HB2	2.15	0.60
1:A:373:SER:O	1:A:374:PHE:HB3	2.01	0.60
1:A:1023:LYS:O	1:A:1025:ASN:N	2.34	0.60
1:B:133:CYS:O	1:B:135:ALA:N	2.34	0.60
1:B:185:LYS:HZ3	1:B:186:ILE:N	1.97	0.60
1:B:429:LYS:HD2	1:B:430:SER:H	1.65	0.60
1:B:604:GLU:OE1	1:B:616:GLY:HA3	2.01	0.60
1:B:742:GLU:O	1:B:746:GLN:HG2	2.00	0.60
1:A:210:LEU:C	1:A:210:LEU:HD13	2.26	0.60
1:A:268:LYS:NZ	1:A:272:ARG:HD3	2.16	0.60
1:A:365:ILE:HG22	1:A:366:ASP:N	2.14	0.60
1:A:733:GLY:HA3	1:A:968:GLU:HG3	1.83	0.60
1:A:1144:ALA:CA	1:A:1186:LEU:HD11	2.29	0.60
1:A:1148:ALA:O	1:A:1149:ASN:HB2	2.01	0.60
1:B:193:MET:HE3	1:B:197:PHE:HE2	1.67	0.60
1:B:1079:LEU:CD2	1:B:1194:LEU:HD21	2.29	0.60
1:A:731:VAL:HG22	1:A:750:LEU:HB3	1.82	0.60
1:A:766:PHE:O	1:A:769:GLN:HG2	2.01	0.60
1:B:906:LEU:HD23	1:B:906:LEU:O	2.00	0.60
1:B:931:ALA:O	1:B:932:HIS:C	2.43	0.60
1:B:959:LEU:O	1:B:964:LEU:HB3	2.01	0.60
1:B:1148:ALA:O	1:B:1149:ASN:HB2	2.02	0.60
1:A:268:LYS:HZ2	1:A:272:ARG:HD3	1.66	0.60
1:B:125:ALA:O	1:B:128:GLN:HG2	2.01	0.60
1:B:993:ASP:C	1:B:995:ALA:H	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1038:PHE:O	1:B:1049:LEU:HB2	2.01	0.60
1:B:1097:ILE:O	1:B:1098:LYS:HB3	2.01	0.60
1:B:1106:ARG:O	1:B:1109:LEU:HD22	2.01	0.60
1:A:267:LYS:HB3	1:A:790:LYS:CE	2.29	0.60
1:B:53:GLY:O	1:B:54:THR:C	2.45	0.60
1:B:59:ILE:CG1	1:B:124:VAL:HG11	2.32	0.60
1:B:268:LYS:NZ	1:B:272:ARG:HD3	2.17	0.60
1:B:288:ALA:CA	1:B:291:ALA:HB3	2.25	0.60
1:B:427:CYS:O	1:B:599:GLY:HA2	2.01	0.60
1:B:689:PRO:HG2	1:B:690:PRO:HD3	1.84	0.60
1:B:849:TYR:CB	1:B:854:THR:OG1	2.49	0.60
1:A:211:THR:O	1:A:214:ILE:HB	2.01	0.60
1:A:1193:LEU:HB2	1:A:1223:CYS:CB	2.32	0.60
1:A:1196:ASP:CG	1:A:1226:ILE:HD11	2.26	0.60
1:B:64:LEU:O	1:B:67:MET:HB3	2.02	0.60
1:B:213:VAL:O	1:B:217:ILE:HG12	2.01	0.60
1:B:256:ALA:O	1:B:260:VAL:HG23	2.02	0.60
1:A:59:ILE:CG1	1:A:124:VAL:HG11	2.31	0.60
1:A:197:PHE:O	1:A:201:ILE:HD13	2.01	0.60
1:A:324:ILE:C	1:A:326:GLN:N	2.59	0.60
1:A:548:LEU:HD23	1:A:549:LEU:N	2.17	0.60
1:A:886:LEU:HD12	1:A:887:GLU:N	2.17	0.60
1:B:357:ALA:O	1:B:361:VAL:HG22	2.01	0.60
1:B:720:LEU:O	1:B:723:ALA:HB3	2.01	0.60
1:B:1048:VAL:C	1:B:1049:LEU:HD22	2.27	0.60
1:A:291:ALA:HA	1:A:294:SER:HB2	1.83	0.60
1:B:1202:LEU:HG	1:B:1206:SER:HB2	1.83	0.60
1:A:910:GLN:O	1:A:911:LYS:C	2.44	0.60
1:A:1063:ALA:HB3	1:A:1239:ILE:CA	2.26	0.60
1:B:65:PRO:O	1:B:66:LEU:C	2.43	0.60
1:B:133:CYS:CB	1:B:931:ALA:HB1	2.32	0.60
1:B:197:PHE:O	1:B:201:ILE:HD13	2.01	0.60
1:B:388:LEU:HD11	1:B:547:ILE:HD12	1.84	0.60
1:B:406:LEU:HD12	1:B:409:LEU:HB2	1.84	0.60
1:A:608:HIS:ND1	1:A:618:TYR:HE2	1.97	0.60
1:A:1038:PHE:O	1:A:1049:LEU:HB2	2.02	0.60
1:A:41:TYR:HE1	1:A:143:ILE:HD11	1.67	0.59
1:A:235:PHE:O	1:A:239:GLU:HG2	2.02	0.59
1:A:387:ASN:O	1:A:450:ASP:O	2.20	0.59
1:A:468:VAL:HG22	1:A:549:LEU:HD13	1.84	0.59
1:A:540:ALA:O	1:A:543:ARG:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:THR:O	1:A:811:THR:HG23	2.01	0.59
1:A:810:LEU:O	1:A:811:THR:C	2.45	0.59
1:A:826:GLY:O	1:A:829:LEU:HB2	2.02	0.59
1:A:900:PHE:O	1:A:903:VAL:HG12	2.00	0.59
1:A:902:THR:O	1:A:904:VAL:N	2.35	0.59
1:B:41:TYR:HE1	1:B:143:ILE:HD11	1.67	0.59
1:B:156:ILE:HD11	1:B:373:SER:HB3	1.83	0.59
1:B:188:MET:O	1:B:189:PHE:C	2.44	0.59
1:B:731:VAL:HG22	1:B:750:LEU:HB3	1.84	0.59
1:B:978:VAL:CG1	2:B:6002:OJZ:H35B	2.30	0.59
1:A:193:MET:HE3	1:A:197:PHE:HE2	1.67	0.59
1:A:762:SER:O	1:A:765:THR:HG22	2.02	0.59
1:B:1042:THR:C	1:B:1044:PRO:HD2	2.26	0.59
1:B:1120:ASP:HA	1:B:1165:VAL:HG21	1.84	0.59
1:A:279:GLU:HG2	1:A:782:LYS:CD	2.32	0.59
1:A:1079:LEU:C	1:A:1081:ARG:H	2.09	0.59
1:A:1100:LEU:HG	1:A:1101:ASN:N	2.16	0.59
1:B:938:PHE:O	1:B:941:THR:HB	2.02	0.59
1:A:207:GLY:HA3	1:A:211:THR:N	2.17	0.59
1:A:585:LEU:HD22	1:A:585:LEU:H	1.68	0.59
1:A:718:GLY:O	1:A:722:PRO:CD	2.48	0.59
1:B:81:VAL:HG13	1:B:99:MET:HG3	1.85	0.59
1:B:210:LEU:HD13	1:B:210:LEU:C	2.26	0.59
1:B:1022:LEU:O	1:B:1022:LEU:HD23	2.02	0.59
1:A:37:THR:O	1:A:38:MET:C	2.45	0.59
1:A:254:LEU:HD23	1:A:811:THR:CG2	2.30	0.59
1:A:359:TYR:O	1:A:362:PHE:HB3	2.02	0.59
1:A:388:LEU:HD11	1:A:547:ILE:HD12	1.84	0.59
1:B:235:PHE:O	1:B:239:GLU:HG2	2.02	0.59
1:B:492:THR:C	1:B:494:ASP:N	2.57	0.59
1:B:528:SER:OG	1:B:531:GLN:HG3	2.02	0.59
1:B:900:PHE:O	1:B:903:VAL:HG12	2.01	0.59
1:B:1144:ALA:HB1	1:B:1183:ALA:HB1	1.85	0.59
1:A:138:ARG:NH2	1:B:515:GLN:NE2	2.50	0.59
1:A:725:SER:HA	2:A:6001:OJZ:C36	2.32	0.59
1:A:938:PHE:O	1:A:941:THR:HB	2.02	0.59
1:A:968:GLU:O	1:A:971:LEU:HD23	2.02	0.59
1:A:1018:SER:O	1:A:1101:ASN:HB2	2.02	0.59
1:B:617:ILE:O	1:B:621:LEU:HD23	2.03	0.59
1:B:913:GLU:HA	1:B:913:GLU:OE2	2.03	0.59
1:B:1020:GLN:HG2	1:B:1021:GLY:N	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:6001:OJZ:O27	2:A:6001:OJZ:H36B	2.02	0.59
1:B:51:LEU:O	1:B:52:VAL:C	2.46	0.59
1:B:958:TYR:O	1:B:966:THR:OG1	2.19	0.59
1:B:1079:LEU:C	1:B:1081:ARG:H	2.10	0.59
1:B:1267:VAL:O	1:B:1270:GLN:HB3	2.02	0.59
1:A:51:LEU:O	1:A:52:VAL:C	2.46	0.59
1:A:1020:GLN:HB3	1:A:1100:LEU:HD12	1.85	0.59
1:B:70:ILE:C	1:B:72:GLY:N	2.59	0.59
1:B:107:MET:HA	1:B:110:TYR:CD2	2.38	0.59
1:B:239:GLU:CB	1:B:285:ILE:HG12	2.33	0.59
1:B:359:TYR:O	1:B:362:PHE:HB3	2.02	0.59
1:B:370:SER:C	1:B:372:ASP:H	2.10	0.59
1:B:390:PHE:HB2	1:B:411:LEU:O	2.03	0.59
1:B:1109:LEU:HD21	1:B:1188:ARG:NH1	2.17	0.59
1:A:170:ARG:HH11	1:A:170:ARG:HB2	1.67	0.59
1:A:198:GLY:O	1:A:202:ILE:HG13	2.02	0.59
1:B:263:PHE:CE1	1:B:1129:TYR:HB3	2.36	0.59
1:B:536:ALA:O	1:B:537:ILE:C	2.46	0.59
1:A:129:VAL:O	1:A:132:TRP:HB3	2.03	0.59
1:A:617:ILE:O	1:A:621:LEU:HD23	2.03	0.59
1:A:720:LEU:O	1:A:723:ALA:HB3	2.02	0.59
1:A:1109:LEU:HD21	1:A:1188:ARG:NH1	2.18	0.59
1:B:49:TYR:OH	1:B:130:SER:HB2	2.03	0.59
1:B:812:THR:O	1:B:813:ARG:C	2.44	0.59
1:B:1120:ASP:HA	1:B:1165:VAL:CG2	2.33	0.59
1:A:779:ILE:HG13	1:A:780:LEU:H	1.66	0.58
1:A:812:THR:O	1:A:813:ARG:C	2.45	0.58
1:A:1016:SER:O	1:A:1017:TYR:HB2	2.02	0.58
1:A:1071:GLY:O	1:A:1075:VAL:HG23	2.03	0.58
1:B:302:ILE:O	1:B:305:SER:HB3	2.02	0.58
1:B:324:ILE:C	1:B:326:GLN:N	2.59	0.58
1:B:327:VAL:HB	1:B:331:PHE:CE1	2.38	0.58
1:A:59:ILE:C	1:A:59:ILE:HD12	2.27	0.58
1:A:536:ALA:O	1:A:537:ILE:C	2.46	0.58
1:A:902:THR:OG1	1:A:908:ARG:HD3	2.03	0.58
1:B:199:GLY:HA2	1:B:202:ILE:HD11	1.86	0.58
1:B:507:ASP:OD1	1:B:508:PHE:N	2.35	0.58
1:B:1261:GLY:H	1:B:1264:PHE:HB3	1.68	0.58
1:A:81:VAL:HG13	1:A:99:MET:HG3	1.86	0.58
1:A:213:VAL:O	1:A:217:ILE:HG12	2.02	0.58
1:A:945:MET:O	1:A:949:TYR:HD1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:993:ASP:N	1:A:996:LYS:HZ1	2.01	0.58
1:B:131:PHE:O	1:B:132:TRP:C	2.46	0.58
1:B:217:ILE:O	1:B:221:LEU:HG	2.02	0.58
1:B:255:ALA:C	1:B:257:ILE:N	2.60	0.58
1:B:479:THR:O	1:B:482:GLU:HB2	2.03	0.58
1:B:520:VAL:HG12	1:B:523:ARG:O	2.04	0.58
1:B:886:LEU:HD12	1:B:887:GLU:N	2.18	0.58
1:B:1005:ILE:O	1:B:1008:ILE:HG22	2.03	0.58
1:B:1053:SER:C	1:B:1054:LEU:HD22	2.28	0.58
1:A:64:LEU:O	1:A:67:MET:HB3	2.03	0.58
1:A:215:LEU:C	1:A:219:PRO:HD2	2.28	0.58
1:A:520:VAL:HG12	1:A:523:ARG:O	2.04	0.58
1:A:541:LEU:O	1:A:544:ASN:N	2.35	0.58
1:A:804:LYS:HD3	1:A:804:LYS:N	2.19	0.58
1:B:438:ARG:O	1:B:439:LEU:C	2.44	0.58
1:B:585:LEU:H	1:B:585:LEU:HD22	1.68	0.58
1:B:1037:VAL:HG22	1:B:1087:ALA:H	1.68	0.58
1:B:1199:THR:CG2	1:B:1210:VAL:HG11	2.34	0.58
1:A:199:GLY:HA2	1:A:202:ILE:HD11	1.85	0.58
1:A:604:GLU:OE1	1:A:616:GLY:HA3	2.03	0.58
1:A:1009:GLU:O	1:A:1010:LYS:HG3	2.03	0.58
1:B:37:THR:O	1:B:40:ARG:N	2.34	0.58
1:B:170:ARG:HB2	1:B:170:ARG:HH11	1.68	0.58
1:B:359:TYR:HA	1:B:362:PHE:HB3	1.86	0.58
1:B:478:THR:CG2	1:B:482:GLU:HG3	2.34	0.58
1:B:492:THR:HG22	1:B:494:ASP:H	1.67	0.58
1:B:535:ILE:O	1:B:538:ALA:HB3	2.04	0.58
1:B:540:ALA:O	1:B:543:ARG:HB3	2.03	0.58
1:B:902:THR:OG1	1:B:908:ARG:HD3	2.03	0.58
1:A:798:SER:HB3	1:A:1041:PRO:HG2	1.85	0.58
1:A:1048:VAL:C	1:A:1049:LEU:HD22	2.28	0.58
1:B:318:ILE:HD13	1:B:327:VAL:CG1	2.23	0.58
1:B:500:VAL:HG23	1:B:501:LYS:N	2.19	0.58
1:B:762:SER:O	1:B:765:THR:HG22	2.04	0.58
1:A:257:ILE:HG13	1:A:800:PHE:CG	2.38	0.58
1:A:602:ILE:O	1:A:603:VAL:HG13	2.04	0.58
1:B:537:ILE:O	1:B:541:LEU:HB2	2.03	0.58
1:A:305:SER:O	1:A:306:TYR:C	2.47	0.58
1:A:528:SER:OG	1:A:531:GLN:HG3	2.03	0.58
1:B:263:PHE:HE1	1:B:1129:TYR:HB3	1.67	0.58
1:B:429:LYS:HD3	1:B:581:ILE:HG12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:VAL:HG22	1:B:549:LEU:HD13	1.85	0.58
1:A:70:ILE:C	1:A:72:GLY:N	2.59	0.58
1:A:125:ALA:O	1:A:128:GLN:HG2	2.04	0.58
1:A:478:THR:CG2	1:A:482:GLU:HG3	2.33	0.58
1:A:500:VAL:HG23	1:A:501:LYS:N	2.19	0.58
1:A:931:ALA:O	1:A:932:HIS:C	2.46	0.58
1:A:1184:ARG:O	1:A:1187:VAL:HB	2.03	0.58
1:B:864:ILE:HD12	1:B:864:ILE:C	2.28	0.58
1:B:1197:GLU:O	1:B:1198:ALA:C	2.46	0.58
1:A:203:GLY:C	1:A:211:THR:OG1	2.47	0.58
1:A:207:GLY:HA2	1:A:210:LEU:HB3	1.85	0.58
1:A:239:GLU:CB	1:A:285:ILE:HG12	2.32	0.58
1:A:327:VAL:HB	1:A:331:PHE:CE1	2.38	0.58
1:A:507:ASP:OD1	1:A:508:PHE:N	2.36	0.58
1:B:303:TYR:O	1:B:304:ALA:C	2.46	0.58
1:B:711:ILE:HG13	1:B:832:ILE:HG21	1.85	0.58
1:B:810:LEU:O	1:B:811:THR:C	2.46	0.58
1:B:1132:ASN:OD1	1:B:1134:ARG:HG2	2.03	0.58
1:B:1137:SER:CB	1:B:1140:GLU:HB2	2.33	0.58
1:A:158:TRP:CZ2	1:A:900:PHE:HB2	2.39	0.57
1:A:245:LYS:HA	1:A:245:LYS:HZ1	1.68	0.57
1:A:278:GLU:OE2	1:A:785:ARG:HD2	2.03	0.57
1:A:359:TYR:HA	1:A:362:PHE:HB3	1.86	0.57
1:A:784:LEU:HD12	1:A:1004:ILE:CD1	2.34	0.57
1:A:993:ASP:N	1:A:996:LYS:NZ	2.52	0.57
1:A:1037:VAL:HG22	1:A:1087:ALA:H	1.68	0.57
1:A:1077:GLN:O	1:A:1080:GLU:N	2.36	0.57
1:B:129:VAL:O	1:B:132:TRP:HB3	2.04	0.57
1:B:379:HIS:CD2	1:B:380:LYS:H	2.22	0.57
1:B:1037:VAL:HG22	1:B:1087:ALA:N	2.19	0.57
1:A:151:ILE:C	1:A:153:ASN:H	2.12	0.57
1:A:217:ILE:O	1:A:221:LEU:HG	2.04	0.57
1:A:492:THR:C	1:A:494:ASP:N	2.56	0.57
1:A:708:VAL:O	1:A:711:ILE:HG22	2.04	0.57
1:A:834:GLN:HG3	1:A:835:ASN:N	2.19	0.57
1:A:853:LEU:CG	1:A:973:VAL:HG21	2.29	0.57
1:A:961:THR:O	1:A:962:GLN:HB3	2.04	0.57
1:A:1214:LEU:HD23	1:A:1214:LEU:O	2.03	0.57
1:B:212:LEU:HD12	1:B:215:LEU:HD12	1.86	0.57
1:B:548:LEU:HD23	1:B:549:LEU:N	2.20	0.57
1:B:850:GLY:O	1:B:852:GLN:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PHE:CE2	1:A:358:ALA:HB3	2.38	0.57
1:A:324:ILE:HD13	1:A:326:GLN:HB3	1.85	0.57
1:A:1031:VAL:HB	1:A:1056:VAL:CG1	2.35	0.57
1:A:1148:ALA:HB1	1:A:1179:ARG:O	2.04	0.57
1:B:356:GLY:HA2	1:B:359:TYR:CE1	2.39	0.57
1:B:434:GLN:C	1:B:436:MET:H	2.13	0.57
1:B:465:ILE:O	1:B:465:ILE:HG22	2.04	0.57
1:B:603:VAL:HG21	1:B:617:ILE:HG12	1.86	0.57
1:A:111:ALA:HA	1:A:114:TYR:HE1	1.70	0.57
1:A:118:GLY:O	1:A:119:ALA:C	2.45	0.57
1:A:1199:THR:CG2	1:A:1210:VAL:HG11	2.34	0.57
1:B:195:THR:HG23	1:B:196:PHE:N	2.19	0.57
1:B:311:TRP:HZ2	1:B:728:PHE:CE2	2.22	0.57
1:A:345:SER:HB3	1:A:346:PRO:HD3	1.87	0.57
1:A:405:ILE:HG22	1:A:406:LEU:HD22	1.87	0.57
1:A:727:ILE:HD13	1:A:754:LEU:HD23	1.85	0.57
1:A:1120:ASP:HA	1:A:1165:VAL:CG2	2.34	0.57
1:A:1197:GLU:O	1:A:1198:ALA:C	2.47	0.57
1:A:1261:GLY:H	1:A:1264:PHE:HB3	1.69	0.57
1:B:246:ALA:HB2	1:B:281:LYS:NZ	2.20	0.57
1:A:61:GLY:O	1:A:65:PRO:CD	2.43	0.57
1:A:295:MET:HE3	1:A:295:MET:HA	1.87	0.57
1:A:479:THR:O	1:A:482:GLU:HB2	2.04	0.57
1:A:780:LEU:O	1:A:784:LEU:HB2	2.05	0.57
1:A:1120:ASP:HA	1:A:1165:VAL:HG21	1.87	0.57
1:A:1132:ASN:OD1	1:A:1134:ARG:HG2	2.04	0.57
1:B:291:ALA:HA	1:B:294:SER:HB2	1.87	0.57
1:A:107:MET:HA	1:A:110:TYR:CD2	2.38	0.57
1:A:233:SER:O	1:A:236:THR:HB	2.05	0.57
1:A:337:GLY:O	1:A:341:VAL:HG23	2.05	0.57
1:A:358:ALA:O	1:A:362:PHE:CB	2.52	0.57
1:A:459:VAL:O	1:A:462:LEU:HB3	2.04	0.57
1:A:707:PHE:HZ	1:A:775:LYS:HE2	1.69	0.57
1:A:816:ASN:CG	1:A:817:ASP:N	2.63	0.57
1:A:1053:SER:C	1:A:1054:LEU:HD22	2.29	0.57
1:B:39:PHE:CE2	1:B:358:ALA:HB3	2.39	0.57
1:B:59:ILE:HD11	1:B:124:VAL:CG1	2.34	0.57
1:B:309:ALA:O	1:B:310:PHE:O	2.23	0.57
1:B:342:GLY:O	1:B:345:SER:N	2.37	0.57
1:B:527:LEU:HD23	1:B:527:LEU:N	2.19	0.57
1:B:618:TYR:O	1:B:622:VAL:HG23	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:GLY:O	1:B:722:PRO:CD	2.47	0.57
1:B:784:LEU:HD12	1:B:1004:ILE:CD1	2.34	0.57
1:B:818:ALA:O	1:B:821:VAL:HG22	2.05	0.57
1:B:1252:THR:HG23	1:B:1255:GLN:HB2	1.86	0.57
1:A:65:PRO:O	1:A:66:LEU:C	2.46	0.57
1:A:212:LEU:HD12	1:A:215:LEU:HD12	1.87	0.57
1:A:246:ALA:HB2	1:A:281:LYS:NZ	2.19	0.57
1:A:342:GLY:O	1:A:345:SER:N	2.38	0.57
1:A:362:PHE:O	1:A:365:ILE:HB	2.05	0.57
1:A:384:ILE:HG22	1:A:385:GLN:N	2.19	0.57
1:B:59:ILE:C	1:B:59:ILE:HD12	2.29	0.57
1:B:110:TYR:HA	1:B:113:TYR:HD2	1.70	0.57
1:B:151:ILE:C	1:B:153:ASN:H	2.12	0.57
1:B:713:CYS:O	1:B:716:ILE:HG13	2.05	0.57
1:A:49:TYR:OH	1:A:130:SER:HB2	2.03	0.57
1:A:195:THR:HG23	1:A:196:PHE:N	2.19	0.57
1:A:286:LYS:HE3	1:A:822:LYS:HZ1	1.70	0.57
1:B:245:LYS:HA	1:B:245:LYS:NZ	2.19	0.57
1:B:816:ASN:CG	1:B:817:ASP:N	2.62	0.57
1:A:70:ILE:O	1:A:72:GLY:N	2.38	0.57
1:A:207:GLY:HA3	1:A:211:THR:HB	1.87	0.57
1:A:711:ILE:HG13	1:A:832:ILE:HG21	1.86	0.57
1:A:827:SER:O	1:A:828:ARG:C	2.48	0.57
1:A:1137:SER:CB	1:A:1140:GLU:HB2	2.35	0.57
1:B:136:ALA:HB2	1:B:182:ILE:CB	2.33	0.57
1:B:156:ILE:HG22	1:B:160:ASP:OD1	2.05	0.57
1:B:387:ASN:O	1:B:450:ASP:O	2.22	0.57
1:B:492:THR:O	1:B:494:ASP:N	2.38	0.57
1:B:548:LEU:C	1:B:549:LEU:HD12	2.30	0.57
1:B:773:PHE:HB2	1:B:829:LEU:CD1	2.35	0.57
1:B:857:LEU:CD1	1:B:976:ALA:HB3	2.32	0.57
1:A:156:ILE:HG22	1:A:160:ASP:OD1	2.05	0.56
1:A:548:LEU:C	1:A:549:LEU:HD12	2.30	0.56
1:A:786:TYR:HE2	1:A:790:LYS:NZ	2.03	0.56
1:A:1011:THR:O	1:A:1012:PRO:C	2.48	0.56
1:A:1037:VAL:HG22	1:A:1087:ALA:N	2.19	0.56
1:B:186:ILE:CG1	1:B:187:GLY:N	2.68	0.56
1:B:253:VAL:O	1:B:254:LEU:HD13	2.05	0.56
1:B:341:VAL:O	1:B:344:ALA:HB3	2.05	0.56
1:B:460:ARG:O	1:B:461:TYR:C	2.47	0.56
1:B:482:GLU:O	1:B:484:ILE:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:945:MET:O	1:B:949:TYR:HD1	1.87	0.56
1:A:354:ALA:O	1:A:358:ALA:HB3	2.05	0.56
1:A:810:LEU:O	1:A:813:ARG:HB2	2.05	0.56
1:A:834:GLN:O	1:A:837:ALA:HB3	2.05	0.56
1:A:864:ILE:HD12	1:A:864:ILE:C	2.30	0.56
1:A:902:THR:O	1:A:903:VAL:C	2.47	0.56
1:A:1212:GLU:O	1:A:1215:ASP:HB3	2.05	0.56
1:A:1252:THR:HG23	1:A:1255:GLN:HB2	1.86	0.56
1:B:693:PHE:N	1:B:693:PHE:CD2	2.71	0.56
1:B:761:ILE:N	1:B:761:ILE:HD12	2.20	0.56
1:B:862:PRO:O	1:B:866:ILE:HG13	2.05	0.56
1:A:166:GLU:O	1:A:169:THR:HB	2.05	0.56
1:A:406:LEU:HD12	1:A:409:LEU:HB2	1.87	0.56
1:A:432:THR:O	1:A:433:VAL:C	2.48	0.56
1:A:858:LEU:HD12	1:A:858:LEU:C	2.30	0.56
1:A:1027:LEU:HD12	1:A:1027:LEU:H	1.70	0.56
1:A:1144:ALA:HB1	1:A:1183:ALA:HB1	1.86	0.56
1:A:1195:LEU:O	1:A:1226:ILE:HG12	2.05	0.56
1:B:185:LYS:HB3	1:B:185:LYS:HZ2	1.71	0.56
1:B:318:ILE:CG1	1:B:325:GLY:H	2.19	0.56
1:B:401:LYS:HB3	1:B:401:LYS:HZ2	1.70	0.56
1:B:543:ARG:HH21	1:B:907:THR:HG23	1.70	0.56
1:B:565:VAL:O	1:B:566:GLN:C	2.48	0.56
1:B:711:ILE:CG1	1:B:832:ILE:HG21	2.35	0.56
1:B:810:LEU:O	1:B:813:ARG:HB2	2.05	0.56
1:B:834:GLN:HG3	1:B:835:ASN:N	2.19	0.56
1:B:1031:VAL:HB	1:B:1056:VAL:CG1	2.34	0.56
1:A:290:THR:HG22	1:A:770:GLY:C	2.31	0.56
1:A:419:VAL:HG23	1:A:593:VAL:HG13	1.88	0.56
1:A:800:PHE:C	1:A:803:PRO:HD3	2.31	0.56
1:A:1106:ARG:O	1:A:1109:LEU:HD22	2.04	0.56
1:B:295:MET:HA	1:B:295:MET:HE3	1.87	0.56
1:B:519:LEU:H	1:B:519:LEU:CD1	2.13	0.56
1:B:707:PHE:HZ	1:B:775:LYS:HE2	1.69	0.56
1:B:727:ILE:HD13	1:B:754:LEU:HD23	1.86	0.56
1:B:1144:ALA:CA	1:B:1186:LEU:HD11	2.27	0.56
1:A:245:LYS:HA	1:A:245:LYS:NZ	2.20	0.56
1:A:460:ARG:O	1:A:461:TYR:C	2.48	0.56
1:A:508:PHE:O	1:A:512:LEU:HB2	2.06	0.56
1:A:603:VAL:HG21	1:A:617:ILE:HG12	1.87	0.56
1:A:795:GLN:O	1:A:796:ASP:CB	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ILE:O	1:B:72:GLY:N	2.39	0.56
1:B:286:LYS:HE2	1:B:778:GLU:HG2	1.86	0.56
1:B:550:LEU:N	1:B:550:LEU:HD12	2.20	0.56
1:B:708:VAL:O	1:B:711:ILE:HG22	2.05	0.56
1:B:716:ILE:HD11	1:B:765:THR:OG1	2.06	0.56
1:B:795:GLN:HE21	1:B:796:ASP:N	2.03	0.56
1:B:1076:VAL:HG13	1:B:1194:LEU:HD22	1.88	0.56
1:B:1229:ARG:C	1:B:1231:SER:H	2.13	0.56
1:A:552:GLU:O	1:A:555:SER:HB2	2.06	0.56
1:A:618:TYR:O	1:A:622:VAL:HG23	2.05	0.56
1:B:290:THR:HG22	1:B:770:GLY:O	2.04	0.56
1:B:1166:GLY:O	1:B:1167:ASP:HB3	2.05	0.56
1:A:550:LEU:HD12	1:A:550:LEU:N	2.21	0.56
1:A:611:LEU:HB3	1:A:618:TYR:HB3	1.86	0.56
1:A:697:LEU:C	1:A:697:LEU:HD12	2.30	0.56
1:A:722:PRO:HB2	1:A:841:THR:CG2	2.34	0.56
1:A:839:LEU:O	1:A:843:ILE:HG12	2.04	0.56
1:A:1080:GLU:CD	1:A:1109:LEU:HD12	2.31	0.56
1:A:1260:LYS:HD2	1:A:1260:LYS:N	2.20	0.56
1:B:480:ILE:O	1:B:481:ALA:C	2.48	0.56
1:B:549:LEU:N	1:B:549:LEU:HD12	2.20	0.56
1:A:318:ILE:HG23	1:A:735:PHE:CZ	2.41	0.56
1:A:1090:VAL:HG13	1:A:1097:ILE:CB	2.31	0.56
1:B:233:SER:O	1:B:236:THR:HB	2.06	0.56
1:B:541:LEU:O	1:B:544:ASN:N	2.37	0.56
1:B:697:LEU:C	1:B:697:LEU:HD12	2.31	0.56
1:B:1035:GLY:C	1:B:1052:LEU:O	2.49	0.56
1:A:257:ILE:HG23	1:A:258:ARG:H	1.71	0.56
1:A:405:ILE:HG23	1:A:427:CYS:O	2.05	0.56
1:A:461:TYR:O	1:A:465:ILE:HG12	2.05	0.56
1:A:465:ILE:HG22	1:A:465:ILE:O	2.05	0.56
1:A:711:ILE:CG1	1:A:832:ILE:HG21	2.36	0.56
1:A:821:VAL:O	1:A:824:ALA:N	2.39	0.56
1:A:853:LEU:HD22	1:A:853:LEU:N	2.19	0.56
1:B:345:SER:HB3	1:B:346:PRO:HD3	1.88	0.56
1:B:383:ASN:C	1:B:384:ILE:O	2.41	0.56
1:B:733:GLY:HA3	1:B:968:GLU:HG3	1.86	0.56
1:A:908:ARG:HH21	1:A:908:ARG:HG3	1.71	0.56
1:A:952:CYS:SG	1:A:977:ILE:HD11	2.47	0.56
1:A:1096:GLU:HB2	1:A:1099:GLN:HE21	1.71	0.56
1:B:362:PHE:O	1:B:365:ILE:HB	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:ILE:O	1:B:487:GLY:N	2.39	0.56
1:B:534:ARG:O	1:B:537:ILE:HB	2.05	0.56
1:B:769:GLN:HG3	1:B:770:GLY:N	2.21	0.56
1:B:800:PHE:C	1:B:803:PRO:HD3	2.31	0.56
1:B:1192:ILE:HA	1:B:1222:THR:O	2.06	0.56
1:B:1255:GLN:O	1:B:1258:ALA:HB3	2.05	0.56
1:A:110:TYR:HA	1:A:113:TYR:HD2	1.71	0.55
1:A:158:TRP:NE1	1:A:900:PHE:CB	2.66	0.55
1:A:818:ALA:O	1:A:821:VAL:HG22	2.06	0.55
1:B:724:PHE:CD1	1:B:754:LEU:HD22	2.41	0.55
1:B:780:LEU:O	1:B:784:LEU:HB2	2.05	0.55
1:B:907:THR:C	1:B:908:ARG:HE	2.15	0.55
1:B:978:VAL:HG13	2:B:6002:OJZ:C35	2.29	0.55
1:A:186:ILE:CG1	1:A:187:GLY:N	2.69	0.55
1:A:318:ILE:HD11	1:A:325:GLY:N	2.21	0.55
1:A:761:ILE:N	1:A:761:ILE:HD12	2.21	0.55
1:A:861:VAL:HB	1:A:862:PRO:CD	2.36	0.55
1:A:1260:LYS:H	1:A:1260:LYS:CD	2.17	0.55
1:B:111:ALA:HA	1:B:114:TYR:HE1	1.70	0.55
1:B:257:ILE:HG23	1:B:258:ARG:H	1.72	0.55
1:B:496:ILE:O	1:B:500:VAL:HG22	2.05	0.55
1:B:617:ILE:N	1:B:617:ILE:HD12	2.20	0.55
1:B:834:GLN:O	1:B:837:ALA:HB3	2.06	0.55
1:B:1064:LEU:HB3	1:B:1226:ILE:HG22	1.87	0.55
1:B:1206:SER:O	1:B:1210:VAL:HG23	2.06	0.55
1:A:310:PHE:CZ	1:A:331:PHE:HB3	2.42	0.55
1:A:519:LEU:H	1:A:519:LEU:CD1	2.13	0.55
1:A:773:PHE:HB2	1:A:829:LEU:CD1	2.36	0.55
1:A:795:GLN:HE21	1:A:796:ASP:N	2.04	0.55
1:A:1127:ILE:CD1	1:A:1180:ILE:HG23	2.36	0.55
1:B:314:THR:O	1:B:315:SER:C	2.49	0.55
1:B:401:LYS:HD2	1:B:401:LYS:N	2.19	0.55
1:B:711:ILE:O	1:B:715:ILE:HG13	2.07	0.55
1:B:907:THR:N	1:B:908:ARG:HE	2.04	0.55
1:B:1080:GLU:CD	1:B:1109:LEU:HD12	2.31	0.55
1:A:68:MET:HG3	1:A:336:ILE:HD12	1.89	0.55
1:A:356:GLY:HA2	1:A:359:TYR:CE1	2.41	0.55
1:A:496:ILE:O	1:A:500:VAL:HG22	2.06	0.55
1:A:716:ILE:HD11	1:A:765:THR:OG1	2.06	0.55
1:A:925:ARG:CZ	1:B:519:LEU:HD12	2.37	0.55
1:B:419:VAL:HG23	1:B:593:VAL:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:ILE:O	1:B:485:ARG:C	2.50	0.55
1:B:721:GLN:O	1:B:722:PRO:C	2.48	0.55
1:B:804:LYS:HD3	1:B:804:LYS:N	2.21	0.55
1:B:993:ASP:N	1:B:996:LYS:NZ	2.54	0.55
1:B:1011:THR:H	1:B:1012:PRO:HD3	1.70	0.55
1:B:1064:LEU:C	1:B:1064:LEU:HD13	2.32	0.55
1:B:1104:TRP:CD1	1:B:1108:GLN:HE22	2.23	0.55
1:B:1137:SER:HB3	1:B:1140:GLU:CB	2.37	0.55
1:A:103:LEU:HD13	1:A:960:VAL:HG22	1.86	0.55
1:A:260:VAL:O	1:A:263:PHE:HB3	2.05	0.55
1:A:302:ILE:O	1:A:305:SER:HB3	2.06	0.55
1:A:584:ARG:O	1:A:588:VAL:HG23	2.06	0.55
1:B:318:ILE:HG13	1:B:325:GLY:H	1.72	0.55
1:B:1037:VAL:CG2	1:B:1087:ALA:HB3	2.36	0.55
1:A:88:SER:O	1:A:90:ASN:N	2.39	0.55
1:A:550:LEU:HD13	1:A:580:VAL:HB	1.89	0.55
1:A:601:VAL:HG13	1:A:601:VAL:O	2.06	0.55
1:A:721:GLN:HB3	1:A:722:PRO:CD	2.37	0.55
1:A:724:PHE:CD1	1:A:754:LEU:HD22	2.42	0.55
1:A:882:ASP:O	1:A:886:LEU:HG	2.07	0.55
1:A:1005:ILE:O	1:A:1008:ILE:HG22	2.06	0.55
1:A:1037:VAL:CG2	1:A:1087:ALA:HB3	2.37	0.55
1:A:1202:LEU:HG	1:A:1206:SER:HB2	1.87	0.55
1:B:908:ARG:HH21	1:B:908:ARG:HG3	1.70	0.55
1:A:78:PHE:CZ	1:A:967:PHE:O	2.59	0.55
1:A:214:ILE:HG12	1:A:331:PHE:CZ	2.42	0.55
1:A:617:ILE:N	1:A:617:ILE:HD12	2.22	0.55
1:B:146:LYS:O	1:B:150:ALA:HB2	2.07	0.55
1:B:601:VAL:O	1:B:601:VAL:HG13	2.06	0.55
1:B:839:LEU:O	1:B:843:ILE:HG12	2.06	0.55
1:B:888:GLY:O	1:B:892:ILE:HG12	2.06	0.55
1:A:289:ILE:O	1:A:292:ASN:HB3	2.07	0.55
1:A:405:ILE:CG2	1:A:427:CYS:O	2.55	0.55
1:A:492:THR:O	1:A:494:ASP:N	2.40	0.55
1:A:713:CYS:O	1:A:716:ILE:HG13	2.07	0.55
1:A:769:GLN:HG3	1:A:770:GLY:N	2.21	0.55
1:A:1064:LEU:HB3	1:A:1226:ILE:HG22	1.89	0.55
1:A:1203:ASP:O	1:A:1206:SER:HB2	2.07	0.55
1:B:216:ALA:O	1:B:220:VAL:HG23	2.06	0.55
1:B:239:GLU:HG3	1:B:288:ALA:CB	2.37	0.55
1:B:602:ILE:O	1:B:603:VAL:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1139:GLU:H	1:B:1139:GLU:CD	2.14	0.55
1:B:1183:ALA:O	1:B:1187:VAL:HG23	2.07	0.55
1:A:434:GLN:O	1:A:436:MET:N	2.39	0.55
1:A:484:ILE:O	1:A:485:ARG:C	2.50	0.55
1:A:697:LEU:HB3	1:A:828:ARG:NH2	2.22	0.55
1:B:111:ALA:HA	1:B:114:TYR:CE1	2.42	0.55
1:B:203:GLY:C	1:B:211:THR:OG1	2.49	0.55
1:B:209:LYS:O	1:B:213:VAL:HG23	2.07	0.55
1:B:1137:SER:O	1:B:1141:ILE:HG23	2.06	0.55
1:B:1260:LYS:H	1:B:1260:LYS:CD	2.19	0.55
1:A:210:LEU:HD23	1:A:317:VAL:CG1	2.37	0.55
1:A:401:LYS:HD2	1:A:401:LYS:N	2.20	0.55
1:A:433:VAL:HG13	1:A:549:LEU:HD23	1.89	0.55
1:A:860:ILE:O	1:A:864:ILE:HG13	2.07	0.55
1:A:892:ILE:O	1:A:893:ALA:C	2.50	0.55
1:A:1104:TRP:CD1	1:A:1108:GLN:HE22	2.24	0.55
1:A:1166:GLY:O	1:A:1167:ASP:HB3	2.06	0.55
1:A:1183:ALA:O	1:A:1187:VAL:HG23	2.07	0.55
1:B:74:MET:O	1:B:78:PHE:HB2	2.07	0.55
1:B:282:ARG:HG3	1:B:782:LYS:HD3	1.89	0.55
1:B:688:VAL:HG23	1:B:688:VAL:O	2.07	0.55
1:B:838:ASN:O	1:B:839:LEU:C	2.50	0.55
1:B:1071:GLY:O	1:B:1075:VAL:HG23	2.07	0.55
1:A:472:GLU:OE1	1:A:473:PRO:HD2	2.07	0.54
1:A:888:GLY:O	1:A:892:ILE:HG12	2.07	0.54
1:A:1164:ARG:C	1:A:1166:GLY:N	2.65	0.54
1:B:207:GLY:C	1:B:209:LYS:H	2.15	0.54
1:B:708:VAL:HG13	1:B:709:VAL:N	2.22	0.54
1:B:720:LEU:HD22	1:B:761:ILE:HG22	1.90	0.54
1:B:1077:GLN:O	1:B:1080:GLU:N	2.40	0.54
1:B:1151:HIS:HA	1:B:1154:ILE:HB	1.88	0.54
1:B:1195:LEU:O	1:B:1226:ILE:HG12	2.07	0.54
1:A:59:ILE:HD11	1:A:124:VAL:CG1	2.34	0.54
1:A:209:LYS:O	1:A:213:VAL:HG23	2.06	0.54
1:A:691:ALA:O	1:A:692:SER:HB3	2.06	0.54
1:B:100:PHE:HB2	1:B:961:THR:HG23	1.88	0.54
1:B:342:GLY:O	1:B:346:PRO:CD	2.56	0.54
1:B:532:LYS:O	1:B:533:GLN:C	2.49	0.54
1:B:716:ILE:HD11	1:B:765:THR:CB	2.37	0.54
1:B:1058:LYS:HA	1:B:1222:THR:OG1	2.07	0.54
1:A:117:ILE:O	1:A:121:VAL:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ALA:C	1:A:257:ILE:N	2.62	0.54
1:A:480:ILE:O	1:A:481:ALA:C	2.49	0.54
1:A:485:ARG:O	1:A:488:ARG:C	2.51	0.54
1:A:791:SER:N	1:A:794:ARG:HH21	2.05	0.54
1:A:859:ALA:O	1:A:863:ILE:HG12	2.08	0.54
1:A:1011:THR:O	1:A:1011:THR:HG23	2.07	0.54
1:A:1058:LYS:HA	1:A:1222:THR:OG1	2.07	0.54
1:A:1063:ALA:CB	1:A:1239:ILE:HG12	2.37	0.54
1:A:1255:GLN:O	1:A:1258:ALA:HB3	2.06	0.54
1:B:61:GLY:O	1:B:65:PRO:CD	2.42	0.54
1:B:254:LEU:HD22	1:B:254:LEU:N	2.22	0.54
1:B:611:LEU:HB3	1:B:618:TYR:HB3	1.90	0.54
1:B:1097:ILE:O	1:B:1098:LYS:CB	2.55	0.54
1:A:120:GLY:O	1:A:121:VAL:C	2.51	0.54
1:A:239:GLU:HG3	1:A:288:ALA:CB	2.37	0.54
1:A:317:VAL:HG12	1:A:317:VAL:O	2.07	0.54
1:A:527:LEU:N	1:A:527:LEU:HD23	2.21	0.54
1:A:693:PHE:C	1:A:695:ARG:H	2.14	0.54
1:A:705:PRO:O	1:A:706:TYR:HB3	2.07	0.54
1:B:431:THR:O	1:B:435:LEU:HD23	2.07	0.54
1:B:850:GLY:C	1:B:852:GLN:H	2.15	0.54
1:A:70:ILE:O	1:A:71:PHE:C	2.50	0.54
1:A:136:ALA:HB2	1:A:182:ILE:CB	2.32	0.54
1:A:311:TRP:HB2	1:A:751:PHE:HB2	1.89	0.54
1:A:315:SER:OG	1:A:747:ASN:HB3	2.08	0.54
1:A:336:ILE:CG1	2:A:6001:OJZ:SE1	2.99	0.54
1:A:549:LEU:N	1:A:549:LEU:HD12	2.22	0.54
1:A:722:PRO:HG2	1:A:841:THR:HB	1.89	0.54
1:A:853:LEU:H	1:A:853:LEU:CD2	2.19	0.54
1:A:969:ASN:ND2	1:A:970:VAL:N	2.54	0.54
1:B:139:GLN:O	1:B:140:ILE:C	2.50	0.54
1:B:419:VAL:O	1:B:579:ILE:HA	2.08	0.54
1:B:1011:THR:N	1:B:1012:PRO:HD2	2.22	0.54
1:B:1033:PHE:HB3	1:B:1036:VAL:CG2	2.36	0.54
1:B:1090:VAL:HG13	1:B:1097:ILE:CB	2.31	0.54
1:A:174:ASP:O	1:A:175:VAL:C	2.51	0.54
1:A:401:LYS:HB3	1:A:401:LYS:HZ2	1.71	0.54
1:A:443:LEU:HD23	1:A:443:LEU:O	2.07	0.54
1:B:247:GLY:O	1:B:250:ALA:HB3	2.06	0.54
1:B:297:ALA:O	1:B:301:LEU:HB2	2.08	0.54
1:B:583:HIS:O	1:B:585:LEU:HD22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:858:LEU:HD12	1:B:858:LEU:C	2.33	0.54
1:B:861:VAL:HB	1:B:862:PRO:CD	2.38	0.54
1:B:1054:LEU:CD1	1:B:1240:VAL:HG11	2.38	0.54
1:B:305:SER:O	1:B:306:TYR:C	2.50	0.54
1:B:461:TYR:O	1:B:465:ILE:HG12	2.07	0.54
1:B:721:GLN:HB3	1:B:722:PRO:CD	2.37	0.54
1:B:1195:LEU:N	1:B:1195:LEU:HD12	2.22	0.54
1:A:103:LEU:HB2	1:A:960:VAL:HG23	1.89	0.54
1:A:907:THR:C	1:A:908:ARG:HE	2.16	0.54
1:A:1076:VAL:HG13	1:A:1194:LEU:HD22	1.88	0.54
1:B:472:GLU:OE1	1:B:473:PRO:HD2	2.07	0.54
1:B:722:PRO:HB2	1:B:841:THR:CG2	2.36	0.54
1:B:1108:GLN:HE21	1:B:1108:GLN:H	1.56	0.54
1:B:1143:ARG:HG2	1:B:1143:ARG:HH11	1.73	0.54
1:A:34:SER:O	1:A:38:MET:HB2	2.08	0.54
1:A:68:MET:HA	1:A:68:MET:HE2	1.90	0.54
1:A:279:GLU:HG2	1:A:782:LYS:NZ	2.22	0.54
1:A:482:GLU:O	1:A:484:ILE:N	2.40	0.54
1:A:583:HIS:O	1:A:585:LEU:HD22	2.07	0.54
1:A:992:PRO:C	1:A:994:TYR:H	2.16	0.54
1:A:1137:SER:HB3	1:A:1140:GLU:CB	2.37	0.54
1:A:1140:GLU:O	1:A:1143:ARG:HB3	2.08	0.54
1:B:215:LEU:O	1:B:219:PRO:CD	2.54	0.54
1:B:358:ALA:O	1:B:362:PHE:CB	2.53	0.54
1:B:1221:ARG:HD2	1:B:1221:ARG:N	2.22	0.54
1:A:111:ALA:HA	1:A:114:TYR:CE1	2.42	0.54
1:A:191:GLN:O	1:A:195:THR:HG22	2.08	0.54
1:A:215:LEU:O	1:A:219:PRO:CD	2.56	0.54
1:A:239:GLU:HG3	1:A:288:ALA:HB2	1.90	0.54
1:A:716:ILE:HD11	1:A:765:THR:CB	2.38	0.54
1:A:954:ARG:HH11	1:A:954:ARG:HG3	1.73	0.54
1:A:1035:GLY:C	1:A:1052:LEU:O	2.51	0.54
1:B:117:ILE:O	1:B:121:VAL:HG13	2.07	0.54
1:B:185:LYS:HG3	1:B:351:PHE:CD2	2.43	0.54
1:B:317:VAL:O	1:B:317:VAL:HG12	2.07	0.54
1:B:550:LEU:HD13	1:B:580:VAL:HB	1.89	0.54
1:B:697:LEU:HB3	1:B:828:ARG:NH2	2.23	0.54
1:A:188:MET:HB2	1:A:347:ASN:HB3	1.89	0.53
1:A:852:GLN:HB2	1:A:853:LEU:HD22	1.90	0.53
1:A:969:ASN:ND2	1:A:970:VAL:H	2.05	0.53
1:A:1108:GLN:HE21	1:A:1108:GLN:H	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:GLU:O	1:B:169:THR:HB	2.07	0.53
1:B:508:PHE:O	1:B:512:LEU:HB2	2.08	0.53
1:B:705:PRO:O	1:B:706:TYR:HB3	2.08	0.53
1:B:792:MET:HE1	1:B:810:LEU:HB3	1.90	0.53
1:B:1019:THR:HG22	1:B:1100:LEU:HD12	1.89	0.53
1:B:1214:LEU:HD23	1:B:1214:LEU:C	2.32	0.53
1:A:901:ARG:O	1:A:902:THR:C	2.51	0.53
1:A:1033:PHE:HB3	1:A:1036:VAL:CG2	2.36	0.53
1:A:1221:ARG:HD2	1:A:1221:ARG:N	2.23	0.53
1:B:152:MET:HG3	1:B:913:GLU:OE1	2.08	0.53
1:B:617:ILE:HD12	1:B:617:ILE:H	1.74	0.53
1:B:969:ASN:ND2	1:B:970:VAL:N	2.57	0.53
1:A:335:LEU:HD23	1:A:335:LEU:C	2.34	0.53
1:A:342:GLY:O	1:A:346:PRO:CD	2.56	0.53
1:A:1229:ARG:C	1:A:1231:SER:H	2.14	0.53
1:B:337:GLY:O	1:B:341:VAL:HG23	2.08	0.53
1:B:388:LEU:HB2	1:B:413:VAL:HG13	1.88	0.53
1:B:821:VAL:O	1:B:824:ALA:N	2.40	0.53
1:B:907:THR:C	1:B:908:ARG:NE	2.65	0.53
1:B:1063:ALA:CB	1:B:1239:ILE:HG12	2.38	0.53
1:B:1142:VAL:HA	1:B:1161:TYR:OH	2.08	0.53
1:A:48:LEU:O	1:A:52:VAL:HG23	2.08	0.53
1:A:146:LYS:O	1:A:150:ALA:HB2	2.07	0.53
1:A:284:GLY:O	1:A:287:LYS:HB3	2.08	0.53
1:A:437:GLN:NE2	1:A:468:VAL:HG21	2.23	0.53
1:A:792:MET:HE1	1:A:810:LEU:HB3	1.89	0.53
1:A:1039:ASN:HB2	1:A:1047:PRO:CA	2.37	0.53
1:A:1124:ALA:HB2	1:A:1161:TYR:O	2.08	0.53
1:A:1206:SER:O	1:A:1210:VAL:HG23	2.09	0.53
1:B:191:GLN:O	1:B:195:THR:HG22	2.07	0.53
1:B:909:GLU:O	1:B:912:PHE:HB2	2.08	0.53
1:A:185:LYS:HG3	1:A:351:PHE:CD2	2.43	0.53
1:A:310:PHE:CE2	1:A:331:PHE:HB3	2.43	0.53
1:A:434:GLN:NE2	1:A:439:LEU:HG	2.21	0.53
1:A:1144:ALA:HA	1:A:1186:LEU:CD1	2.32	0.53
1:B:533:GLN:O	1:B:536:ALA:HB3	2.09	0.53
1:A:148:PHE:HD2	1:A:913:GLU:OE2	1.92	0.53
1:A:620:LYS:HD3	1:A:624:THR:OG1	2.09	0.53
1:A:697:LEU:O	1:A:700:ASN:HB3	2.09	0.53
1:A:1028:GLU:OE1	1:A:1058:LYS:HD2	2.08	0.53
1:A:1142:VAL:HA	1:A:1161:TYR:OH	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:LEU:HD23	1:B:167:LEU:C	2.34	0.53
1:B:853:LEU:HD22	1:B:853:LEU:H	1.73	0.53
1:B:1005:ILE:HA	1:B:1008:ILE:HG22	1.89	0.53
1:B:1127:ILE:CD1	1:B:1180:ILE:HG23	2.38	0.53
1:A:300:LEU:HA	1:A:303:TYR:HB2	1.90	0.53
1:A:388:LEU:HB2	1:A:413:VAL:HG13	1.89	0.53
1:A:532:LYS:O	1:A:533:GLN:C	2.50	0.53
1:A:565:VAL:O	1:A:566:GLN:C	2.51	0.53
1:A:1060:GLN:HB2	1:A:1237:ASP:OD1	2.09	0.53
1:B:200:PHE:O	1:B:201:ILE:C	2.51	0.53
1:B:405:ILE:HG22	1:B:406:LEU:HD22	1.91	0.53
1:B:1060:GLN:HB2	1:B:1237:ASP:OD1	2.09	0.53
1:B:1140:GLU:O	1:B:1143:ARG:HB3	2.09	0.53
1:A:419:VAL:O	1:A:579:ILE:HA	2.09	0.53
1:A:1204:THR:C	1:A:1206:SER:H	2.16	0.53
1:B:543:ARG:NH2	1:B:907:THR:HG23	2.24	0.53
1:B:1092:LEU:HD22	1:B:1097:ILE:CD1	2.37	0.53
1:A:209:LYS:C	1:A:212:LEU:HB3	2.34	0.53
1:A:279:GLU:HG2	1:A:782:LYS:HD2	1.91	0.53
1:B:552:GLU:O	1:B:555:SER:HB2	2.09	0.53
1:B:620:LYS:HD3	1:B:624:THR:OG1	2.09	0.53
1:B:717:ASN:O	1:B:720:LEU:HB3	2.09	0.53
1:B:781:THR:HG23	1:B:818:ALA:CB	2.39	0.53
1:A:52:VAL:O	1:A:53:GLY:C	2.52	0.53
1:A:195:THR:HB	1:A:340:SER:HG	1.73	0.53
1:A:341:VAL:O	1:A:344:ALA:HB3	2.08	0.53
1:A:483:ASN:O	1:A:486:TYR:HB2	2.08	0.53
1:A:1092:LEU:HD22	1:A:1097:ILE:CD1	2.37	0.53
1:A:1123:ILE:O	1:A:1127:ILE:HG12	2.08	0.53
1:A:1195:LEU:HD12	1:A:1195:LEU:N	2.24	0.53
1:A:1254:GLN:N	1:A:1254:GLN:OE1	2.42	0.53
1:B:68:MET:HG3	1:B:336:ILE:HD12	1.90	0.53
1:B:129:VAL:HG11	1:B:935:GLY:HA2	1.91	0.53
1:B:300:LEU:O	1:B:303:TYR:HB3	2.08	0.53
1:B:443:LEU:O	1:B:443:LEU:HD23	2.09	0.53
1:B:1124:ALA:HB2	1:B:1161:TYR:O	2.09	0.53
1:B:1186:LEU:C	1:B:1186:LEU:HD12	2.34	0.53
1:A:139:GLN:O	1:A:140:ILE:C	2.52	0.52
1:A:161:VAL:O	1:A:162:HIS:HB2	2.08	0.52
1:A:894:THR:O	1:A:895:GLU:C	2.52	0.52
1:A:1186:LEU:C	1:A:1186:LEU:HD12	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:PHE:C	1:B:131:PHE:CD2	2.86	0.52
1:B:335:LEU:HD23	1:B:335:LEU:C	2.35	0.52
1:B:722:PRO:HG2	1:B:841:THR:HB	1.90	0.52
1:B:1212:GLU:O	1:B:1215:ASP:HB3	2.08	0.52
1:A:141:HIS:O	1:A:144:ARG:HB3	2.10	0.52
1:A:155:GLU:O	1:A:157:GLY:N	2.41	0.52
1:A:420:ALA:HA	1:A:580:VAL:O	2.09	0.52
1:A:731:VAL:HG22	1:A:750:LEU:CB	2.39	0.52
1:A:753:LEU:O	1:A:754:LEU:C	2.52	0.52
1:A:857:LEU:CD1	1:A:977:ILE:HG13	2.39	0.52
1:A:978:VAL:HG21	2:A:6001:OJZ:C35	2.38	0.52
1:B:779:ILE:O	1:B:780:LEU:C	2.53	0.52
1:B:882:ASP:O	1:B:886:LEU:HG	2.09	0.52
1:B:954:ARG:HH11	1:B:954:ARG:HG3	1.74	0.52
1:A:254:LEU:HD22	1:A:254:LEU:N	2.25	0.52
1:A:390:PHE:HB2	1:A:411:LEU:O	2.09	0.52
1:A:398:PRO:HD3	1:A:440:TYR:CE2	2.44	0.52
1:A:907:THR:C	1:A:908:ARG:NE	2.68	0.52
1:A:1054:LEU:CD1	1:A:1240:VAL:HG11	2.37	0.52
1:A:1196:ASP:HA	1:A:1226:ILE:HG12	1.92	0.52
1:B:68:MET:HE2	1:B:68:MET:HA	1.90	0.52
1:B:240:LEU:O	1:B:243:TYR:HB3	2.09	0.52
1:B:318:ILE:CD1	1:B:325:GLY:N	2.67	0.52
1:B:354:ALA:O	1:B:358:ALA:HB3	2.09	0.52
1:B:458:ASN:ND2	1:B:459:VAL:N	2.57	0.52
1:B:795:GLN:O	1:B:796:ASP:CB	2.50	0.52
1:B:1079:LEU:C	1:B:1081:ARG:N	2.68	0.52
1:B:1186:LEU:HD12	1:B:1187:VAL:N	2.24	0.52
1:A:74:MET:O	1:A:78:PHE:HB2	2.09	0.52
1:A:314:THR:O	1:A:315:SER:C	2.51	0.52
1:A:534:ARG:O	1:A:535:ILE:C	2.50	0.52
1:A:907:THR:N	1:A:908:ARG:HE	2.07	0.52
1:A:1064:LEU:HD13	1:A:1064:LEU:C	2.34	0.52
1:A:1109:LEU:O	1:A:1109:LEU:HD23	2.10	0.52
1:A:1143:ARG:HG2	1:A:1143:ARG:HH11	1.73	0.52
1:A:1144:ALA:HB2	1:A:1187:VAL:CG2	2.40	0.52
1:B:202:ILE:HG12	1:B:333:SER:OG	2.09	0.52
1:B:318:ILE:CD1	1:B:324:ILE:H	2.22	0.52
1:B:420:ALA:HA	1:B:580:VAL:O	2.09	0.52
1:B:1144:ALA:HA	1:B:1186:LEU:CD1	2.30	0.52
1:A:573:ARG:HD2	1:A:578:THR:CG2	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:ASN:O	1:A:720:LEU:HB3	2.10	0.52
1:A:718:GLY:HA3	1:A:837:ALA:CB	2.39	0.52
1:A:862:PRO:O	1:A:866:ILE:HG13	2.09	0.52
1:B:188:MET:HB2	1:B:347:ASN:HB3	1.91	0.52
1:B:483:ASN:O	1:B:486:TYR:HB2	2.10	0.52
1:B:860:ILE:O	1:B:864:ILE:HG13	2.09	0.52
1:B:875:LEU:HD23	1:B:875:LEU:C	2.34	0.52
1:B:969:ASN:ND2	1:B:970:VAL:H	2.07	0.52
1:A:258:ARG:O	1:A:259:THR:C	2.52	0.52
1:A:267:LYS:CA	1:A:790:LYS:HE2	2.40	0.52
1:B:418:THR:HG22	1:B:578:THR:CG2	2.40	0.52
1:B:1027:LEU:H	1:B:1027:LEU:CD2	2.22	0.52
1:B:1208:LYS:C	1:B:1208:LYS:HD3	2.35	0.52
1:A:37:THR:O	1:A:40:ARG:N	2.37	0.52
1:A:69:LEU:HA	1:A:329:THR:HG21	1.91	0.52
1:A:170:ARG:HB2	1:A:170:ARG:NH1	2.25	0.52
1:A:240:LEU:O	1:A:243:TYR:HB3	2.09	0.52
1:A:254:LEU:CD2	1:A:811:THR:HG22	2.39	0.52
1:A:311:TRP:HD1	1:A:754:LEU:HD12	1.74	0.52
1:A:1095:LYS:HD2	1:A:1095:LYS:N	2.24	0.52
1:A:1097:ILE:O	1:A:1098:LYS:CB	2.57	0.52
1:A:1139:GLU:CD	1:A:1139:GLU:H	2.17	0.52
1:B:258:ARG:O	1:B:259:THR:C	2.51	0.52
1:B:349:GLU:O	1:B:352:ALA:N	2.42	0.52
1:B:406:LEU:HD12	1:B:409:LEU:CB	2.40	0.52
1:B:753:LEU:O	1:B:754:LEU:C	2.53	0.52
1:A:291:ALA:HA	1:A:294:SER:CB	2.39	0.52
1:A:418:THR:HG22	1:A:578:THR:CG2	2.39	0.52
1:A:458:ASN:ND2	1:A:459:VAL:N	2.57	0.52
1:A:724:PHE:CE1	1:A:754:LEU:HD22	2.45	0.52
1:A:967:PHE:HD1	1:A:968:GLU:H	1.58	0.52
1:A:979:PHE:HA	1:A:982:MET:SD	2.50	0.52
1:A:1108:GLN:HE21	1:A:1108:GLN:N	2.07	0.52
1:A:1214:LEU:HD23	1:A:1214:LEU:C	2.35	0.52
1:B:103:LEU:HD13	1:B:960:VAL:HG22	1.91	0.52
1:B:141:HIS:O	1:B:144:ARG:HB3	2.10	0.52
1:B:210:LEU:HD23	1:B:317:VAL:CG1	2.37	0.52
1:B:239:GLU:HG3	1:B:288:ALA:HB2	1.90	0.52
1:B:584:ARG:NE	1:B:584:ARG:HA	2.24	0.52
1:B:859:ALA:O	1:B:863:ILE:HG12	2.10	0.52
1:B:1092:LEU:HB3	1:B:1097:ILE:CD1	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1102:VAL:HG13	1:B:1103:GLN:N	2.24	0.52
1:A:133:CYS:CB	1:A:931:ALA:HB1	2.39	0.52
1:A:484:ILE:O	1:A:487:GLY:N	2.43	0.52
1:A:486:TYR:O	1:A:908:ARG:NH1	2.43	0.52
1:A:781:THR:HG23	1:A:818:ALA:CB	2.40	0.52
1:A:827:SER:O	1:A:830:ALA:N	2.43	0.52
1:A:1091:PHE:CE1	1:A:1096:GLU:HG2	2.32	0.52
1:A:1202:LEU:CD2	1:A:1206:SER:HB3	2.40	0.52
1:B:116:GLY:O	1:B:117:ILE:C	2.52	0.52
1:B:267:LYS:CA	1:B:270:LEU:HD21	2.39	0.52
1:B:289:ILE:O	1:B:292:ASN:HB3	2.10	0.52
1:B:900:PHE:O	1:B:901:ARG:C	2.53	0.52
1:B:957:ALA:O	1:B:958:TYR:C	2.53	0.52
1:A:138:ARG:NH2	1:B:515:GLN:HG2	2.25	0.52
1:A:188:MET:O	1:A:189:PHE:C	2.50	0.52
1:A:796:ASP:O	1:A:797:VAL:C	2.52	0.52
1:A:806:THR:HG23	1:A:809:ALA:H	1.75	0.52
1:A:1026:MET:HE3	1:A:1095:LYS:CD	2.40	0.52
1:A:1027:LEU:HD12	1:A:1027:LEU:N	2.25	0.52
1:A:1108:GLN:N	1:A:1108:GLN:NE2	2.58	0.52
1:B:437:GLN:NE2	1:B:468:VAL:HG21	2.23	0.52
1:B:485:ARG:O	1:B:488:ARG:C	2.53	0.52
1:B:731:VAL:HG22	1:B:750:LEU:CB	2.40	0.52
1:B:766:PHE:HA	1:B:769:GLN:HG2	1.91	0.52
1:B:777:GLY:HA3	1:B:822:LYS:HG3	1.92	0.52
1:B:901:ARG:H	1:B:901:ARG:HD3	1.74	0.52
1:B:1124:ALA:HB2	1:B:1161:TYR:HB3	1.91	0.52
1:A:125:ALA:O	1:A:126:TYR:C	2.52	0.51
1:A:158:TRP:NE1	1:A:900:PHE:HB2	2.25	0.51
1:A:185:LYS:O	1:A:186:ILE:C	2.52	0.51
1:A:206:ARG:O	1:A:330:VAL:HG11	2.10	0.51
1:A:349:GLU:O	1:A:352:ALA:N	2.43	0.51
1:A:373:SER:O	1:A:374:PHE:CB	2.57	0.51
1:A:534:ARG:O	1:A:537:ILE:HB	2.09	0.51
1:A:708:VAL:HG13	1:A:709:VAL:N	2.24	0.51
1:A:843:ILE:HA	1:A:846:SER:CB	2.40	0.51
1:B:174:ASP:O	1:B:175:VAL:C	2.51	0.51
1:B:260:VAL:O	1:B:263:PHE:HB3	2.10	0.51
1:B:352:ALA:O	1:B:355:ARG:N	2.42	0.51
1:B:503:ALA:O	1:B:504:ASN:C	2.53	0.51
1:B:584:ARG:O	1:B:588:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:998:THR:O	1:B:1001:ALA:HB3	2.10	0.51
1:B:1219:GLU:HG3	1:B:1219:GLU:O	2.09	0.51
1:B:1260:LYS:HD2	1:B:1260:LYS:N	2.22	0.51
1:A:59:ILE:HG12	1:A:124:VAL:HG11	1.92	0.51
1:A:106:GLU:OE2	1:A:109:THR:HB	2.09	0.51
1:A:175:VAL:CG1	1:A:176:SER:N	2.73	0.51
1:A:202:ILE:HG12	1:A:333:SER:OG	2.10	0.51
1:A:247:GLY:O	1:A:250:ALA:HB3	2.09	0.51
1:A:354:ALA:O	1:A:358:ALA:CB	2.58	0.51
1:A:711:ILE:O	1:A:715:ILE:HG13	2.10	0.51
1:A:875:LEU:C	1:A:875:LEU:HD23	2.34	0.51
1:B:133:CYS:HB3	1:B:931:ALA:CB	2.40	0.51
1:B:716:ILE:HD11	1:B:765:THR:HB	1.92	0.51
1:B:853:LEU:HD22	1:B:853:LEU:N	2.25	0.51
1:B:895:GLU:O	1:B:899:ASN:ND2	2.43	0.51
1:A:144:ARG:HH12	1:A:175:VAL:HG11	1.76	0.51
1:A:539:ARG:O	1:A:540:ALA:C	2.53	0.51
1:A:720:LEU:HD22	1:A:761:ILE:HG22	1.91	0.51
1:A:981:ALA:HB3	2:A:6001:OJZ:H33	1.93	0.51
1:A:1202:LEU:HG	1:A:1203:ASP:H	1.75	0.51
1:B:106:GLU:HG3	1:B:110:TYR:CZ	2.46	0.51
1:B:427:CYS:O	1:B:599:GLY:CA	2.57	0.51
1:B:434:GLN:C	1:B:436:MET:N	2.68	0.51
1:B:724:PHE:CE1	1:B:754:LEU:HD22	2.45	0.51
1:B:915:MET:O	1:B:918:GLN:HB2	2.11	0.51
1:A:297:ALA:O	1:A:301:LEU:HB2	2.10	0.51
1:A:379:HIS:HB2	1:A:456:THR:O	2.10	0.51
1:A:464:GLU:HG2	1:A:543:ARG:HH21	1.76	0.51
1:A:901:ARG:HD3	1:A:901:ARG:H	1.75	0.51
1:A:1178:GLN:O	1:A:1181:ALA:HB3	2.11	0.51
1:B:275:ASN:HA	1:B:278:GLU:HB2	1.92	0.51
1:B:543:ARG:NH1	1:B:905:SER:HA	2.24	0.51
1:B:615:LYS:HA	1:B:619:PHE:CG	2.45	0.51
1:B:757:ILE:O	1:B:761:ILE:HD13	2.09	0.51
1:B:802:ASP:OD2	1:B:1041:PRO:HB2	2.10	0.51
1:B:902:THR:O	1:B:904:VAL:N	2.44	0.51
1:B:933:VAL:C	1:B:935:GLY:N	2.68	0.51
1:B:1014:ILE:O	1:B:1014:ILE:HG23	2.10	0.51
1:B:1144:ALA:HB2	1:B:1187:VAL:HG23	1.92	0.51
1:A:118:GLY:HA3	1:A:946:TYR:CD2	2.45	0.51
1:A:291:ALA:O	1:A:295:MET:SD	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LEU:O	1:A:304:ALA:HB3	2.09	0.51
1:A:418:THR:HG22	1:A:578:THR:HG22	1.92	0.51
1:B:1225:VAL:O	1:B:1225:VAL:HG13	2.09	0.51
1:A:113:TYR:CG	1:A:114:TYR:N	2.79	0.51
1:A:200:PHE:O	1:A:201:ILE:C	2.54	0.51
1:A:318:ILE:HD13	1:A:327:VAL:CG1	2.41	0.51
1:A:374:PHE:CD2	1:A:375:SER:N	2.76	0.51
1:A:1151:HIS:HA	1:A:1154:ILE:HB	1.92	0.51
1:A:1192:ILE:HA	1:A:1222:THR:O	2.10	0.51
1:A:1196:ASP:HA	1:A:1226:ILE:HD11	1.91	0.51
1:B:59:ILE:HG12	1:B:124:VAL:HG11	1.93	0.51
1:B:383:ASN:O	1:B:384:ILE:C	2.53	0.51
1:B:421:LEU:HD23	1:B:429:LYS:HA	1.92	0.51
1:B:902:THR:O	1:B:903:VAL:C	2.54	0.51
1:B:1056:VAL:CG2	1:B:1062:LEU:HB2	2.41	0.51
1:B:1123:ILE:O	1:B:1127:ILE:HG12	2.10	0.51
1:B:1254:GLN:OE1	1:B:1254:GLN:N	2.44	0.51
1:A:420:ALA:C	1:A:421:LEU:HD12	2.35	0.51
1:A:716:ILE:HD11	1:A:765:THR:HB	1.93	0.51
1:A:878:GLN:NE2	1:A:881:LYS:HD3	2.26	0.51
1:A:887:GLU:O	1:A:888:GLY:C	2.53	0.51
1:A:959:LEU:HD23	1:A:959:LEU:C	2.34	0.51
1:A:1079:LEU:C	1:A:1081:ARG:N	2.66	0.51
1:A:1218:ARG:HB2	1:A:1223:CYS:SG	2.51	0.51
1:B:55:LEU:HD23	1:B:55:LEU:C	2.36	0.51
1:B:464:GLU:HG2	1:B:543:ARG:HH21	1.75	0.51
1:B:1096:GLU:HB2	1:B:1099:GLN:HE21	1.75	0.51
1:B:1108:GLN:HE21	1:B:1108:GLN:N	2.08	0.51
1:B:1120:ASP:O	1:B:1164:ARG:NE	2.43	0.51
1:A:167:LEU:HD23	1:A:167:LEU:C	2.36	0.51
1:A:615:LYS:HA	1:A:619:PHE:CG	2.46	0.51
1:A:857:LEU:HG	1:A:977:ILE:HG12	1.92	0.51
1:A:881:LYS:HB2	1:A:881:LYS:HZ3	1.74	0.51
1:A:962:GLN:HG2	1:A:962:GLN:O	2.11	0.51
1:A:1144:ALA:HB2	1:A:1187:VAL:HG23	1.91	0.51
1:B:106:GLU:OE2	1:B:109:THR:HB	2.10	0.51
1:B:125:ALA:O	1:B:126:TYR:C	2.53	0.51
1:B:133:CYS:HB3	1:B:931:ALA:HB1	1.91	0.51
1:B:291:ALA:C	1:B:294:SER:H	2.19	0.51
1:B:498:LYS:HE2	1:B:499:ALA:N	2.26	0.51
1:B:573:ARG:HD2	1:B:578:THR:CG2	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:GLY:HA3	1:B:837:ALA:CB	2.40	0.51
1:B:831:VAL:O	1:B:832:ILE:C	2.54	0.51
1:B:1218:ARG:HB2	1:B:1223:CYS:SG	2.51	0.51
1:B:1243:GLN:O	1:B:1244:ASN:C	2.53	0.51
1:A:55:LEU:C	1:A:55:LEU:HD23	2.35	0.51
1:A:762:SER:CA	1:A:765:THR:HG22	2.40	0.51
1:A:949:TYR:N	1:A:949:TYR:CD1	2.79	0.51
1:A:1005:ILE:HA	1:A:1008:ILE:HG22	1.92	0.51
1:A:1120:ASP:O	1:A:1164:ARG:NE	2.44	0.51
1:B:48:LEU:O	1:B:52:VAL:HG23	2.10	0.51
1:B:52:VAL:O	1:B:53:GLY:C	2.53	0.51
1:B:86:LYS:HG2	1:B:738:GLY:O	2.11	0.51
1:B:113:TYR:CG	1:B:114:TYR:N	2.78	0.51
1:B:175:VAL:CG1	1:B:176:SER:N	2.74	0.51
1:B:295:MET:C	1:B:297:ALA:N	2.68	0.51
1:B:826:GLY:O	1:B:829:LEU:HB2	2.10	0.51
1:B:1176:GLN:O	1:B:1179:ARG:N	2.44	0.51
1:A:93:GLU:CD	1:A:93:GLU:H	2.19	0.51
1:A:409:LEU:HD13	1:A:410:ASN:N	2.26	0.51
1:A:1032:GLN:HE21	1:A:1055:GLU:HG3	1.76	0.51
1:A:1056:VAL:CG2	1:A:1060:GLN:HE22	2.23	0.51
1:B:34:SER:O	1:B:38:MET:HB2	2.11	0.51
1:B:70:ILE:O	1:B:71:PHE:C	2.53	0.51
1:B:161:VAL:O	1:B:162:HIS:HB2	2.11	0.51
1:B:418:THR:HA	1:B:578:THR:O	2.11	0.51
1:B:902:THR:HG23	1:B:903:VAL:N	2.25	0.51
1:A:158:TRP:O	1:A:164:VAL:HG12	2.10	0.50
1:A:430:SER:O	1:A:434:GLN:HB2	2.11	0.50
1:A:431:THR:O	1:A:434:GLN:HB3	2.11	0.50
1:A:449:ILE:O	1:A:450:ASP:C	2.53	0.50
1:A:467:GLY:O	1:A:548:LEU:HA	2.12	0.50
1:A:801:ASP:OD2	1:A:1082:PHE:HB3	2.11	0.50
1:A:1020:GLN:CG	1:A:1101:ASN:HB3	2.41	0.50
1:B:35:VAL:HG12	1:B:359:TYR:CZ	2.46	0.50
1:B:248:ALA:O	1:B:251:GLU:HB2	2.11	0.50
1:B:286:LYS:HG2	1:B:778:GLU:HG3	1.89	0.50
1:B:788:VAL:HG21	1:B:1004:ILE:HG13	1.94	0.50
1:B:845:ILE:O	1:B:848:ILE:HG12	2.12	0.50
1:B:1109:LEU:HD23	1:B:1109:LEU:O	2.11	0.50
1:B:1202:LEU:HG	1:B:1203:ASP:H	1.76	0.50
1:A:33:VAL:O	1:A:34:SER:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ALA:C	1:A:294:SER:H	2.18	0.50
1:A:499:ALA:CB	1:A:542:VAL:HG22	2.41	0.50
1:A:702:THR:HB	1:A:703:GLU:OE1	2.10	0.50
1:A:717:ASN:HB3	1:A:833:PHE:CE1	2.46	0.50
1:A:838:ASN:O	1:A:839:LEU:C	2.52	0.50
1:A:915:MET:O	1:A:918:GLN:HB2	2.11	0.50
1:A:1102:VAL:HG13	1:A:1103:GLN:N	2.24	0.50
1:B:35:VAL:HG21	1:B:355:ARG:HH21	1.76	0.50
1:B:121:VAL:CG2	1:B:122:LEU:N	2.74	0.50
1:B:467:GLY:O	1:B:548:LEU:HA	2.12	0.50
1:B:791:SER:N	1:B:794:ARG:HH21	2.08	0.50
1:B:838:ASN:C	1:B:838:ASN:HD22	2.18	0.50
1:B:894:THR:O	1:B:895:GLU:C	2.54	0.50
1:B:905:SER:HB2	1:B:908:ARG:CZ	2.41	0.50
1:B:1144:ALA:HB2	1:B:1187:VAL:CG2	2.41	0.50
1:A:131:PHE:C	1:A:131:PHE:CD2	2.89	0.50
1:A:147:PHE:O	1:A:148:PHE:C	2.54	0.50
1:A:214:ILE:HD11	1:A:330:VAL:HB	1.92	0.50
1:A:248:ALA:O	1:A:251:GLU:HB2	2.12	0.50
1:A:766:PHE:HA	1:A:769:GLN:HG2	1.92	0.50
1:B:33:VAL:O	1:B:34:SER:C	2.54	0.50
1:B:415:SER:HA	1:B:577:THR:HG21	1.93	0.50
1:B:466:ILE:HG22	1:B:468:VAL:HG23	1.94	0.50
1:B:534:ARG:O	1:B:535:ILE:C	2.53	0.50
1:B:702:THR:HB	1:B:703:GLU:OE1	2.10	0.50
1:B:728:PHE:C	1:B:728:PHE:CD1	2.89	0.50
1:B:786:TYR:HE2	1:B:790:LYS:NZ	2.03	0.50
1:A:61:GLY:HA3	1:A:194:ALA:HB2	1.94	0.50
1:A:85:SER:HA	1:A:963:GLN:OE1	2.11	0.50
1:A:121:VAL:CG2	1:A:122:LEU:N	2.74	0.50
1:A:314:THR:CG2	1:A:327:VAL:HG21	2.36	0.50
1:A:318:ILE:CD1	1:A:324:ILE:H	2.24	0.50
1:A:584:ARG:HA	1:A:584:ARG:NE	2.26	0.50
1:A:617:ILE:HD12	1:A:617:ILE:H	1.74	0.50
1:A:886:LEU:HD12	1:A:886:LEU:C	2.37	0.50
1:B:118:GLY:HA3	1:B:946:TYR:CD2	2.46	0.50
1:B:901:ARG:O	1:B:902:THR:C	2.55	0.50
1:B:978:VAL:HG22	2:B:6002:OJZ:H35B	1.93	0.50
1:B:1023:LYS:HB3	1:B:1026:MET:CG	2.37	0.50
1:B:1108:GLN:N	1:B:1108:GLN:NE2	2.59	0.50
1:B:1196:ASP:HA	1:B:1226:ILE:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ILE:HG22	1:A:202:ILE:N	2.27	0.50
1:A:318:ILE:HD11	1:A:325:GLY:H	1.74	0.50
1:A:534:ARG:O	1:A:537:ILE:N	2.45	0.50
1:A:716:ILE:C	1:A:716:ILE:HD12	2.37	0.50
1:A:721:GLN:O	1:A:722:PRO:C	2.49	0.50
1:A:797:VAL:CG1	1:A:798:SER:N	2.69	0.50
1:A:824:ALA:O	1:A:828:ARG:HG2	2.11	0.50
1:A:1186:LEU:HD12	1:A:1187:VAL:N	2.26	0.50
1:B:69:LEU:HA	1:B:329:THR:HG21	1.93	0.50
1:B:300:LEU:HA	1:B:303:TYR:HB2	1.92	0.50
1:B:398:PRO:HD3	1:B:440:TYR:CE2	2.45	0.50
1:B:697:LEU:HA	1:B:700:ASN:CB	2.41	0.50
1:B:816:ASN:O	1:B:819:ALA:HB3	2.11	0.50
1:A:309:ALA:O	1:A:310:PHE:O	2.30	0.50
1:A:312:TYR:HB2	1:A:751:PHE:CE2	2.46	0.50
1:A:406:LEU:HD12	1:A:409:LEU:CB	2.41	0.50
1:A:502:GLU:C	1:A:504:ASN:N	2.68	0.50
1:A:691:ALA:O	1:A:692:SER:CB	2.60	0.50
1:A:757:ILE:O	1:A:761:ILE:HD13	2.11	0.50
1:A:838:ASN:C	1:A:838:ASN:HD22	2.17	0.50
1:A:972:LEU:H	1:A:972:LEU:CD1	2.23	0.50
1:B:170:ARG:HB2	1:B:170:ARG:NH1	2.26	0.50
1:B:757:ILE:HA	1:B:761:ILE:HD13	1.94	0.50
1:B:766:PHE:O	1:B:769:GLN:N	2.44	0.50
1:B:1092:LEU:CD2	1:B:1097:ILE:HD11	2.40	0.50
1:A:57:ALA:O	1:A:60:HIS:HB3	2.11	0.50
1:A:267:LYS:HG2	1:A:793:LEU:HG	1.93	0.50
1:A:531:GLN:O	1:A:534:ARG:HB3	2.12	0.50
1:A:959:LEU:O	1:A:964:LEU:HB3	2.12	0.50
1:B:271:GLU:O	1:B:274:ASN:HB2	2.12	0.50
1:B:717:ASN:HD21	1:B:766:PHE:HE1	1.57	0.50
1:B:887:GLU:O	1:B:888:GLY:C	2.55	0.50
1:A:106:GLU:HG3	1:A:110:TYR:CZ	2.46	0.50
1:A:842:GLY:HA2	1:A:979:PHE:CE2	2.47	0.50
1:A:1243:GLN:O	1:A:1244:ASN:C	2.54	0.50
1:B:421:LEU:O	1:B:581:ILE:HD12	2.11	0.50
1:B:878:GLN:NE2	1:B:881:LYS:HD3	2.26	0.50
1:B:1037:VAL:HG21	1:B:1087:ALA:HB3	1.94	0.50
1:A:35:VAL:HG21	1:A:355:ARG:HH21	1.76	0.50
1:A:227:ILE:HG22	1:A:228:TRP:N	2.27	0.50
1:A:533:GLN:O	1:A:536:ALA:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:LYS:O	1:A:623:MET:N	2.45	0.50
1:A:902:THR:HG23	1:A:903:VAL:N	2.26	0.50
1:A:1124:ALA:HB2	1:A:1161:TYR:HB3	1.93	0.50
1:B:284:GLY:O	1:B:287:LYS:HB3	2.12	0.50
1:B:291:ALA:O	1:B:295:MET:SD	2.70	0.50
1:B:394:HIS:O	1:B:443:LEU:HB3	2.11	0.50
1:B:485:ARG:O	1:B:488:ARG:N	2.43	0.50
1:B:705:PRO:HG2	1:B:706:TYR:N	2.27	0.50
1:B:750:LEU:O	1:B:753:LEU:HB3	2.12	0.50
1:B:937:THR:O	1:B:938:PHE:C	2.54	0.50
1:B:962:GLN:HG2	1:B:962:GLN:O	2.10	0.50
1:B:991:ALA:HB1	1:B:992:PRO:HD2	1.93	0.50
1:B:1197:GLU:OE2	1:B:1228:HIS:HB2	2.12	0.50
1:A:135:ALA:O	1:A:136:ALA:C	2.54	0.49
1:A:777:GLY:HA3	1:A:822:LYS:HG3	1.93	0.49
1:A:943:ALA:O	1:A:944:MET:C	2.55	0.49
1:B:155:GLU:O	1:B:156:ILE:C	2.55	0.49
1:B:201:ILE:HG22	1:B:202:ILE:N	2.27	0.49
1:B:762:SER:CA	1:B:765:THR:HG22	2.42	0.49
1:B:967:PHE:HD1	1:B:968:GLU:H	1.56	0.49
1:B:1164:ARG:C	1:B:1166:GLY:N	2.68	0.49
1:A:238:LYS:HZ1	1:A:242:ALA:HB2	1.76	0.49
1:A:311:TRP:CD1	1:A:754:LEU:HD12	2.47	0.49
1:A:466:ILE:HG22	1:A:468:VAL:HG23	1.93	0.49
1:A:1037:VAL:HG21	1:A:1087:ALA:HB3	1.94	0.49
1:A:1056:VAL:CG2	1:A:1062:LEU:HB2	2.41	0.49
1:B:158:TRP:HZ2	1:B:900:PHE:HB2	1.75	0.49
1:B:411:LEU:HD23	1:B:411:LEU:C	2.37	0.49
1:B:425:SER:HB2	1:B:598:ASP:O	2.12	0.49
1:B:706:TYR:O	1:B:707:PHE:CG	2.66	0.49
1:B:717:ASN:HB3	1:B:833:PHE:CE1	2.46	0.49
1:B:1095:LYS:HD2	1:B:1095:LYS:N	2.26	0.49
1:A:136:ALA:O	1:A:139:GLN:HB2	2.12	0.49
1:A:307:ALA:O	1:A:308:LEU:O	2.30	0.49
1:A:409:LEU:HD21	1:A:597:PHE:CE1	2.47	0.49
1:B:129:VAL:HG11	1:B:935:GLY:N	2.27	0.49
1:B:308:LEU:O	1:B:309:ALA:C	2.55	0.49
1:B:418:THR:HG22	1:B:578:THR:HG22	1.92	0.49
1:B:843:ILE:HA	1:B:846:SER:CB	2.40	0.49
1:B:892:ILE:O	1:B:893:ALA:C	2.54	0.49
1:B:1128:ALA:HB2	1:B:1141:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1196:ASP:HA	1:B:1226:ILE:HD11	1.93	0.49
1:A:147:PHE:O	1:A:150:ALA:HB3	2.13	0.49
1:A:158:TRP:CE2	1:A:900:PHE:HB2	2.48	0.49
1:A:318:ILE:HD11	1:A:324:ILE:H	1.78	0.49
1:A:492:THR:C	1:A:494:ASP:H	2.19	0.49
1:A:838:ASN:C	1:A:838:ASN:ND2	2.70	0.49
1:A:857:LEU:HD11	1:A:977:ILE:N	2.28	0.49
1:A:1164:ARG:O	1:A:1166:GLY:N	2.44	0.49
1:B:238:LYS:HZ1	1:B:242:ALA:HB2	1.75	0.49
1:B:499:ALA:CB	1:B:542:VAL:HG22	2.42	0.49
1:B:1056:VAL:CG2	1:B:1060:GLN:HE22	2.23	0.49
1:A:35:VAL:HG12	1:A:359:TYR:CZ	2.47	0.49
1:A:291:ALA:CA	1:A:294:SER:HB2	2.42	0.49
1:A:620:LYS:HD2	1:A:621:LEU:HD22	1.95	0.49
1:A:1023:LYS:C	1:A:1025:ASN:N	2.71	0.49
1:A:1202:LEU:HG	1:A:1206:SER:CB	2.42	0.49
1:B:144:ARG:HG2	1:B:920:LEU:HD11	1.93	0.49
1:B:206:ARG:O	1:B:330:VAL:HG11	2.12	0.49
1:B:291:ALA:HA	1:B:294:SER:CB	2.42	0.49
1:B:311:TRP:CE3	1:B:311:TRP:CA	2.96	0.49
1:B:620:LYS:HD2	1:B:621:LEU:HD22	1.95	0.49
1:B:842:GLY:HA2	1:B:979:PHE:CE2	2.47	0.49
1:B:942:GLN:O	1:B:943:ALA:C	2.56	0.49
1:A:253:VAL:O	1:A:254:LEU:HD13	2.11	0.49
1:A:270:LEU:HG	1:A:271:GLU:H	1.78	0.49
1:A:750:LEU:O	1:A:753:LEU:HB3	2.12	0.49
1:A:895:GLU:O	1:A:899:ASN:ND2	2.45	0.49
1:A:905:SER:HB2	1:A:908:ARG:CZ	2.42	0.49
1:A:909:GLU:O	1:A:912:PHE:HB2	2.13	0.49
1:A:1095:LYS:H	1:A:1095:LYS:CD	2.24	0.49
1:A:1189:GLN:N	1:A:1190:PRO:CD	2.76	0.49
1:B:144:ARG:HH12	1:B:175:VAL:HG11	1.74	0.49
1:B:301:LEU:O	1:B:304:ALA:HB3	2.13	0.49
1:B:824:ALA:O	1:B:828:ARG:HG2	2.12	0.49
1:B:827:SER:O	1:B:828:ARG:C	2.55	0.49
1:B:949:TYR:N	1:B:949:TYR:CD1	2.80	0.49
1:B:972:LEU:H	1:B:972:LEU:CD1	2.22	0.49
1:B:1166:GLY:HA3	1:B:1171:GLN:OE1	2.12	0.49
1:B:1178:GLN:O	1:B:1181:ALA:HB3	2.13	0.49
1:A:44:TRP:C	1:A:46:ASP:N	2.71	0.49
1:A:157:GLY:HA2	1:A:160:ASP:CB	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:VAL:HG13	1:A:176:SER:H	1.75	0.49
1:A:269:GLU:O	1:A:270:LEU:C	2.54	0.49
1:A:295:MET:C	1:A:297:ALA:N	2.69	0.49
1:A:352:ALA:O	1:A:355:ARG:N	2.46	0.49
1:B:314:THR:CG2	1:B:327:VAL:CG2	2.81	0.49
1:B:492:THR:C	1:B:494:ASP:H	2.19	0.49
1:B:795:GLN:NE2	1:B:796:ASP:H	2.08	0.49
1:B:872:MET:HE2	1:B:873:LYS:HA	1.95	0.49
1:A:209:LYS:HA	1:A:212:LEU:HB3	1.95	0.49
1:A:505:ALA:HB1	1:A:508:PHE:CZ	2.47	0.49
1:A:843:ILE:CA	1:A:846:SER:HB3	2.39	0.49
1:A:1080:GLU:OE1	1:A:1109:LEU:HD12	2.12	0.49
1:A:1147:GLU:OE1	1:A:1216:LYS:HB2	2.11	0.49
1:B:57:ALA:O	1:B:60:HIS:HB3	2.13	0.49
1:B:120:GLY:O	1:B:121:VAL:C	2.55	0.49
1:B:434:GLN:O	1:B:436:MET:N	2.46	0.49
1:B:843:ILE:CA	1:B:846:SER:HB3	2.39	0.49
1:B:886:LEU:HD12	1:B:886:LEU:C	2.37	0.49
1:B:1020:GLN:O	1:B:1021:GLY:O	2.30	0.49
1:B:1193:LEU:HB2	1:B:1223:CYS:CB	2.34	0.49
1:A:216:ALA:O	1:A:220:VAL:HG23	2.13	0.49
1:A:300:LEU:O	1:A:303:TYR:HB3	2.12	0.49
1:A:429:LYS:O	1:A:432:THR:N	2.46	0.49
1:A:485:ARG:O	1:A:488:ARG:N	2.42	0.49
1:A:816:ASN:O	1:A:819:ALA:HB3	2.13	0.49
1:A:1125:GLU:O	1:A:1126:ASN:C	2.56	0.49
1:A:1197:GLU:OE2	1:A:1228:HIS:HB2	2.12	0.49
1:B:110:TYR:HA	1:B:113:TYR:CD2	2.47	0.49
1:B:147:PHE:O	1:B:148:PHE:C	2.54	0.49
1:B:409:LEU:HD13	1:B:410:ASN:N	2.26	0.49
1:B:583:HIS:HB2	1:B:584:ARG:HH12	1.78	0.49
1:B:762:SER:O	1:B:763:PHE:C	2.55	0.49
1:B:853:LEU:HB3	1:B:973:VAL:CG2	2.43	0.49
1:B:1205:GLU:HA	1:B:1208:LYS:HB3	1.94	0.49
1:A:411:LEU:HD23	1:A:411:LEU:C	2.38	0.49
1:A:498:LYS:HE2	1:A:499:ALA:N	2.28	0.49
1:A:620:LYS:HD3	1:A:624:THR:HG1	1.78	0.49
1:A:706:TYR:O	1:A:707:PHE:CG	2.66	0.49
1:A:722:PRO:HA	1:A:979:PHE:HE1	1.78	0.49
1:A:773:PHE:CD1	1:A:773:PHE:C	2.91	0.49
1:A:830:ALA:O	1:A:833:PHE:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:TRP:CD1	1:B:45:LEU:HD22	2.48	0.49
1:B:93:GLU:H	1:B:93:GLU:CD	2.21	0.49
1:B:255:ALA:O	1:B:257:ILE:N	2.45	0.49
1:B:420:ALA:C	1:B:421:LEU:HD12	2.37	0.49
1:B:539:ARG:O	1:B:540:ALA:C	2.54	0.49
1:B:570:ASP:HA	1:B:573:ARG:NH1	2.28	0.49
1:B:1076:VAL:HG13	1:B:1194:LEU:HB3	1.94	0.49
1:B:1147:GLU:OE1	1:B:1216:LYS:HB2	2.12	0.49
1:A:207:GLY:C	1:A:209:LYS:H	2.21	0.48
1:A:394:HIS:O	1:A:443:LEU:HB3	2.12	0.48
1:A:401:LYS:HB3	1:A:401:LYS:HZ3	1.78	0.48
1:A:728:PHE:CD1	1:A:728:PHE:C	2.91	0.48
1:B:61:GLY:HA3	1:B:194:ALA:HB2	1.95	0.48
1:B:218:SER:CB	1:B:219:PRO:HD3	2.42	0.48
1:B:342:GLY:O	1:B:345:SER:HB3	2.12	0.48
1:B:415:SER:HA	1:B:577:THR:CG2	2.43	0.48
1:B:462:LEU:O	1:B:465:ILE:N	2.45	0.48
1:B:1080:GLU:OE1	1:B:1109:LEU:HD12	2.13	0.48
1:B:1102:VAL:HG13	1:B:1103:GLN:H	1.77	0.48
1:A:132:TRP:CD2	1:A:183:GLY:HA3	2.47	0.48
1:A:214:ILE:HG12	1:A:331:PHE:CE2	2.48	0.48
1:A:570:ASP:HA	1:A:573:ARG:NH1	2.28	0.48
1:A:778:GLU:C	1:A:782:LYS:HE2	2.39	0.48
1:A:883:LYS:HA	1:A:886:LEU:HG	1.95	0.48
1:A:933:VAL:C	1:A:935:GLY:N	2.69	0.48
1:B:270:LEU:HG	1:B:271:GLU:H	1.78	0.48
1:B:793:LEU:HD13	1:B:793:LEU:C	2.37	0.48
1:B:933:VAL:O	1:B:935:GLY:N	2.46	0.48
1:A:781:THR:O	1:A:782:LYS:C	2.56	0.48
1:A:900:PHE:O	1:A:901:ARG:C	2.56	0.48
1:B:281:LYS:HD2	1:B:281:LYS:N	2.28	0.48
1:B:409:LEU:HD21	1:B:597:PHE:CE1	2.47	0.48
1:B:505:ALA:HB1	1:B:508:PHE:CZ	2.49	0.48
1:B:538:ALA:O	1:B:539:ARG:C	2.57	0.48
1:B:560:GLU:O	1:B:561:SER:C	2.56	0.48
1:B:777:GLY:CA	1:B:822:LYS:HG3	2.44	0.48
1:B:781:THR:O	1:B:782:LYS:C	2.56	0.48
1:B:911:LYS:C	1:B:911:LYS:HD3	2.38	0.48
1:A:213:VAL:O	1:A:216:ALA:HB3	2.13	0.48
1:A:418:THR:HA	1:A:578:THR:O	2.12	0.48
1:A:1043:ARG:N	1:A:1044:PRO:HD2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:SER:O	1:B:372:ASP:N	2.44	0.48
1:B:371:ILE:O	1:B:371:ILE:HG22	2.13	0.48
1:B:722:PRO:HA	1:B:979:PHE:HE1	1.78	0.48
1:B:741:PRO:O	1:B:742:GLU:HB2	2.13	0.48
1:B:959:LEU:HD23	1:B:959:LEU:C	2.39	0.48
1:A:44:TRP:CD1	1:A:45:LEU:HD22	2.48	0.48
1:A:163:ASP:C	1:A:164:VAL:HG22	2.38	0.48
1:A:831:VAL:O	1:A:832:ILE:C	2.57	0.48
1:A:911:LYS:C	1:A:911:LYS:HD3	2.38	0.48
1:A:914:THR:O	1:A:917:ALA:HB3	2.14	0.48
1:B:132:TRP:CD2	1:B:183:GLY:HA3	2.48	0.48
1:B:147:PHE:O	1:B:150:ALA:HB3	2.14	0.48
1:B:269:GLU:O	1:B:270:LEU:C	2.55	0.48
1:B:318:ILE:HD11	1:B:324:ILE:C	2.38	0.48
1:B:552:GLU:O	1:B:553:ALA:C	2.57	0.48
1:B:620:LYS:HD3	1:B:624:THR:HG1	1.78	0.48
1:B:761:ILE:HD12	1:B:761:ILE:H	1.78	0.48
1:B:1091:PHE:CE1	1:B:1096:GLU:HG2	2.32	0.48
1:A:429:LYS:C	1:A:431:THR:N	2.69	0.48
1:A:434:GLN:C	1:A:436:MET:H	2.20	0.48
1:A:437:GLN:HE21	1:A:468:VAL:HG21	1.79	0.48
1:A:788:VAL:HG21	1:A:1004:ILE:HG13	1.95	0.48
1:A:795:GLN:NE2	1:A:796:ASP:H	2.10	0.48
1:A:837:ALA:HB1	1:A:982:MET:CE	2.44	0.48
1:A:1128:ALA:CB	1:A:1136:VAL:HG13	2.43	0.48
1:A:1128:ALA:HB2	1:A:1141:ILE:HG21	1.96	0.48
1:A:1166:GLY:HA3	1:A:1171:GLN:OE1	2.13	0.48
1:B:534:ARG:O	1:B:537:ILE:N	2.46	0.48
1:B:697:LEU:O	1:B:700:ASN:HB3	2.13	0.48
1:B:773:PHE:HB2	1:B:829:LEU:HD13	1.95	0.48
1:B:837:ALA:HB1	1:B:982:MET:CE	2.43	0.48
1:B:846:SER:HA	1:B:849:TYR:CG	2.49	0.48
1:B:881:LYS:HB2	1:B:881:LYS:HZ3	1.78	0.48
1:B:992:PRO:C	1:B:994:TYR:H	2.21	0.48
1:B:1032:GLN:HE21	1:B:1055:GLU:HG3	1.77	0.48
1:A:846:SER:HA	1:A:849:TYR:CE1	2.49	0.48
1:A:872:MET:HE2	1:A:873:LYS:HA	1.95	0.48
1:A:1090:VAL:CG1	1:A:1097:ILE:HB	2.36	0.48
1:B:806:THR:HG23	1:B:809:ALA:H	1.78	0.48
1:B:979:PHE:HA	1:B:982:MET:SD	2.54	0.48
1:B:1135:VAL:O	1:B:1137:SER:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LYS:HD3	1:A:429:LYS:N	2.19	0.48
1:A:583:HIS:HB2	1:A:584:ARG:HH12	1.78	0.48
1:A:846:SER:HA	1:A:849:TYR:CG	2.48	0.48
1:A:1101:ASN:O	1:A:1102:VAL:C	2.57	0.48
1:B:221:LEU:HD13	1:B:306:TYR:HA	1.95	0.48
1:B:309:ALA:O	1:B:310:PHE:C	2.56	0.48
1:B:322:TYR:CE2	1:B:324:ILE:HD11	2.49	0.48
1:B:566:GLN:HA	1:B:569:LEU:HD12	1.96	0.48
1:B:704:TRP:CZ2	1:B:707:PHE:N	2.82	0.48
1:B:833:PHE:O	1:B:834:GLN:C	2.56	0.48
1:B:852:GLN:HB3	1:B:853:LEU:HD22	1.96	0.48
1:B:1014:ILE:HD12	1:B:1106:ARG:NH1	2.29	0.48
1:B:1036:VAL:HB	1:B:1052:LEU:CB	2.35	0.48
1:B:1149:ASN:O	1:B:1179:ARG:HD3	2.14	0.48
1:A:175:VAL:CG1	1:A:176:SER:H	2.27	0.48
1:A:204:PHE:HA	1:A:211:THR:CG2	2.41	0.48
1:A:265:GLY:C	1:A:267:LYS:HG3	2.39	0.48
1:A:425:SER:HB2	1:A:598:ASP:O	2.14	0.48
1:A:470:SER:HB2	1:A:471:GLN:OE1	2.14	0.48
1:A:1098:LYS:O	1:A:1099:GLN:HB2	2.14	0.48
1:B:838:ASN:C	1:B:838:ASN:ND2	2.71	0.48
1:B:1149:ASN:OD1	1:B:1213:ALA:HB2	2.14	0.48
1:B:1192:ILE:HD13	1:B:1193:LEU:N	2.29	0.48
1:A:43:GLY:HA3	1:A:46:ASP:HB2	1.96	0.48
1:A:134:LEU:O	1:A:138:ARG:HG3	2.14	0.48
1:A:221:LEU:HD13	1:A:306:TYR:HA	1.96	0.48
1:A:281:LYS:N	1:A:281:LYS:HD2	2.28	0.48
1:A:761:ILE:HD12	1:A:761:ILE:H	1.79	0.48
1:A:991:ALA:HB1	1:A:992:PRO:HD2	1.96	0.48
1:A:1137:SER:HB3	1:A:1140:GLU:HB2	1.96	0.48
1:B:175:VAL:HG13	1:B:176:SER:H	1.78	0.48
1:B:316:LEU:C	1:B:318:ILE:H	2.22	0.48
1:B:318:ILE:CD1	1:B:325:GLY:H	2.26	0.48
1:B:476:PHE:O	1:B:478:THR:N	2.41	0.48
1:B:568:ALA:O	1:B:569:LEU:C	2.56	0.48
1:B:1022:LEU:O	1:B:1023:LYS:C	2.57	0.48
1:A:116:GLY:O	1:A:117:ILE:C	2.56	0.47
1:A:217:ILE:HG13	1:A:218:SER:N	2.28	0.47
1:A:255:ALA:O	1:A:256:ALA:C	2.57	0.47
1:A:409:LEU:CD2	1:A:602:ILE:HB	2.44	0.47
1:A:453:ASP:HB3	1:A:456:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:THR:O	1:A:493:MET:C	2.57	0.47
1:A:751:PHE:CD1	1:A:752:SER:N	2.82	0.47
1:A:1076:VAL:HG13	1:A:1194:LEU:HB3	1.96	0.47
1:A:1078:LEU:HD23	1:A:1083:TYR:O	2.14	0.47
1:A:1092:LEU:CD2	1:A:1097:ILE:HD11	2.40	0.47
1:A:1225:VAL:O	1:A:1225:VAL:HG13	2.13	0.47
1:B:217:ILE:HG13	1:B:218:SER:N	2.29	0.47
1:B:318:ILE:HG12	1:B:325:GLY:HA2	1.96	0.47
1:B:909:GLU:OE2	1:B:909:GLU:N	2.44	0.47
1:B:930:LYS:HA	1:B:933:VAL:CG2	2.44	0.47
1:A:278:GLU:HB3	1:A:782:LYS:HG2	1.96	0.47
1:A:307:ALA:O	1:A:308:LEU:C	2.55	0.47
1:A:421:LEU:O	1:A:581:ILE:HD12	2.14	0.47
1:A:817:ASP:OD1	1:A:1000:SER:HB3	2.14	0.47
1:B:449:ILE:O	1:B:450:ASP:C	2.57	0.47
1:B:453:ASP:HB3	1:B:456:THR:HG23	1.96	0.47
1:B:724:PHE:HA	1:B:727:ILE:CG2	2.43	0.47
1:B:727:ILE:HG21	1:B:754:LEU:HD23	1.96	0.47
1:B:821:VAL:O	1:B:824:ALA:HB3	2.14	0.47
1:B:892:ILE:HB	1:B:916:TYR:HE1	1.75	0.47
1:B:1038:PHE:CD1	1:B:1039:ASN:N	2.82	0.47
1:B:1043:ARG:N	1:B:1044:PRO:HD2	2.29	0.47
1:B:1193:LEU:HD21	1:B:1221:ARG:HH11	1.78	0.47
1:A:110:TYR:HA	1:A:113:TYR:CD2	2.48	0.47
1:A:275:ASN:HA	1:A:278:GLU:HB2	1.95	0.47
1:A:560:GLU:O	1:A:561:SER:C	2.56	0.47
1:A:561:SER:O	1:A:562:GLU:C	2.56	0.47
1:A:723:ALA:O	1:A:724:PHE:C	2.57	0.47
1:A:933:VAL:O	1:A:935:GLY:N	2.47	0.47
1:A:943:ALA:C	1:A:945:MET:N	2.71	0.47
1:A:1107:ALA:HB3	1:A:1108:GLN:NE2	2.29	0.47
1:B:209:LYS:C	1:B:212:LEU:HB3	2.38	0.47
1:B:1032:GLN:HE21	1:B:1055:GLU:CG	2.27	0.47
1:B:1123:ILE:HG13	1:B:1124:ALA:N	2.29	0.47
1:B:1202:LEU:HG	1:B:1206:SER:CB	2.44	0.47
1:A:157:GLY:HA2	1:A:160:ASP:OD2	2.15	0.47
1:A:311:TRP:CE3	1:A:311:TRP:CA	2.97	0.47
1:A:1149:ASN:OD1	1:A:1213:ALA:HB2	2.14	0.47
1:A:1193:LEU:HD21	1:A:1221:ARG:HH11	1.78	0.47
1:B:405:ILE:N	1:B:405:ILE:HD12	2.29	0.47
1:B:409:LEU:CD2	1:B:602:ILE:HB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:GLN:HE21	1:B:468:VAL:HG21	1.79	0.47
1:B:468:VAL:HG12	1:B:469:VAL:N	2.29	0.47
1:B:561:SER:O	1:B:562:GLU:C	2.56	0.47
1:B:686:GLU:HB2	1:B:813:ARG:HH21	1.79	0.47
1:B:808:GLY:O	1:B:810:LEU:N	2.47	0.47
1:A:315:SER:C	1:A:318:ILE:HG22	2.39	0.47
1:A:352:ALA:O	1:A:353:ASN:C	2.57	0.47
1:A:704:TRP:CZ2	1:A:707:PHE:N	2.82	0.47
1:A:1077:GLN:O	1:A:1078:LEU:C	2.56	0.47
1:B:185:LYS:O	1:B:186:ILE:C	2.58	0.47
1:B:374:PHE:HD1	1:B:375:SER:H	1.61	0.47
1:B:396:SER:HB3	1:B:443:LEU:HD12	1.97	0.47
1:B:401:LYS:HB3	1:B:401:LYS:HZ3	1.75	0.47
1:B:533:GLN:O	1:B:537:ILE:HG12	2.15	0.47
1:B:959:LEU:O	1:B:964:LEU:CB	2.62	0.47
1:B:967:PHE:CD1	1:B:968:GLU:N	2.82	0.47
1:B:1031:VAL:H	1:B:1056:VAL:HG13	1.78	0.47
1:B:1137:SER:HB3	1:B:1140:GLU:HB2	1.95	0.47
1:A:53:GLY:O	1:A:56:ALA:N	2.48	0.47
1:A:58:ILE:C	1:A:60:HIS:N	2.72	0.47
1:A:435:LEU:HD23	1:A:435:LEU:H	1.80	0.47
1:A:438:ARG:O	1:A:439:LEU:O	2.31	0.47
1:A:724:PHE:HA	1:A:727:ILE:CG2	2.44	0.47
1:A:793:LEU:C	1:A:793:LEU:HD13	2.39	0.47
1:A:1032:GLN:HE21	1:A:1055:GLU:CG	2.27	0.47
1:B:273:TYR:O	1:B:274:ASN:O	2.33	0.47
1:B:352:ALA:O	1:B:353:ASN:C	2.57	0.47
1:B:1107:ALA:HB3	1:B:1108:GLN:NE2	2.29	0.47
1:A:258:ARG:HH22	1:A:1113:SER:CB	2.27	0.47
1:A:348:ILE:O	1:A:349:GLU:C	2.57	0.47
1:A:468:VAL:HG12	1:A:469:VAL:N	2.29	0.47
1:A:533:GLN:O	1:A:537:ILE:HG12	2.14	0.47
1:A:589:ARG:HG2	1:A:589:ARG:HH11	1.80	0.47
1:A:705:PRO:HG2	1:A:706:TYR:N	2.27	0.47
1:A:777:GLY:CA	1:A:822:LYS:HG3	2.43	0.47
1:A:785:ARG:O	1:A:786:TYR:C	2.57	0.47
1:A:797:VAL:HG13	1:A:1082:PHE:O	2.15	0.47
1:A:957:ALA:O	1:A:958:TYR:C	2.58	0.47
1:A:1092:LEU:HB3	1:A:1097:ILE:CD1	2.37	0.47
1:A:1097:ILE:O	1:A:1098:LYS:HB3	2.13	0.47
1:A:1116:PRO:HB3	1:A:1178:GLN:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1204:THR:O	1:A:1206:SER:N	2.48	0.47
1:B:136:ALA:O	1:B:137:GLY:C	2.57	0.47
1:B:314:THR:HG22	1:B:315:SER:N	2.29	0.47
1:B:315:SER:C	1:B:318:ILE:HG22	2.40	0.47
1:B:318:ILE:HD11	1:B:325:GLY:H	1.77	0.47
1:B:354:ALA:O	1:B:358:ALA:CB	2.62	0.47
1:B:432:THR:O	1:B:433:VAL:C	2.56	0.47
1:B:502:GLU:OE1	1:B:541:LEU:HD11	2.14	0.47
1:B:1077:GLN:O	1:B:1078:LEU:C	2.58	0.47
1:B:1095:LYS:H	1:B:1095:LYS:CD	2.27	0.47
1:B:1176:GLN:O	1:B:1177:LYS:C	2.56	0.47
1:B:1229:ARG:C	1:B:1231:SER:N	2.73	0.47
1:A:55:LEU:O	1:A:56:ALA:C	2.58	0.47
1:A:188:MET:SD	1:A:188:MET:C	2.97	0.47
1:A:218:SER:CB	1:A:219:PRO:HD3	2.42	0.47
1:A:415:SER:HA	1:A:577:THR:HG21	1.97	0.47
1:A:727:ILE:HG21	1:A:754:LEU:HD23	1.97	0.47
1:A:1123:ILE:HG13	1:A:1124:ALA:N	2.30	0.47
1:B:348:ILE:O	1:B:349:GLU:C	2.57	0.47
1:B:436:MET:O	1:B:436:MET:HE3	2.15	0.47
1:B:778:GLU:C	1:B:782:LYS:HE2	2.40	0.47
1:B:1203:ASP:O	1:B:1206:SER:HB2	2.13	0.47
1:A:58:ILE:O	1:A:60:HIS:N	2.48	0.47
1:A:308:LEU:O	1:A:309:ALA:C	2.55	0.47
1:A:502:GLU:OE1	1:A:541:LEU:HD11	2.14	0.47
1:B:59:ILE:HD11	1:B:124:VAL:CG2	2.45	0.47
1:B:64:LEU:O	1:B:65:PRO:C	2.50	0.47
1:B:135:ALA:O	1:B:136:ALA:C	2.57	0.47
1:B:157:GLY:HA2	1:B:160:ASP:OD2	2.15	0.47
1:B:320:LYS:O	1:B:323:SER:OG	2.32	0.47
1:B:531:GLN:O	1:B:534:ARG:HB3	2.14	0.47
1:B:722:PRO:HA	1:B:979:PHE:CE1	2.50	0.47
1:B:853:LEU:HG	1:B:973:VAL:HG21	1.97	0.47
1:B:943:ALA:C	1:B:945:MET:N	2.73	0.47
1:B:972:LEU:HD12	1:B:972:LEU:N	2.25	0.47
1:A:249:VAL:O	1:A:273:TYR:HB3	2.15	0.47
1:A:315:SER:O	1:A:318:ILE:HG22	2.15	0.47
1:A:566:GLN:HA	1:A:569:LEU:HD12	1.97	0.47
1:B:249:VAL:O	1:B:273:TYR:HB3	2.14	0.47
1:B:942:GLN:O	1:B:945:MET:N	2.48	0.47
1:A:207:GLY:CA	1:A:210:LEU:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:PHE:O	1:A:478:THR:N	2.45	0.46
1:A:541:LEU:C	1:A:543:ARG:N	2.71	0.46
1:A:833:PHE:O	1:A:834:GLN:C	2.57	0.46
1:A:868:GLY:O	1:A:871:GLU:HB3	2.14	0.46
1:A:998:THR:O	1:A:1001:ALA:HB3	2.15	0.46
1:A:1101:ASN:OD1	1:A:1103:GLN:HB3	2.15	0.46
1:A:1135:VAL:O	1:A:1137:SER:N	2.47	0.46
1:B:291:ALA:CA	1:B:294:SER:HB2	2.45	0.46
1:B:468:VAL:HG22	1:B:549:LEU:HB2	1.97	0.46
1:B:492:THR:O	1:B:493:MET:C	2.58	0.46
1:B:709:VAL:HG13	1:B:710:GLY:N	2.30	0.46
1:B:846:SER:HA	1:B:849:TYR:CE1	2.50	0.46
1:B:1125:GLU:O	1:B:1126:ASN:C	2.58	0.46
1:A:64:LEU:O	1:A:65:PRO:C	2.52	0.46
1:A:78:PHE:CE2	1:A:967:PHE:O	2.69	0.46
1:A:151:ILE:C	1:A:153:ASN:N	2.72	0.46
1:A:274:ASN:O	1:A:278:GLU:HG3	2.15	0.46
1:A:405:ILE:HD12	1:A:405:ILE:N	2.30	0.46
1:A:468:VAL:HG22	1:A:549:LEU:HB2	1.97	0.46
1:A:973:VAL:O	1:A:976:ALA:N	2.47	0.46
1:A:1218:ARG:NH1	1:A:1235:ASN:HD22	2.14	0.46
1:B:144:ARG:HG2	1:B:920:LEU:CD1	2.45	0.46
1:B:199:GLY:O	1:B:203:GLY:HA3	2.15	0.46
1:B:315:SER:O	1:B:318:ILE:HG22	2.16	0.46
1:B:342:GLY:O	1:B:346:PRO:HD3	2.15	0.46
1:B:536:ALA:O	1:B:539:ARG:N	2.49	0.46
1:B:1250:HIS:C	1:B:1256:LEU:HD21	2.40	0.46
1:A:121:VAL:HG23	1:A:122:LEU:H	1.78	0.46
1:A:538:ALA:O	1:A:539:ARG:C	2.58	0.46
1:A:697:LEU:HA	1:A:700:ASN:CB	2.43	0.46
1:A:762:SER:O	1:A:763:PHE:C	2.57	0.46
1:A:773:PHE:HB2	1:A:829:LEU:HD13	1.96	0.46
1:A:779:ILE:O	1:A:780:LEU:C	2.58	0.46
1:A:845:ILE:O	1:A:848:ILE:HG12	2.14	0.46
1:B:207:GLY:CA	1:B:210:LEU:HB3	2.45	0.46
1:B:751:PHE:CD1	1:B:752:SER:N	2.83	0.46
1:B:1116:PRO:HB3	1:B:1178:GLN:OE1	2.15	0.46
1:A:278:GLU:HA	1:A:282:ARG:NH1	2.31	0.46
1:A:297:ALA:HB1	1:A:763:PHE:CD2	2.51	0.46
1:A:322:TYR:CE2	1:A:324:ILE:HD11	2.50	0.46
1:A:434:GLN:C	1:A:436:MET:N	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1149:ASN:O	1:A:1179:ARG:HD3	2.15	0.46
1:A:1167:ASP:O	1:A:1168:LYS:HB2	2.15	0.46
1:A:1229:ARG:C	1:A:1231:SER:N	2.74	0.46
1:B:227:ILE:HG22	1:B:228:TRP:N	2.30	0.46
1:B:714:ALA:HB1	1:B:833:PHE:HB2	1.98	0.46
1:B:852:GLN:HG3	1:B:955:PHE:CZ	2.51	0.46
1:B:957:ALA:O	1:B:958:TYR:O	2.33	0.46
1:B:1039:ASN:HD22	1:B:1048:VAL:N	2.14	0.46
1:B:1157:LEU:HD22	1:B:1157:LEU:N	2.30	0.46
1:B:1164:ARG:O	1:B:1166:GLY:N	2.49	0.46
1:A:158:TRP:HA	1:A:162:HIS:CD2	2.43	0.46
1:A:165:GLY:H	1:A:167:LEU:H	1.63	0.46
1:A:992:PRO:O	1:A:994:TYR:N	2.49	0.46
1:B:470:SER:HA	1:B:551:ASP:HB3	1.97	0.46
1:B:550:LEU:HD23	1:B:569:LEU:HD13	1.97	0.46
1:B:589:ARG:HG2	1:B:589:ARG:HH11	1.80	0.46
1:B:1020:GLN:O	1:B:1026:MET:CE	2.64	0.46
1:B:1032:GLN:NE2	1:B:1055:GLU:HB2	2.30	0.46
1:B:1170:THR:O	1:B:1170:THR:HG22	2.15	0.46
1:A:38:MET:HE2	1:A:38:MET:HA	1.98	0.46
1:A:144:ARG:O	1:A:145:GLN:C	2.59	0.46
1:A:210:LEU:HG	1:A:322:TYR:CD2	2.51	0.46
1:A:268:LYS:O	1:A:269:GLU:C	2.59	0.46
1:A:462:LEU:O	1:A:465:ILE:N	2.48	0.46
1:A:550:LEU:HD23	1:A:569:LEU:HD13	1.97	0.46
1:A:709:VAL:HG13	1:A:710:GLY:N	2.31	0.46
1:A:766:PHE:O	1:A:769:GLN:N	2.49	0.46
1:A:892:ILE:HB	1:A:916:TYR:HE1	1.74	0.46
1:A:1164:ARG:O	1:A:1165:VAL:C	2.57	0.46
1:A:1218:ARG:O	1:A:1219:GLU:HB3	2.16	0.46
1:B:34:SER:O	1:B:35:VAL:C	2.59	0.46
1:B:138:ARG:O	1:B:139:GLN:C	2.58	0.46
1:B:144:ARG:O	1:B:145:GLN:C	2.57	0.46
1:B:204:PHE:HA	1:B:211:THR:HG21	1.98	0.46
1:B:286:LYS:HG2	1:B:778:GLU:CD	2.41	0.46
1:B:702:THR:C	1:B:704:TRP:H	2.23	0.46
1:B:765:THR:HG23	1:B:766:PHE:N	2.30	0.46
1:B:969:ASN:HD22	1:B:969:ASN:N	2.12	0.46
1:A:83:ASN:O	1:A:86:LYS:HB3	2.16	0.46
1:A:324:ILE:CD1	1:A:326:GLN:H	2.26	0.46
1:A:342:GLY:O	1:A:345:SER:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:ALA:O	1:A:543:ARG:CB	2.63	0.46
1:A:710:GLY:O	1:A:711:ILE:C	2.57	0.46
1:A:901:ARG:O	1:A:904:VAL:HG12	2.16	0.46
1:A:972:LEU:HD12	1:A:972:LEU:N	2.24	0.46
1:A:1036:VAL:HB	1:A:1052:LEU:CB	2.36	0.46
1:A:1176:GLN:O	1:A:1177:LYS:C	2.59	0.46
1:B:129:VAL:HG11	1:B:934:PHE:C	2.41	0.46
1:B:293:ILE:CD1	1:B:773:PHE:HZ	2.29	0.46
1:B:310:PHE:HB3	1:B:311:TRP:H	1.47	0.46
1:B:773:PHE:C	1:B:773:PHE:CD1	2.93	0.46
1:B:808:GLY:O	1:B:809:ALA:C	2.58	0.46
1:B:940:PHE:O	1:B:944:MET:HG2	2.16	0.46
1:A:429:LYS:O	1:A:431:THR:N	2.49	0.46
1:A:443:LEU:HD23	1:A:443:LEU:C	2.41	0.46
1:A:722:PRO:HA	1:A:979:PHE:CE1	2.50	0.46
1:A:925:ARG:HG2	1:B:514:HIS:ND1	2.31	0.46
1:A:967:PHE:CD1	1:A:968:GLU:N	2.82	0.46
1:A:1102:VAL:HG13	1:A:1103:GLN:H	1.81	0.46
1:B:38:MET:HE2	1:B:38:MET:HA	1.97	0.46
1:B:188:MET:SD	1:B:188:MET:C	2.98	0.46
1:B:223:LEU:O	1:B:224:SER:C	2.59	0.46
1:B:313:GLY:O	1:B:317:VAL:HG23	2.16	0.46
1:B:686:GLU:HB2	1:B:813:ARG:NH2	2.30	0.46
1:B:1101:ASN:OD1	1:B:1103:GLN:HB3	2.16	0.46
1:A:155:GLU:O	1:A:156:ILE:C	2.58	0.46
1:A:429:LYS:H	1:A:429:LYS:CD	2.18	0.46
1:A:536:ALA:O	1:A:539:ARG:N	2.48	0.46
1:A:770:GLY:HA2	1:A:773:PHE:CE2	2.51	0.46
1:A:900:PHE:C	1:A:902:THR:N	2.73	0.46
1:A:902:THR:C	1:A:904:VAL:N	2.68	0.46
1:A:1039:ASN:CG	1:A:1047:PRO:HA	2.41	0.46
1:A:1114:GLN:O	1:A:1116:PRO:HD3	2.15	0.46
1:A:1170:THR:O	1:A:1170:THR:HG22	2.15	0.46
1:B:44:TRP:C	1:B:46:ASP:N	2.71	0.46
1:B:258:ARG:C	1:B:260:VAL:N	2.74	0.46
1:B:383:ASN:O	1:B:384:ILE:O	2.34	0.46
1:B:704:TRP:CZ2	1:B:707:PHE:HB2	2.51	0.46
1:B:716:ILE:C	1:B:716:ILE:HD12	2.41	0.46
1:B:990:PHE:O	1:B:991:ALA:C	2.58	0.46
1:B:1145:ALA:HA	1:B:1150:ILE:HG22	1.98	0.46
1:A:309:ALA:O	1:A:310:PHE:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:PHE:HB3	1:A:311:TRP:H	1.50	0.46
1:A:314:THR:HG22	1:A:315:SER:N	2.31	0.46
1:A:315:SER:CA	1:A:318:ILE:HG22	2.46	0.46
1:A:334:VAL:O	1:A:335:LEU:C	2.59	0.46
1:A:356:GLY:HA2	1:A:359:TYR:HE1	1.79	0.46
1:A:459:VAL:O	1:A:460:ARG:C	2.56	0.46
1:A:570:ASP:O	1:A:573:ARG:N	2.46	0.46
1:A:585:LEU:HA	1:A:588:VAL:HB	1.97	0.46
1:B:136:ALA:O	1:B:139:GLN:HB2	2.16	0.46
1:B:195:THR:HB	1:B:340:SER:HG	1.80	0.46
1:B:307:ALA:O	1:B:308:LEU:C	2.58	0.46
1:B:345:SER:O	1:B:346:PRO:C	2.57	0.46
1:B:459:VAL:O	1:B:460:ARG:C	2.57	0.46
1:B:614:GLU:O	1:B:615:LYS:C	2.59	0.46
1:B:620:LYS:O	1:B:623:MET:N	2.48	0.46
1:B:1078:LEU:HD23	1:B:1083:TYR:O	2.16	0.46
1:B:1128:ALA:CB	1:B:1136:VAL:HG13	2.46	0.46
1:A:75:THR:HB	1:A:326:GLN:OE1	2.16	0.45
1:A:386:GLY:CA	1:A:450:ASP:HA	2.44	0.45
1:A:500:VAL:HG23	1:A:501:LYS:H	1.81	0.45
1:A:503:ALA:O	1:A:504:ASN:C	2.58	0.45
1:A:808:GLY:O	1:A:809:ALA:C	2.59	0.45
1:A:833:PHE:CG	1:A:834:GLN:N	2.83	0.45
1:A:930:LYS:HA	1:A:933:VAL:CG2	2.46	0.45
1:A:1048:VAL:HG23	1:A:1049:LEU:HD22	1.97	0.45
1:A:1048:VAL:HG23	1:A:1049:LEU:HD23	1.97	0.45
1:A:1144:ALA:O	1:A:1148:ALA:CB	2.64	0.45
1:A:1250:HIS:C	1:A:1256:LEU:HD21	2.40	0.45
1:B:214:ILE:HG12	1:B:331:PHE:CZ	2.50	0.45
1:B:255:ALA:O	1:B:256:ALA:C	2.59	0.45
1:B:692:SER:CB	1:B:695:ARG:HD3	2.47	0.45
1:B:770:GLY:HA2	1:B:773:PHE:CE2	2.52	0.45
1:B:943:ALA:O	1:B:944:MET:C	2.56	0.45
1:B:1020:GLN:CG	1:B:1021:GLY:N	2.66	0.45
1:B:1090:VAL:CG1	1:B:1097:ILE:HB	2.35	0.45
1:B:1155:ASP:O	1:B:1160:LYS:HE3	2.16	0.45
1:B:1246:LYS:HD2	1:B:1246:LYS:H	1.81	0.45
1:A:312:TYR:O	1:A:313:GLY:C	2.59	0.45
1:A:463:ARG:HH11	1:A:463:ARG:HG3	1.82	0.45
1:A:568:ALA:O	1:A:569:LEU:C	2.57	0.45
1:A:942:GLN:O	1:A:943:ALA:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:993:ASP:C	1:A:995:ALA:N	2.74	0.45
1:A:1196:ASP:HA	1:A:1226:ILE:CD1	2.46	0.45
1:B:207:GLY:HA3	1:B:211:THR:CB	2.44	0.45
1:B:282:ARG:O	1:B:286:LYS:CB	2.63	0.45
1:B:286:LYS:HA	1:B:289:ILE:CB	2.29	0.45
1:B:399:SER:O	1:B:402:GLU:N	2.46	0.45
1:B:817:ASP:OD1	1:B:1000:SER:HB3	2.15	0.45
1:B:868:GLY:O	1:B:871:GLU:HB3	2.16	0.45
1:B:1036:VAL:O	1:B:1052:LEU:HB3	2.17	0.45
1:B:1121:CYS:O	1:B:1165:VAL:HG13	2.16	0.45
1:B:1218:ARG:O	1:B:1219:GLU:HB3	2.16	0.45
1:A:51:LEU:O	1:A:54:THR:HB	2.16	0.45
1:A:55:LEU:O	1:A:58:ILE:HB	2.16	0.45
1:A:255:ALA:O	1:A:257:ILE:N	2.49	0.45
1:A:282:ARG:O	1:A:286:LYS:CB	2.61	0.45
1:A:291:ALA:C	1:A:294:SER:HB2	2.41	0.45
1:A:396:SER:HB3	1:A:443:LEU:HD12	1.98	0.45
1:A:415:SER:HA	1:A:577:THR:CG2	2.46	0.45
1:A:765:THR:HG23	1:A:766:PHE:N	2.30	0.45
1:A:969:ASN:HD22	1:A:969:ASN:N	2.12	0.45
1:A:1037:VAL:O	1:A:1086:MET:N	2.50	0.45
1:A:1218:ARG:CZ	1:A:1235:ASN:HD22	2.29	0.45
1:B:142:LYS:O	1:B:143:ILE:C	2.60	0.45
1:B:157:GLY:HA2	1:B:160:ASP:CB	2.43	0.45
1:B:218:SER:CB	1:B:219:PRO:CD	2.94	0.45
1:B:570:ASP:O	1:B:573:ARG:N	2.48	0.45
1:B:900:PHE:C	1:B:902:THR:N	2.73	0.45
1:A:454:ILE:HG23	1:A:455:ARG:N	2.32	0.45
1:A:727:ILE:O	1:A:731:VAL:HG23	2.17	0.45
1:A:927:ALA:HA	1:A:930:LYS:CE	2.37	0.45
1:A:1039:ASN:HD22	1:A:1048:VAL:N	2.14	0.45
1:B:134:LEU:O	1:B:138:ARG:HG3	2.16	0.45
1:B:788:VAL:CG2	1:B:1004:ILE:HG13	2.46	0.45
1:B:809:ALA:O	1:B:813:ARG:HG2	2.16	0.45
1:B:1261:GLY:H	1:B:1264:PHE:CB	2.30	0.45
1:A:68:MET:HG3	1:A:336:ILE:CD1	2.46	0.45
1:A:151:ILE:HD12	1:A:167:LEU:HD11	1.99	0.45
1:A:183:GLY:O	1:A:184:ASP:C	2.60	0.45
1:A:779:ILE:CG1	1:A:780:LEU:N	2.79	0.45
1:A:981:ALA:CB	2:A:6001:OJZ:H33	2.46	0.45
1:A:1039:ASN:O	1:A:1040:TYR:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:MET:HB3	1:B:960:VAL:O	2.16	0.45
1:B:311:TRP:HZ2	1:B:728:PHE:HE2	1.62	0.45
1:B:528:SER:O	1:B:532:LYS:HG3	2.17	0.45
1:B:697:LEU:CA	1:B:700:ASN:HB2	2.45	0.45
1:B:748:SER:HA	1:B:751:PHE:CD1	2.51	0.45
1:A:154:GLN:O	1:A:154:GLN:HG2	2.17	0.45
1:A:238:LYS:HZ3	1:A:242:ALA:HB2	1.82	0.45
1:A:316:LEU:C	1:A:318:ILE:H	2.24	0.45
1:A:942:GLN:O	1:A:945:MET:N	2.49	0.45
1:A:1208:LYS:HD3	1:A:1208:LYS:C	2.41	0.45
1:B:60:HIS:O	1:B:63:ALA:N	2.50	0.45
1:B:500:VAL:HG23	1:B:501:LYS:H	1.82	0.45
1:B:801:ASP:HB3	1:B:1083:TYR:CE2	2.51	0.45
1:B:860:ILE:HG21	1:B:948:SER:HB3	1.97	0.45
1:B:901:ARG:O	1:B:904:VAL:HG12	2.16	0.45
1:B:1048:VAL:HG23	1:B:1049:LEU:HD22	1.97	0.45
1:B:1132:ASN:C	1:B:1134:ARG:H	2.25	0.45
1:B:1202:LEU:CD2	1:B:1206:SER:HB3	2.44	0.45
1:B:1218:ARG:CZ	1:B:1235:ASN:HD22	2.29	0.45
2:B:6002:OJZ:H29B	2:B:6002:OJZ:O25	2.16	0.45
1:A:218:SER:CB	1:A:219:PRO:CD	2.95	0.45
1:A:271:GLU:O	1:A:274:ASN:HB2	2.16	0.45
1:A:369:PRO:O	1:A:370:SER:C	2.60	0.45
1:A:740:PRO:N	1:A:741:PRO:HD2	2.32	0.45
1:A:860:ILE:HG21	1:A:948:SER:HB3	1.97	0.45
1:A:1150:ILE:O	1:A:1150:ILE:HG13	2.16	0.45
1:B:140:ILE:O	1:B:141:HIS:C	2.60	0.45
1:B:249:VAL:O	1:B:249:VAL:HG12	2.17	0.45
1:B:302:ILE:O	1:B:303:TYR:C	2.59	0.45
1:B:386:GLY:CA	1:B:450:ASP:HA	2.45	0.45
1:B:470:SER:HB2	1:B:471:GLN:OE1	2.16	0.45
1:B:792:MET:CA	1:B:795:GLN:HB2	2.46	0.45
1:B:1048:VAL:HG23	1:B:1049:LEU:HD23	1.97	0.45
1:B:1092:LEU:CB	1:B:1097:ILE:HD11	2.38	0.45
1:A:60:HIS:O	1:A:63:ALA:N	2.50	0.45
1:A:62:VAL:O	1:A:65:PRO:HG2	2.17	0.45
1:A:302:ILE:O	1:A:303:TYR:C	2.57	0.45
1:A:345:SER:O	1:A:346:PRO:C	2.56	0.45
1:A:614:GLU:O	1:A:615:LYS:C	2.60	0.45
1:A:714:ALA:HB1	1:A:833:PHE:HB2	1.98	0.45
1:A:835:ASN:O	1:A:836:ILE:C	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:971:LEU:O	1:A:972:LEU:C	2.60	0.45
1:A:1013:GLU:C	1:A:1014:ILE:HG12	2.42	0.45
1:A:1159:ASP:O	1:A:1160:LYS:C	2.60	0.45
1:B:151:ILE:C	1:B:153:ASN:N	2.73	0.45
1:B:359:TYR:HA	1:B:362:PHE:CB	2.45	0.45
1:B:696:ILE:O	1:B:700:ASN:CB	2.60	0.45
1:B:883:LYS:HA	1:B:886:LEU:HG	1.99	0.45
1:B:902:THR:C	1:B:904:VAL:N	2.75	0.45
1:B:1114:GLN:O	1:B:1116:PRO:HD3	2.17	0.45
1:A:796:ASP:CG	1:A:797:VAL:H	2.24	0.45
1:A:848:ILE:O	1:A:848:ILE:HG13	2.17	0.45
1:A:853:LEU:HG	1:A:973:VAL:CG2	2.33	0.45
1:A:960:VAL:HG12	1:A:966:THR:HG1	1.81	0.45
1:A:993:ASP:O	1:A:995:ALA:N	2.47	0.45
1:A:1157:LEU:HD22	1:A:1157:LEU:N	2.32	0.45
1:A:1193:LEU:HD21	1:A:1221:ARG:NH1	2.32	0.45
1:A:1195:LEU:HB2	1:A:1225:VAL:HA	1.98	0.45
1:B:207:GLY:CA	1:B:211:THR:H	2.28	0.45
1:B:257:ILE:C	1:B:257:ILE:CD1	2.86	0.45
1:B:443:LEU:HD23	1:B:443:LEU:C	2.42	0.45
1:B:463:ARG:HH11	1:B:463:ARG:HG3	1.81	0.45
1:B:689:PRO:HG2	1:B:690:PRO:CD	2.46	0.45
1:B:885:GLU:HB3	1:B:923:PRO:HG3	1.97	0.45
1:B:996:LYS:HD3	1:B:996:LYS:N	2.19	0.45
1:A:59:ILE:HD11	1:A:124:VAL:CG2	2.45	0.45
1:A:69:LEU:O	1:A:72:GLY:N	2.49	0.45
1:A:150:ALA:O	1:A:151:ILE:C	2.58	0.45
1:A:304:ALA:O	1:A:307:ALA:HB3	2.17	0.45
1:A:908:ARG:O	1:A:911:LYS:HB3	2.17	0.45
1:A:1020:GLN:OE1	1:A:1020:GLN:C	2.59	0.45
1:A:1178:GLN:OE1	1:A:1178:GLN:HA	2.17	0.45
1:B:36:LEU:HD12	1:B:36:LEU:C	2.42	0.45
1:B:441:ASP:CG	1:B:442:PRO:HD2	2.42	0.45
1:B:527:LEU:HB2	1:B:531:GLN:OE1	2.17	0.45
1:B:732:VAL:O	1:B:736:THR:HG23	2.16	0.45
1:B:792:MET:O	1:B:795:GLN:N	2.50	0.45
1:B:830:ALA:O	1:B:833:PHE:HB3	2.17	0.45
1:B:1037:VAL:HG23	1:B:1086:MET:HB2	1.98	0.45
1:B:1150:ILE:O	1:B:1150:ILE:HG13	2.16	0.45
1:A:132:TRP:C	1:A:132:TRP:CD1	2.95	0.44
1:A:717:ASN:HD21	1:A:766:PHE:HE1	1.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1072:LYS:HB3	1:A:1226:ILE:HD12	1.98	0.44
1:A:1168:LYS:N	1:A:1168:LYS:HD2	2.31	0.44
1:A:1205:GLU:HA	1:A:1208:LYS:HB3	1.97	0.44
1:B:35:VAL:HG21	1:B:355:ARG:NH2	2.32	0.44
1:B:121:VAL:HG23	1:B:122:LEU:H	1.80	0.44
1:B:215:LEU:CA	1:B:219:PRO:HD2	2.47	0.44
1:B:268:LYS:O	1:B:269:GLU:C	2.60	0.44
1:B:304:ALA:O	1:B:307:ALA:HB3	2.17	0.44
1:B:388:LEU:N	1:B:388:LEU:CD1	2.81	0.44
1:B:454:ILE:HG23	1:B:455:ARG:N	2.32	0.44
1:B:480:ILE:C	1:B:482:GLU:N	2.75	0.44
1:B:612:MET:HA	1:B:619:PHE:HB2	1.99	0.44
1:B:945:MET:O	1:B:949:TYR:CD1	2.69	0.44
1:B:1056:VAL:HG21	1:B:1062:LEU:HB2	1.99	0.44
1:B:1189:GLN:N	1:B:1190:PRO:CD	2.78	0.44
1:B:1218:ARG:NH1	1:B:1235:ASN:HD22	2.14	0.44
1:A:71:PHE:HA	1:A:74:MET:HG2	1.99	0.44
1:A:270:LEU:HB3	1:A:789:PHE:CE1	2.53	0.44
1:A:382:ASP:O	1:A:384:ILE:HG13	2.18	0.44
1:A:478:THR:O	1:A:520:VAL:HG23	2.17	0.44
1:A:821:VAL:O	1:A:824:ALA:HB3	2.16	0.44
1:A:821:VAL:HG23	1:A:822:LYS:N	2.32	0.44
1:A:911:LYS:O	1:A:914:THR:HB	2.17	0.44
1:A:1246:LYS:HD2	1:A:1246:LYS:H	1.82	0.44
1:B:131:PHE:C	1:B:131:PHE:HD2	2.25	0.44
1:B:486:TYR:O	1:B:908:ARG:NH1	2.50	0.44
1:B:690:PRO:HG2	1:B:1006:ARG:CZ	2.47	0.44
1:B:693:PHE:N	1:B:693:PHE:HD2	2.13	0.44
1:B:740:PRO:N	1:B:741:PRO:HD2	2.32	0.44
1:B:833:PHE:CG	1:B:834:GLN:N	2.83	0.44
1:B:945:MET:O	1:B:946:TYR:C	2.59	0.44
1:B:957:ALA:O	1:B:960:VAL:HG13	2.17	0.44
1:B:1037:VAL:O	1:B:1086:MET:N	2.50	0.44
1:B:1097:ILE:HG23	1:B:1105:LEU:HD22	1.98	0.44
1:B:1167:ASP:O	1:B:1168:LYS:HB2	2.16	0.44
1:A:393:ILE:HG13	1:A:393:ILE:O	2.17	0.44
1:A:467:GLY:H	1:A:545:PRO:CB	2.31	0.44
1:A:732:VAL:O	1:A:736:THR:HG23	2.18	0.44
1:A:1032:GLN:NE2	1:A:1055:GLU:HB2	2.32	0.44
1:A:1037:VAL:HG23	1:A:1086:MET:HB2	1.98	0.44
1:A:1145:ALA:HA	1:A:1150:ILE:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ILE:O	1:B:128:GLN:C	2.60	0.44
1:B:318:ILE:CG1	1:B:325:GLY:N	2.80	0.44
1:B:433:VAL:HG13	1:B:549:LEU:HD23	1.99	0.44
1:B:541:LEU:C	1:B:543:ARG:N	2.73	0.44
1:B:1168:LYS:N	1:B:1168:LYS:HD2	2.33	0.44
1:B:1249:GLU:O	1:B:1250:HIS:HB3	2.16	0.44
1:A:88:SER:OG	1:A:89:THR:N	2.51	0.44
1:A:217:ILE:HG13	1:A:218:SER:H	1.82	0.44
1:A:257:ILE:C	1:A:257:ILE:CD1	2.83	0.44
1:A:306:TYR:CG	1:A:307:ALA:N	2.85	0.44
1:A:407:LYS:O	1:A:407:LYS:HG3	2.18	0.44
1:A:716:ILE:HD12	1:A:717:ASN:N	2.32	0.44
1:A:740:PRO:HG2	1:A:741:PRO:CD	2.44	0.44
1:A:757:ILE:HA	1:A:761:ILE:HD13	1.98	0.44
1:A:940:PHE:O	1:A:944:MET:HG2	2.16	0.44
1:A:1027:LEU:H	1:A:1027:LEU:CD1	2.29	0.44
1:A:1038:PHE:CZ	1:A:1040:TYR:N	2.85	0.44
1:A:1092:LEU:CB	1:A:1097:ILE:HD11	2.40	0.44
1:A:1192:ILE:HD13	1:A:1193:LEU:N	2.32	0.44
1:A:1267:VAL:HG13	1:A:1270:GLN:OE1	2.17	0.44
1:B:255:ALA:C	1:B:257:ILE:H	2.22	0.44
1:B:265:GLY:C	1:B:267:LYS:HG3	2.41	0.44
1:B:306:TYR:CG	1:B:307:ALA:N	2.84	0.44
1:B:723:ALA:O	1:B:724:PHE:C	2.59	0.44
1:B:914:THR:O	1:B:917:ALA:HB3	2.17	0.44
1:B:1072:LYS:HB3	1:B:1226:ILE:HD12	1.98	0.44
1:A:35:VAL:HG21	1:A:355:ARG:NH2	2.33	0.44
1:A:342:GLY:O	1:A:346:PRO:HD3	2.17	0.44
1:A:508:PHE:CE1	1:A:509:ILE:HG23	2.53	0.44
1:A:533:GLN:O	1:A:534:ARG:C	2.59	0.44
1:A:547:ILE:HG22	1:A:549:LEU:HD11	1.99	0.44
1:A:730:LYS:O	1:A:731:VAL:C	2.61	0.44
1:A:928:MET:O	1:A:929:LYS:C	2.59	0.44
1:A:943:ALA:O	1:A:945:MET:N	2.51	0.44
1:A:1266:MET:HE2	1:A:1266:MET:HA	1.99	0.44
1:B:58:ILE:C	1:B:60:HIS:N	2.72	0.44
1:B:151:ILE:HD12	1:B:167:LEU:HD11	2.00	0.44
1:B:278:GLU:HB3	1:B:782:LYS:CG	2.44	0.44
1:B:303:TYR:O	1:B:306:TYR:HB3	2.17	0.44
1:B:356:GLY:HA2	1:B:359:TYR:HE1	1.80	0.44
1:B:727:ILE:O	1:B:731:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:849:TYR:HD1	1:B:854:THR:HA	1.83	0.44
1:B:1101:ASN:O	1:B:1102:VAL:C	2.57	0.44
1:B:1149:ASN:C	1:B:1179:ARG:HD3	2.43	0.44
1:A:110:TYR:O	1:A:111:ALA:C	2.60	0.44
1:A:199:GLY:O	1:A:203:GLY:HA3	2.17	0.44
1:A:384:ILE:HG23	1:A:546:LYS:HE2	2.00	0.44
1:A:441:ASP:CG	1:A:442:PRO:HD2	2.43	0.44
1:A:690:PRO:O	1:A:1006:ARG:NH2	2.50	0.44
1:A:723:ALA:O	1:A:727:ILE:HG22	2.18	0.44
1:A:739:GLY:C	1:A:741:PRO:HD2	2.43	0.44
1:A:788:VAL:CG2	1:A:1004:ILE:HG13	2.47	0.44
1:A:932:HIS:C	1:A:932:HIS:ND1	2.75	0.44
1:A:937:THR:O	1:A:938:PHE:C	2.59	0.44
1:A:1261:GLY:H	1:A:1264:PHE:CB	2.30	0.44
1:B:88:SER:OG	1:B:89:THR:N	2.51	0.44
1:B:393:ILE:O	1:B:393:ILE:HG13	2.17	0.44
1:B:438:ARG:O	1:B:439:LEU:O	2.34	0.44
1:B:723:ALA:O	1:B:727:ILE:HG22	2.17	0.44
1:B:916:TYR:O	1:B:920:LEU:HB2	2.17	0.44
1:B:1090:VAL:CG2	1:B:1091:PHE:N	2.80	0.44
1:B:1178:GLN:OE1	1:B:1178:GLN:HA	2.18	0.44
1:B:1196:ASP:HA	1:B:1226:ILE:CD1	2.48	0.44
1:A:58:ILE:HG22	1:A:59:ILE:N	2.33	0.44
1:A:364:ILE:HG22	1:A:364:ILE:O	2.17	0.44
1:A:382:ASP:C	1:A:384:ILE:N	2.75	0.44
1:A:527:LEU:HB2	1:A:531:GLN:OE1	2.18	0.44
1:A:539:ARG:C	1:A:541:LEU:N	2.75	0.44
1:A:769:GLN:O	1:A:770:GLY:C	2.60	0.44
1:A:1041:PRO:O	1:A:1042:THR:HB	2.18	0.44
1:B:274:ASN:O	1:B:275:ASN:C	2.59	0.44
1:B:306:TYR:HE1	1:B:310:PHE:CE1	2.36	0.44
1:B:307:ALA:O	1:B:308:LEU:O	2.35	0.44
1:B:363:LYS:O	1:B:367:ASN:CB	2.66	0.44
1:B:508:PHE:CE1	1:B:509:ILE:HG23	2.53	0.44
1:B:615:LYS:HA	1:B:619:PHE:CD2	2.53	0.44
1:B:710:GLY:O	1:B:711:ILE:C	2.57	0.44
1:B:730:LYS:O	1:B:731:VAL:C	2.61	0.44
1:A:121:VAL:CG2	1:A:122:LEU:H	2.31	0.44
1:A:138:ARG:O	1:A:139:GLN:C	2.61	0.44
1:A:313:GLY:O	1:A:317:VAL:HG23	2.18	0.44
1:A:466:ILE:HG22	1:A:466:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:ILE:HG12	1:A:603:VAL:N	2.32	0.44
1:A:706:TYR:CD1	1:A:706:TYR:C	2.96	0.44
1:A:708:VAL:HA	1:A:711:ILE:HG22	2.00	0.44
1:A:821:VAL:O	1:A:822:LYS:C	2.61	0.44
1:A:993:ASP:O	1:A:994:TYR:HB3	2.18	0.44
1:A:1119:PHE:C	1:A:1121:CYS:H	2.26	0.44
1:A:1159:ASP:HB3	1:A:1162:ASN:HB2	2.00	0.44
2:A:6001:0JZ:H35B	2:A:6001:0JZ:SE3	2.68	0.44
1:B:129:VAL:HG11	1:B:935:GLY:CA	2.48	0.44
1:B:855:LEU:HA	1:B:858:LEU:HG	2.00	0.44
1:B:996:LYS:H	1:B:996:LYS:CD	2.16	0.44
1:B:1132:ASN:C	1:B:1134:ARG:N	2.74	0.44
1:A:306:TYR:HE1	1:A:310:PHE:CE1	2.36	0.44
1:A:573:ARG:O	1:A:575:GLY:N	2.46	0.44
1:A:704:TRP:CZ2	1:A:707:PHE:HB2	2.53	0.44
1:A:798:SER:CB	1:A:1041:PRO:HG2	2.47	0.44
1:B:478:THR:O	1:B:520:VAL:HG23	2.17	0.44
1:B:479:THR:HA	1:B:518:THR:O	2.18	0.44
1:B:810:LEU:O	1:B:813:ARG:N	2.51	0.44
1:B:1037:VAL:HG22	1:B:1087:ALA:HB3	2.00	0.44
1:B:1193:LEU:HD21	1:B:1221:ARG:NH1	2.33	0.44
1:A:44:TRP:C	1:A:46:ASP:H	2.26	0.43
1:A:144:ARG:CZ	1:A:175:VAL:HG21	2.48	0.43
1:A:195:THR:HA	1:A:337:GLY:HA2	2.00	0.43
1:A:272:ARG:O	1:A:276:ASN:HB2	2.18	0.43
1:A:278:GLU:HA	1:A:282:ARG:CZ	2.48	0.43
1:A:297:ALA:HB1	1:A:763:PHE:HA	2.00	0.43
1:A:470:SER:HA	1:A:551:ASP:HB3	1.98	0.43
1:A:689:PRO:HB2	1:A:690:PRO:CD	2.43	0.43
1:A:748:SER:HA	1:A:751:PHE:CD1	2.53	0.43
1:A:945:MET:O	1:A:949:TYR:CD1	2.68	0.43
1:A:1131:ASP:OD2	1:A:1188:ARG:NE	2.51	0.43
1:B:55:LEU:O	1:B:58:ILE:HB	2.17	0.43
1:B:60:HIS:O	1:B:61:GLY:C	2.60	0.43
1:B:68:MET:HG3	1:B:336:ILE:CD1	2.48	0.43
1:B:69:LEU:O	1:B:72:GLY:N	2.50	0.43
1:B:75:THR:HB	1:B:326:GLN:OE1	2.17	0.43
1:B:129:VAL:CG1	1:B:935:GLY:HA2	2.48	0.43
1:B:267:LYS:HA	1:B:790:LYS:HE2	2.00	0.43
1:B:370:SER:C	1:B:372:ASP:N	2.76	0.43
1:B:547:ILE:HG22	1:B:549:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:LYS:HD3	1:B:620:LYS:C	2.43	0.43
1:B:756:LEU:HD12	1:B:757:ILE:H	1.78	0.43
1:B:756:LEU:O	1:B:760:ILE:HB	2.18	0.43
1:B:841:THR:O	1:B:845:ILE:HG13	2.17	0.43
1:A:88:SER:C	1:A:90:ASN:N	2.75	0.43
1:A:96:LYS:O	1:A:100:PHE:HB2	2.18	0.43
1:A:363:LYS:O	1:A:367:ASN:CB	2.66	0.43
1:A:612:MET:HA	1:A:619:PHE:HB2	2.00	0.43
1:A:731:VAL:HA	1:A:750:LEU:HD12	2.00	0.43
1:A:797:VAL:O	1:A:801:ASP:OD1	2.36	0.43
1:A:846:SER:O	1:A:849:TYR:HB2	2.17	0.43
1:A:1036:VAL:O	1:A:1052:LEU:HB3	2.17	0.43
1:A:1097:ILE:HG23	1:A:1105:LEU:HD22	2.00	0.43
1:A:1149:ASN:C	1:A:1179:ARG:HD3	2.42	0.43
1:B:51:LEU:O	1:B:54:THR:HB	2.18	0.43
1:B:195:THR:HA	1:B:337:GLY:HA2	1.99	0.43
1:B:207:GLY:CA	1:B:211:THR:HB	2.45	0.43
1:B:716:ILE:HD12	1:B:717:ASN:N	2.32	0.43
1:B:791:SER:O	1:B:795:GLN:HB2	2.18	0.43
1:A:60:HIS:O	1:A:61:GLY:C	2.61	0.43
1:A:266:GLN:HB2	1:A:270:LEU:CD2	2.49	0.43
1:A:308:LEU:HD13	1:A:755:PHE:CD1	2.53	0.43
1:A:727:ILE:HD12	1:A:753:LEU:HD23	2.00	0.43
1:A:912:PHE:O	1:A:915:MET:N	2.51	0.43
1:A:960:VAL:CG1	1:A:966:THR:OG1	2.67	0.43
1:A:1090:VAL:CG2	1:A:1091:PHE:N	2.80	0.43
1:B:44:TRP:CD1	1:B:45:LEU:N	2.86	0.43
1:B:62:VAL:O	1:B:65:PRO:HG2	2.18	0.43
1:B:65:PRO:HG3	1:B:198:GLY:CA	2.48	0.43
1:B:217:ILE:HG13	1:B:218:SER:H	1.83	0.43
1:B:266:GLN:HB2	1:B:270:LEU:CD2	2.48	0.43
1:B:384:ILE:HG23	1:B:546:LYS:HE2	1.98	0.43
1:B:419:VAL:CG2	1:B:593:VAL:HG13	2.48	0.43
1:A:46:ASP:O	1:A:47:ARG:C	2.61	0.43
1:A:65:PRO:HG3	1:A:198:GLY:CA	2.48	0.43
1:A:142:LYS:O	1:A:143:ILE:C	2.62	0.43
1:A:249:VAL:O	1:A:249:VAL:HG12	2.17	0.43
1:A:265:GLY:CA	1:A:793:LEU:HD21	2.45	0.43
1:A:359:TYR:HA	1:A:362:PHE:CB	2.46	0.43
1:A:796:ASP:HA	1:A:800:PHE:CD2	2.54	0.43
1:A:957:ALA:O	1:A:960:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:GLU:O	1:A:1010:LYS:CG	2.65	0.43
1:B:43:GLY:HA3	1:B:46:ASP:HB2	2.01	0.43
1:B:175:VAL:CG1	1:B:176:SER:H	2.30	0.43
1:B:218:SER:O	1:B:219:PRO:C	2.61	0.43
1:B:270:LEU:O	1:B:274:ASN:CG	2.62	0.43
1:B:1106:ARG:O	1:B:1109:LEU:CD2	2.66	0.43
1:A:59:ILE:O	1:A:63:ALA:HB2	2.19	0.43
1:A:91:MET:H	1:A:91:MET:HG3	1.61	0.43
1:A:273:TYR:O	1:A:274:ASN:O	2.36	0.43
1:A:478:THR:HG22	1:A:479:THR:N	2.20	0.43
1:A:615:LYS:HA	1:A:619:PHE:CD2	2.53	0.43
1:A:773:PHE:CD1	1:A:774:GLY:N	2.87	0.43
1:A:796:ASP:O	1:A:797:VAL:O	2.35	0.43
1:B:83:ASN:O	1:B:86:LYS:HB3	2.19	0.43
1:B:213:VAL:O	1:B:216:ALA:HB3	2.19	0.43
1:B:312:TYR:O	1:B:313:GLY:C	2.61	0.43
1:B:315:SER:CA	1:B:318:ILE:HG22	2.49	0.43
1:B:379:HIS:HB2	1:B:457:ILE:HA	1.95	0.43
1:B:532:LYS:O	1:B:535:ILE:N	2.52	0.43
1:B:706:TYR:CD1	1:B:706:TYR:C	2.96	0.43
1:B:1039:ASN:HB2	1:B:1047:PRO:CA	2.37	0.43
1:B:1144:ALA:O	1:B:1148:ALA:CB	2.65	0.43
1:B:1147:GLU:HB3	1:B:1186:LEU:HD22	2.00	0.43
1:A:1252:THR:CG2	1:A:1255:GLN:HB2	2.49	0.43
1:B:58:ILE:HG22	1:B:59:ILE:N	2.33	0.43
1:B:70:ILE:C	1:B:72:GLY:H	2.25	0.43
1:B:163:ASP:C	1:B:164:VAL:HG22	2.43	0.43
1:B:207:GLY:O	1:B:209:LYS:N	2.51	0.43
1:B:248:ALA:C	1:B:250:ALA:H	2.25	0.43
1:B:308:LEU:HD12	1:B:751:PHE:CE2	2.54	0.43
1:B:321:GLU:O	1:B:323:SER:N	2.51	0.43
1:B:346:PRO:O	1:B:349:GLU:HB3	2.18	0.43
1:B:1116:PRO:O	1:B:1117:ILE:HB	2.19	0.43
1:B:1195:LEU:HB2	1:B:1225:VAL:HG23	2.01	0.43
1:A:36:LEU:HD12	1:A:36:LEU:C	2.43	0.43
1:A:127:ILE:O	1:A:128:GLN:C	2.61	0.43
1:A:282:ARG:O	1:A:286:LYS:N	2.50	0.43
1:A:322:TYR:CZ	1:A:324:ILE:HG12	2.54	0.43
1:A:388:LEU:N	1:A:388:LEU:CD1	2.81	0.43
1:A:415:SER:C	1:A:417:GLN:H	2.27	0.43
1:A:618:TYR:CE2	1:A:622:VAL:HG21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:GLY:CA	1:A:968:GLU:HG3	2.49	0.43
1:A:765:THR:HG23	1:A:766:PHE:HD1	1.84	0.43
1:A:808:GLY:O	1:A:810:LEU:N	2.52	0.43
1:A:949:TYR:HD1	1:A:949:TYR:H	1.67	0.43
1:A:1031:VAL:H	1:A:1056:VAL:HG13	1.83	0.43
1:B:68:MET:O	1:B:69:LEU:C	2.61	0.43
1:B:110:TYR:O	1:B:111:ALA:C	2.61	0.43
1:B:279:GLU:O	1:B:282:ARG:HB2	2.18	0.43
1:B:463:ARG:NH1	1:B:903:VAL:HG22	2.33	0.43
1:B:684:LEU:C	1:B:684:LEU:HD12	2.43	0.43
1:A:257:ILE:HG13	1:A:800:PHE:CD2	2.54	0.43
1:A:389:GLU:OE1	1:A:412:LYS:HB2	2.17	0.43
1:A:796:ASP:OD2	1:A:1014:ILE:HD11	2.19	0.43
1:A:1195:LEU:HB2	1:A:1225:VAL:HG23	2.01	0.43
1:A:1213:ALA:O	1:A:1217:ALA:HB2	2.19	0.43
2:A:6001:OJZ:H29B	2:A:6001:OJZ:O25	2.19	0.43
1:B:58:ILE:O	1:B:60:HIS:N	2.51	0.43
1:B:156:ILE:HG12	1:B:439:LEU:O	2.18	0.43
1:B:171:LEU:HD13	1:B:172:THR:N	2.34	0.43
1:B:272:ARG:O	1:B:276:ASN:HB2	2.19	0.43
1:B:291:ALA:C	1:B:294:SER:HB2	2.42	0.43
1:B:312:TYR:O	1:B:314:THR:N	2.52	0.43
1:B:407:LYS:HG3	1:B:407:LYS:O	2.18	0.43
1:B:431:THR:HG22	1:B:435:LEU:HD23	2.00	0.43
1:B:433:VAL:O	1:B:436:MET:HB3	2.18	0.43
1:B:513:PRO:O	1:B:514:HIS:HB2	2.19	0.43
1:B:936:ILE:O	1:B:939:SER:OG	2.37	0.43
1:B:946:TYR:O	1:B:947:PHE:C	2.62	0.43
1:B:993:ASP:O	1:B:995:ALA:N	2.52	0.43
1:B:1039:ASN:O	1:B:1040:TYR:C	2.61	0.43
1:B:1040:TYR:O	1:B:1042:THR:HG22	2.19	0.43
1:B:1076:VAL:CG1	1:B:1194:LEU:HD13	2.49	0.43
1:B:1252:THR:CG2	1:B:1255:GLN:HB2	2.49	0.43
1:A:78:PHE:HZ	1:A:967:PHE:O	1.99	0.43
1:A:223:LEU:O	1:A:224:SER:C	2.62	0.43
1:A:258:ARG:C	1:A:260:VAL:N	2.75	0.43
1:A:362:PHE:HA	1:A:365:ILE:HD12	2.01	0.43
1:A:809:ALA:O	1:A:813:ARG:HG2	2.19	0.43
1:A:1014:ILE:CD1	1:A:1106:ARG:HH22	2.31	0.43
1:B:163:ASP:O	1:B:164:VAL:C	2.61	0.43
1:B:182:ILE:O	1:B:186:ILE:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:ILE:CD1	1:B:326:GLN:H	2.24	0.43
1:B:740:PRO:O	1:B:743:THR:HG23	2.19	0.43
1:B:908:ARG:O	1:B:911:LYS:HB3	2.19	0.43
1:B:1007:ILE:C	1:B:1009:GLU:N	2.75	0.43
1:B:1076:VAL:HG13	1:B:1194:LEU:HD13	2.01	0.43
1:B:1092:LEU:HD22	1:B:1100:LEU:HD22	2.01	0.43
1:B:1218:ARG:NH1	1:B:1235:ASN:ND2	2.65	0.43
1:A:34:SER:O	1:A:35:VAL:C	2.62	0.43
1:A:67:MET:HE2	1:A:117:ILE:HG21	2.01	0.43
1:A:103:LEU:HD22	1:A:960:VAL:HG22	2.01	0.43
1:A:155:GLU:HB3	1:A:156:ILE:CD1	2.34	0.43
1:A:203:GLY:HA2	1:A:211:THR:OG1	2.17	0.43
1:A:252:GLU:OE1	1:A:252:GLU:N	2.52	0.43
1:A:861:VAL:CB	1:A:862:PRO:HD3	2.48	0.43
1:A:1028:GLU:HB2	1:A:1093:ASP:OD1	2.19	0.43
1:A:1116:PRO:O	1:A:1117:ILE:HB	2.19	0.43
1:A:1176:GLN:O	1:A:1179:ARG:N	2.52	0.43
1:B:498:LYS:O	1:B:499:ALA:C	2.62	0.43
1:B:519:LEU:HD22	1:B:526:GLN:HE22	1.84	0.43
1:B:773:PHE:CB	1:B:829:LEU:HD13	2.49	0.43
1:B:852:GLN:HE22	1:B:966:THR:CG2	2.31	0.43
1:B:875:LEU:HD23	1:B:875:LEU:O	2.19	0.43
1:B:943:ALA:O	1:B:945:MET:N	2.52	0.43
1:A:59:ILE:HD12	1:A:59:ILE:O	2.19	0.42
1:A:74:MET:HG3	1:A:75:THR:N	2.34	0.42
1:A:151:ILE:O	1:A:153:ASN:N	2.51	0.42
1:A:171:LEU:HD13	1:A:172:THR:N	2.34	0.42
1:A:215:LEU:CA	1:A:219:PRO:HD2	2.49	0.42
1:A:288:ALA:O	1:A:292:ASN:N	2.52	0.42
1:A:401:LYS:O	1:A:402:GLU:C	2.63	0.42
1:A:697:LEU:HD12	1:A:698:LYS:N	2.34	0.42
1:A:909:GLU:OE2	1:A:909:GLU:N	2.45	0.42
1:B:53:GLY:O	1:B:56:ALA:N	2.52	0.42
1:B:55:LEU:O	1:B:56:ALA:C	2.60	0.42
1:B:121:VAL:O	1:B:122:LEU:C	2.62	0.42
1:B:151:ILE:O	1:B:153:ASN:N	2.52	0.42
1:B:158:TRP:HA	1:B:162:HIS:CD2	2.45	0.42
1:B:252:GLU:N	1:B:252:GLU:OE1	2.52	0.42
1:B:348:ILE:O	1:B:351:PHE:HB3	2.19	0.42
1:B:362:PHE:HA	1:B:365:ILE:HD12	2.01	0.42
1:B:540:ALA:O	1:B:543:ARG:CB	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:ILE:O	1:B:700:ASN:N	2.52	0.42
1:B:705:PRO:CG	1:B:706:TYR:H	2.30	0.42
1:B:820:GLN:CB	1:B:1000:SER:HB2	2.49	0.42
1:B:821:VAL:HG23	1:B:822:LYS:N	2.34	0.42
1:B:857:LEU:C	1:B:857:LEU:CD2	2.91	0.42
1:B:1041:PRO:O	1:B:1042:THR:HB	2.19	0.42
1:B:1131:ASP:OD2	1:B:1188:ARG:NE	2.52	0.42
1:B:1267:VAL:HG13	1:B:1270:GLN:OE1	2.18	0.42
1:A:327:VAL:O	1:A:328:LEU:C	2.62	0.42
1:A:342:GLY:O	1:A:343:GLN:C	2.60	0.42
1:A:401:LYS:H	1:A:401:LYS:CD	2.24	0.42
1:A:711:ILE:HD11	1:A:832:ILE:HG21	2.01	0.42
1:A:779:ILE:HA	1:A:782:LYS:HE3	2.01	0.42
1:A:942:GLN:O	1:A:945:MET:CB	2.64	0.42
1:A:1018:SER:C	1:A:1019:THR:HG1	2.26	0.42
1:A:1035:GLY:O	1:A:1036:VAL:C	2.62	0.42
1:A:1084:ASP:HA	1:A:1085:PRO:HD2	1.89	0.42
1:A:1121:CYS:O	1:A:1165:VAL:HG13	2.19	0.42
1:A:1144:ALA:O	1:A:1148:ALA:HB3	2.19	0.42
1:B:132:TRP:C	1:B:132:TRP:CD1	2.96	0.42
1:B:283:LEU:HD12	1:B:283:LEU:C	2.44	0.42
1:B:299:PHE:O	1:B:303:TYR:N	2.51	0.42
1:B:331:PHE:O	1:B:332:PHE:C	2.61	0.42
1:B:381:PRO:HG3	1:B:457:ILE:HB	2.00	0.42
1:B:506:TYR:CD1	1:B:509:ILE:HD11	2.54	0.42
1:B:1026:MET:O	1:B:1026:MET:HG3	2.18	0.42
1:B:1159:ASP:HB3	1:B:1162:ASN:HB2	2.00	0.42
1:B:1176:GLN:OE1	1:B:1176:GLN:N	2.52	0.42
1:B:1266:MET:HE2	1:B:1266:MET:HA	2.00	0.42
1:A:157:GLY:HA2	1:A:160:ASP:CG	2.45	0.42
1:A:182:ILE:O	1:A:186:ILE:HG23	2.20	0.42
1:A:460:ARG:O	1:A:462:LEU:N	2.52	0.42
1:A:513:PRO:O	1:A:514:HIS:HB2	2.18	0.42
1:A:519:LEU:HD22	1:A:526:GLN:HE22	1.84	0.42
1:A:726:VAL:O	1:A:727:ILE:C	2.62	0.42
1:A:883:LYS:HA	1:A:886:LEU:CG	2.49	0.42
1:A:990:PHE:O	1:A:991:ALA:C	2.63	0.42
1:A:1076:VAL:CG1	1:A:1194:LEU:HD13	2.50	0.42
1:A:1179:ARG:CZ	1:A:1209:VAL:HG11	2.49	0.42
1:A:1182:ILE:N	1:A:1182:ILE:HD12	2.34	0.42
1:B:74:MET:HG3	1:B:75:THR:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:VAL:CG2	1:B:122:LEU:H	2.32	0.42
1:B:195:THR:O	1:B:196:PHE:C	2.63	0.42
1:B:324:ILE:O	1:B:326:GLN:HB2	2.19	0.42
1:B:389:GLU:OE1	1:B:412:LYS:HB2	2.19	0.42
1:B:471:GLN:HG2	1:B:472:GLU:H	1.80	0.42
1:B:573:ARG:O	1:B:575:GLY:N	2.44	0.42
1:B:692:SER:HB2	1:B:695:ARG:HD3	2.01	0.42
1:B:827:SER:O	1:B:830:ALA:N	2.53	0.42
1:B:964:LEU:C	1:B:966:THR:H	2.27	0.42
1:B:1195:LEU:HB2	1:B:1225:VAL:HA	2.01	0.42
1:A:60:HIS:O	1:A:63:ALA:CB	2.65	0.42
1:A:144:ARG:HG2	1:A:920:LEU:CD1	2.49	0.42
1:A:447:VAL:HG13	1:A:454:ILE:HG22	2.01	0.42
1:A:490:ASP:O	1:A:491:VAL:HB	2.19	0.42
1:A:792:MET:O	1:A:795:GLN:N	2.53	0.42
1:A:981:ALA:HB1	2:A:6001:OJZ:H32	2.02	0.42
1:A:1037:VAL:HG22	1:A:1087:ALA:HB3	2.00	0.42
1:A:1063:ALA:HB3	1:A:1239:ILE:HG12	2.01	0.42
1:B:90:ASN:O	1:B:91:MET:C	2.63	0.42
1:B:154:GLN:O	1:B:154:GLN:HG2	2.19	0.42
1:B:974:PHE:HB3	2:B:6002:OJZ:C30	2.49	0.42
1:B:1207:GLU:OE2	1:B:1229:ARG:NH2	2.52	0.42
1:A:206:ARG:C	1:A:211:THR:HB	2.44	0.42
1:A:209:LYS:CA	1:A:212:LEU:HB3	2.49	0.42
1:A:283:LEU:HD12	1:A:283:LEU:C	2.43	0.42
1:A:293:ILE:CG2	1:A:766:PHE:HB3	2.31	0.42
1:A:474:VAL:HG11	1:A:901:ARG:CB	2.48	0.42
1:A:900:PHE:O	1:A:903:VAL:N	2.51	0.42
1:A:962:GLN:O	1:A:963:GLN:HB2	2.19	0.42
1:B:54:THR:O	1:B:58:ILE:HD13	2.19	0.42
1:B:238:LYS:HZ3	1:B:242:ALA:HB2	1.83	0.42
1:B:286:LYS:O	1:B:290:THR:CG2	2.63	0.42
1:B:548:LEU:HD22	1:B:550:LEU:HD11	2.02	0.42
1:B:727:ILE:HD12	1:B:753:LEU:HD23	1.99	0.42
1:B:1031:VAL:O	1:B:1055:GLU:HA	2.19	0.42
1:B:1119:PHE:HD2	1:B:1121:CYS:SG	2.42	0.42
1:B:1129:TYR:CD2	1:B:1184:ARG:HG3	2.54	0.42
1:A:471:GLN:HG2	1:A:472:GLU:H	1.80	0.42
1:A:506:TYR:CD1	1:A:509:ILE:HD11	2.54	0.42
1:A:541:LEU:C	1:A:541:LEU:HD13	2.44	0.42
1:A:796:ASP:CG	1:A:797:VAL:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1207:GLU:OE2	1:A:1229:ARG:NH2	2.52	0.42
1:B:39:PHE:CD2	1:B:355:ARG:HA	2.55	0.42
1:B:72:GLY:O	1:B:73:ASP:C	2.63	0.42
1:B:178:ILE:HG12	1:B:358:ALA:HB1	2.00	0.42
1:B:278:GLU:HA	1:B:282:ARG:NH1	2.34	0.42
1:B:278:GLU:CB	1:B:782:LYS:HG2	2.43	0.42
1:B:415:SER:C	1:B:417:GLN:H	2.26	0.42
1:B:467:GLY:H	1:B:545:PRO:CB	2.33	0.42
1:B:703:GLU:HA	1:B:783:ARG:HH12	1.84	0.42
1:B:905:SER:HB3	1:B:907:THR:OG1	2.18	0.42
1:B:1090:VAL:HG22	1:B:1097:ILE:HG13	2.01	0.42
1:A:279:GLU:O	1:A:282:ARG:HB2	2.19	0.42
1:A:279:GLU:CG	1:A:782:LYS:HD2	2.49	0.42
1:A:303:TYR:O	1:A:306:TYR:HB3	2.19	0.42
1:A:406:LEU:O	1:A:408:GLY:N	2.47	0.42
1:A:437:GLN:C	1:A:439:LEU:H	2.27	0.42
1:A:532:LYS:O	1:A:535:ILE:N	2.53	0.42
1:A:696:ILE:O	1:A:700:ASN:N	2.53	0.42
1:A:1164:ARG:C	1:A:1166:GLY:H	2.28	0.42
1:B:150:ALA:O	1:B:151:ILE:C	2.62	0.42
1:B:261:ILE:C	1:B:263:PHE:H	2.26	0.42
1:B:539:ARG:C	1:B:541:LEU:N	2.76	0.42
1:B:618:TYR:CE2	1:B:622:VAL:HG21	2.54	0.42
1:B:1039:ASN:CG	1:B:1047:PRO:HA	2.44	0.42
1:A:107:MET:HE2	1:A:954:ARG:HD2	2.01	0.42
1:A:419:VAL:CG2	1:A:593:VAL:HG13	2.48	0.42
1:A:620:LYS:HD3	1:A:620:LYS:C	2.44	0.42
1:A:912:PHE:O	1:A:913:GLU:C	2.63	0.42
1:A:922:ILE:HB	1:A:923:PRO:CD	2.46	0.42
1:A:970:VAL:HG23	1:A:971:LEU:HD22	2.02	0.42
1:A:1020:GLN:CG	1:A:1101:ASN:CB	2.92	0.42
1:A:1249:GLU:O	1:A:1250:HIS:HB3	2.20	0.42
1:B:278:GLU:OE2	1:B:785:ARG:HD2	2.20	0.42
1:B:406:LEU:C	1:B:408:GLY:H	2.27	0.42
1:B:691:ALA:HA	1:B:1002:SER:HB3	2.01	0.42
1:B:708:VAL:HA	1:B:711:ILE:HG22	2.00	0.42
1:B:731:VAL:HA	1:B:750:LEU:HD12	2.02	0.42
1:B:942:GLN:O	1:B:945:MET:CB	2.64	0.42
1:B:1073:SER:O	1:B:1077:GLN:HG3	2.20	0.42
1:B:1178:GLN:O	1:B:1181:ALA:N	2.53	0.42
1:A:137:GLY:O	1:A:138:ARG:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:GLY:O	1:A:721:GLN:N	2.53	0.42
1:A:756:LEU:O	1:A:760:ILE:HB	2.19	0.42
1:A:945:MET:SD	1:A:946:TYR:N	2.93	0.42
1:B:130:SER:O	1:B:131:PHE:C	2.63	0.42
1:B:266:GLN:HB2	1:B:270:LEU:HD22	2.01	0.42
1:B:328:LEU:HD11	1:B:728:PHE:HZ	1.84	0.42
1:B:384:ILE:O	1:B:385:GLN:C	2.63	0.42
1:B:447:VAL:HG13	1:B:454:ILE:HG22	2.00	0.42
1:B:541:LEU:C	1:B:541:LEU:HD13	2.45	0.42
1:B:765:THR:HG23	1:B:766:PHE:HD1	1.84	0.42
1:B:1032:GLN:HB3	1:B:1091:PHE:HD2	1.85	0.42
1:B:1164:ARG:O	1:B:1165:VAL:C	2.61	0.42
1:B:1185:ALA:O	1:B:1190:PRO:CD	2.67	0.42
1:A:43:GLY:CA	1:A:46:ASP:HB2	2.49	0.42
1:A:44:TRP:CD1	1:A:45:LEU:N	2.88	0.42
1:A:54:THR:O	1:A:55:LEU:C	2.62	0.42
1:A:114:TYR:O	1:A:115:THR:C	2.63	0.42
1:A:406:LEU:C	1:A:408:GLY:H	2.27	0.42
1:A:625:GLN:O	1:A:626:THR:HB	2.20	0.42
1:A:692:SER:HB2	1:A:695:ARG:HB3	2.02	0.42
1:A:1076:VAL:O	1:A:1077:GLN:C	2.62	0.42
1:B:238:LYS:C	1:B:238:LYS:HD3	2.45	0.42
1:B:257:ILE:CG2	1:B:258:ARG:N	2.82	0.42
1:B:312:TYR:C	1:B:314:THR:N	2.78	0.42
1:B:533:GLN:O	1:B:534:ARG:C	2.63	0.42
1:B:585:LEU:HA	1:B:588:VAL:HB	2.02	0.42
1:B:1179:ARG:CZ	1:B:1209:VAL:HG11	2.50	0.42
1:A:54:THR:O	1:A:58:ILE:HD13	2.20	0.41
1:A:99:MET:N	1:A:99:MET:SD	2.93	0.41
1:A:121:VAL:O	1:A:122:LEU:C	2.60	0.41
1:A:281:LYS:O	1:A:285:ILE:HG22	2.21	0.41
1:A:773:PHE:CB	1:A:829:LEU:HD13	2.50	0.41
1:A:820:GLN:CB	1:A:1000:SER:HB2	2.50	0.41
1:A:948:SER:O	1:A:952:CYS:SG	2.75	0.41
1:A:1092:LEU:HD22	1:A:1100:LEU:HD22	2.01	0.41
1:A:1129:TYR:CD2	1:A:1184:ARG:HG3	2.54	0.41
1:A:1156:SER:OG	1:A:1157:LEU:HD22	2.20	0.41
1:B:59:ILE:HD12	1:B:59:ILE:O	2.20	0.41
1:B:132:TRP:CE2	1:B:183:GLY:HA3	2.55	0.41
1:B:144:ARG:CZ	1:B:175:VAL:HG21	2.49	0.41
1:B:212:LEU:CD1	1:B:215:LEU:HD12	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:GLN:C	1:B:439:LEU:H	2.27	0.41
1:B:498:LYS:HE2	1:B:498:LYS:C	2.45	0.41
1:B:529:GLY:HA2	1:B:532:LYS:HD3	2.01	0.41
1:B:932:HIS:C	1:B:932:HIS:ND1	2.77	0.41
1:A:81:VAL:HG13	1:A:99:MET:HE2	2.03	0.41
1:A:178:ILE:HG12	1:A:358:ALA:HB1	2.00	0.41
1:A:697:LEU:CA	1:A:700:ASN:HB2	2.47	0.41
1:A:718:GLY:CA	1:A:837:ALA:HB2	2.50	0.41
1:A:741:PRO:O	1:A:742:GLU:HB2	2.20	0.41
1:B:96:LYS:O	1:B:100:PHE:HB2	2.20	0.41
1:B:773:PHE:CD1	1:B:774:GLY:N	2.88	0.41
1:B:832:ILE:O	1:B:835:ASN:HB3	2.20	0.41
1:B:846:SER:O	1:B:849:TYR:HB2	2.20	0.41
1:A:130:SER:O	1:A:131:PHE:C	2.61	0.41
1:A:312:TYR:O	1:A:314:THR:N	2.53	0.41
1:A:702:THR:C	1:A:704:TRP:H	2.29	0.41
1:A:856:LEU:O	1:A:860:ILE:HG12	2.20	0.41
1:A:861:VAL:O	1:A:862:PRO:C	2.62	0.41
1:A:885:GLU:HB3	1:A:923:PRO:HG3	2.02	0.41
1:A:887:GLU:O	1:A:890:GLY:N	2.53	0.41
1:A:1076:VAL:O	1:A:1079:LEU:HB3	2.20	0.41
1:B:215:LEU:HA	1:B:219:PRO:HD2	2.01	0.41
1:B:439:LEU:HB3	1:B:440:TYR:H	1.74	0.41
1:B:466:ILE:HG22	1:B:466:ILE:O	2.20	0.41
1:B:701:SER:O	1:B:702:THR:C	2.63	0.41
1:B:718:GLY:O	1:B:719:GLY:C	2.64	0.41
1:B:808:GLY:C	1:B:810:LEU:N	2.78	0.41
1:B:945:MET:SD	1:B:946:TYR:N	2.93	0.41
1:B:970:VAL:HG23	1:B:971:LEU:HD22	2.02	0.41
1:B:1076:VAL:O	1:B:1079:LEU:HB3	2.19	0.41
1:A:39:PHE:CD2	1:A:355:ARG:HA	2.54	0.41
1:A:388:LEU:HD12	1:A:388:LEU:H	1.83	0.41
1:A:513:PRO:O	1:A:518:THR:OG1	2.39	0.41
1:A:740:PRO:O	1:A:743:THR:HG23	2.20	0.41
1:A:756:LEU:HD12	1:A:757:ILE:H	1.79	0.41
1:A:889:SER:OG	1:A:919:SER:HB2	2.20	0.41
1:A:905:SER:HB3	1:A:907:THR:OG1	2.21	0.41
1:A:1050:GLN:HG3	1:A:1050:GLN:O	2.21	0.41
1:A:1076:VAL:HG13	1:A:1194:LEU:HD13	2.01	0.41
1:A:1234:GLN:HA	1:A:1253:HIS:CD2	2.50	0.41
1:B:59:ILE:O	1:B:63:ALA:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:MET:CG	1:B:913:GLU:OE1	2.69	0.41
1:B:617:ILE:H	1:B:617:ILE:CD1	2.33	0.41
1:B:740:PRO:HG2	1:B:741:PRO:CD	2.45	0.41
1:B:883:LYS:HD3	1:B:886:LEU:HD21	2.02	0.41
1:B:910:GLN:O	1:B:912:PHE:N	2.53	0.41
1:B:911:LYS:O	1:B:914:THR:HB	2.19	0.41
1:B:918:GLN:O	1:B:919:SER:C	2.62	0.41
1:B:1119:PHE:C	1:B:1121:CYS:H	2.28	0.41
1:B:1229:ARG:O	1:B:1231:SER:N	2.53	0.41
1:A:245:LYS:NZ	1:A:245:LYS:CA	2.83	0.41
1:A:324:ILE:O	1:A:326:GLN:HB2	2.20	0.41
1:A:583:HIS:HB2	1:A:584:ARG:NH1	2.35	0.41
1:A:620:LYS:O	1:A:621:LEU:C	2.63	0.41
1:A:705:PRO:CG	1:A:706:TYR:H	2.31	0.41
1:A:918:GLN:O	1:A:919:SER:C	2.64	0.41
1:A:1090:VAL:HG22	1:A:1097:ILE:HG13	2.03	0.41
1:A:1176:GLN:N	1:A:1176:GLN:OE1	2.53	0.41
1:A:1189:GLN:O	1:A:1190:PRO:O	2.39	0.41
1:B:86:LYS:HE2	1:B:739:GLY:N	2.35	0.41
1:B:156:ILE:HG23	1:B:439:LEU:HD12	2.02	0.41
1:B:198:GLY:C	1:B:200:PHE:N	2.77	0.41
1:B:322:TYR:CZ	1:B:324:ILE:HG12	2.55	0.41
1:B:391:LYS:O	1:B:392:ASN:C	2.64	0.41
1:B:409:LEU:HD13	1:B:409:LEU:C	2.45	0.41
1:B:476:PHE:CE2	1:B:912:PHE:HZ	2.38	0.41
1:B:531:GLN:O	1:B:532:LYS:C	2.61	0.41
1:B:583:HIS:HB2	1:B:584:ARG:NH1	2.35	0.41
1:B:928:MET:O	1:B:929:LYS:C	2.63	0.41
1:B:1129:TYR:O	1:B:1131:ASP:N	2.52	0.41
1:A:92:SER:OG	1:A:962:GLN:NE2	2.51	0.41
1:A:382:ASP:C	1:A:384:ILE:H	2.28	0.41
1:A:391:LYS:O	1:A:392:ASN:C	2.63	0.41
1:A:617:ILE:H	1:A:617:ILE:CD1	2.33	0.41
1:A:718:GLY:O	1:A:719:GLY:C	2.63	0.41
1:A:740:PRO:N	1:A:741:PRO:CD	2.84	0.41
1:A:745:ARG:O	1:A:749:ASN:HB2	2.21	0.41
1:A:1176:GLN:O	1:A:1179:ARG:HB2	2.20	0.41
1:B:44:TRP:C	1:B:46:ASP:H	2.28	0.41
1:B:88:SER:C	1:B:90:ASN:N	2.78	0.41
1:B:278:GLU:HA	1:B:282:ARG:CZ	2.51	0.41
1:B:286:LYS:HG2	1:B:778:GLU:HG2	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:LEU:HD21	1:B:597:PHE:CZ	2.56	0.41
1:B:848:ILE:O	1:B:848:ILE:HG13	2.21	0.41
1:B:889:SER:OG	1:B:919:SER:HB2	2.21	0.41
1:B:992:PRO:C	1:B:996:LYS:HZ1	2.28	0.41
1:B:1079:LEU:O	1:B:1105:LEU:HD21	2.21	0.41
1:B:1243:GLN:HG3	1:B:1246:LYS:HZ2	1.84	0.41
1:A:70:ILE:C	1:A:72:GLY:H	2.26	0.41
1:A:118:GLY:C	1:A:120:GLY:N	2.78	0.41
1:A:147:PHE:CE2	1:A:365:ILE:HG12	2.56	0.41
1:A:374:PHE:CG	1:A:375:SER:N	2.89	0.41
1:A:494:ASP:O	1:A:497:GLU:HB3	2.21	0.41
1:A:708:VAL:O	1:A:709:VAL:C	2.63	0.41
1:A:731:VAL:HA	1:A:750:LEU:CD1	2.50	0.41
1:A:1031:VAL:O	1:A:1055:GLU:HA	2.21	0.41
1:B:43:GLY:CA	1:B:46:ASP:HB2	2.50	0.41
1:B:711:ILE:HD11	1:B:832:ILE:HG21	2.02	0.41
1:B:727:ILE:HD13	1:B:754:LEU:CD2	2.50	0.41
1:B:728:PHE:O	1:B:729:SER:C	2.63	0.41
1:B:733:GLY:CA	1:B:968:GLU:HG3	2.51	0.41
1:B:835:ASN:O	1:B:836:ILE:C	2.63	0.41
1:B:900:PHE:O	1:B:902:THR:N	2.53	0.41
1:A:211:THR:HA	1:A:214:ILE:CD1	2.44	0.41
1:A:248:ALA:C	1:A:250:ALA:H	2.28	0.41
1:A:267:LYS:HA	1:A:270:LEU:HD21	2.00	0.41
1:A:315:SER:HA	1:A:318:ILE:HG22	2.02	0.41
1:A:368:LYS:O	1:A:369:PRO:C	2.63	0.41
1:A:531:GLN:O	1:A:532:LYS:C	2.64	0.41
1:A:816:ASN:O	1:A:820:GLN:HG2	2.21	0.41
1:A:1178:GLN:O	1:A:1181:ALA:N	2.54	0.41
1:B:46:ASP:O	1:B:49:TYR:N	2.54	0.41
1:B:67:MET:HE2	1:B:117:ILE:HG21	2.01	0.41
1:B:71:PHE:C	1:B:71:PHE:CD1	2.99	0.41
1:B:296:GLY:O	1:B:300:LEU:HG	2.20	0.41
1:B:422:VAL:O	1:B:597:PHE:O	2.39	0.41
1:B:739:GLY:C	1:B:741:PRO:HD2	2.45	0.41
1:B:779:ILE:HA	1:B:782:LYS:HE3	2.03	0.41
1:B:843:ILE:C	1:B:846:SER:HB3	2.45	0.41
1:B:906:LEU:HA	1:B:909:GLU:OE2	2.21	0.41
1:B:922:ILE:HB	1:B:923:PRO:CD	2.45	0.41
1:A:131:PHE:C	1:A:131:PHE:HD2	2.28	0.41
1:A:209:LYS:HA	1:A:212:LEU:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:HA	1:A:219:PRO:HD2	2.03	0.41
1:A:238:LYS:HD3	1:A:238:LYS:C	2.46	0.41
1:A:255:ALA:C	1:A:257:ILE:H	2.28	0.41
1:A:261:ILE:C	1:A:263:PHE:H	2.29	0.41
1:A:266:GLN:HB2	1:A:270:LEU:HD22	2.03	0.41
1:A:286:LYS:HA	1:A:289:ILE:CB	2.31	0.41
1:A:342:GLY:O	1:A:346:PRO:HD2	2.20	0.41
1:A:406:LEU:C	1:A:408:GLY:N	2.79	0.41
1:A:441:ASP:OD1	1:A:442:PRO:HD2	2.21	0.41
1:A:504:ASN:O	1:A:504:ASN:CG	2.64	0.41
1:A:787:MET:SD	1:A:1008:ILE:HD11	2.61	0.41
1:A:792:MET:CA	1:A:795:GLN:HB2	2.47	0.41
1:A:799:TRP:O	1:A:803:PRO:CB	2.62	0.41
1:A:845:ILE:O	1:A:849:TYR:CD2	2.74	0.41
1:A:883:LYS:HD3	1:A:886:LEU:HD21	2.02	0.41
1:A:933:VAL:O	1:A:936:ILE:HG22	2.21	0.41
1:A:946:TYR:O	1:A:947:PHE:C	2.64	0.41
1:A:1038:PHE:CD2	1:A:1078:LEU:HD21	2.56	0.41
1:A:1056:VAL:HG21	1:A:1062:LEU:HB2	2.01	0.41
1:A:1073:SER:O	1:A:1077:GLN:HG3	2.21	0.41
1:A:1147:GLU:HB3	1:A:1186:LEU:HD22	2.02	0.41
1:A:1252:THR:O	1:A:1255:GLN:HB3	2.21	0.41
1:B:54:THR:O	1:B:57:ALA:HB3	2.20	0.41
1:B:157:GLY:HA2	1:B:160:ASP:CG	2.46	0.41
1:B:168:ASN:O	1:B:169:THR:C	2.64	0.41
1:B:300:LEU:O	1:B:303:TYR:CB	2.68	0.41
1:B:388:LEU:HD12	1:B:388:LEU:H	1.83	0.41
1:B:449:ILE:O	1:B:450:ASP:HB3	2.21	0.41
1:B:482:GLU:C	1:B:484:ILE:N	2.78	0.41
1:B:535:ILE:O	1:B:536:ALA:C	2.63	0.41
1:B:551:ASP:HA	1:B:581:ILE:HG23	2.03	0.41
1:B:689:PRO:CD	1:B:690:PRO:HD2	2.51	0.41
1:B:693:PHE:HD2	1:B:693:PHE:H	1.65	0.41
1:B:726:VAL:O	1:B:727:ILE:C	2.63	0.41
1:B:731:VAL:O	1:B:734:VAL:HG12	2.21	0.41
1:B:761:ILE:H	1:B:761:ILE:CD1	2.33	0.41
1:B:892:ILE:O	1:B:895:GLU:HB3	2.21	0.41
1:B:912:PHE:O	1:B:915:MET:N	2.54	0.41
1:B:948:SER:O	1:B:952:CYS:SG	2.76	0.41
1:B:974:PHE:CD1	2:B:6002:OJZ:H30B	2.56	0.41
1:B:1005:ILE:C	1:B:1007:ILE:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1107:ALA:O	1:B:1188:ARG:HD3	2.21	0.41
1:B:1126:ASN:O	1:B:1127:ILE:C	2.64	0.41
1:B:1156:SER:OG	1:B:1157:LEU:HD22	2.20	0.41
1:B:1203:ASP:O	1:B:1207:GLU:HG3	2.21	0.41
1:A:174:ASP:O	1:A:178:ILE:HG13	2.21	0.41
1:A:348:ILE:O	1:A:351:PHE:HB3	2.20	0.41
1:A:471:GLN:OE1	1:A:471:GLN:N	2.52	0.41
1:A:899:ASN:OD1	1:A:901:ARG:NH2	2.54	0.41
1:B:140:ILE:O	1:B:143:ILE:N	2.53	0.41
1:B:462:LEU:O	1:B:463:ARG:C	2.62	0.41
1:B:480:ILE:O	1:B:482:GLU:N	2.54	0.41
1:B:785:ARG:O	1:B:786:TYR:C	2.64	0.41
1:B:796:ASP:HA	1:B:800:PHE:CD2	2.56	0.41
1:B:973:VAL:O	1:B:976:ALA:N	2.51	0.41
1:B:1003:HIS:O	1:B:1007:ILE:HG13	2.21	0.41
1:B:1067:SER:OG	1:B:1244:ASN:ND2	2.54	0.41
1:B:1213:ALA:O	1:B:1217:ALA:HB2	2.21	0.41
1:A:90:ASN:O	1:A:91:MET:C	2.64	0.40
1:A:168:ASN:O	1:A:169:THR:C	2.63	0.40
1:A:170:ARG:O	1:A:171:LEU:C	2.63	0.40
1:A:327:VAL:O	1:A:331:PHE:HD1	2.04	0.40
1:A:346:PRO:O	1:A:349:GLU:HB3	2.21	0.40
1:A:703:GLU:HA	1:A:783:ARG:HH12	1.86	0.40
1:A:853:LEU:HD11	1:A:956:GLY:HA2	2.03	0.40
1:A:892:ILE:HG12	1:A:892:ILE:H	1.49	0.40
1:A:901:ARG:O	1:A:904:VAL:N	2.44	0.40
1:A:928:MET:O	1:A:931:ALA:CB	2.65	0.40
1:A:1067:SER:OG	1:A:1244:ASN:ND2	2.54	0.40
1:A:1107:ALA:HB3	1:A:1108:GLN:HE22	1.86	0.40
1:A:1132:ASN:C	1:A:1134:ARG:N	2.79	0.40
1:A:1255:GLN:O	1:A:1258:ALA:N	2.54	0.40
1:B:147:PHE:CE2	1:B:365:ILE:HG12	2.56	0.40
1:B:270:LEU:O	1:B:274:ASN:HB2	2.22	0.40
1:B:288:ALA:O	1:B:292:ASN:N	2.54	0.40
1:B:381:PRO:CG	1:B:457:ILE:HB	2.50	0.40
1:B:534:ARG:O	1:B:537:ILE:CB	2.68	0.40
1:B:900:PHE:C	1:B:900:PHE:CD1	3.00	0.40
1:B:936:ILE:C	1:B:939:SER:HG	2.27	0.40
1:A:212:LEU:CD1	1:A:215:LEU:HD12	2.50	0.40
1:A:218:SER:O	1:A:219:PRO:C	2.64	0.40
1:A:429:LYS:O	1:A:430:SER:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:LEU:HD12	1:A:466:ILE:CD1	2.51	0.40
1:A:714:ALA:O	1:A:715:ILE:C	2.65	0.40
1:A:727:ILE:HD13	1:A:754:LEU:CD2	2.50	0.40
1:A:761:ILE:H	1:A:761:ILE:CD1	2.34	0.40
1:A:810:LEU:O	1:A:813:ARG:N	2.54	0.40
1:A:945:MET:O	1:A:946:TYR:C	2.63	0.40
1:A:1155:ASP:O	1:A:1160:LYS:HE3	2.21	0.40
1:B:279:GLU:HG2	1:B:782:LYS:NZ	2.35	0.40
1:B:310:PHE:CE2	1:B:331:PHE:HB3	2.55	0.40
1:B:471:GLN:OE1	1:B:471:GLN:N	2.49	0.40
1:B:500:VAL:CG2	1:B:501:LYS:N	2.84	0.40
1:B:745:ARG:O	1:B:749:ASN:HB2	2.21	0.40
1:B:912:PHE:O	1:B:913:GLU:C	2.64	0.40
1:B:1038:PHE:CZ	1:B:1040:TYR:N	2.89	0.40
1:B:1076:VAL:O	1:B:1077:GLN:C	2.64	0.40
1:A:38:MET:O	1:A:39:PHE:C	2.63	0.40
1:A:68:MET:O	1:A:69:LEU:C	2.63	0.40
1:A:253:VAL:HB	1:A:1119:PHE:CE1	2.52	0.40
1:A:282:ARG:HA	1:A:282:ARG:HD3	1.83	0.40
1:A:387:ASN:ND2	1:A:415:SER:H	2.20	0.40
1:A:403:VAL:O	1:A:405:ILE:HD12	2.21	0.40
1:A:449:ILE:O	1:A:450:ASP:HB3	2.21	0.40
1:A:693:PHE:C	1:A:695:ARG:N	2.80	0.40
1:A:714:ALA:O	1:A:717:ASN:HB3	2.22	0.40
1:A:791:SER:O	1:A:795:GLN:HB2	2.21	0.40
1:A:847:LEU:C	1:A:849:TYR:H	2.28	0.40
1:A:925:ARG:NE	1:B:519:LEU:HD12	2.36	0.40
1:A:1014:ILE:HA	1:A:1017:TYR:HE2	1.86	0.40
1:A:1032:GLN:HB3	1:A:1091:PHE:HD2	1.85	0.40
1:B:108:THR:O	1:B:109:THR:C	2.64	0.40
1:B:206:ARG:O	1:B:211:THR:HB	2.21	0.40
1:B:332:PHE:HE1	2:B:6002:OJZ:N24	2.19	0.40
1:B:342:GLY:O	1:B:346:PRO:HD2	2.21	0.40
1:B:358:ALA:O	1:B:362:PHE:N	2.53	0.40
1:B:504:ASN:O	1:B:504:ASN:CG	2.64	0.40
1:B:519:LEU:HD13	1:B:519:LEU:N	2.19	0.40
1:B:690:PRO:O	1:B:691:ALA:C	2.65	0.40
1:B:899:ASN:OD1	1:B:901:ARG:NH2	2.54	0.40
1:A:58:ILE:O	1:A:59:ILE:C	2.65	0.40
1:A:110:TYR:CA	1:A:113:TYR:HD2	2.34	0.40
1:A:140:ILE:O	1:A:141:HIS:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:LEU:HD21	1:A:597:PHE:CZ	2.56	0.40
1:A:480:ILE:C	1:A:482:GLU:N	2.78	0.40
1:A:770:GLY:HA2	1:A:773:PHE:CZ	2.56	0.40
1:A:815:ALA:O	1:A:816:ASN:C	2.65	0.40
1:A:857:LEU:C	1:A:857:LEU:CD2	2.91	0.40
1:A:901:ARG:HD3	1:A:901:ARG:N	2.36	0.40
1:A:961:THR:O	1:A:962:GLN:CB	2.69	0.40
1:A:1191:HIS:HA	1:A:1221:ARG:HB2	2.02	0.40
1:B:92:SER:O	1:B:96:LYS:HG3	2.21	0.40
1:B:406:LEU:C	1:B:408:GLY:N	2.80	0.40
1:B:436:MET:HB3	1:B:549:LEU:HD21	2.03	0.40
1:B:462:LEU:HD12	1:B:466:ILE:CD1	2.51	0.40
1:B:688:VAL:HB	1:B:1006:ARG:HH12	1.87	0.40
1:B:756:LEU:HD12	1:B:757:ILE:HG12	2.04	0.40
1:B:770:GLY:HA2	1:B:773:PHE:CZ	2.56	0.40
1:B:1212:GLU:C	1:B:1212:GLU:CD	2.90	0.40
1:A:92:SER:O	1:A:96:LYS:HG3	2.22	0.40
1:A:136:ALA:O	1:A:137:GLY:C	2.64	0.40
1:A:195:THR:O	1:A:196:PHE:C	2.64	0.40
1:A:203:GLY:O	1:A:215:LEU:HD21	2.21	0.40
1:A:203:GLY:CA	1:A:211:THR:OG1	2.70	0.40
1:A:299:PHE:O	1:A:303:TYR:N	2.53	0.40
1:A:479:THR:HA	1:A:518:THR:O	2.21	0.40
1:A:498:LYS:HE2	1:A:498:LYS:C	2.47	0.40
1:A:693:PHE:O	1:A:695:ARG:N	2.55	0.40
1:A:724:PHE:CD1	1:A:758:LEU:HD12	2.57	0.40
1:A:900:PHE:C	1:A:900:PHE:CD1	3.00	0.40
1:B:129:VAL:CB	1:B:935:GLY:HA2	2.51	0.40
1:B:155:GLU:HA	1:B:158:TRP:CZ3	2.56	0.40
1:B:170:ARG:O	1:B:171:LEU:C	2.64	0.40
1:B:327:VAL:O	1:B:331:PHE:HD1	2.04	0.40
1:B:342:GLY:O	1:B:343:GLN:C	2.64	0.40
1:B:439:LEU:HB3	1:B:440:TYR:HD1	1.86	0.40
1:B:500:VAL:O	1:B:503:ALA:N	2.55	0.40
1:B:901:ARG:HD3	1:B:901:ARG:N	2.35	0.40
1:B:990:PHE:O	1:B:991:ALA:O	2.40	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	1178/1284 (92%)	704 (60%)	302 (26%)	172 (15%)	0	3
1	B	1178/1284 (92%)	707 (60%)	305 (26%)	166 (14%)	0	3
All	All	2356/2568 (92%)	1411 (60%)	607 (26%)	338 (14%)	0	3

All (338) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	35	VAL
1	A	52	VAL
1	A	89	THR
1	A	133	CYS
1	A	134	LEU
1	A	135	ALA
1	A	156	ILE
1	A	190	PHE
1	A	201	ILE
1	A	274	ASN
1	A	308	LEU
1	A	310	PHE
1	A	371	ILE
1	A	385	GLN
1	A	400	ARG
1	A	439	LEU
1	A	489	GLU
1	A	521	GLY
1	A	539	ARG
1	A	574	GLU
1	A	598	ASP
1	A	603	VAL
1	A	692	SER
1	A	757	ILE

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Mol	Chain	Res	Type
1	A	796	ASP
1	A	797	VAL
1	A	833	PHE
1	A	837	ALA
1	A	849	TYR
1	A	909	GLU
1	A	958	TYR
1	A	959	LEU
1	A	1014	ILE
1	A	1042	THR
1	A	1098	LYS
1	A	1099	GLN
1	A	1114	GLN
1	A	1136	VAL
1	A	1155	ASP
1	A	1161	TYR
1	A	1198	ALA
1	A	1201	ALA
1	A	1204	THR
1	A	1205	GLU
1	A	1244	ASN
1	B	34	SER
1	B	35	VAL
1	B	52	VAL
1	B	89	THR
1	B	133	CYS
1	B	134	LEU
1	B	135	ALA
1	B	156	ILE
1	B	164	VAL
1	B	190	PHE
1	B	201	ILE
1	B	208	TRP
1	B	274	ASN
1	B	308	LEU
1	B	310	PHE
1	B	371	ILE
1	B	377	SER
1	B	385	GLN
1	B	400	ARG
1	B	439	LEU
1	B	489	GLU

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Mol	Chain	Res	Type
1	B	521	GLY
1	B	574	GLU
1	B	598	ASP
1	B	603	VAL
1	B	757	ILE
1	B	796	ASP
1	B	797	VAL
1	B	833	PHE
1	B	839	LEU
1	B	849	TYR
1	B	851	TRP
1	B	909	GLU
1	B	958	TYR
1	B	959	LEU
1	B	1014	ILE
1	B	1015	ASP
1	B	1016	SER
1	B	1021	GLY
1	B	1042	THR
1	B	1098	LYS
1	B	1136	VAL
1	B	1155	ASP
1	B	1198	ALA
1	B	1201	ALA
1	B	1204	THR
1	B	1205	GLU
1	B	1244	ASN
1	A	91	MET
1	A	132	TRP
1	A	137	GLY
1	A	144	ARG
1	A	152	MET
1	A	216	ALA
1	A	227	ILE
1	A	325	GLY
1	A	373	SER
1	A	384	ILE
1	A	429	LYS
1	A	434	GLN
1	A	435	LEU
1	A	491	VAL
1	A	707	PHE

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Mol	Chain	Res	Type
1	A	758	LEU
1	A	799	TRP
1	A	806	THR
1	A	835	ASN
1	A	839	LEU
1	A	840	GLY
1	A	851	TRP
1	A	906	LEU
1	A	908	ARG
1	A	933	VAL
1	A	965	MET
1	A	993	ASP
1	A	995	ALA
1	A	1020	GLN
1	A	1024	PRO
1	A	1027	LEU
1	A	1069	GLY
1	A	1190	PRO
1	B	44	TRP
1	B	132	TRP
1	B	137	GLY
1	B	144	ARG
1	B	152	MET
1	B	155	GLU
1	B	209	LYS
1	B	216	ALA
1	B	227	ILE
1	B	272	ARG
1	B	322	TYR
1	B	325	GLY
1	B	384	ILE
1	B	392	ASN
1	B	491	VAL
1	B	539	ARG
1	B	555	SER
1	B	691	ALA
1	B	707	PHE
1	B	758	LEU
1	B	814	LEU
1	B	835	ASN
1	B	837	ALA
1	B	840	GLY

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Mol	Chain	Res	Type
1	B	908	ARG
1	B	933	VAL
1	B	965	MET
1	B	993	ASP
1	B	995	ALA
1	B	1019	THR
1	B	1069	GLY
1	B	1114	GLN
1	B	1161	TYR
1	B	1190	PRO
1	B	1230	LEU
1	A	44	TRP
1	A	123	ILE
1	A	131	PHE
1	A	139	GLN
1	A	160	ASP
1	A	169	THR
1	A	272	ARG
1	A	276	ASN
1	A	278	GLU
1	A	329	THR
1	A	374	PHE
1	A	392	ASN
1	A	424	ASN
1	A	504	ASN
1	A	522	GLU
1	A	526	GLN
1	A	532	LYS
1	A	545	PRO
1	A	555	SER
1	A	615	LYS
1	A	687	ASP
1	A	781	THR
1	A	814	LEU
1	A	815	ALA
1	A	838	ASN
1	A	903	VAL
1	A	1017	TYR
1	A	1046	ILE
1	A	1117	ILE
1	A	1130	GLY
1	A	1134	ARG

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Mol	Chain	Res	Type
1	A	1156	SER
1	A	1158	PRO
1	A	1230	LEU
1	B	91	MET
1	B	123	ILE
1	B	131	PHE
1	B	139	GLN
1	B	160	ASP
1	B	267	LYS
1	B	276	ASN
1	B	278	GLU
1	B	329	THR
1	B	424	ASN
1	B	435	LEU
1	B	477	ALA
1	B	493	MET
1	B	504	ASN
1	B	522	GLU
1	B	526	GLN
1	B	532	LYS
1	B	545	PRO
1	B	693	PHE
1	B	781	THR
1	B	799	TRP
1	B	806	THR
1	B	809	ALA
1	B	838	ASN
1	B	906	LEU
1	B	992	PRO
1	B	1036	VAL
1	B	1046	ILE
1	B	1119	PHE
1	B	1130	GLY
1	B	1134	ARG
1	B	1156	SER
1	B	1158	PRO
1	B	1253	HIS
1	A	209	LYS
1	A	223	LEU
1	A	266	GLN
1	A	267	LYS
1	A	369	PRO

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Mol	Chain	Res	Type
1	A	477	ALA
1	A	483	ASN
1	A	493	MET
1	A	523	ARG
1	A	573	ARG
1	A	620	LYS
1	A	809	ALA
1	A	912	PHE
1	A	963	GLN
1	A	1036	VAL
1	A	1041	PRO
1	A	1093	ASP
1	A	1094	GLY
1	A	1119	PHE
1	A	1120	ASP
1	A	1170	THR
1	A	1253	HIS
1	B	71	PHE
1	B	169	THR
1	B	223	LEU
1	B	256	ALA
1	B	258	ARG
1	B	266	GLN
1	B	369	PRO
1	B	483	ASN
1	B	523	ARG
1	B	573	ARG
1	B	615	LYS
1	B	620	LYS
1	B	731	VAL
1	B	815	ALA
1	B	903	VAL
1	B	931	ALA
1	B	957	ALA
1	B	963	GLN
1	B	1093	ASP
1	B	1094	GLY
1	B	1117	ILE
1	B	1120	ASP
1	B	1146	LYS
1	B	1170	THR
1	A	162	HIS

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Mol	Chain	Res	Type
1	A	196	PHE
1	A	258	ARG
1	A	312	TYR
1	A	317	VAL
1	A	370	SER
1	A	691	ALA
1	A	726	VAL
1	A	731	VAL
1	A	931	ALA
1	A	992	PRO
1	A	1012	PRO
1	A	1028	GLU
1	A	1039	ASN
1	A	1129	TYR
1	A	1157	LEU
1	A	1184	ARG
1	B	196	PHE
1	B	312	TYR
1	B	912	PHE
1	B	1011	THR
1	B	1012	PRO
1	B	1023	LYS
1	B	1041	PRO
1	B	1157	LEU
1	A	71	PHE
1	A	381	PRO
1	A	428	GLY
1	A	694	TRP
1	A	895	GLU
1	A	1146	LYS
1	B	116	GLY
1	B	772	THR
1	B	895	GLU
1	B	1100	LEU
1	B	1129	TYR
1	A	118	GLY
1	B	140	ILE
1	B	203	GLY
1	B	317	VAL
1	B	380	LYS
1	B	726	VAL
1	A	116	GLY

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Mol	Chain	Res	Type
1	A	140	ILE
1	A	164	VAL
1	A	593	VAL
1	B	118	GLY
1	A	58	ILE
1	A	365	ILE
1	A	1165	VAL
1	B	313	GLY
1	B	705	PRO
1	A	121	VAL
1	A	199	GLY
1	A	203	GLY
1	A	356	GLY
1	A	705	PRO
1	B	58	ILE
1	B	365	ILE
1	B	593	VAL
1	A	165	GLY
1	B	161	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	976/1065 (92%)	889 (91%)	87 (9%)	9	28
1	B	976/1065 (92%)	892 (91%)	84 (9%)	10	29
All	All	1952/2130 (92%)	1781 (91%)	171 (9%)	9	29

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	MET
1	A	59	ILE
1	A	64	LEU
1	A	91	MET

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Mol	Chain	Res	Type
1	A	102	LYS
1	A	113	TYR
1	A	131	PHE
1	A	138	ARG
1	A	155	GLU
1	A	156	ILE
1	A	158	TRP
1	A	163	ASP
1	A	173	ASP
1	A	185	LYS
1	A	186	ILE
1	A	210	LEU
1	A	219	PRO
1	A	228	TRP
1	A	238	LYS
1	A	245	LYS
1	A	252	GLU
1	A	254	LEU
1	A	257	ILE
1	A	270	LEU
1	A	285	ILE
1	A	289	ILE
1	A	295	MET
1	A	306	TYR
1	A	310	PHE
1	A	311	TRP
1	A	330	VAL
1	A	397	TYR
1	A	401	LYS
1	A	402	GLU
1	A	404	GLN
1	A	435	LEU
1	A	438	ARG
1	A	439	LEU
1	A	447	VAL
1	A	519	LEU
1	A	581	ILE
1	A	697	LEU
1	A	703	GLU
1	A	722	PRO
1	A	751	PHE
1	A	795	GLN

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Mol	Chain	Res	Type
1	A	799	TRP
1	A	804	LYS
1	A	816	ASN
1	A	851	TRP
1	A	853	LEU
1	A	862	PRO
1	A	872	MET
1	A	881	LYS
1	A	892	ILE
1	A	902	THR
1	A	908	ARG
1	A	912	PHE
1	A	932	HIS
1	A	968	GLU
1	A	969	ASN
1	A	978	VAL
1	A	996	LYS
1	A	1010	LYS
1	A	1013	GLU
1	A	1014	ILE
1	A	1020	GLN
1	A	1027	LEU
1	A	1036	VAL
1	A	1037	VAL
1	A	1060	GLN
1	A	1090	VAL
1	A	1099	GLN
1	A	1108	GLN
1	A	1118	LEU
1	A	1131	ASP
1	A	1139	GLU
1	A	1140	GLU
1	A	1158	PRO
1	A	1176	GLN
1	A	1192	ILE
1	A	1204	THR
1	A	1214	LEU
1	A	1223	CYS
1	A	1246	LYS
1	A	1248	LYS
1	A	1259	GLN
1	B	38	MET

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Mol	Chain	Res	Type
1	B	59	ILE
1	B	64	LEU
1	B	91	MET
1	B	102	LYS
1	B	113	TYR
1	B	131	PHE
1	B	138	ARG
1	B	155	GLU
1	B	156	ILE
1	B	158	TRP
1	B	163	ASP
1	B	173	ASP
1	B	185	LYS
1	B	186	ILE
1	B	210	LEU
1	B	219	PRO
1	B	228	TRP
1	B	238	LYS
1	B	245	LYS
1	B	252	GLU
1	B	254	LEU
1	B	257	ILE
1	B	270	LEU
1	B	285	ILE
1	B	289	ILE
1	B	295	MET
1	B	306	TYR
1	B	310	PHE
1	B	311	TRP
1	B	330	VAL
1	B	374	PHE
1	B	397	TYR
1	B	401	LYS
1	B	402	GLU
1	B	404	GLN
1	B	429	LYS
1	B	438	ARG
1	B	439	LEU
1	B	447	VAL
1	B	519	LEU
1	B	581	ILE
1	B	693	PHE

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Mol	Chain	Res	Type
1	B	697	LEU
1	B	703	GLU
1	B	722	PRO
1	B	751	PHE
1	B	795	GLN
1	B	799	TRP
1	B	803	PRO
1	B	804	LYS
1	B	816	ASN
1	B	851	TRP
1	B	862	PRO
1	B	872	MET
1	B	881	LYS
1	B	892	ILE
1	B	902	THR
1	B	908	ARG
1	B	912	PHE
1	B	932	HIS
1	B	968	GLU
1	B	969	ASN
1	B	978	VAL
1	B	996	LYS
1	B	1010	LYS
1	B	1036	VAL
1	B	1037	VAL
1	B	1060	GLN
1	B	1090	VAL
1	B	1108	GLN
1	B	1118	LEU
1	B	1131	ASP
1	B	1139	GLU
1	B	1140	GLU
1	B	1158	PRO
1	B	1176	GLN
1	B	1192	ILE
1	B	1204	THR
1	B	1214	LEU
1	B	1223	CYS
1	B	1246	LYS
1	B	1248	LYS
1	B	1259	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	83	ASN
1	A	87	ASN
1	A	128	GLN
1	A	154	GLN
1	A	191	GLN
1	A	274	ASN
1	A	347	ASN
1	A	379	HIS
1	A	385	GLN
1	A	387	ASN
1	A	394	HIS
1	A	404	GLN
1	A	434	GLN
1	A	437	GLN
1	A	458	ASN
1	A	605	GLN
1	A	721	GLN
1	A	746	GLN
1	A	747	ASN
1	A	769	GLN
1	A	795	GLN
1	A	805	ASN
1	A	816	ASN
1	A	838	ASN
1	A	852	GLN
1	A	878	GLN
1	A	932	HIS
1	A	962	GLN
1	A	963	GLN
1	A	969	ASN
1	A	1032	GLN
1	A	1039	ASN
1	A	1099	GLN
1	A	1108	GLN
1	A	1114	GLN
1	A	1126	ASN
1	A	1149	ASN
1	A	1191	HIS
1	A	1235	ASN
1	A	1244	ASN
1	A	1253	HIS

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Mol	Chain	Res	Type
1	B	60	HIS
1	B	83	ASN
1	B	87	ASN
1	B	128	GLN
1	B	145	GLN
1	B	154	GLN
1	B	191	GLN
1	B	274	ASN
1	B	347	ASN
1	B	379	HIS
1	B	385	GLN
1	B	387	ASN
1	B	394	HIS
1	B	404	GLN
1	B	434	GLN
1	B	437	GLN
1	B	458	ASN
1	B	515	GLN
1	B	605	GLN
1	B	721	GLN
1	B	746	GLN
1	B	747	ASN
1	B	769	GLN
1	B	795	GLN
1	B	805	ASN
1	B	816	ASN
1	B	834	GLN
1	B	838	ASN
1	B	852	GLN
1	B	878	GLN
1	B	932	HIS
1	B	963	GLN
1	B	969	ASN
1	B	1032	GLN
1	B	1039	ASN
1	B	1099	GLN
1	B	1108	GLN
1	B	1114	GLN
1	B	1126	ASN
1	B	1235	ASN
1	B	1244	ASN
1	B	1253	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	OJZ	B	6002	-	33,39,39	1.52	5 (15%)	51,57,57	1.62	11 (21%)
2	OJZ	A	6001	-	33,39,39	1.79	6 (18%)	51,57,57	1.77	9 (17%)

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	OJZ	B	6002	-	-	4/42/48/48	0/4/4/4
2	OJZ	A	6001	-	-	4/42/48/48	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6001	OJZ	C16-N17	5.70	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6002	OJZ	C09-N10	4.62	1.43	1.34
2	A	6001	OJZ	C02-N03	4.57	1.43	1.34
2	A	6001	OJZ	C09-N10	4.04	1.42	1.34
2	B	6002	OJZ	C02-N03	3.85	1.42	1.34
2	A	6001	OJZ	C18-N17	3.14	1.52	1.45
2	B	6002	OJZ	C16-N17	2.65	1.39	1.34
2	B	6002	OJZ	C15-C16	-2.24	1.44	1.48
2	A	6001	OJZ	C04-N03	2.23	1.50	1.45
2	A	6001	OJZ	C34-C18	2.18	1.60	1.54
2	B	6002	OJZ	C01-N22	2.00	1.42	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6001	OJZ	C04-N03-C02	4.67	131.07	121.57
2	A	6001	OJZ	C18-N17-C16	4.47	130.66	121.57
2	A	6001	OJZ	SE2-C14-C15	3.72	116.41	111.07
2	A	6001	OJZ	SE3-C21-C01	3.59	116.22	111.07
2	B	6002	OJZ	C01-C02-N03	3.57	120.29	115.22
2	B	6002	OJZ	SE3-C21-C01	3.42	115.98	111.07
2	B	6002	OJZ	SE1-C07-C08	3.37	115.91	111.07
2	A	6001	OJZ	C15-C16-N17	3.33	119.96	115.22
2	B	6002	OJZ	C18-C19-N22	3.30	128.24	123.89
2	A	6001	OJZ	C11-N10-C09	3.18	128.04	121.57
2	B	6002	OJZ	C04-N03-C02	3.07	127.82	121.57
2	A	6001	OJZ	SE1-C07-C08	2.96	115.31	111.07
2	B	6002	OJZ	C08-C09-N10	2.77	119.16	115.22
2	A	6001	OJZ	C05-C04-N03	-2.75	103.80	108.05
2	B	6002	OJZ	C11-N10-C09	2.69	127.04	121.57
2	B	6002	OJZ	C02-C01-N22	2.54	125.49	120.67
2	B	6002	OJZ	C18-N17-C16	2.46	126.58	121.57
2	B	6002	OJZ	C34-C18-C19	2.26	115.25	111.76
2	B	6002	OJZ	SE2-C14-C15	2.20	114.23	111.07
2	A	6001	OJZ	C01-C02-N03	2.10	118.21	115.22

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	6001	OJZ	C19-C18-N17-C16
2	A	6001	OJZ	C34-C18-C19-N22
2	B	6002	OJZ	N03-C04-C05-N24

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Mol	Chain	Res	Type	Atoms
2	B	6002	OJZ	C28-C04-C05-N24
2	A	6001	OJZ	C34-C18-N17-C16
2	A	6001	OJZ	C28-C04-N03-C02
2	B	6002	OJZ	C28-C04-N03-C02
2	B	6002	OJZ	C31-C11-N10-C09

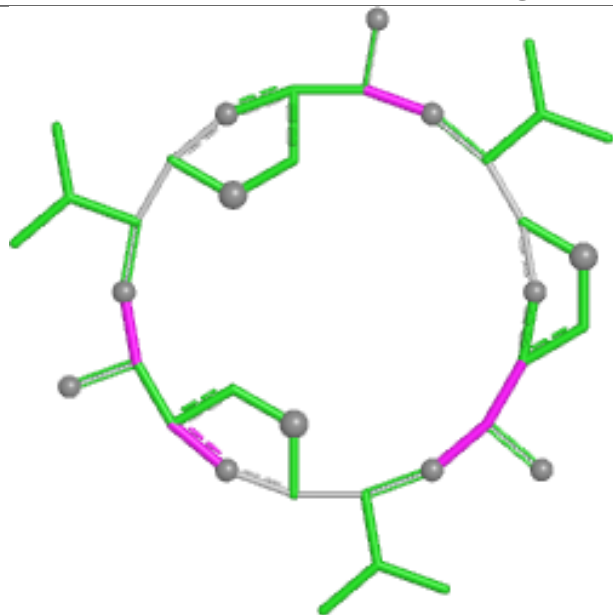
There are no ring outliers.

2 monomers are involved in 22 short contacts:

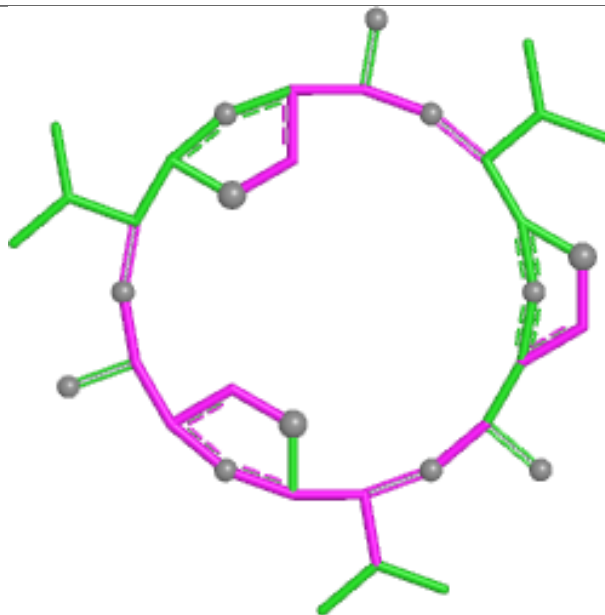
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	6002	OJZ	10	0
2	A	6001	OJZ	12	0

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.

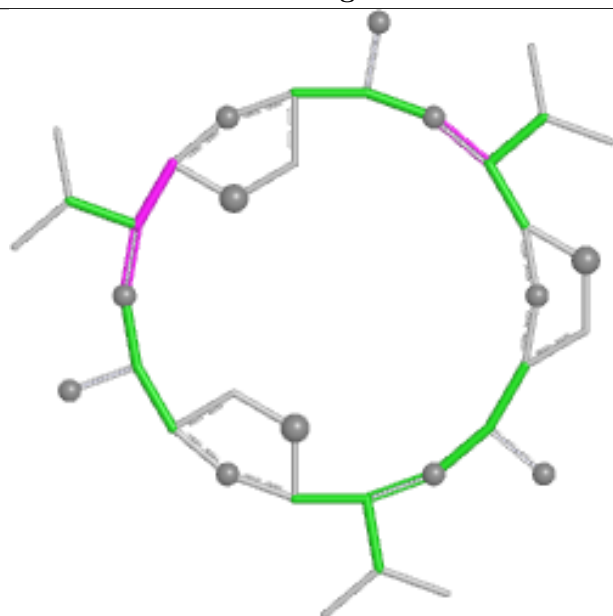
Ligand 0JZ B 6002



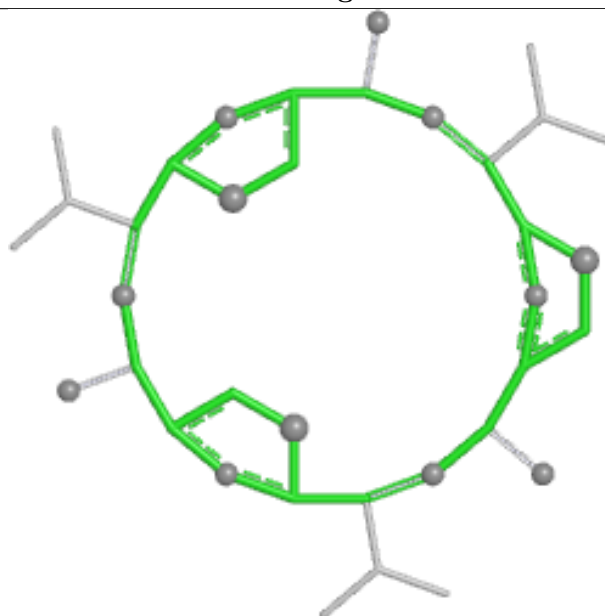
Bond lengths



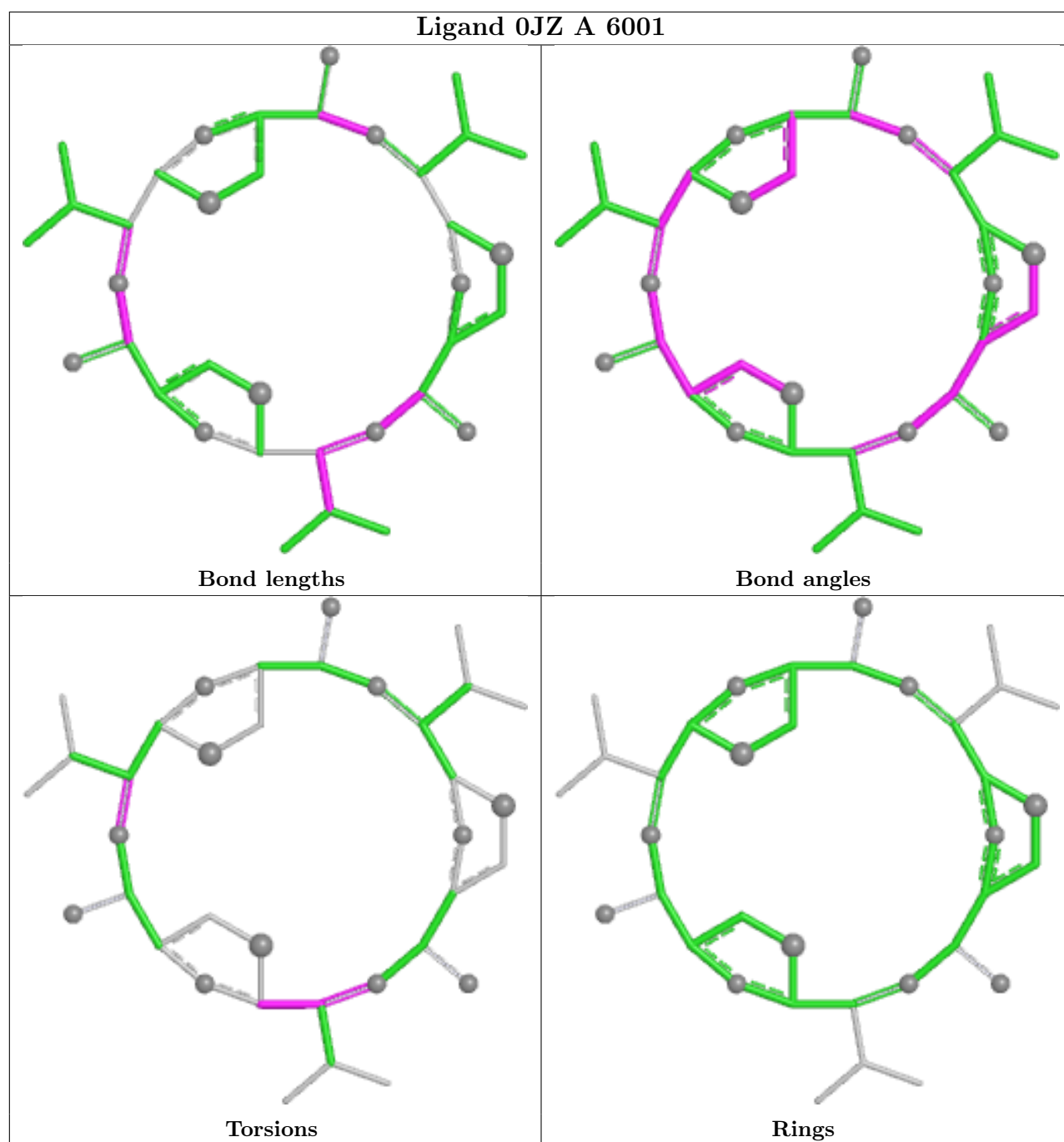
Bond angles



Torsions



Rings



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	1182/1284 (92%)	-0.04	27 (2%) 61 48	118, 194, 243, 306	0
1	B	1182/1284 (92%)	-0.04	14 (1%) 76 62	123, 200, 243, 301	0
All	All	2364/2568 (92%)	-0.04	41 (1%) 69 55	118, 197, 244, 306	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	205	THR	5.3
1	B	1241	VAL	4.1
1	B	217	ILE	3.9
1	B	982	MET	3.9
1	A	288	ALA	3.4
1	A	720	LEU	3.4
1	B	228	TRP	3.1
1	B	474	VAL	3.1
1	A	314	THR	3.0
1	A	236	THR	3.0
1	A	577	THR	2.9
1	A	1163	THR	2.9
1	A	340	SER	2.7
1	A	207	GLY	2.6
1	B	617	ILE	2.6
1	A	867	ALA	2.6
1	A	69	LEU	2.5
1	A	983	ALA	2.5
1	B	415	SER	2.4
1	A	1081	ARG	2.4
1	A	977	ILE	2.4
1	A	1196	ASP	2.3
1	A	902	THR	2.3
1	B	1249	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	194	ALA	2.3
1	A	980	GLY	2.2
1	B	887	GLU	2.2
1	A	158	TRP	2.2
1	A	1084	ASP	2.2
1	A	329	THR	2.2
1	A	623	MET	2.2
1	B	1141	ILE	2.1
1	B	81	VAL	2.1
1	A	373	SER	2.1
1	A	449	ILE	2.1
1	A	838	ASN	2.1
1	A	108	THR	2.1
1	A	191	GLN	2.1
1	A	554	THR	2.1
1	B	603	VAL	2.1
1	A	328	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

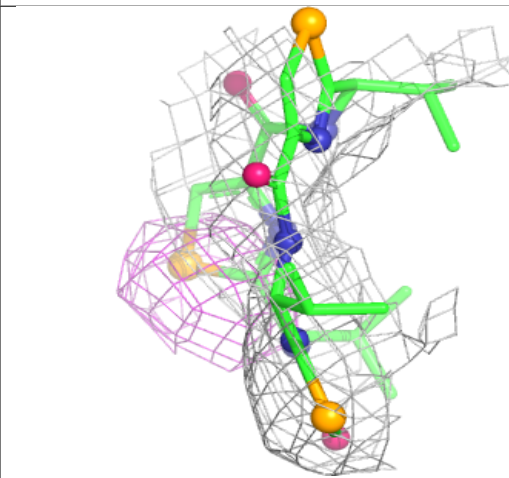
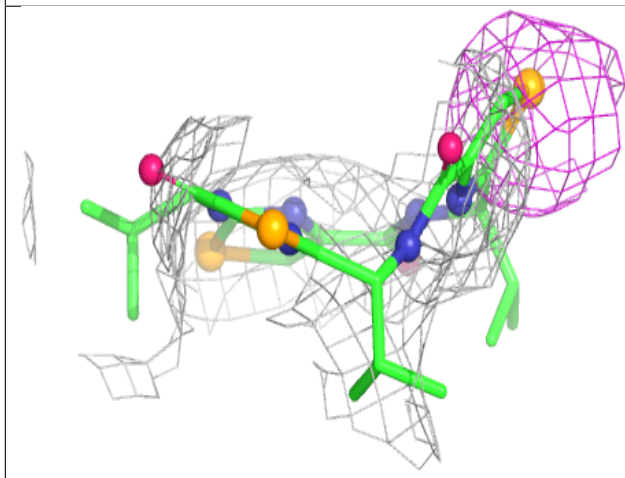
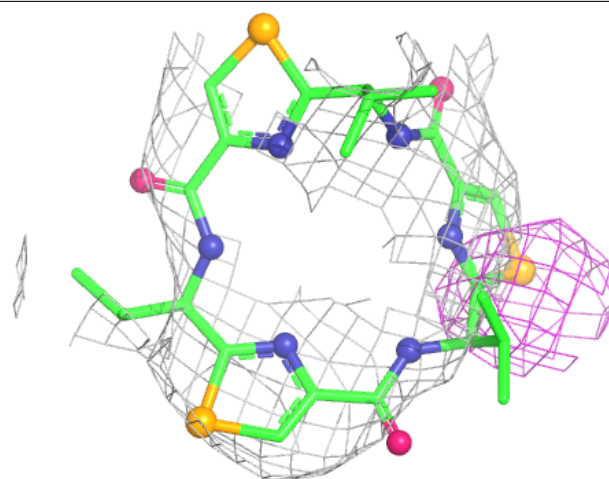
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

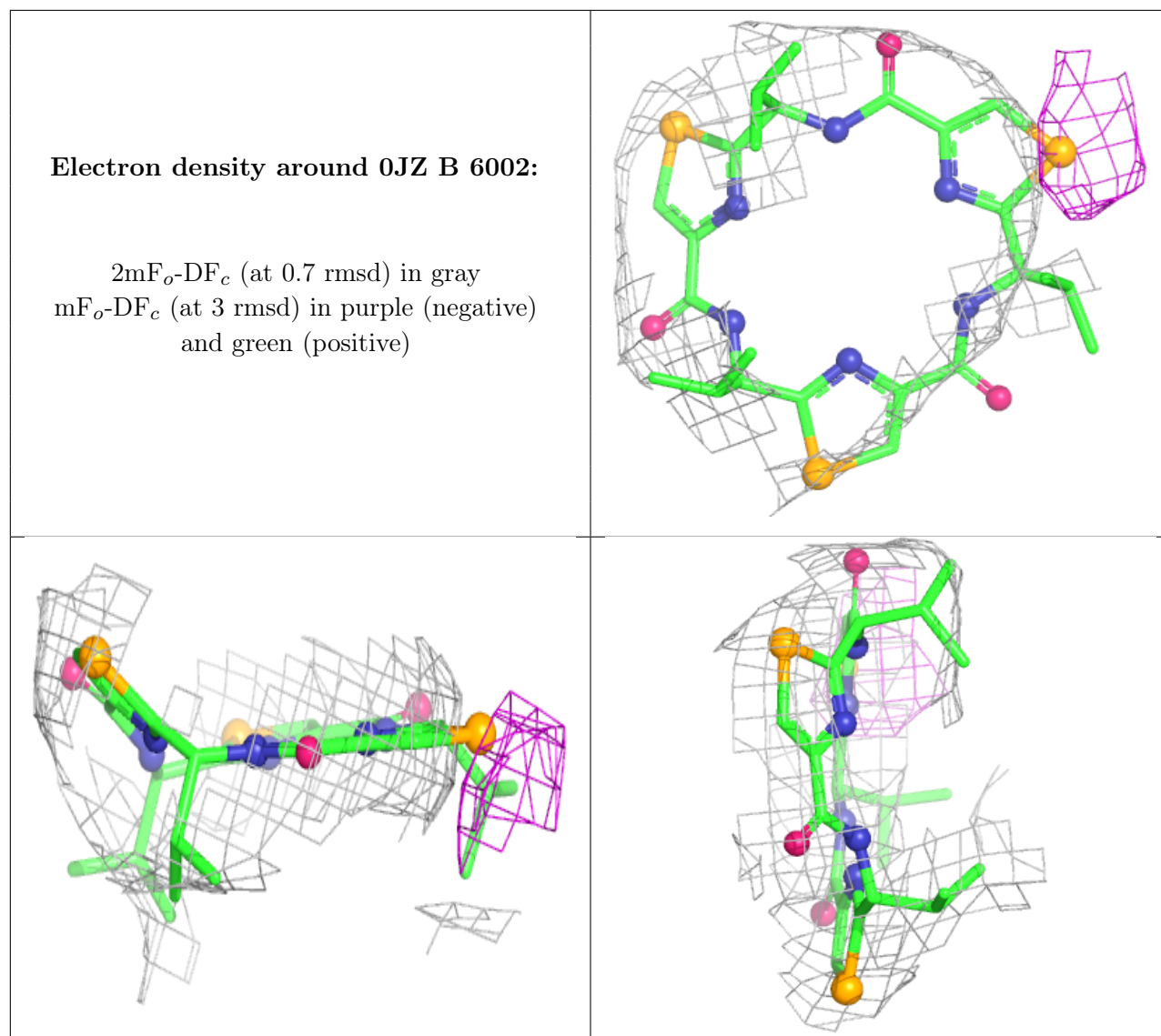
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	0JZ	A	6001	36/36	0.65	0.13	196,196,196,196	0
2	0JZ	B	6002	36/36	0.70	0.12	196,196,196,196	0

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 0JZ A 6001:

$2mF_o-DF_c$ (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.