



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:32 am BST

PDB ID : 3G60
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

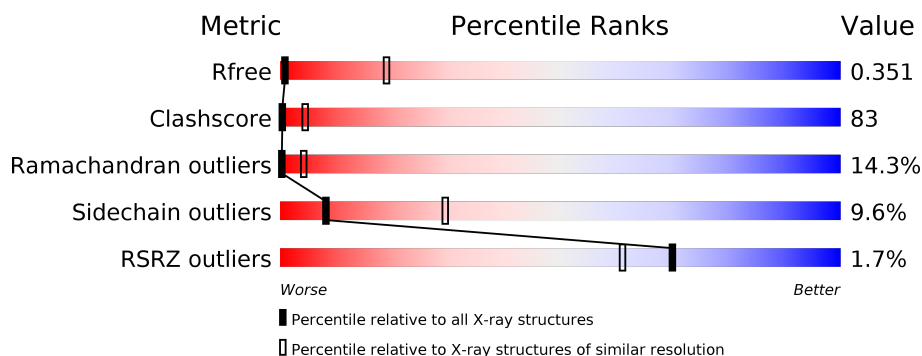
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1043 (5.00-3.80)
Clashscore	141614	1111 (5.00-3.80)
Ramachandran outliers	138981	1059 (5.00-3.80)
Sidechain outliers	138945	1041 (5.00-3.80)
RSRZ outliers	127900	1095 (5.08-3.70)

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

Mol	Chain	Length	Quality of chain
1	A	1284	<div> <div>2%</div> <div>16% 59% 15% 8%</div> </div>
1	B	1284	<div> <div>2%</div> <div>16% 59% 16% 8%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	0JZ	A	6001	-	-	-	X
2	0JZ	B	6002	-	-	-	X

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.

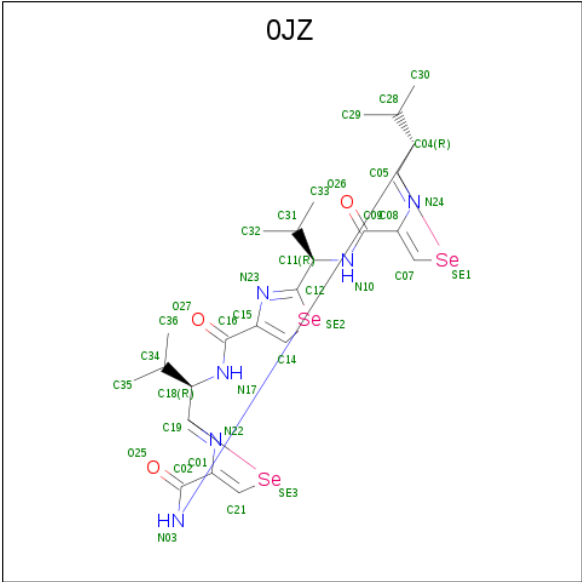
- Molecule 1 is a protein called Multidrug resistance protein 1a.

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			

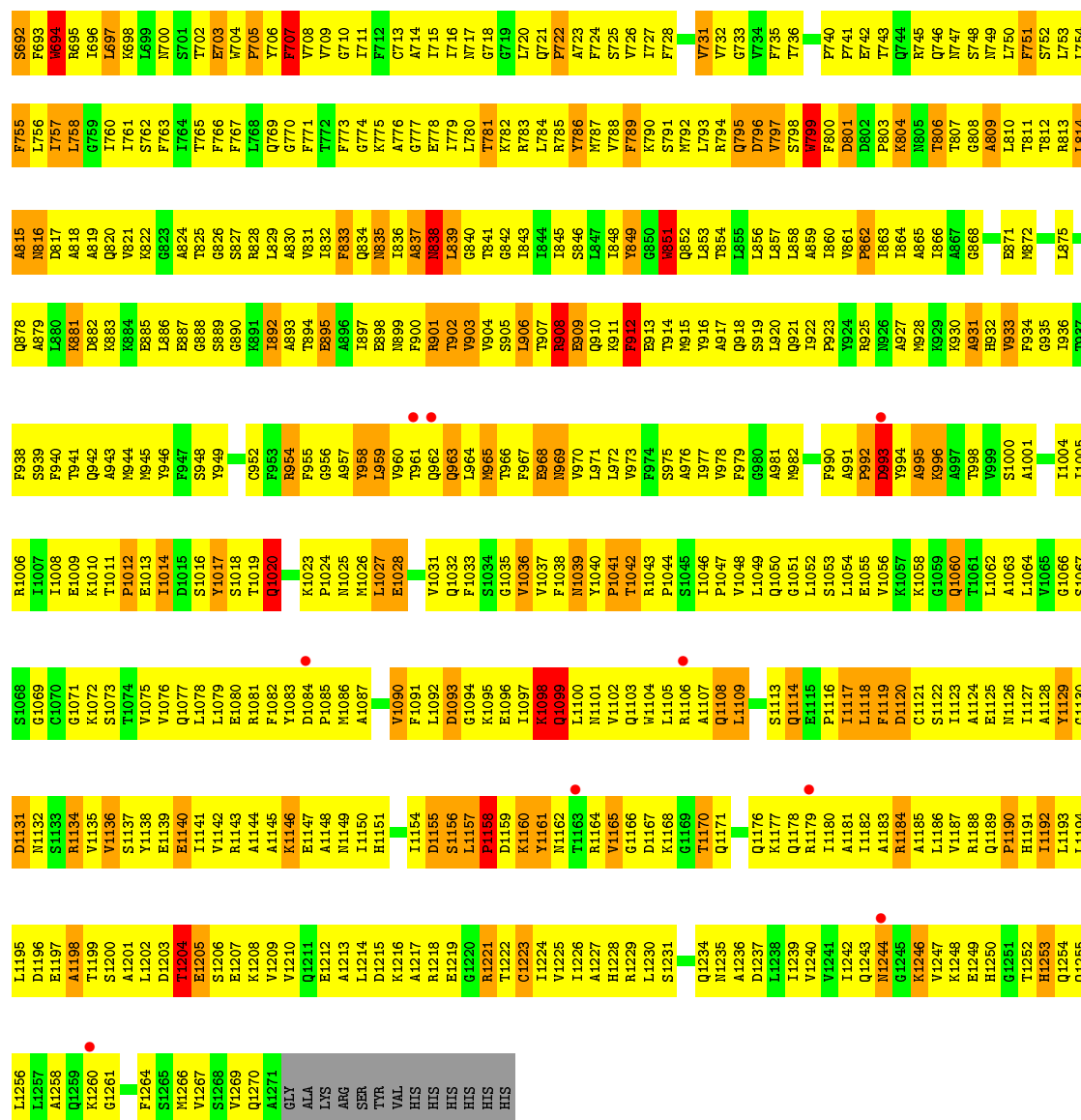
There are 16 discrepancies between the modelled and reference sequences:

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 (three-letter code: 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		



N1126	N1127	N1128	N1129	N1130	N1131	N1132	N1133	N1134	N1135	N1136	N1137	N1138	N1139	N1140	N1141	N1142	N1143	N1144	N1145	N1146	N1147	N1148	N1149	N1150	N1151		I1154	D1155	S1156	L1157	P1158	D1159	K1160	N1161	N1162	N1163	R1164	V1165	G1166	D1167	K1168	G1169	T1170	Q1171		Q1176	K1177	Q1178	R1179	I1180	A1181	I1182	A1183	C1121	A1185	I1186	V1187	R1188												
A1063	L1064	V1065	G1066	S1067	S1068	G1069	G1070	G1071	K1072	S1073	T1074	K1010	K1011	P1012	E1013	I1014	L1078	L1079	E1080	R1081	F1082	F1083	G1084	P1085	M1086	A1087		M1026	Q1020	G1021	L1022	K1023		M1026	L1027	V1031	Q1032	I1033	G1034	G1035	E1096	K1097	K1098	Q1099	F1037	M1038	L1100	N1101	Y1040	P1041	T1042	R1043	P1044	S1045	I1046	P1047	V1048	Q1050	G1051	L1052	S1053	L1054	E1055	V1056	K1057	R1058	G1059	Q1060	T1061	L1062
F934	G935	I936	T937	F938	S939	F940	T941	Q942	A943	N944	N945	Y946	F947	S948	Y949		Q952	F953	R954	F955	G956	A957	Y958	L959	V960	T961	Q962	L963	L964	T965	N966	F967	E968	N969	V970	L971	L972	V973	F974	S975	A976	I977	V978	F979	G980	A981	N982		S988	S989	F990	A991	F992	D993	Y994	A995	R996	A997	T998											
G808	A809	T810	T811	T812	R813	L814	A815	N816	D817	A818	L819	Q820	V821	G822	G823	A824	T825	G826	S827	R828	L829	A830	V831	I832	F833	Q834	N835	I836	A837	G838	N839	G840	S841	I842	I843	I844	I845	S846	L847	Y848	G850	R851	Q852	L853	T854	L855	L856	L857	L858	A859	I860	V861	P862	I863	I864	A865	I866	A867												
G868		E871	M872		L875		Q878	A879	L880	K881	D882	K883	K884	E885	L886	E887	G888	S889		I892	A893	T894	E895	A896	I897	E898	N899	F900	R901	Q902	V903	V904	S905	L906	T907	R908	E909	Q910	Q918	S919	L920	Q921	I922		A927	M928	K929	R930	A931	H932		V933																		
S748	N749	F751	P752	S753	A754	F755	L756	I757	L758	G759	I760	I761		F762	F763	I764	T765	F766	F767	R768	Q769	G770	F771	T772	F773	G774	K775	A776	G777	E778	I779	L780	K781	G782	R783	L784	R785	T786	V787	V788	F789	K790	S791	M792	L793	R794	Q795	D796	V797	S798	F799	F800	D801	D802	P803	K804	R805	T806	T807											
G808	A809	T810	T811	T812	R813	L814	A815	N816	D817	A818	L819	Q820	V821	G822	G823	A824	T825	G826	S827	R828	L829	A830	V831	I832	F833	Q834	N835	I836	A837	G838	N839	G840	S841	I842	I843	I844	I845	S846	L847	Y848	G850	R851	Q852	L853	T854	L855	L856	L857	L858	A859	I860	V861	P862	I863	I864	A865	I866	A867												
G868		E871	M872		L875		Q878	A879	L880	K881	D882	K883	K884	E885	L886	E887	G888	S889		I892	A893	T894	E895	A896	I897	E898	N899	F900	R901	Q902	V903	V904	S905	L906	T907	R908	E909	Q910	Q918	S919	L920	Q921	I922		A927	M928	K929	R930	A931	H932		V933																		
F934	G935	I936	T937	F938	S939	F940	T941	Q942	A943	N944	N945	Y946	F947	S948	Y949		Q952	F953	R954	F955	G956	A957	Y958	L959	V960	T961	Q962	L963	L964	T965	N966	F967	E968	N969	V970	L971	L972	V973	F974	S975	A976	I977	V978	F979	G980	A981	N982		S988	S989	F990	A991	F992	D993	Y994	A995	R996	A997	T998											
V999	S1000	A1001	S1002	H1003	I1004	I1005	K1006	I1007	Q942	A943	N944	N945	Y946	F947	S948	Y949		Q952	F953	R954	F955	G956	A957	Y958	L959	V960	T961	Q962	L963	L964	T965	N966	F967	E968	N969	V970	L971	L972	V973	F974	S975	A976	I977	V978	F979	G980	A981	N982		S988	S989	F990	A991	F992	D993	Y994	A995	R996	A997	T998										
A1063	L1064	V1065	G1066	S1067	S1068	G1069	G1070	G1071	K1072	S1073	T1074	K1010	K1011	P1012	E1013	I1014	L1078	L1079	E1080	R1081	F1082	F1083	G1084	P1085	M1086	A1087		M1026	Q1020	G1021	L1022	K1023		M1026	L1027	V1031	Q1032	I1033	G1034	G1035	E1096	K1097	K1098	Q1099	F1037	M1038	L1100	N1101	Y1040	P1041	T1042	R1043	P1044	S1045	I1046	P1047	V1048	Q1050	G1051	L1052	S1053	L1054	E1055	V1056	K1057	R1058	G1059	Q1060	T1061	L1062
N1126	N1127	N1128	N1129	N1130	N1131	N1132	N1133	N1134	N1135	N1136	N1137	N1138	N1139	N1140	N1141	N1142	N1143	N1144	N1145	N1146	N1147	N1148	N1149	N1150	N1151		I1154	D1155	S1156	L1157	P1158	D1159	K1160	N1161	N1162	N1163	R1164	V1165	G1166	D1167	K1168	G1169	T1170	Q1171		Q1176	K1177	Q1178	R1179	I1180	A1181	I1182	A1183	C1121	A1185	I1186	V1187	R1188												

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

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 49.02 – 4.31	Depositor EDS
% Data completeness (in resolution range)	94.7 (19.99-4.40) 93.3 (49.02-4.31)	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 0.297 , 0.351	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)	0.21 , 103.6	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	0.87	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 ⓘ

5.1 Standard geometry ⓘ

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	0.41	1/9339 (0.0%)	0.70	13/12626 (0.1%)
1	B	0.41	0/9339	0.68	8/12626 (0.1%)
All	All	0.41	1/18678 (0.0%)	0.69	21/25252 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	851	TRP	CB-CG	5.17	1.59	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	427	CYS	N-CA-C	9.35	136.24	111.00
1	A	1098	LYS	N-CA-C	-7.80	89.94	111.00
1	A	164	VAL	N-CA-C	-7.79	89.98	111.00
1	A	267	LYS	N-CA-C	7.23	130.52	111.00
1	A	165	GLY	N-CA-C	-7.16	95.21	113.10
1	A	603	VAL	N-CA-C	7.01	129.92	111.00
1	A	450	ASP	N-CA-C	-6.87	92.46	111.00
1	B	267	LYS	N-CA-C	6.55	128.68	111.00
1	B	450	ASP	N-CA-C	-6.48	93.51	111.00
1	A	64	LEU	C-N-CD	6.36	141.75	128.40
1	B	64	LEU	C-N-CD	6.27	141.57	128.40
1	B	852	GLN	N-CA-C	-5.96	94.92	111.00
1	A	42	ALA	N-CA-C	5.64	126.24	111.00
1	A	574	GLU	N-CA-C	5.63	126.21	111.00
1	A	384	ILE	N-CA-C	-5.50	96.15	111.00
1	B	165	GLY	N-CA-C	-5.49	99.38	113.10
1	B	377	SER	N-CA-C	5.46	125.76	111.00
1	B	208	TRP	CB-CA-C	-5.19	100.02	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1020	GLN	N-CA-C	5.18	125.00	111.00
1	A	851	TRP	N-CA-C	5.18	124.99	111.00
1	A	1160	LYS	N-CA-C	-5.13	97.15	111.00

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	1558	0
1	B	9171	0	9344	1534	0
2	A	36	0	27	12	0
2	B	36	0	27	10	0
All	All	18414	0	18742	3089	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 83.

All (3089) 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:H	1:A:270:LEU:HD23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:B:270:LEU:HD23	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
1:B:979:PHE:O	1:B:982:MET:HG2	1.62	0.99
1:A:164:VAL:O	1:A:164:VAL:HG23	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:1114:GLN:HE22	1:A:1200:SER:HB3	1.27	0.97
1:A:686:GLU:HG2	1:A:813:ARG:HH22	1.29	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:B:58:ILE:HG13	1:B:193:MET:HG3	1.49	0.94
1:A:853:LEU:HG	1:A:973:VAL:HG21	1.48	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:155:GLU:HB3	1:A:156:ILE:HD12	1.48	0.93
1:A:58:ILE:HG13	1:A:193:MET:HG3	1.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HE2	1:B:1216:LYS:HA	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:HD3	1:A:996:LYS:H	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:1091:PHE:HE1	1:B:1096:GLU:HG2	1.41	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:1037:VAL:HG12	1:A:1051:GLY:H	1.42	0.84
1:A:976:ALA:HA	1:A:979:PHE:CD2	2.12	0.84
1:B:1014:ILE:HA	1:B:1102:VAL:HG11	1.59	0.84
1:B:401:LYS:HD2	1:B:401:LYS:H	1.42	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:1091:PHE:HE1	1:A:1096:GLU:HG2	1.41	0.83
1:A:725:SER:HA	2:A:6001:OJZ:H36	1.59	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:1179:ARG:NH2	1:A:1209:VAL:HG11	1.94	0.82
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: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:773:PHE:O	1:B:776:ALA:HB3	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1218:ARG:HH22	1:A:1235:ASN:HD22	1.28	0.82
1:A:358:ALA:O	1:A:362:PHE:HB2	1.79	0.82
1:B:1179:ARG:NH2	1:B:1209:VAL:HG11	1.95	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: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:A:163:ASP:O	1:A:164:VAL:C	2.19	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:1121:CYS:HB2	1:A:1126:ASN:HD21	1.46	0.81
1:B:1121:CYS:HB2	1:B:1126:ASN:HD21	1.44	0.81
1:B:318:ILE:HD11	1:B:324:ILE:HD12	1.62	0.81
1:B:802:ASP:CG	1:B:1041:PRO:HB2	2.01	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:HD2	1:A:401:LYS:H	1.44	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:1142:VAL:O	1:A:1146:LYS:HG2	1.82	0.79
1:A:59:ILE:HD11	1:A:124:VAL:HG11	1.62	0.79
1:A:278:GLU:C	1:A:282:ARG:HG2	2.03	0.79
1:A:508:PHE:HE2	1:A:534:ARG:HD2	1.47	0.79
1:A:286:LYS:O	1:A:290:THR:HG23	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:VAL:HG23	1:A:36:LEU:N	1.97	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:1062:LEU:HD12	1:A:1224:ILE:HG23	1.65	0.78
1:A:689:PRO:HB2	1:A:690:PRO:HD3	1.66	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:A:905:SER:C	1:A:907:THR:H	1.86	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:1113:SER:HA	1:B:1196:ASP:HB3	1.66	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:A:797:VAL:O	1:A:801:ASP:CB	2.32	0.78
1:A:1260:LYS:HD2	1:A:1260:LYS:H	1.48	0.78
1:A:864:ILE:HD12	1:A:865:ALA:N	1.99	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:1181:ALA:O	1:B:1184:ARG:HB3	1.84	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: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:91:MET:HB2	1:A:94:ALA:HB3	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:1014:ILE:HB	1:A:1102:VAL:HG21	1.66	0.76
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1260:LYS:HD2	1:B:1260:LYS:H	1.50	0.76
1:B:91:MET:HB2	1:B:94:ALA:HB3	1.68	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:324:ILE:HD12	1:B:326:GLN:H	1.51	0.76
1:B:286:LYS:HG2	1:B:778:GLU:CG	2.15	0.76
1:B:1062:LEU:HD12	1:B:1224:ILE:HG23	1.66	0.76
1:B:504:ASN:O	1:B:534:ARG:HD3	1.85	0.76
1:B:797:VAL:O	1:B:801:ASP:CG	2.23	0.76
1:A:753:LEU:HD12	1:A:756:LEU:HD11	1.68	0.76
1:A:722:PRO:HB2	1:A:841:THR:HG21	1.68	0.76
1:B:1056:VAL:HG23	1:B:1060:GLN:HE22	1.50	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:A:1181:ALA:O	1:A:1184:ARG:HB3	1.85	0.76
1:A:740:PRO:HG2	1:A:741:PRO:HD3	1.68	0.76
1:B:278:GLU:C	1:B:282:ARG:HG2	2.05	0.76
1:B:905:SER:C	1:B:907:THR:H	1.88	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:B:797:VAL:HG12	1:B:798:SER:N	2.01	0.75
1:A:608:HIS:HD1	1:A:618:TYR:HE2	1.33	0.75
1:A:853:LEU:H	1:A:853:LEU:HD22	1.51	0.75
1:B:1033:PHE:HB3	1:B:1036:VAL:HG21	1.68	0.75
1:B:270:LEU:HD23	1:B:270:LEU:N	1.98	0.75
1:B:35:VAL:HG12	1:B:359:TYR:CE2	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:N	1:A:270:LEU:HD23	1.99	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
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: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:1199:THR:HG23	1:B:1210:VAL:HG11	1.67	0.74
1:B:401:LYS:NZ	1:B:401:LYS:HB3	2.02	0.74
1:A:1056:VAL:HG23	1:A:1060:GLN:HE22	1.50	0.74
1:A:686:GLU:HG2	1:A:813:ARG:NH2	2.02	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: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: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: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:A:128:GLN:O	1:A:131:PHE:HB3	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:1100:LEU:HG	1:B:1101:ASN:H	1.53	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: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:1027:LEU:H	1:B:1027:LEU:HD23	1.53	0.73
1:B:282:ARG:O	1:B:286:LYS:HB2	1.87	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:B:993:ASP:N	1:B:996:LYS:HZ1	1.86	0.73
1:B:1063:ALA:HB2	1:B:1236:ALA:HB1	1.69	0.73
1:B:722:PRO:O	1:B:725:SER:HB2	1.87	0.73
1:A:1242:ILE:HA	1:A:1247:VAL:HA	1.70	0.73
1:A:972:LEU:HD12	1:A:972:LEU:H	1.52	0.73
1:B:407:LYS:HZ1	1:B:601:VAL:HA	1.54	0.73
1:A:1013:GLU:O	1:A:1014:ILE:HG23	1.89	0.73
1:A:332:PHE:O	1:A:335:LEU:HB3	1.88	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:1242:ILE:HA	1:B:1247:VAL:HA	1.69	0.73
1:B:930:LYS:O	1:B:933:VAL:HB	1.88	0.73
1:B:972:LEU:HD12	1:B:972:LEU:H	1.52	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:B:992:PRO:HB2	1:B:996:LYS:HZ1	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:PHE:HA	1:A:211:THR:HG21	1.71	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
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: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:A:1218:ARG:HH22	1:A:1235:ASN:ND2	1.87	0.71
1:B:1121:CYS:HB2	1:B:1126:ASN:ND2	2.05	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: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:1150:ILE:HB	1:B:1179:ARG:HB3	1.72	0.71
1:B:795:GLN:HE21	1:B:796:ASP:H	1.38	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: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:A:1100:LEU:HG	1:A:1101:ASN:H	1.56	0.71
1:A:187:GLY:O	1:A:190:PHE:HB3	1.89	0.71
1:B:288:ALA:HA	1:B:291:ALA:CB	2.18	0.71
1:A:186:ILE:HG13	1:A:187:GLY:N	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:122:LEU:HD12	1:A:939:SER:HB2	1.72	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:688:VAL:HB	1:A:1006:ARG:HH12	1.56	0.70
1:A:471:GLN:O	1:A:473:PRO:HD3	1.91	0.70
1:B:211:THR:O	1:B:215:LEU:HG	1.91	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:A:59:ILE:CD1	1:A:124:VAL:HG11	2.21	0.70
1:B:239:GLU:HB3	1:B:285:ILE:HG12	1.73	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: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:A:1218:ARG:NH2	1:A:1235:ASN:HD22	1.88	0.70
1:A:482:GLU:O	1:A:485:ARG:N	2.25	0.70
1:A:416:GLY:N	1:A:577:THR:HG22	2.05	0.70
1:B:1218:ARG:NH2	1:B:1235:ASN:HD22	1.88	0.70
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:A:386:GLY:HA3	1:A:450:ASP:HA	1.73	0.69
1:A:482:GLU:O	1:A:483:ASN:C	2.29	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:779:ILE:HG13	1:B:780:LEU:N	2.08	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:B:802:ASP:CB	1:B:1041:PRO:HB2	2.22	0.69
1:B:1031:VAL:HB	1:B:1056:VAL:HG12	1.75	0.69
1:A:1193:LEU:HD11	1:A:1217:ALA:O	1.93	0.69
1:A:158:TRP:O	1:A:164:VAL:HG11	1.91	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:905:SER:O	1:A:907:THR:N	2.26	0.69
1:A:133:CYS:SG	1:A:931:ALA:HA	2.32	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:B:482:GLU:O	1:B:483:ASN:C	2.31	0.69
1:B:254:LEU:HD12	1:B:789:PHE:HZ	1.58	0.69
1:A:1001:ALA:O	1:A:1005:ILE:HG12	1.92	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:B:1248:LYS:HA	1:B:1248:LYS:HE3	1.73	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: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:B:1106:ARG:HA	1:B:1109:LEU:HD13	1.75	0.69
1:A:1138:TYR:O	1:A:1141:ILE:HG12	1.92	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:B:1127:ILE:HD13	1:B:1180:ILE:HG23	1.75	0.69
1:B:552:GLU:HB3	1:B:555:SER:OG	1.92	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:B:705:PRO:HG2	1:B:706:TYR:H	1.58	0.69
1:A:1020:GLN:HG3	1:A:1101:ASN:CB	2.23	0.69
1:A:195:THR:HG23	1:A:196:PHE:H	1.58	0.69
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1127:ILE:HD13	1:A:1180:ILE:HG23	1.74	0.68
1:A:1031:VAL:HB	1:A:1056:VAL:HG12	1.75	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:60:HIS:O	1:A:63:ALA:HB3	1.93	0.68
1:A:762:SER:HA	1:A:765:THR:HG22	1.74	0.68
1:A:39:PHE:HE2	1:A:358:ALA:HB3	1.58	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:A:99:MET:HB3	1:A:960:VAL:O	1.93	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:1054:LEU:HD11	1:A:1240:VAL:HG11	1.75	0.68
1:A:390:PHE:HE1	1:A:432:THR:HB	1.59	0.68
1:B:1048:VAL:O	1:B:1049:LEU:HD22	1.94	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:A:1106:ARG:HA	1:A:1109:LEU:HD13	1.76	0.68
1:A:388:LEU:HB2	1:A:413:VAL:HG12	1.76	0.68
1:A:138:ARG:HH22	1:B:515:GLN:HE21	1.40	0.68
1:A:164:VAL:O	1:A:164:VAL:CG2	2.32	0.68
1:A:257:ILE:HD13	1:A:257:ILE:C	2.14	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: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:285:ILE:O	1:A:285:ILE:HD13	1.94	0.67
1:A:178:ILE:HG12	1:A:358:ALA:HB2	1.76	0.67
1:A:35:VAL:O	1:A:39:PHE:HB2	1.95	0.67
1:A:405:ILE:CG2	1:A:428:GLY:HA2	2.25	0.67
1:A:251:GLU:OE1	1:A:811:THR:HB	1.94	0.67
1:B:1054:LEU:HD11	1:B:1240:VAL:HG11	1.75	0.67
1:A:1039:ASN:ND2	1:A:1047:PRO:HA	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:766:PHE:HA	1:B:769:GLN:HE21	1.59	0.67
1:A:1039:ASN:CB	1:A:1047:PRO:HA	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:B:133:CYS:O	1:B:134:LEU:C	2.31	0.67
1:B:303:TYR:O	1:B:306:TYR:N	2.27	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: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:A:856:LEU:HD22	1:A:955:PHE:CD1	2.28	0.67
1:B:1266:MET:O	1:B:1269:VAL:HG12	1.94	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: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: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:B:60:HIS:O	1:B:63:ALA:HB3	1.94	0.66
1:A:1218:ARG:HH12	1:A:1235:ASN:ND2	1.93	0.66
1:A:178:ILE:HG12	1:A:358:ALA:CB	2.25	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: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: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
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:283:LEU:HD12	1:B:284:GLY:N	2.10	0.66
1:B:502:GLU:C	1:B:504:ASN:H	1.97	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ILE:HD11	1:B:124:VAL:HG21	1.78	0.66
1:A:1189:GLN:N	1:A:1190:PRO:HD3	2.09	0.66
1:A:447:VAL:HG13	1:A:454:ILE:HG21	1.77	0.66
1:A:96:LYS:HG2	1:A:962:GLN:HB2	1.75	0.66
1:B:185:LYS:HZ2	1:B:185:LYS:HB3	1.61	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:1150:ILE:O	1:A:1154:ILE:HD13	1.95	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: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:B:218:SER:HB2	1:B:219:PRO:CD	2.26	0.66
1:B:603:VAL:HG23	1:B:604:GLU:H	1.61	0.66
1:A:133:CYS:O	1:A:134:LEU:C	2.34	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: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: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: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:290:THR:HG22	1:B:770:GLY:C	2.17	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:384:ILE:HG22	1:B:385:GLN:H	1.60	0.65
1:B:39:PHE:HE2	1:B:358:ALA:HB3	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
1:A:1039:ASN:HD22	1:A:1047:PRO:HA	1.62	0.65
1:A:324:ILE:O	1:A:326:GLN:N	2.30	0.65
1:B:1202:LEU:HD21	1:B:1206:SER:HB3	1.77	0.65
1:B:178:ILE:HG12	1:B:358:ALA:CB	2.26	0.65
1:A:246:ALA:CB	1:A:277:LEU:HB3	2.23	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1137:SER:OG	1:A:1140:GLU:HB2	1.96	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:B:1195:LEU:HD23	1:B:1214:LEU:HD11	1.78	0.65
1:B:324:ILE:O	1:B:326:GLN:N	2.29	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:1138:TYR:O	1:B:1141:ILE:HG12	1.97	0.65
1:B:311:TRP:HE3	1:B:311:TRP:HA	1.61	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: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:1185:ALA:O	1:A:1190:PRO:HD3	1.97	0.65
1:A:902:THR:HG23	1:A:903:VAL:H	1.62	0.65
1:B:424:ASN:HB3	1:B:598:ASP:OD1	1.97	0.65
1:B:465:ILE:C	1:B:466:ILE:HD12	2.17	0.65
1:A:1048:VAL:O	1:A:1049:LEU:HD22	1.97	0.65
1:A:458:ASN:HD22	1:A:459:VAL:N	1.94	0.65
1:B:1058:LYS:O	1:B:1060:GLN:HG3	1.96	0.65
1:B:478:THR:HG21	1:B:482:GLU:HG3	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:B:421:LEU:HB3	1:B:429:LYS:HB3	1.78	0.65
1:B:88:SER:O	1:B:90:ASN:N	2.30	0.65
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
1:A:35:VAL:CG2	1:A:36:LEU:H	2.02	0.64
1:B:121:VAL:HG23	1:B:122:LEU:N	2.12	0.64
1:B:49:TYR:CE2	1:B:134:LEU:HD12	2.32	0.64
1:B:311:TRP:CE3	1:B:311:TRP:HA	2.32	0.64
1:A:270:LEU:CD2	1:A:270:LEU:H	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:B:270:LEU:CD2	1:B:270:LEU:H	2.01	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:257:ILE:HD13	1:B:257:ILE:C	2.17	0.64
1:B:423:GLY:HA2	1:B:597:PHE:O	1.97	0.64
1:A:1234:GLN:HA	1:A:1253:HIS:HD2	1.62	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:B:1203:ASP:O	1:B:1204:THR:O	2.15	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:158:TRP:CZ2	1:B:900:PHE:HB2	2.33	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:1080:GLU:OE2	1:A:1109:LEU:HD12	1.97	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:B:1080:GLU:OE2	1:B:1109:LEU:HD12	1.97	0.64
1:B:1014:ILE:HD12	1:B:1106:ARG:HH11	1.62	0.64
1:B:881:LYS:HB2	1:B:881:LYS:NZ	2.12	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:A:502:GLU:C	1:A:504:ASN:H	2.01	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:A:766:PHE:HA	1:A:769:GLN:HE21	1.62	0.64
1:B:1039:ASN:HD22	1:B:1047:PRO:HA	1.63	0.64
1:B:185:LYS:HB3	1:B:185:LYS:NZ	2.11	0.64
1:B:207:GLY:HA2	1:B:210:LEU:HB3	1.80	0.64
1:B:207:GLY:HA3	1:B:211:THR:N	2.12	0.64
1:B:331:PHE:O	1:B:334:VAL:HG12	1.97	0.64
1:B:293:ILE:HG22	1:B:766:PHE:HB3	1.78	0.64
1:A:458:ASN:HD22	1:A:459:VAL:H	1.45	0.64
1:A:49:TYR:CE2	1:A:134:LEU:HD12	2.33	0.64
1:A:90:ASN:HB2	1:A:91:MET:HE2	1.80	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:HE3	1:A:311:TRP:HA	1.63	0.63
1:A:478:THR:HG21	1:A:482:GLU:HG3	1.78	0.63
1:A:799:TRP:HE3	1:A:799:TRP:HA	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:881:LYS:NZ	1:A:881:LYS:HB2	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:879:ALA:O	1:A:883:LYS:HG2	1.99	0.63
1:B:1039:ASN:ND2	1:B:1047:PRO:HA	2.12	0.63
1:B:569:LEU:O	1:B:573:ARG:HG3	1.98	0.63
1:A:611:LEU:HD23	1:A:618:TYR:HB2	1.80	0.63
1:B:1214:LEU:HD23	1:B:1214:LEU:O	1.98	0.63
1:B:175:VAL:HG13	1:B:176:SER:N	2.13	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:A:465:ILE:C	1:A:466:ILE:HD12	2.19	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:B:981:ALA:HB3	2:B:6002:OJZ:H35	1.78	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
1:A:1095:LYS:HD2	1:A:1095:LYS:H	1.62	0.63
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: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:A:45:LEU:H	1:A:45:LEU:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1214:LEU:HA	1:A:1217:ALA:HB3	1.81	0.62
1:A:428:GLY:O	1:A:431:THR:HB	1.99	0.62
1:B:375:SER:C	1:B:376:LYS:HD2	2.19	0.62
1:B:696:ILE:HD13	1:B:998:THR:HG23	1.79	0.62
1:A:253:VAL:HB	1:A:1119:PHE:HE1	1.63	0.62
1:A:39:PHE:CE2	1:A:355:ARG:HA	2.34	0.62
1:B:1048:VAL:HG23	1:B:1049:LEU:CD2	2.30	0.62
1:B:807:THR:O	1:B:811:THR:HG23	2.00	0.62
1:A:1019:THR:OG1	1:A:1101:ASN:HA	1.99	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: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:HD2	1:B:1221:ARG:H	1.64	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:HE3	1:B:799:TRP:HA	1.64	0.62
1:B:857:LEU:HD12	1:B:973:VAL:CG1	2.29	0.62
1:A:195:THR:HB	1:A:340:SER:OG	1.99	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:N	1:B:388:LEU:HD12	2.14	0.62
1:B:608:HIS:ND1	1:B:618:TYR:HE2	1.97	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:A:696:ILE:HD13	1:A:998:THR:HG23	1.80	0.62
1:B:1158:PRO:O	1:B:1159:ASP:HB2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:PRO:O	1:B:68:MET:N	2.33	0.62
1:A:1048:VAL:HG23	1:A:1049:LEU:CD2	2.29	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:1179:ARG:HH21	1:A:1209:VAL:HG11	1.60	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:B:1037:VAL:HG12	1:B:1051:GLY:N	2.14	0.62
1:B:846:SER:HA	1:B:849:TYR:CD1	2.35	0.62
1:B:158:TRP:HE1	1:B:900:PHE:HB3	1.65	0.62
1:A:107:MET:HA	1:A:110:TYR:HD2	1.63	0.62
1:A:185:LYS:HZ3	1:A:186:ILE:N	1.98	0.62
1:B:1216:LYS:CE	1:B:1216:LYS:HA	2.30	0.62
1:B:905:SER:O	1:B:907:THR:N	2.33	0.62
1:B:722:PRO:HD3	1:B:982:MET:HE1	1.82	0.62
1:A:537:ILE:O	1:A:541:LEU:HB2	1.99	0.61
1:B:217:ILE:HD11	1:B:331:PHE:HE2	1.64	0.61
1:B:39:PHE:CE2	1:B:355:ARG:HA	2.35	0.61
1:B:916:TYR:O	1:B:920:LEU:HD23	1.99	0.61
1:B:1196:ASP:HA	1:B:1226:ILE:CG1	2.30	0.61
1:B:155:GLU:O	1:B:157:GLY:N	2.33	0.61
1:B:50:MET:HG3	1:B:131:PHE:CE2	2.33	0.61
1:B:538:ALA:O	1:B:541:LEU:HB3	1.99	0.61
1:B:574:GLU:HG3	1:B:574:GLU:O	1.98	0.61
1:B:956:GLY:O	1:B:966:THR:CB	2.46	0.61
1:A:1037:VAL:HG12	1:A:1051:GLY:N	2.14	0.61
1:A:806:THR:O	1:A:810:LEU:HG	2.00	0.61
1:B:1095:LYS:HD2	1:B:1095:LYS:H	1.64	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:A:282:ARG:O	1:A:286:LYS:HD3	2.00	0.61
1:A:913:GLU:HA	1:A:913:GLU:OE2	2.00	0.61
1:B:67:MET:SD	1:B:113:TYR:HE1	2.23	0.61
1:B:1184:ARG:O	1:B:1187:VAL:HB	2.00	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:A:204:PHE:CA	1:A:211:THR:HG21	2.30	0.61
1:A:67:MET:SD	1:A:113:TYR:HE1	2.24	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1216:LYS:CE	1:A:1216:LYS:HA	2.30	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:217:ILE:HD11	1:A:331:PHE:HE2	1.65	0.61
1:B:154:GLN:NE2	1:B:162:HIS:NE2	2.42	0.61
1:B:321:GLU:O	1:B:322:TYR:C	2.38	0.61
1:B:969:ASN:HD22	1:B:970:VAL:N	1.98	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:268:LYS:HZ2	1:A:272:ARG:HD3	1.66	0.61
1:B:1075:VAL:O	1:B:1076:VAL:C	2.39	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:A:722:PRO:HD3	1:A:982:MET:HE1	1.81	0.61
1:B:1038:PHE:CG	1:B:1039:ASN:N	2.68	0.61
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:A:1148:ALA:O	1:A:1149:ASN:HB2	2.01	0.61
1:A:1158:PRO:O	1:A:1159:ASP:HB2	2.01	0.61
1:A:492:THR:HG22	1:A:494:ASP:H	1.66	0.61
1:B:968:GLU:O	1:B:971:LEU:HD23	2.01	0.61
1:A:287:LYS:O	1:A:291:ALA:HB2	2.01	0.61
1:A:843:ILE:O	1:A:846:SER:HB3	2.00	0.61
1:B:1148:ALA:HB1	1:B:1179:ARG:O	2.01	0.61
1:B:154:GLN:HE22	1:B:162:HIS:CD2	2.19	0.61
1:A:1023:LYS:O	1:A:1025:ASN:N	2.34	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:B:133:CYS:O	1:B:135:ALA:N	2.34	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:1144:ALA:CA	1:A:1186:LEU:HD11	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:766:PHE:O	1:A:769:GLN:HG2	2.01	0.60
1:B:1148:ALA:O	1:B:1149:ASN:HB2	2.02	0.60
1:B:906:LEU:O	1:B:906:LEU:HD23	2.00	0.60
1:B:959:LEU:O	1:B:964:LEU:HB3	2.01	0.60
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:B:125:ALA:O	1:B:128:GLN:HG2	2.01	0.60
1:A:1075:VAL:O	1:A:1076:VAL:C	2.40	0.60
1:A:267:LYS:HB3	1:A:790:LYS:CE	2.29	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:59:ILE:CG1	1:B:124:VAL:HG11	2.32	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:1193:LEU:HB2	1:A:1223:CYS:CB	2.32	0.60
1:A:211:THR:O	1:A:214:ILE:HB	2.01	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:B:64:LEU:O	1:B:67:MET:HB3	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: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:857:LEU:C	1:B:857:LEU:HD23	2.22	0.60
1:A:291:ALA:HA	1:A:294:SER:HB2	1.83	0.60
1:A:905:SER:C	1:A:907:THR:N	2.54	0.60
1:B:1202:LEU:HG	1:B:1206:SER:HB2	1.83	0.60
1:A:1063:ALA:HB3	1:A:1239:ILE:CA	2.26	0.60
1:B:197:PHE:O	1:B:201:ILE:HD13	2.01	0.60
1:B:406:LEU:HD12	1:B:409:LEU:HB2	1.84	0.60
1:B:388:LEU:HD11	1:B:547:ILE:HD12	1.84	0.60
1:B:133:CYS:CB	1:B:931:ALA:HB1	2.32	0.60
1:A:1038:PHE:O	1:A:1049:LEU:HB2	2.02	0.60
1:A:608:HIS:ND1	1:A:618:TYR:HE2	1.97	0.60
1:B:163:ASP:C	1:B:165:GLY:H	2.05	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:TYR:HE1	1:A:143:ILE:HD11	1.67	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
1:A:807:THR:O	1:A:811:THR:HG23	2.01	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:1020:GLN:CD	1:B:1020:GLN:N	2.56	0.59
1:B:268:LYS:HZ2	1:B:272:ARG:HD3	1.67	0.59
1:B:156:ILE:HD11	1:B:373:SER:HB3	1.83	0.59
1:B:41:TYR:HE1	1:B:143:ILE:HD11	1.67	0.59
1:B:978:VAL:CG1	2:B:6002:OJZ:H35B	2.30	0.59
1:B:731:VAL:HG22	1:B:750:LEU:HB3	1.84	0.59
1:A:1023:LYS:C	1:A:1025:ASN:H	2.06	0.59
1:A:762:SER:O	1:A:765:THR:HG22	2.02	0.59
1:B:1120:ASP:HA	1:B:1165:VAL:HG21	1.84	0.59
1:A:1009:GLU:C	1:A:1010:LYS:HG3	2.22	0.59
1:A:1100:LEU:HG	1:A:1101:ASN:N	2.16	0.59
1:A:279:GLU:HG2	1:A:782:LYS:CD	2.32	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:A:857:LEU:HD23	1:A:857:LEU:C	2.22	0.59
1:B:1022:LEU:HD23	1:B:1022:LEU:O	2.02	0.59
1:B:81:VAL:HG13	1:B:99:MET:HG3	1.85	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:A:254:LEU:HD23	1:A:811:THR:CG2	2.30	0.59
1:B:1144:ALA:HB1	1:B:1183:ALA:HB1	1.85	0.59
1:B:235:PHE:O	1:B:239:GLU:HG2	2.02	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:A:1018:SER:O	1:A:1101:ASN:HB2	2.02	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:B:1020:GLN:HG2	1:B:1021:GLY:N	2.02	0.59
1:B:617:ILE:O	1:B:621:LEU:HD23	2.03	0.59
1:B:913:GLU:OE2	1:B:913:GLU:HA	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:933:VAL:O	1:B:934:PHE:C	2.40	0.59
2:A:6001:OJZ:H36B	2:A:6001:OJZ:O27	2.02	0.59
1:B:1267:VAL:O	1:B:1270:GLN:HB3	2.02	0.59
1:B:185:LYS:HZ3	1:B:186:ILE:N	1.99	0.59
1:A:1020:GLN:HB3	1:A:1100:LEU:HD12	1.85	0.59
1:B:107:MET:HA	1:B:110:TYR:CD2	2.38	0.59
1:B:1109:LEU:HD21	1:B:1188:ARG:NH1	2.17	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:390:PHE:HB2	1:B:411:LEU:O	2.03	0.59
1:A:170:ARG:HB2	1:A:170:ARG:HH11	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:A:1109:LEU:HD21	1:A:1188:ARG:NH1	2.18	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:148:PHE:HB3	1:A:913:GLU:CD	2.24	0.59
1:B:1120:ASP:HA	1:B:1165:VAL:CG2	2.33	0.59
1:B:49:TYR:OH	1:B:130:SER:HB2	2.03	0.59
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:A:779:ILE:HG13	1:A:780:LEU:H	1.66	0.58
1:A:797:VAL:O	1:A:801:ASP:CG	2.40	0.58
1:B:302:ILE:O	1:B:305:SER:HB3	2.02	0.58
1:B:327:VAL:HB	1:B:331:PHE:CE1	2.38	0.58
1:B:766:PHE:O	1:B:767:PHE:C	2.41	0.58
1:A:902:THR:OG1	1:A:908:ARG:HD3	2.03	0.58
1:B:1261:GLY:H	1:B:1264:PHE:HB3	1.68	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: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
1:A:993:ASP:N	1:A:996:LYS:HZ1	2.01	0.58
1:A:81:VAL:HG13	1:A:99:MET:HG3	1.86	0.58
1:B:1005:ILE:O	1:B:1008:ILE:HG22	2.03	0.58
1:B:217:ILE:O	1:B:221:LEU:HG	2.02	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:905:SER:C	1:B:907:THR:N	2.55	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:64:LEU:O	1:A:67:MET:HB3	2.03	0.58
1:A:804:LYS:HD3	1:A:804:LYS:N	2.19	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:B:585:LEU:H	1:B:585:LEU:HD22	1.68	0.58
1:A:1009:GLU:O	1:A:1010:LYS:HG3	2.03	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: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:37:THR:O	1:B:40:ARG:N	2.34	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: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:602:ILE:O	1:A:603:VAL:HG13	2.04	0.58
1:A:257:ILE:HG13	1:A:800:PHE:CG	2.38	0.58
1:B:537:ILE:O	1:B:541:LEU:HB2	2.03	0.58
1:A:528:SER:OG	1:A:531:GLN:HG3	2.03	0.58
1:A:993:ASP:C	1:A:995:ALA:H	2.07	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
1:B:468:VAL:HG22	1:B:549:LEU:HD13	1.85	0.58
1:A:1184:ARG:O	1:A:1187:VAL:HB	2.03	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: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:A:766:PHE:O	1:A:767:PHE:C	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:ILE:HG13	1:B:832:ILE:HG21	1.85	0.58
1:A:784:LEU:HD12	1:A:1004:ILE:CD1	2.34	0.57
1:A:1037:VAL:HG22	1:A:1087:ALA:H	1.68	0.57
1:A:1042:THR:C	1:A:1044:PRO:HD2	2.24	0.57
1:A:1077:GLN:O	1:A:1080:GLU:N	2.36	0.57
1:A:245:LYS:HZ1	1:A:245:LYS:HA	1.68	0.57
1:A:359:TYR:HA	1:A:362:PHE:HB3	1.86	0.57
1:A:278:GLU:OE2	1:A:785:ARG:HD2	2.03	0.57
1:A:158:TRP:CZ2	1:A:900:PHE:HB2	2.39	0.57
1:A:993:ASP:N	1:A:996:LYS:NZ	2.52	0.57
1:B:1037:VAL:HG22	1:B:1087:ALA:N	2.19	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:A:1214:LEU:HD23	1:A:1214:LEU:O	2.03	0.57
1:A:217:ILE:O	1:A:221:LEU:HG	2.04	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:961:THR:O	1:A:962:GLN:HB3	2.04	0.57
1:A:853:LEU:CG	1:A:973:VAL:HG21	2.29	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
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:A:324:ILE:HD13	1:A:326:GLN:HB3	1.85	0.57
1:A:39:PHE:CE2	1:A:358:ALA:HB3	2.38	0.57
1:B:356:GLY:HA2	1:B:359:TYR:CE1	2.39	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:B:908:ARG:O	1:B:909:GLU:C	2.41	0.57
1:A:111:ALA:HA	1:A:114:TYR:HE1	1.70	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:1120:ASP:HA	1:A:1165:VAL:CG2	2.34	0.57
1:A:1261:GLY:H	1:A:1264:PHE:HB3	1.69	0.57
1:A:246:ALA:HB2	1:A:281:LYS:NZ	2.19	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:B:246:ALA:HB2	1:B:281:LYS:NZ	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1132:ASN:OD1	1:A:1134:ARG:HG2	2.04	0.57
1:A:1120:ASP:HA	1:A:1165:VAL:HG21	1.87	0.57
1:A:479:THR:O	1:A:482:GLU:HB2	2.04	0.57
1:A:61:GLY:O	1:A:65:PRO:CD	2.43	0.57
1:A:780:LEU:O	1:A:784:LEU:HB2	2.05	0.57
1:A:933:VAL:O	1:A:934:PHE:C	2.43	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:B:1252:THR:HG23	1:B:1255:GLN:HB2	1.86	0.57
1:B:309:ALA:O	1:B:310:PHE:O	2.23	0.57
1:B:324:ILE:O	1:B:325:GLY:C	2.43	0.57
1:B:342:GLY:O	1:B:345:SER:N	2.37	0.57
1:B:39:PHE:CE2	1:B:358:ALA:HB3	2.39	0.57
1:B:527:LEU:N	1:B:527:LEU:HD23	2.19	0.57
1:B:59:ILE:HD11	1:B:124:VAL:CG1	2.34	0.57
1:B:618:TYR:O	1:B:622:VAL:HG23	2.03	0.57
1:B:718:GLY:O	1:B:722:PRO:CD	2.47	0.57
1:B:725:SER:HG	1:B:979:PHE:HE1	1.52	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:A:212:LEU:HD12	1:A:215:LEU:HD12	1.87	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:A:465:ILE:HG22	1:A:465:ILE:O	2.05	0.57
1:B:110:TYR:HA	1:B:113:TYR:HD2	1.70	0.57
1:B:492:THR:C	1:B:494:ASP:N	2.57	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:B:215:LEU:C	1:B:219:PRO:HD2	2.25	0.57
1:B:245:LYS:HA	1:B:245:LYS:NZ	2.19	0.57
1:B:379:HIS:C	1:B:381:PRO:HD3	2.24	0.57
1:A:1137:SER:CB	1:A:1140:GLU:HB2	2.35	0.57
1:A:207:GLY:HA3	1:A:211:THR:HB	1.87	0.57
1:A:492:THR:C	1:A:494:ASP:N	2.56	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ILE:O	1:A:72:GLY:N	2.38	0.57
1:A:711:ILE:HG13	1:A:832:ILE:HG21	1.86	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: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:1037:VAL:HG22	1:A:1087:ALA:N	2.19	0.56
1:A:1119:PHE:HD2	1:A:1121:CYS:HG	1.51	0.56
1:A:156:ILE:HG22	1:A:160:ASP:OD1	2.05	0.56
1:A:786:TYR:HE2	1:A:790:LYS:NZ	2.03	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:482:GLU:O	1:B:484:ILE:N	2.38	0.56
1:B:910:GLN:O	1:B:911:LYS:C	2.43	0.56
1:B:945:MET:O	1:B:949:TYR:HD1	1.87	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:A:303:TYR:O	1:A:304:ALA:C	2.43	0.56
1:A:324:ILE:O	1:A:325:GLY:C	2.43	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:B:1020:GLN:CG	1:B:1021:GLY:N	2.66	0.56
1:B:693:PHE:N	1:B:693:PHE:CD2	2.71	0.56
1:B:761:ILE:HD12	1:B:761:ILE:N	2.20	0.56
1:B:862:PRO:O	1:B:866:ILE:HG13	2.05	0.56
1:A:1195:LEU:O	1:A:1226:ILE:HG12	2.05	0.56
1:A:131:PHE:O	1:A:132:TRP:C	2.44	0.56
1:B:401:LYS:HZ2	1:B:401:LYS:HB3	1.70	0.56
1:B:543:ARG:HH21	1:B:907:THR:HG23	1.70	0.56
1:A:1027:LEU:H	1:A:1027:LEU:HD12	1.70	0.56
1:A:1144:ALA:HB1	1:A:1183:ALA:HB1	1.86	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:B:1031:VAL:HB	1:B:1056:VAL:CG1	2.34	0.56
1:B:1196:ASP:CG	1:B:1226:ILE:HD11	2.26	0.56
1:B:318:ILE:CG1	1:B:325:GLY:H	2.19	0.56
1:B:711:ILE:CG1	1:B:832:ILE:HG21	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1106:ARG:O	1:A:1109:LEU:HD22	2.04	0.56
1:A:419:VAL:HG23	1:A:593:VAL:HG13	1.88	0.56
1:A:908:ARG:O	1:A:909:GLU:C	2.42	0.56
1:B:1144:ALA:CA	1:B:1186:LEU:HD11	2.27	0.56
1:B:118:GLY:O	1:B:119:ALA:C	2.44	0.56
1:B:519:LEU:CD1	1:B:519:LEU:H	2.13	0.56
1:B:727:ILE:HD13	1:B:754:LEU:HD23	1.86	0.56
1:B:707:PHE:HZ	1:B:775:LYS:HE2	1.69	0.56
1:A:245:LYS:HA	1:A:245:LYS:NZ	2.20	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
1:B:1076:VAL:HG13	1:B:1194:LEU:HD22	1.88	0.56
1:B:37:THR:O	1:B:38:MET:C	2.43	0.56
1:B:550:LEU:N	1:B:550:LEU:HD12	2.20	0.56
1:B:70:ILE:O	1:B:72:GLY:N	2.39	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:286:LYS:HE2	1:B:778:GLU:HG2	1.86	0.56
1:B:795:GLN:HE21	1:B:796:ASP:N	2.03	0.56
1:A:438:ARG:O	1:A:439:LEU:C	2.41	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:1166:GLY:O	1:B:1167:ASP:HB3	2.05	0.56
1:B:163:ASP:C	1:B:165:GLY:N	2.59	0.56
1:B:290:THR:HG22	1:B:770:GLY:O	2.04	0.56
1:A:1260:LYS:HD2	1:A:1260:LYS:N	2.20	0.56
1:A:53:GLY:O	1:A:54:THR:C	2.42	0.56
1:A:550:LEU:N	1:A:550:LEU:HD12	2.21	0.56
1:A:611:LEU:HB3	1:A:618:TYR:HB3	1.86	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:B:549:LEU:HD12	1:B:549:LEU:N	2.20	0.56
1:A:1090:VAL:HG13	1:A:1097:ILE:CB	2.31	0.56
1:A:210:LEU:C	1:A:210:LEU:HD13	2.26	0.56
1:A:318:ILE:HG23	1:A:735:PHE:CZ	2.41	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:A:257:ILE:HG23	1:A:258:ARG:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:N	1:A:853:LEU:HD22	2.19	0.56
1:B:345:SER:HB3	1:B:346:PRO:HD3	1.88	0.56
1:B:931:ALA:O	1:B:932:HIS:C	2.43	0.56
1:B:733:GLY:HA3	1:B:968:GLU:HG3	1.86	0.56
1:A:1096:GLU:HB2	1:A:1099:GLN:HE21	1.71	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: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:B:362:PHE:O	1:B:365:ILE:HB	2.05	0.56
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:993:ASP:C	1:B:995:ALA:H	2.09	0.56
1:A:110:TYR:HA	1:A:113:TYR:HD2	1.71	0.55
1:A:601:VAL:HG13	1:A:601:VAL:O	2.06	0.55
1:A:818:ALA:O	1:A:821:VAL:HG22	2.06	0.55
1:A:158:TRP:NE1	1:A:900:PHE:CB	2.66	0.55
1:B:53:GLY:O	1:B:54:THR:C	2.45	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:978:VAL:HG13	2:B:6002:OJZ:C35	2.29	0.55
1:A:1196:ASP:CG	1:A:1226:ILE:HD11	2.26	0.55
1:A:1260:LYS:CD	1:A:1260:LYS:H	2.17	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:HD12	1:A:761:ILE:N	2.21	0.55
1:A:861:VAL:HB	1:A:862:PRO:CD	2.36	0.55
1:B:1048:VAL:C	1:B:1049:LEU:HD22	2.27	0.55
1:B:1064:LEU:HB3	1:B:1226:ILE:HG22	1.87	0.55
1:B:111:ALA:HA	1:B:114:TYR:HE1	1.70	0.55
1:B:1206:SER:O	1:B:1210:VAL:HG23	2.06	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:HD12	1:B:617:ILE:N	2.20	0.55
1:B:834:GLN:O	1:B:837:ALA:HB3	2.06	0.55
1:B:958:TYR:O	1:B:966:THR:OG1	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1127:ILE:CD1	1:A:1180:ILE:HG23	2.36	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:795:GLN:HE21	1:A:796:ASP:N	2.04	0.55
1:A:773:PHE:HB2	1:A:829:LEU:CD1	2.36	0.55
1:A:849:TYR:HD1	1:A:854:THR:HG1	1.53	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:A:324:ILE:C	1:A:326:GLN:N	2.59	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:68:MET:HG3	1:A:336:ILE:HD12	1.89	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:1011:THR:H	1:B:1012:PRO:HD3	1.70	0.55
1:B:1137:SER:HB3	1:B:1140:GLU:CB	2.37	0.55
1:B:419:VAL:HG23	1:B:593:VAL:HG13	1.88	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: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:A:103:LEU:HD13	1:A:960:VAL:HG22	1.86	0.55
1:B:1037:VAL:CG2	1:B:1087:ALA:HB3	2.36	0.55
1:B:318:ILE:HG13	1:B:325:GLY:H	1.72	0.55
1:B:65:PRO:O	1:B:66:LEU:C	2.43	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:A:550:LEU:HD13	1:A:580:VAL:HB	1.89	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:88:SER:O	1:A:90:ASN:N	2.39	0.55
1:A:910:GLN:O	1:A:911:LYS:C	2.44	0.55
1:B:908:ARG:HH21	1:B:908:ARG:HG3	1.70	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:A:810:LEU:O	1:A:811:THR:C	2.45	0.55
1:A:78:PHE:CZ	1:A:967:PHE:O	2.59	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:LYS:O	1:B:150:ALA:HB2	2.07	0.55
1:B:188:MET:O	1:B:189:PHE:C	2.44	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:1064:LEU:HB3	1:A:1226:ILE:HG22	1.89	0.55
1:A:1079:LEU:C	1:A:1081:ARG:H	2.09	0.55
1:A:1203:ASP:O	1:A:1206:SER:HB2	2.07	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:B:1042:THR:C	1:B:1044:PRO:HD2	2.26	0.55
1:B:1183:ALA:O	1:B:1187:VAL:HG23	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
1:A:434:GLN:O	1:A:436:MET:N	2.39	0.55
1:A:691:ALA:O	1:A:692:SER:HB3	2.06	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:1137:SER:O	1:B:1141:ILE:HG23	2.06	0.55
1:B:1260:LYS:CD	1:B:1260:LYS:H	2.19	0.55
1:B:209:LYS:O	1:B:213:VAL:HG23	2.07	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: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:B:1071:GLY:O	1:B:1075:VAL:HG23	2.07	0.55
1:B:210:LEU:HD13	1:B:210:LEU:C	2.26	0.55
1:B:255:ALA:C	1:B:257:ILE:N	2.60	0.55
1:B:688:VAL:O	1:B:688:VAL:HG23	2.07	0.55
1:B:282:ARG:HG3	1:B:782:LYS:HD3	1.89	0.55
1:B:74:MET:O	1:B:78:PHE:HB2	2.07	0.55
1:A:37:THR:O	1:A:38:MET:C	2.45	0.54
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:B:1077:GLN:O	1:B:1080:GLU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:209:LYS:O	1:A:213:VAL:HG23	2.06	0.54
1:A:401:LYS:HB3	1:A:401:LYS:HZ3	1.72	0.54
1:A:59:ILE:HD11	1:A:124:VAL:CG1	2.34	0.54
1:B:100:PHE:HB2	1:B:961:THR:HG23	1.88	0.54
1:B:1058:LYS:HA	1:B:1222:THR:OG1	2.07	0.54
1:B:342:GLY:O	1:B:346:PRO:CD	2.56	0.54
1:B:716:ILE:HD11	1:B:765:THR:CB	2.37	0.54
1:A:1011:THR:HG23	1:A:1011:THR:O	2.07	0.54
1:A:1063:ALA:CB	1:A:1239:ILE:HG12	2.37	0.54
1:A:117:ILE:O	1:A:121:VAL:HG13	2.08	0.54
1:A:1058:LYS:HA	1:A:1222:THR:OG1	2.07	0.54
1:A:1255:GLN:O	1:A:1258:ALA:HB3	2.06	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:B:1097:ILE:O	1:B:1098:LYS:CB	2.55	0.54
1:B:254:LEU:HD22	1:B:254:LEU:N	2.22	0.54
1:B:51:LEU:O	1:B:52:VAL:C	2.46	0.54
1:B:611:LEU:HB3	1:B:618:TYR:HB3	1.90	0.54
1:B:61:GLY:O	1:B:65:PRO:CD	2.42	0.54
1:B:70:ILE:C	1:B:72:GLY:N	2.59	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:705:PRO:O	1:A:706:TYR:HB3	2.07	0.54
1:B:370:SER:C	1:B:372:ASP:H	2.10	0.54
1:B:431:THR:O	1:B:435:LEU:HD23	2.07	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:51:LEU:O	1:A:52:VAL:C	2.46	0.54
1:A:549:LEU:N	1:A:549:LEU:HD12	2.22	0.54
1:A:336:ILE:CG1	2:A:6001:OJZ:SE1	2.99	0.54
1:A:315:SER:OG	1:A:747:ASN:HB3	2.08	0.54
1:A:722:PRO:HG2	1:A:841:THR:HB	1.89	0.54
1:A:853:LEU:CD2	1:A:853:LEU:H	2.19	0.54
1:A:969:ASN:ND2	1:A:970:VAL:N	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1090:VAL:HG13	1:B:1097:ILE:CB	2.31	0.54
1:B:324:ILE:C	1:B:326:GLN:N	2.59	0.54
1:B:536:ALA:O	1:B:537:ILE:C	2.46	0.54
1:B:419:VAL:O	1:B:579:ILE:HA	2.08	0.54
1:A:443:LEU:HD23	1:A:443:LEU:O	2.07	0.54
1:B:1054:LEU:CD1	1:B:1240:VAL:HG11	2.38	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
1:B:812:THR:O	1:B:813:ARG:C	2.44	0.54
1:B:861:VAL:HB	1:B:862:PRO:CD	2.38	0.54
1:A:812:THR:O	1:A:813:ARG:C	2.45	0.54
1:B:1195:LEU:HD12	1:B:1195:LEU:N	2.22	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:A:103:LEU:HB2	1:A:960:VAL:HG23	1.89	0.54
1:A:1076:VAL:HG13	1:A:1194:LEU:HD22	1.88	0.54
1:A:536:ALA:O	1:A:537:ILE:C	2.46	0.54
1:B:1108:GLN:H	1:B:1108:GLN:HE21	1.56	0.54
1:B:1143:ARG:HG2	1:B:1143:ARG:HH11	1.73	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: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:A:279:GLU:HG2	1:A:782:LYS:NZ	2.22	0.54
1:A:34:SER:O	1:A:38:MET:HB2	2.08	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:59:ILE:HD12	1:A:59:ILE:C	2.27	0.54
1:B:1053:SER:C	1:B:1054:LEU:HD22	2.28	0.54
1:B:1079:LEU:C	1:B:1081:ARG:H	2.10	0.54
1:B:1221:ARG:N	1:B:1221:ARG:HD2	2.22	0.54
1:B:131:PHE:O	1:B:132:TRP:C	2.46	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: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:215:LEU:C	1:A:219:PRO:HD2	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:ARG:HH11	1:A:954:ARG:HG3	1.73	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:HG12	1:B:317:VAL:O	2.07	0.54
1:B:438:ARG:O	1:B:439:LEU:C	2.44	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:B:90:ASN:HB2	1:B:91:MET:HE2	1.89	0.54
1:A:1048:VAL:C	1:A:1049:LEU:HD22	2.28	0.53
1:A:1108:GLN:H	1:A:1108:GLN:HE21	1.56	0.53
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:B:1019:THR:HG22	1:B:1100:LEU:HD12	1.89	0.53
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:A:1033:PHE:HB3	1:A:1036:VAL:CG2	2.36	0.53
1:A:1221:ARG:N	1:A:1221:ARG:HD2	2.23	0.53
1:A:185:LYS:HZ2	1:A:185:LYS:HB3	1.73	0.53
1:B:245:LYS:HA	1:B:245:LYS:HZ1	1.74	0.53
1:B:617:ILE:HD12	1:B:617:ILE:H	1.74	0.53
1:B:152:MET:HG3	1:B:913:GLU:OE1	2.08	0.53
1:B:969:ASN:ND2	1:B:970:VAL:N	2.57	0.53
1:A:342:GLY:O	1:A:346:PRO:CD	2.56	0.53
1:A:70:ILE:C	1:A:72:GLY:N	2.59	0.53
1:B:1142:VAL:HA	1:B:1161:TYR:OH	2.08	0.53
1:B:1063:ALA:CB	1:B:1239:ILE:HG12	2.38	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: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: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:48:LEU:O	1:A:52:VAL:HG23	2.08	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:1144:ALA:HA	1:A:1186:LEU:CD1	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LYS:HG3	1:A:351:PHE:CD2	2.43	0.53
1:A:305:SER:O	1:A:306:TYR:C	2.47	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:931:ALA:O	1:A:932:HIS:C	2.46	0.53
1:B:1197:GLU:O	1:B:1198:ALA:C	2.46	0.53
1:B:533:GLN:O	1:B:536:ALA:HB3	2.09	0.53
1:B:864:ILE:HD12	1:B:864:ILE:C	2.28	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
1:A:151:ILE:C	1:A:153:ASN:H	2.12	0.53
1:A:203:GLY:C	1:A:211:THR:OG1	2.47	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:148:PHE:HD2	1:A:913:GLU:OE2	1.92	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:B:810:LEU:O	1:B:811:THR:C	2.46	0.53
1:B:853:LEU:HD22	1:B:853:LEU:H	1.73	0.53
1:A:1060:GLN:HB2	1:A:1237:ASP:OD1	2.09	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:B:1140:GLU:O	1:B:1143:ARG:HB3	2.09	0.53
1:B:1060:GLN:HB2	1:B:1237:ASP:OD1	2.09	0.53
1:B:303:TYR:O	1:B:304:ALA:C	2.46	0.53
1:B:405:ILE:HG22	1:B:406:LEU:HD22	1.91	0.53
1:A:419:VAL:O	1:A:579:ILE:HA	2.09	0.53
1:B:1092:LEU:HD22	1:B:1097:ILE:CD1	2.37	0.53
1:B:383:ASN:C	1:B:384:ILE:O	2.41	0.53
1:B:543:ARG:NH2	1:B:907:THR:HG23	2.24	0.53
1:A:279:GLU:HG2	1:A:782:LYS:HD2	1.91	0.53
1:B:434:GLN:C	1:B:436:MET:H	2.13	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: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:118:GLY:O	1:A:119:ALA:C	2.45	0.53
1:A:1254:GLN:N	1:A:1254:GLN:OE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1124:ALA:HB2	1:B:1161:TYR:O	2.09	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:68:MET:HG3	1:B:336:ILE:HD12	1.90	0.53
1:A:161:VAL:O	1:A:162:HIS:HB2	2.08	0.52
1:B:1212:GLU:O	1:B:1215:ASP:HB3	2.08	0.52
1:B:722:PRO:HG2	1:B:841:THR:HB	1.90	0.52
1:A:1197:GLU:O	1:A:1198:ALA:C	2.47	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: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: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:1053:SER:C	1:A:1054:LEU:HD22	2.29	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:A:254:LEU:N	1:A:254:LEU:HD22	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:B:1186:LEU:HD12	1:B:1187:VAL:N	2.24	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:59:ILE:C	1:B:59:ILE:HD12	2.29	0.52
1:B:795:GLN:O	1:B:796:ASP:CB	2.50	0.52
1:A:1109:LEU:O	1:A:1109:LEU:HD23	2.10	0.52
1:A:1143:ARG:HH11	1:A:1143:ARG:HG2	1.73	0.52
1:A:1144:ALA:HB2	1:A:1187:VAL:CG2	2.40	0.52
1:A:65:PRO:O	1:A:66:LEU:C	2.46	0.52
1:A:74:MET:O	1:A:78:PHE:HB2	2.09	0.52
1:A:816:ASN:CG	1:A:817:ASP:N	2.63	0.52
1:A:907:THR:N	1:A:908:ARG:HE	2.07	0.52
1:B:1144:ALA:HA	1:B:1186:LEU:CD1	2.30	0.52
1:B:318:ILE:CD1	1:B:324:ILE:H	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ILE:HG12	1:B:333:SER:OG	2.09	0.52
1:B:420:ALA:HA	1:B:580:VAL:O	2.09	0.52
1:A:573:ARG:HD2	1:A:578:THR:CG2	2.33	0.52
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:816:ASN:CG	1:B:817:ASP:N	2.62	0.52
1:B:860:ILE:O	1:B:864:ILE:HG13	2.09	0.52
1:B:969:ASN:ND2	1:B:970:VAL:H	2.07	0.52
1:A:267:LYS:CA	1:A:790:LYS:HE2	2.40	0.52
1:B:1027:LEU:H	1:B:1027:LEU:CD2	2.22	0.52
1:B:418:THR:HG22	1:B:578:THR:CG2	2.40	0.52
1:A:1011:THR:O	1:A:1012:PRO:C	2.48	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:170:ARG:NH1	1:A:170:ARG:HB2	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:37:THR:O	1:A:40:ARG:N	2.37	0.52
1:A:548:LEU:C	1:A:549:LEU:HD12	2.30	0.52
1:A:69:LEU:HA	1:A:329:THR:HG21	1.91	0.52
1:A:311:TRP:HD1	1:A:754:LEU:HD12	1.74	0.52
1:A:827:SER:O	1:A:828:ARG:C	2.48	0.52
1:B:151:ILE:C	1:B:153:ASN:H	2.12	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:548:LEU:C	1:B:549:LEU:HD12	2.30	0.52
1:A:1108:GLN:N	1:A:1108:GLN:HE21	2.07	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:697:LEU:HD12	1:A:697:LEU:C	2.30	0.52
1:A:724:PHE:CE1	1:A:754:LEU:HD22	2.45	0.52
1:A:864:ILE:C	1:A:864:ILE:HD12	2.30	0.52
1:A:902:THR:O	1:A:903:VAL:C	2.47	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:B:103:LEU:HD13	1:B:960:VAL:HG22	1.91	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: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:460:ARG:O	1:B:461:TYR:C	2.47	0.52
1:B:584:ARG:HA	1:B:584:ARG:NE	2.24	0.52
1:B:859:ALA:O	1:B:863:ILE:HG12	2.10	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: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: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:858:LEU:C	1:A:858:LEU:HD12	2.30	0.52
1:A:486:TYR:O	1:A:908:ARG:NH1	2.43	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:A:1027:LEU:N	1:A:1027:LEU:HD12	2.25	0.52
1:A:1108:GLN:N	1:A:1108:GLN:NE2	2.58	0.52
1:A:138:ARG:NH2	1:B:515:GLN:HG2	2.25	0.52
1:A:432:THR:O	1:A:433:VAL:C	2.48	0.52
1:A:806:THR:HG23	1:A:809:ALA:H	1.75	0.52
1:B:1124:ALA:HB2	1:B:1161:TYR:HB3	1.91	0.52
1:B:437:GLN:NE2	1:B:468:VAL:HG21	2.23	0.52
1:B:565:VAL:O	1:B:566:GLN:C	2.48	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:HD3	1:B:901:ARG:H	1.74	0.52
1:A:158:TRP:NE1	1:A:900:PHE:HB2	2.25	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:290:THR:HG22	1:A:770:GLY:C	2.31	0.51
1:A:843:ILE:HA	1:A:846:SER:CB	2.40	0.51
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:1229:ARG:C	1:B:1231:SER:H	2.13	0.51
1:B:1260:LYS:HD2	1:B:1260:LYS:N	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:584:ARG:O	1:B:588:VAL:HG23	2.10	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:247:GLY:O	1:A:250:ALA:HB3	2.09	0.51
1:A:202:ILE:HG12	1:A:333:SER:OG	2.10	0.51
1:A:354:ALA:O	1:A:358:ALA:CB	2.58	0.51
1:A:460:ARG:O	1:A:461:TYR:C	2.48	0.51
1:A:59:ILE:HG12	1:A:124:VAL:HG11	1.92	0.51
1:A:711:ILE:O	1:A:715:ILE:HG13	2.10	0.51
1:A:800:PHE:C	1:A:803:PRO:HD3	2.31	0.51
1:B:246:ALA:HB2	1:B:281:LYS:HZ2	1.75	0.51
1:B:716:ILE:HD11	1:B:765:THR:HB	1.92	0.51
1:B:853:LEU:N	1:B:853:LEU:HD22	2.25	0.51
1:B:895:GLU:O	1:B:899:ASN:ND2	2.43	0.51
1:B:133:CYS:HB3	1:B:931:ALA:CB	2.40	0.51
1:A:1202:LEU:HG	1:A:1203:ASP:H	1.75	0.51
1:A:144:ARG:HH12	1:A:175:VAL:HG11	1.76	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: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: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:1080:GLU:CD	1:A:1109:LEU:HD12	2.31	0.51
1:A:1178:GLN:O	1:A:1181:ALA:HB3	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:H	1:A:901:ARG:HD3	1.75	0.51
1:B:1014:ILE:HG23	1:B:1014:ILE:O	2.10	0.51
1:B:802:ASP:OD2	1:B:1041:PRO:HB2	2.10	0.51
1:B:1144:ALA:HB2	1:B:1187:VAL:HG23	1.92	0.51
1:B:275:ASN:HA	1:B:278:GLU:HB2	1.92	0.51
1:B:480:ILE:O	1:B:481:ALA:C	2.48	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:902:THR:O	1:B:904:VAL:N	2.44	0.51
1:B:543:ARG:NH1	1:B:905:SER:HA	2.24	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:A:118:GLY:HA3	1:A:946:TYR:CD2	2.45	0.51
1:B:1035:GLY:C	1:B:1052:LEU:O	2.49	0.51
1:B:1225:VAL:HG13	1:B:1225:VAL:O	2.09	0.51
1:B:697:LEU:HD12	1:B:697:LEU:C	2.31	0.51
1:A:113:TYR:CG	1:A:114:TYR:N	2.79	0.51
1:A:1151:HIS:HA	1:A:1154:ILE:HB	1.92	0.51
1:A:1196:ASP:HA	1:A:1226:ILE:HD11	1.91	0.51
1:A:1192:ILE:HA	1:A:1222:THR:O	2.10	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: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:B:421:LEU:HD23	1:B:429:LYS:HA	1.92	0.51
1:B:59:ILE:HG12	1:B:124:VAL:HG11	1.93	0.51
1:A:1218:ARG:HB2	1:A:1223:CYS:SG	2.51	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: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:B:464:GLU:HG2	1:B:543:ARG:HH21	1.75	0.51
1:B:800:PHE:C	1:B:803:PRO:HD3	2.31	0.51
1:A:1144:ALA:HB2	1:A:1187:VAL:HG23	1.91	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:962:GLN:O	1:A:962:GLN:HG2	2.11	0.51
1:B:106:GLU:OE2	1:B:109:THR:HB	2.10	0.51
1:B:1218:ARG:HB2	1:B:1223:CYS:SG	2.51	0.51
1:B:203:GLY:C	1:B:211:THR:OG1	2.49	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
1:B:718:GLY:HA3	1:B:837:ALA:CB	2.40	0.51
1:B:907:THR:C	1:B:908:ARG:HE	2.15	0.51
1:B:133:CYS:HB3	1:B:931:ALA:HB1	1.91	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:A:762:SER:CA	1:A:765:THR:HG22	2.40	0.51
1:A:949:TYR:CD1	1:A:949:TYR:N	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:TYR:CG	1:B:114:TYR:N	2.78	0.51
1:B:1176:GLN:O	1:B:1179:ARG:N	2.44	0.51
1:B:175:VAL:CG1	1:B:176:SER:N	2.74	0.51
1:B:48:LEU:O	1:B:52:VAL:HG23	2.10	0.51
1:B:86:LYS:HG2	1:B:738:GLY:O	2.11	0.51
1:B:826:GLY:O	1:B:829:LEU:HB2	2.10	0.51
1:B:962:GLN:HG2	1:B:962:GLN:O	2.10	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:A:409:LEU:HD13	1:A:410:ASN:N	2.26	0.51
1:B:1080:GLU:CD	1:B:1109:LEU:HD12	2.31	0.51
1:B:161:VAL:O	1:B:162:HIS:HB2	2.11	0.51
1:B:314:THR:O	1:B:315:SER:C	2.49	0.51
1:B:34:SER:O	1:B:38:MET: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:1020:GLN:CG	1:A:1101:ASN:HB3	2.41	0.50
1:A:801:ASP:OD2	1:A:1082:PHE:HB3	2.11	0.50
1:A:1102:VAL:HG13	1:A:1103:GLN:N	2.24	0.50
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:467:GLY:O	1:A:548:LEU:HA	2.12	0.50
1:B:788:VAL:HG21	1:B:1004:ILE:HG13	1.94	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:B:248:ALA:O	1:B:251:GLU:HB2	2.11	0.50
1:B:35:VAL:HG12	1:B:359:TYR:CZ	2.46	0.50
1:B:484:ILE:O	1:B:485:ARG:C	2.50	0.50
1:B:721:GLN:O	1:B:722:PRO:C	2.48	0.50
1:B:286:LYS:HG2	1:B:778:GLU:HG3	1.89	0.50
1:B:845:ILE:O	1:B:848:ILE:HG12	2.12	0.50
1:A:499:ALA:CB	1:A:542:VAL:HG22	2.41	0.50
1:A:693:PHE:C	1:A:695:ARG:H	2.14	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:915:MET:O	1:A:918:GLN:HB2	2.11	0.50
1:B:1144:ALA:HB2	1:B:1187:VAL:CG2	2.41	0.50
1:B:121:VAL:CG2	1:B:122:LEU:N	2.74	0.50
1:B:35:VAL:HG21	1:B:355:ARG:HH21	1.76	0.50
1:B:467:GLY:O	1:B:548:LEU:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:791:SER:N	1:B:794:ARG:HH21	2.08	0.50
1:B:905:SER:HB2	1:B:908:ARG:CZ	2.41	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: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:702:THR:HB	1:B:703:GLU:OE1	2.10	0.50
1:B:786:TYR:HE2	1:B:790:LYS:NZ	2.03	0.50
1:A:121:VAL:CG2	1:A:122:LEU:N	2.74	0.50
1:A:318:ILE:CD1	1:A:324:ILE:H	2.24	0.50
1:A:314:THR:CG2	1:A:327:VAL:HG21	2.36	0.50
1:A:584:ARG:NE	1:A:584:ARG:HA	2.26	0.50
1:A:617:ILE:H	1:A:617:ILE:HD12	1.74	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:B:1023:LYS:HB3	1:B:1026:MET:CG	2.37	0.50
1:B:1108:GLN:NE2	1:B:1108:GLN:N	2.59	0.50
1:B:1196:ASP:HA	1:B:1226:ILE:HG12	1.92	0.50
1:B:978:VAL:HG22	2:B:6002:OJZ:H35B	1.93	0.50
1:B:118:GLY:HA3	1:B:946:TYR:CD2	2.46	0.50
1:A:1186:LEU:HD12	1:A:1187:VAL:N	2.26	0.50
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: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:B:300:LEU:HA	1:B:303:TYR:HB2	1.92	0.50
1:B:69:LEU:HA	1:B:329:THR:HG21	1.93	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:255:ALA:C	1:A:257:ILE:N	2.62	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:484:ILE:O	1:A:485:ARG:C	2.50	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:972:LEU:CD1	1:A:972:LEU:H	2.23	0.50
1:B:1064:LEU:HD13	1:B:1064:LEU:C	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1092:LEU:CD2	1:B:1097:ILE:HD11	2.40	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: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:57:ALA:O	1:A:60:HIS:HB3	2.11	0.50
1:A:892:ILE:O	1:A:893:ALA:C	2.50	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:838:ASN:O	1:B:839:LEU:C	2.50	0.50
1:A:106:GLU:HG3	1:A:110:TYR:CZ	2.46	0.50
1:A:1164:ARG:C	1:A:1166:GLY:N	2.65	0.50
1:A:721:GLN:O	1:A:722:PRO:C	2.49	0.50
1:A:842:GLY:HA2	1:A:979:PHE:CE2	2.47	0.50
1:B:1037:VAL:HG21	1:B:1087:ALA:HB3	1.94	0.50
1:B:207:GLY:C	1:B:209:LYS:H	2.15	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:A:1124:ALA:HB2	1:A:1161:TYR:HB3	1.93	0.50
1:A:227:ILE:HG22	1:A:228:TRP:N	2.27	0.50
1:A:35:VAL:HG21	1:A:355:ARG:HH21	1.76	0.50
1:A:533:GLN:O	1:A:536:ALA:HB3	2.11	0.50
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:B:1197:GLU:OE2	1:B:1228:HIS:HB2	2.12	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:532:LYS:O	1:B:533:GLN:C	2.49	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:991:ALA:HB1	1:B:992:PRO:HD2	1.93	0.50
1:A:480:ILE:O	1:A:481:ALA:C	2.49	0.49
1:A:777:GLY:HA3	1:A:822:LYS:HG3	1.93	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:A:1056:VAL:CG2	1:A:1062:LEU:HB2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1037:VAL:HG21	1:A:1087:ALA:HB3	1.94	0.49
1:A:120:GLY:O	1:A:121:VAL:C	2.51	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:485:ARG:O	1:A:488:ARG:C	2.51	0.49
1:B:1095:LYS:HD2	1:B:1095:LYS:N	2.26	0.49
1:B:1139:GLU:CD	1:B:1139:GLU:H	2.14	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:850:GLY:C	1:B:852:GLN:H	2.15	0.49
1:B:158:TRP:HZ2	1:B:900:PHE:HB2	1.75	0.49
1:A:1229:ARG:C	1:A:1231:SER:H	2.14	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:1128:ALA:HB2	1:B:1141:ILE:HG21	1.94	0.49
1:B:1196:ASP:HA	1:B:1226:ILE:HD11	1.93	0.49
1:B:139:GLN:O	1:B:140:ILE:C	2.50	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:129:VAL:HG11	1:B:935:GLY:N	2.27	0.49
1:A:1164:ARG:O	1:A:1166:GLY:N	2.44	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:174:ASP:O	1:A:175:VAL:C	2.51	0.49
1:A:318:ILE:HD11	1:A:324:ILE:H	1.78	0.49
1:A:70:ILE:O	1:A:71:PHE:C	2.50	0.49
1:A:857:LEU:HD11	1:A:977:ILE:N	2.28	0.49
1:B:1056:VAL:CG2	1:B:1060:GLN:HE22	2.23	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:858:LEU:C	1:B:858:LEU:HD12	2.33	0.49
1:A:1079:LEU:C	1:A:1081:ARG:N	2.66	0.49
1:A:1202:LEU:HG	1:A:1206:SER:CB	2.42	0.49
1:A:291:ALA:CA	1:A:294:SER:HB2	2.42	0.49
1:A:35:VAL:HG12	1:A:359:TYR:CZ	2.47	0.49
1:A:620:LYS:HD2	1:A:621:LEU:HD22	1.95	0.49
1:A:786:TYR:HE2	1:A:790:LYS:HZ1	1.58	0.49
1:B:144:ARG:HG2	1:B:920:LEU:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CA	1:B:311:TRP:CE3	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:A:1095:LYS:CD	1:A:1095:LYS:H	2.24	0.49
1:A:1189:GLN:N	1:A:1190:PRO:CD	2.76	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:907:THR:C	1:A:908:ARG:HE	2.16	0.49
1:A:909:GLU:O	1:A:912:PHE:HB2	2.13	0.49
1:A:992:PRO:C	1:A:994:TYR:H	2.16	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: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:305:SER:O	1:B:306:TYR:C	2.50	0.49
1:B:824:ALA:O	1:B:828:ARG:HG2	2.12	0.49
1:B:949:TYR:CD1	1:B:949:TYR:N	2.80	0.49
1:B:972:LEU:CD1	1:B:972:LEU:H	2.22	0.49
1:A:157:GLY:HA2	1:A:160:ASP:CB	2.41	0.49
1:A:175:VAL:HG13	1:A:176:SER:H	1.75	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:795:GLN:NE2	1:B:796:ASP:H	2.08	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: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: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:B:1214:LEU:HD23	1:B:1214:LEU:C	2.32	0.49
1:B:434:GLN:O	1:B:436:MET:N	2.46	0.49
1:B:57:ALA:O	1:B:60:HIS:HB3	2.13	0.49
1:B:843:ILE:CA	1:B:846:SER:HB3	2.39	0.49
1:B:907:THR:C	1:B:908:ARG:NE	2.65	0.49
1:A:1035:GLY:C	1:A:1052:LEU:O	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1197:GLU:OE2	1:A:1228:HIS:HB2	2.12	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:B:110:TYR:HA	1:B:113:TYR:CD2	2.47	0.49
1:B:1205:GLU:HA	1:B:1208:LYS:HB3	1.94	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:853:LEU:HB3	1:B:973:VAL:CG2	2.43	0.49
1:A:498:LYS:HE2	1:A:499:ALA:N	2.28	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:830:ALA:O	1:A:833:PHE:HB3	2.13	0.49
1:A:901:ARG:O	1:A:902:THR:C	2.51	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:B:255:ALA:O	1:B:257:ILE:N	2.45	0.49
1:B:44:TRP:CD1	1:B:45:LEU:HD22	2.48	0.49
1:B:570:ASP:HA	1:B:573:ARG:NH1	2.28	0.49
1:A:394:HIS:O	1:A:443:LEU:HB3	2.12	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: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: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:883:LYS:HA	1:A:886:LEU:HG	1.95	0.48
1:B:270:LEU:HG	1:B:271:GLU:H	1.78	0.48
1:B:933:VAL:O	1:B:935:GLY:N	2.46	0.48
1:A:401:LYS:HB3	1:A:401:LYS:HZ2	1.77	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:777:GLY:CA	1:B:822:LYS:HG3	2.44	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: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:B:167:LEU:C	1:B:167:LEU:HD23	2.34	0.48
1:B:371:ILE:O	1:B:371:ILE:HG22	2.13	0.48
1:B:370:SER:O	1:B:372:ASP:N	2.44	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:A:286:LYS:HE3	1:A:822:LYS:HZ1	1.78	0.48
1:A:44:TRP:CD1	1:A:45:LEU:HD22	2.48	0.48
1:A:532:LYS:O	1:A:533:GLN:C	2.50	0.48
1:A:565:VAL:O	1:A:566:GLN:C	2.51	0.48
1:A:914:THR:O	1:A:917:ALA:HB3	2.14	0.48
1:B:1091:PHE:CE1	1:B:1096:GLU:HG2	2.32	0.48
1:B:147:PHE:O	1:B:150:ALA:HB3	2.14	0.48
1:B:132:TRP:CD2	1:B:183:GLY:HA3	2.48	0.48
1:B:200:PHE:O	1:B:201:ILE:C	2.51	0.48
1:B:761:ILE:HD12	1:B:761:ILE:H	1.78	0.48
1:B:792:MET:HE3	1:B:810:LEU:HD22	1.95	0.48
1:A:1097:ILE:O	1:A:1098:LYS:HB3	2.13	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:A:1204:THR:C	1:A:1206:SER:H	2.16	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:B:1032:GLN:HE21	1:B:1055:GLU:HG3	1.77	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:HZ3	1:B:881:LYS:HB2	1.78	0.48
1:A:1090:VAL:CG1	1:A:1097:ILE:HB	2.36	0.48
1:A:209:LYS:C	1:A:212:LEU:HB3	2.34	0.48
1:A:246:ALA:HB2	1:A:281:LYS:HZ2	1.77	0.48
1:A:846:SER:HA	1:A:849:TYR:CE1	2.49	0.48
1:B:1135:VAL:O	1:B:1137:SER:N	2.47	0.48
1:B:131:PHE:CD2	1:B:131:PHE:C	2.86	0.48
1:B:806:THR:HG23	1:B:809:ALA:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:979:PHE:HA	1:B:982:MET:SD	2.54	0.48
1:A:429:LYS:HD3	1:A:429:LYS:N	2.19	0.48
1:A:52:VAL:O	1:A:53:GLY:C	2.52	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: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:B:1186:LEU:HD12	1:B:1186:LEU:C	2.34	0.48
1:B:221:LEU:HD13	1:B:306:TYR:HA	1.95	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:852:GLN:HB3	1:B:853:LEU:HD22	1.96	0.48
1:A:1098:LYS:O	1:A:1099:GLN:HB2	2.14	0.48
1:A:1186:LEU:C	1:A:1186:LEU:HD12	2.34	0.48
1:A:1225:VAL:O	1:A:1225:VAL:HG13	2.13	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: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:894:THR:O	1:A:895:GLU:C	2.52	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:B:335:LEU:C	1:B:335:LEU:HD23	2.35	0.48
1:A:1137:SER:HB3	1:A:1140:GLU:HB2	1.96	0.48
1:A:134:LEU:O	1:A:138:ARG:HG3	2.14	0.48
1:A:139:GLN:O	1:A:140:ILE:C	2.52	0.48
1:A:221:LEU:HD13	1:A:306:TYR:HA	1.96	0.48
1:A:281:LYS:HD2	1:A:281:LYS:N	2.28	0.48
1:A:335:LEU:C	1:A:335:LEU:HD23	2.34	0.48
1:A:43:GLY:HA3	1:A:46:ASP:HB2	1.96	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:B:175:VAL:HG13	1:B:176:SER:H	1.78	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:779:ILE:O	1:B:780:LEU:C	2.53	0.48
1:A:1064:LEU:C	1:A:1064:LEU:HD13	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1092:LEU:CD2	1:A:1097:ILE:HD11	2.40	0.47
1:A:217:ILE:HG13	1:A:218:SER:N	2.28	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
1:A:751:PHE:CD1	1:A:752:SER:N	2.82	0.47
1:A:753:LEU:O	1:A:754:LEU:C	2.52	0.47
1:A:907:THR:C	1:A:908:ARG:NE	2.68	0.47
1:A:725:SER:HG	1:A:979:PHE:HE1	1.62	0.47
1:B:1079:LEU:C	1:B:1081:ARG:N	2.68	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:314:THR:O	1:A:315:SER:C	2.51	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: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: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:875:LEU:HD23	1:B:875:LEU:C	2.34	0.47
1:B:892:ILE:HB	1:B:916:TYR:HE1	1.75	0.47
1:A:1107:ALA:HB3	1:A:1108:GLN:NE2	2.29	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:534:ARG:O	1:A:535:ILE:C	2.50	0.47
1:A:933:VAL:O	1:A:935:GLY:N	2.47	0.47
1:A:959:LEU:C	1:A:959:LEU:HD23	2.34	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: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:A:157:GLY:HA2	1:A:160:ASP:OD2	2.15	0.47
1:A:258:ARG:O	1:A:259:THR:C	2.52	0.47
1:A:311:TRP:CA	1:A:311:TRP:CE3	2.97	0.47
1:A:438:ARG:O	1:A:439:LEU:O	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1208:LYS:HD3	1:B:1208:LYS:C	2.35	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
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: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:1139:GLU:CD	1:A:1139:GLU:H	2.17	0.47
1:A:704:TRP:CZ2	1:A:707:PHE: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:B:258:ARG:O	1:B:259:THR:C	2.51	0.47
1:B:295:MET:C	1:B:297:ALA:N	2.68	0.47
1:B:374:PHE:HD1	1:B:375:SER:H	1.61	0.47
1:B:401:LYS:HZ3	1:B:401:LYS:HB3	1.75	0.47
1:B:396:SER:HB3	1:B:443:LEU:HD12	1.97	0.47
1:B:533:GLN:O	1:B:537:ILE:HG12	2.15	0.47
1:B:753:LEU:O	1:B:754:LEU:C	2.53	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:A:1032:GLN:HE21	1:A:1055:GLU:CG	2.27	0.47
1:A:1214:LEU:HD23	1:A:1214:LEU:C	2.35	0.47
1:A:435:LEU:H	1:A:435:LEU:HD23	1.80	0.47
1:A:53:GLY:O	1:A:56:ALA:N	2.48	0.47
1:A:724:PHE:HA	1:A:727:ILE:CG2	2.44	0.47
1:B:1107:ALA:HB3	1:B:1108:GLN:NE2	2.29	0.47
1:B:273:TYR:O	1:B:274:ASN:O	2.33	0.47
1:A:468:VAL:HG12	1:A:469:VAL:N	2.29	0.47
1:A:589:ARG:HG2	1:A:589:ARG:HH11	1.80	0.47
1:A:797:VAL:HG13	1:A:1082:PHE:O	2.15	0.47
1:A:777:GLY:CA	1:A:822:LYS:HG3	2.43	0.47
1:B:1095:LYS:CD	1:B:1095:LYS:H	2.27	0.47
1:B:116:GLY:O	1:B:117:ILE:C	2.52	0.47
1:B:314:THR:HG22	1:B:315:SER:N	2.29	0.47
1:B:900:PHE:O	1:B:901:ARG:C	2.53	0.47
1:B:957:ALA:O	1:B:958:TYR:C	2.53	0.47
1:A:1092:LEU:HB3	1:A:1097:ILE:CD1	2.37	0.47
1:A:1116:PRO:HB3	1:A:1178:GLN:OE1	2.15	0.47
1:A:1204:THR:O	1:A:1206:SER:N	2.48	0.47
1:A:188:MET:O	1:A:189:PHE:C	2.50	0.47
1:A:258:ARG:HH22	1:A:1113:SER:CB	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:GLN:O	1:A:537:ILE:HG12	2.14	0.47
1:A:705:PRO:HG2	1:A:706:TYR:N	2.27	0.47
1:A:796:ASP:O	1:A:797:VAL:C	2.52	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:485:ARG:O	1:B:488:ARG:C	2.53	0.47
1:B:502:GLU:OE1	1:B:541:LEU:HD11	2.14	0.47
1:B:838:ASN:C	1:B:838:ASN:HD22	2.18	0.47
1:A:1123:ILE:HG13	1:A:1124:ALA:N	2.30	0.47
1:A:125:ALA:O	1:A:126:TYR:C	2.52	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:B:1203:ASP:O	1:B:1206:SER:HB2	2.13	0.47
1:B:174:ASP:O	1:B:175:VAL:C	2.51	0.47
1:B:503:ALA:O	1:B:504:ASN:C	2.53	0.47
1:A:185:LYS:O	1:A:186:ILE:C	2.52	0.47
1:A:502:GLU:OE1	1:A:541:LEU:HD11	2.14	0.47
1:A:58:ILE:O	1:A:60:HIS:N	2.48	0.47
1:A:875:LEU:C	1:A:875:LEU:HD23	2.34	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:59:ILE:HD11	1:B:124:VAL:CG2	2.45	0.47
1:B:972:LEU:HD12	1:B:972:LEU:N	2.25	0.47
1:B:853:LEU:HG	1:B:973:VAL:HG21	1.97	0.47
1:B:722:PRO:HA	1:B:979:PHE:CE1	2.50	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:539:ARG:O	1:A:540:ALA:C	2.53	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:434:GLN:C	1:B:436:MET:N	2.68	0.47
1:B:64:LEU:O	1:B:65:PRO:C	2.50	0.47
1:B:942:GLN:O	1:B:945:MET:N	2.48	0.47
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:A:207:GLY:CA	1:A:210:LEU:HB3	2.45	0.46
1:A:476:PHE:O	1:A:478:THR:N	2.45	0.46
1:A:868:GLY:O	1:A:871:GLU:HB3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:933:VAL:C	1:B:935:GLY:N	2.68	0.46
1:A:1218:ARG:NH1	1:A:1235:ASN:HD22	2.14	0.46
1:A:274:ASN:O	1:A:278:GLU:HG3	2.15	0.46
1:A:405:ILE:N	1:A:405:ILE:HD12	2.30	0.46
1:A:468:VAL:HG22	1:A:549:LEU:HB2	1.97	0.46
1:A:78:PHE:CE2	1:A:967:PHE:O	2.69	0.46
1:A:973:VAL:O	1:A:976:ALA:N	2.47	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:A:121:VAL:HG23	1:A:122:LEU:H	1.78	0.46
1:A:200:PHE:O	1:A:201:ILE:C	2.54	0.46
1:A:420:ALA:C	1:A:421:LEU:HD12	2.35	0.46
1:A:697:LEU:HA	1:A:700:ASN:CB	2.43	0.46
1:A:773:PHE:HB2	1:A:829:LEU:HD13	1.96	0.46
1:A:845:ILE:O	1:A:848:ILE:HG12	2.14	0.46
1:B:1116:PRO:HB3	1:B:1178:GLN:OE1	2.15	0.46
1:B:1167:ASP:O	1:B:1168:LYS:HB2	2.16	0.46
1:B:207:GLY:CA	1:B:210:LEU:HB3	2.45	0.46
1:B:383:ASN:O	1:B:384:ILE:C	2.53	0.46
1:B:751:PHE:CD1	1:B:752:SER:N	2.83	0.46
1:B:902:THR:O	1:B:903:VAL:C	2.54	0.46
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: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:887:GLU:O	1:A:888:GLY:C	2.53	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:B:227:ILE:HG22	1:B:228:TRP:N	2.30	0.46
1:B:55:LEU:C	1:B:55:LEU:HD23	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:957:ALA:O	1:B:958:TYR:O	2.33	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:167:LEU:HD23	1:A:167:LEU:C	2.36	0.46
1:A:992:PRO:O	1:A:994:TYR:N	2.49	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:B:1243:GLN:O	1:B:1244:ASN:C	2.53	0.46
1:B:291:ALA:C	1:B:294:SER:H	2.19	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:831:VAL:O	1:B:832:ILE:C	2.54	0.46
1:A:1218:ARG:O	1:A:1219:GLU:HB3	2.16	0.46
1:A:210:LEU:HG	1:A:322:TYR:CD2	2.51	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:B:125:ALA:O	1:B:126:TYR:C	2.53	0.46
1:B:204:PHE:HA	1:B:211:THR:HG21	1.98	0.46
1:B:52:VAL:O	1:B:53:GLY:C	2.53	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:1036:VAL:HB	1:A:1052:LEU:CB	2.36	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
1:A:540:ALA:O	1:A:543:ARG:CB	2.63	0.46
1:A:83:ASN:O	1:A:86:LYS:HB3	2.16	0.46
1:A:901:ARG:O	1:A:904:VAL:HG12	2.16	0.46
1:A:93:GLU:CD	1:A:93:GLU:H	2.19	0.46
1:A:972:LEU:HD12	1:A:972:LEU:N	2.24	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:70:ILE:O	1:B:71:PHE:C	2.53	0.46
1:B:940:PHE:O	1:B:944:MET:HG2	2.16	0.46
1:A:1102:VAL:HG13	1:A:1103:GLN:H	1.81	0.46
1:A:429:LYS:O	1:A:431:THR:N	2.49	0.46
1:A:722:PRO:HA	1:A:979:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:ASN:HD22	1:A:838:ASN:C	2.17	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:B:1101:ASN:OD1	1:B:1103:GLN:HB3	2.16	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:A:1026:MET:HE1	1:A:1104:TRP:CZ3	2.51	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:A:131:PHE:CD2	1:A:131:PHE:C	2.89	0.46
1:A:33:VAL:O	1:A:34:SER:C	2.54	0.46
1:A:429:LYS:H	1:A:429:LYS:CD	2.18	0.46
1:A:449:ILE:O	1:A:450:ASP:C	2.53	0.46
1:A:536:ALA:O	1:A:539:ARG:N	2.48	0.46
1:A:55:LEU:HD23	1:A:55:LEU:C	2.35	0.46
1:A:770:GLY:HA2	1:A:773:PHE:CE2	2.51	0.46
1:A:838:ASN:O	1:A:839:LEU:C	2.52	0.46
1:B:1145:ALA:HA	1:B:1150:ILE:HG22	1.98	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:894:THR:O	1:B:895:GLU:C	2.54	0.46
1:A:147:PHE:O	1:A:148:PHE:C	2.54	0.46
1:A:291:ALA:C	1:A:294:SER:H	2.18	0.46
1:A:310:PHE:HB3	1:A:311:TRP:H	1.50	0.46
1:A:315:SER:CA	1:A:318:ILE:HG22	2.46	0.46
1:A:314:THR:HG22	1:A:315:SER:N	2.31	0.46
1:A:356:GLY:HA2	1:A:359:TYR:HE1	1.79	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: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:B:136:ALA:O	1:B:139:GLN:HB2	2.16	0.46
1:B:33:VAL:O	1:B:34:SER:C	2.54	0.46
1:B:534:ARG:O	1:B:535:ILE:C	2.53	0.46
1:B:620:LYS:O	1:B:623:MET:N	2.48	0.46
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:PHE:CG	1:A:834:GLN:N	2.83	0.45
1:A:886:LEU:C	1:A:886:LEU:HD12	2.37	0.45
1:A:930:LYS:HA	1:A:933:VAL:CG2	2.46	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:B:214:ILE:HG12	1:B:331:PHE:CZ	2.50	0.45
1:B:692:SER:CB	1:B:695:ARG:HD3	2.47	0.45
1:B:728:PHE:CD1	1:B:728:PHE:C	2.89	0.45
1:B:770:GLY:HA2	1:B:773:PHE:CE2	2.52	0.45
1:B:901:ARG:O	1:B:902:THR:C	2.55	0.45
1:A:1196:ASP:HA	1:A:1226:ILE:CD1	2.46	0.45
1:A:463:ARG:HG3	1:A:463:ARG:HH11	1.82	0.45
1:B:817:ASP:OD1	1:B:1000:SER:HB3	2.15	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: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:868:GLY:O	1:B:871:GLU:HB3	2.16	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: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:415:SER:HA	1:A:577:THR:CG2	2.46	0.45
1:A:396:SER:HB3	1:A:443:LEU:HD12	1.98	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:716:ILE:HD12	1:A:716:ILE:C	2.37	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:B:1164:ARG:C	1:B:1166:GLY:N	2.68	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:A:1039:ASN:HD22	1:A:1048:VAL:N	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:788:VAL:CG2	1:B:1004:ILE:HG13	2.46	0.45
1:B:1261:GLY:H	1:B:1264:PHE:CB	2.30	0.45
1:B:134:LEU:O	1:B:138:ARG:HG3	2.16	0.45
1:B:809:ALA:O	1:B:813:ARG:HG2	2.16	0.45
1:B:887:GLU:O	1:B:888:GLY:C	2.55	0.45
1:A:1243:GLN:O	1:A:1244:ASN:C	2.54	0.45
1:A:151:ILE:HD12	1:A:167:LEU:HD11	1.99	0.45
1:A:68:MET:HG3	1:A:336:ILE:CD1	2.46	0.45
1:A:981:ALA:CB	2:A:6001:OJZ:H33	2.46	0.45
1:A:779:ILE:CG1	1:A:780:LEU:N	2.79	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:B:99:MET:HB3	1:B:960:VAL:O	2.16	0.45
1:A:154:GLN:HG2	1:A:154:GLN:O	2.17	0.45
1:A:238:LYS:HZ3	1:A:242:ALA:HB2	1.82	0.45
1:A:942:GLN:O	1:A:945:MET:N	2.49	0.45
1:B:1048:VAL:HG23	1:B:1049:LEU:HD22	1.97	0.45
1:B:801:ASP:HB3	1:B:1083:TYR:CE2	2.51	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
1:B:438:ARG:O	1:B:439:LEU:O	2.34	0.45
1:B:500:VAL:HG23	1:B:501:LYS:H	1.82	0.45
2:B:6002:OJZ:O25	2:B:6002:OJZ:H29B	2.16	0.45
1:B:60:HIS:O	1:B:63:ALA:N	2.50	0.45
1:B:901:ARG:O	1:B:904:VAL:HG12	2.16	0.45
1:B:937:THR:O	1:B:938:PHE:C	2.54	0.45
1:B:860:ILE:HG21	1:B:948:SER:HB3	1.97	0.45
1:A:1150:ILE:HG13	1:A:1150:ILE:O	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:740:PRO:N	1:A:741:PRO:HD2	2.32	0.45
1:A:902:THR:C	1:A:904:VAL:N	2.68	0.45
1:A:943:ALA:O	1:A:944:MET:C	2.55	0.45
1:A:860:ILE:HG21	1:A:948:SER:HB3	1.97	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:B:1249:GLU:O	1:B:1250:HIS:HB3	2.16	0.45
1:B:155:GLU:O	1:B:156:ILE:C	2.55	0.45
1:B:249:VAL:HG12	1:B:249:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:833:PHE:CG	1:B:834:GLN:N	2.83	0.45
1:A:135:ALA:O	1:A:136:ALA:C	2.54	0.45
1:A:492:THR:C	1:A:494:ASP:H	2.19	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:714:ALA:HB1	1:A:833:PHE:HB2	1.98	0.45
1:A:728:PHE:C	1:A:728:PHE:CD1	2.91	0.45
1:B:1114:GLN:O	1:B:1116:PRO:HD3	2.17	0.45
1:B:306:TYR:CG	1:B:307:ALA:N	2.84	0.45
1:B:359:TYR:HA	1:B:362:PHE:CB	2.45	0.45
1:B:411:LEU:C	1:B:411:LEU:HD23	2.37	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: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:A:792:MET:HE3	1:A:810:LEU:HD22	1.98	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:993:ASP:O	1:A:995:ALA:N	2.47	0.45
1:B:207:GLY:CA	1:B:211:THR:H	2.28	0.45
1:B:308:LEU:O	1:B:309:ALA:C	2.55	0.45
1:B:463:ARG:HG3	1:B:463:ARG:HH11	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:892:ILE:O	1:B:893:ALA:C	2.54	0.45
1:B:996:LYS:HD3	1:B:996:LYS:N	2.19	0.45
1:A:1178:GLN:HA	1:A:1178:GLN:OE1	2.17	0.45
1:A:304:ALA:O	1:A:307:ALA:HB3	2.17	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:908:ARG:O	1:A:911:LYS: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:B:492:THR:C	1:B:494:ASP:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:830:ALA:O	1:B:833:PHE:HB3	2.17	0.45
1:A:1023:LYS:C	1:A:1025:ASN:N	2.71	0.44
1:A:1168:LYS:HD2	1:A:1168:LYS:N	2.31	0.44
1:A:1205:GLU:HA	1:A:1208:LYS:HB3	1.97	0.44
1:A:1072:LYS:HB3	1:A:1226:ILE:HD12	1.98	0.44
1:A:295:MET:C	1:A:297:ALA:N	2.69	0.44
1:A:717:ASN:HD21	1:A:766:PHE:HE1	1.56	0.44
1:A:838:ASN:C	1:A:838:ASN:ND2	2.70	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:121:VAL:HG23	1:B:122:LEU:H	1.80	0.44
1:B:1218:ARG:NH1	1:B:1235:ASN:HD22	2.14	0.44
1:B:215:LEU:CA	1:B:219:PRO:HD2	2.47	0.44
1:B:304:ALA:O	1:B:307:ALA:HB3	2.17	0.44
1:B:35:VAL:HG21	1:B:355:ARG:NH2	2.32	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:612:MET:HA	1:B:619:PHE:HB2	1.99	0.44
1:B:942:GLN:O	1:B:943:ALA:C	2.56	0.44
1:B:945:MET:O	1:B:949:TYR:CD1	2.69	0.44
1:A:1246:LYS:H	1:A:1246:LYS:HD2	1.82	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:502:GLU:C	1:A:504:ASN:N	2.68	0.44
1:A:478:THR:O	1:A:520:VAL:HG23	2.17	0.44
1:A:71:PHE:HA	1:A:74:MET:HG2	1.99	0.44
1:A:821:VAL:HG23	1:A:822:LYS:N	2.32	0.44
1:A:821:VAL:O	1:A:824:ALA:HB3	2.16	0.44
1:A:911:LYS:O	1:A:914:THR:HB	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: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:827:SER:O	1:B:828:ARG:C	2.55	0.44
1:B:957:ALA:O	1:B:960:VAL:HG13	2.17	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
1:A:269:GLU:O	1:A:270:LEU:C	2.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ILE:HG13	1:A:393:ILE:O	2.17	0.44
1:A:44:TRP:C	1:A:46:ASP:N	2.71	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:797:VAL:O	1:A:801:ASP:OD1	2.36	0.44
1:B:1168:LYS:N	1:B:1168:LYS:HD2	2.33	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: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:A:217:ILE:HG13	1:A:218:SER:H	1.82	0.44
1:A:306:TYR:CG	1:A:307:ALA:N	2.85	0.44
1:A:407:LYS:HG3	1:A:407:LYS:O	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:88:SER:OG	1:A:89:THR:N	2.51	0.44
1:A:940:PHE:O	1:A:944:MET:HG2	2.16	0.44
1:B:120:GLY:O	1:B:121:VAL:C	2.55	0.44
1:B:1072:LYS:HB3	1:B:1226:ILE:HD12	1.98	0.44
1:B:886:LEU:HD12	1:B:886:LEU:C	2.37	0.44
1:B:914:THR:O	1:B:917:ALA:HB3	2.17	0.44
1:A:1125:GLU:O	1:A:1126:ASN:C	2.56	0.44
1:A:342:GLY:O	1:A:346:PRO:HD3	2.17	0.44
1:A:35:VAL:HG21	1:A:355:ARG:NH2	2.33	0.44
1:A:508:PHE:CE1	1:A:509:ILE:HG23	2.53	0.44
1:A:547:ILE:HG22	1:A:549:LEU:HD11	1.99	0.44
1:A:943:ALA:O	1:A:945:MET:N	2.51	0.44
1:B:147:PHE:O	1:B:148:PHE:C	2.54	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:420:ALA:C	1:B:421:LEU:HD12	2.37	0.44
1:B:727:ILE:O	1:B:731:VAL:HG23	2.17	0.44
1:B:762:SER:O	1:B:763:PHE:C	2.55	0.44
1:B:849:TYR:HD1	1:B:854:THR:HA	1.83	0.44
1:A:788:VAL:CG2	1:A:1004:ILE:HG13	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:PRO:O	1:A:1006:ARG:NH2	2.50	0.44
1:A:1090:VAL:CG2	1:A:1091:PHE:N	2.80	0.44
1:A:1261:GLY:H	1:A:1264:PHE:CB	2.30	0.44
1:A:199:GLY:O	1:A:203:GLY:HA3	2.17	0.44
1:A:249:VAL:HG12	1:A:249:VAL:O	2.17	0.44
1:A:411:LEU:C	1:A:411:LEU:HD23	2.38	0.44
1:A:384:ILE:HG23	1:A:546:LYS:HE2	2.00	0.44
1:A:723:ALA:O	1:A:727:ILE:HG22	2.18	0.44
1:A:773:PHE:CD1	1:A:773:PHE:C	2.91	0.44
1:A:837:ALA:HB1	1:A:982:MET:HE1	2.00	0.44
1:B:1090:VAL:CG2	1:B:1091:PHE:N	2.80	0.44
1:B:1178:GLN:HA	1:B:1178:GLN:OE1	2.18	0.44
1:B:1196:ASP:HA	1:B:1226:ILE:CD1	2.48	0.44
1:B:393:ILE:O	1:B:393:ILE:HG13	2.17	0.44
1:B:539:ARG:O	1:B:540:ALA:C	2.54	0.44
1:B:723:ALA:O	1:B:727:ILE:HG22	2.17	0.44
1:B:88:SER:OG	1:B:89:THR:N	2.51	0.44
1:B:916:TYR:O	1:B:920:LEU:HB2	2.17	0.44
1:B:93:GLU:H	1:B:93:GLU:CD	2.21	0.44
1:A:1041:PRO:O	1:A:1042:THR:HB	2.18	0.44
1:A:207:GLY:C	1:A:209:LYS:H	2.21	0.44
1:A:364:ILE:O	1:A:364:ILE:HG22	2.17	0.44
1:A:527:LEU:HB2	1:A:531:GLN:OE1	2.18	0.44
1:A:58:ILE:HG22	1:A:59:ILE:N	2.33	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:91:MET:HE3	1:B:91:MET:N	2.32	0.44
1:A:1159:ASP:HB3	1:A:1162:ASN:HB2	2.00	0.44
1:A:121:VAL:CG2	1:A:122:LEU:H	2.31	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
1:A:541:LEU:C	1:A:543:ARG:N	2.71	0.44
2:A:6001:0JZ:H35B	2:A:6001:0JZ:SE3	2.68	0.44
1:A:602:ILE:HG12	1:A:603:VAL:N	2.32	0.44
1:A:708:VAL:HA	1:A:711:ILE:HG22	2.00	0.44
1:A:933:VAL:C	1:A:935:GLY:N	2.69	0.44
1:A:993:ASP:O	1:A:994:TYR:HB3	2.18	0.44
1:B:129:VAL:HG11	1:B:935:GLY:CA	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:793:LEU:C	1:B:793:LEU:HD13	2.37	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:A:798:SER:CB	1:A:1041:PRO:HG2	2.47	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:781:THR:O	1:A:782:LYS:C	2.56	0.44
1:A:778:GLU:C	1:A:782:LYS:HE2	2.39	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: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:538:ALA:O	1:B:539:ARG:C	2.57	0.44
1:B:560:GLU:O	1:B:561:SER:C	2.56	0.44
1:B:781:THR:O	1:B:782:LYS:C	2.56	0.44
1:B:810:LEU:O	1:B:813:ARG:N	2.51	0.44
1:B:911:LYS:C	1:B:911:LYS:HD3	2.38	0.44
1:A:1131:ASP:OD2	1:A:1188:ARG:NE	2.51	0.43
1:A:144:ARG:CZ	1:A:175:VAL:HG21	2.48	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:195:THR:HA	1:A:337:GLY:HA2	2.00	0.43
1:A:429:LYS:C	1:A:431:THR:N	2.69	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:900:PHE:O	1:A:901:ARG:C	2.56	0.43
1:A:945:MET:O	1:A:949:TYR:CD1	2.68	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:75:THR:HB	1:B:326:GLN:OE1	2.17	0.43
1:B:547:ILE:HG22	1:B:549:LEU:HD11	1.99	0.43
1:B:55:LEU:O	1:B:58:ILE:HB	2.17	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: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:B:837:ALA:HB1	1:B:982:MET:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LYS:O	1:A:100:PHE:HB2	2.18	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:163:ASP:C	1:A:164:VAL:HG22	2.38	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:846:SER:O	1:A:849:TYR:HB2	2.17	0.43
1:A:911:LYS:C	1:A:911:LYS:HD3	2.38	0.43
1:B:207:GLY:CA	1:B:211:THR:HB	2.45	0.43
1:B:318:ILE:HD11	1:B:324:ILE:C	2.38	0.43
1:B:195:THR:HA	1:B:337:GLY:HA2	1.99	0.43
1:B:51:LEU:O	1:B:54:THR:HB	2.18	0.43
1:B:552:GLU:O	1:B:553:ALA:C	2.57	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:1077:GLN:O	1:A:1078:LEU:C	2.56	0.43
1:A:266:GLN:HB2	1:A:270:LEU:CD2	2.49	0.43
1:A:434:GLN:C	1:A:436:MET:H	2.20	0.43
1:A:727:ILE:HD12	1:A:753:LEU:HD23	2.00	0.43
1:A:308:LEU:HD13	1:A:755:PHE:CD1	2.53	0.43
1:A:831:VAL:O	1:A:832:ILE:C	2.57	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: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:269:GLU:O	1:B:270:LEU:C	2.55	0.43
1:B:384:ILE:HG23	1:B:546:LYS:HE2	1.98	0.43
1:B:44:TRP:CD1	1:B:45:LEU:N	2.86	0.43
1:B:419:VAL:CG2	1:B:593:VAL:HG13	2.48	0.43
1:B:62:VAL:O	1:B:65:PRO:HG2	2.18	0.43
1:A:1009:GLU:O	1:A:1010:LYS:CG	2.65	0.43
1:A:359:TYR:HA	1:A:362:PHE:CB	2.46	0.43
1:A:65:PRO:HG3	1:A:198:GLY:CA	2.48	0.43
1:A:265:GLY:CA	1:A:793:LEU:HD21	2.45	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
1:B:1106:ARG:O	1:B:1109:LEU:CD2	2.66	0.43
1:B:175:VAL:CG1	1:B:176:SER:H	2.30	0.43
1:B:43:GLY:HA3	1:B:46:ASP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:ASN:O	1:A:1102:VAL:C	2.57	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:59:ILE:O	1:A:63:ALA:HB2	2.19	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:A:91:MET:HG3	1:A:91:MET:H	1.61	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:B:213:VAL:O	1:B:216:ALA:HB3	2.19	0.43
1:B:309:ALA:O	1:B:310:PHE:C	2.56	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:561:SER:O	1:B:562:GLU:C	2.56	0.43
1:B:833:PHE:O	1:B:834:GLN:C	2.56	0.43
1:B:83:ASN:O	1:B:86:LYS:HB3	2.19	0.43
1:A:1252:THR:CG2	1:A:1255:GLN:HB2	2.49	0.43
1:A:265:GLY:C	1:A:267:LYS:HG3	2.39	0.43
1:B:1026:MET:O	1:B:1026:MET:HG3	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:B:207:GLY:O	1:B:209:LYS:N	2.51	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:44:TRP:C	1:B:46:ASP:N	2.71	0.43
1:B:58:ILE:HG22	1:B:59:ILE:N	2.33	0.43
1:B:308:LEU:HD12	1:B:751:PHE:CE2	2.54	0.43
1:A:1031:VAL:H	1:A:1056:VAL:HG13	1.83	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:618:TYR:CE2	1:A:622:VAL:HG21	2.53	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:833:PHE:O	1:A:834:GLN:C	2.57	0.43
1:A:949:TYR:H	1:A:949:TYR:HD1	1.67	0.43
1:A:733:GLY:CA	1:A:968:GLU:HG3	2.49	0.43
1:B:1022:LEU:O	1:B:1023:LYS:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1176:GLN:O	1:B:1177:LYS:C	2.56	0.43
1:B:279:GLU:O	1:B:282:ARG:HB2	2.18	0.43
1:B:316:LEU:C	1:B:318:ILE:H	2.22	0.43
1:B:463:ARG:NH1	1:B:903:VAL:HG22	2.33	0.43
1:B:568:ALA:O	1:B:569:LEU:C	2.56	0.43
1:B:992:PRO:C	1:B:994:TYR:H	2.21	0.43
1:A:1119:PHE:HD2	1:A:1121:CYS:SG	2.42	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
1:A:255:ALA:O	1:A:256:ALA:C	2.57	0.43
1:A:389:GLU:OE1	1:A:412:LYS:HB2	2.17	0.43
2:A:6001:OJZ:O25	2:A:6001:OJZ:H29B	2.19	0.43
1:A:796:ASP:OD2	1:A:1014:ILE:HD11	2.19	0.43
1:A:257:ILE:HG13	1:A:800:PHE:CD2	2.54	0.43
1:A:943:ALA:C	1:A:945:MET:N	2.71	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: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:312:TYR:O	1:B:314:THR:N	2.52	0.43
1:B:407:LYS:O	1:B:407:LYS:HG3	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:156:ILE:HG12	1:B:439:LEU:O	2.18	0.43
1:B:513:PRO:O	1:B:514:HIS:HB2	2.19	0.43
1:B:58:ILE:O	1:B:60:HIS:N	2.51	0.43
1:B:936:ILE:O	1:B:939:SER:OG	2.37	0.43
1:B:959:LEU:C	1:B:959:LEU:HD23	2.39	0.43
1:B:993:ASP:O	1:B:995:ALA:N	2.52	0.43
1:A:1014:ILE:CD1	1:A:1106:ARG:HH22	2.31	0.43
1:A:116:GLY:O	1:A:117:ILE:C	2.56	0.43
1:A:307:ALA:O	1:A:308:LEU:C	2.55	0.43
1:A:362:PHE:HA	1:A:365:ILE:HD12	2.01	0.43
1:A:492:THR:O	1:A:493:MET:C	2.57	0.43
1:A:809:ALA:O	1:A:813:ARG:HG2	2.19	0.43
1:A:78:PHE:HZ	1:A:967:PHE:O	1.99	0.43
1:B:1092:LEU:HD22	1:B:1100:LEU:HD22	2.01	0.43
1:B:1076:VAL:HG13	1:B:1194:LEU:HD13	2.01	0.43
1:B:1218:ARG:NH1	1:B:1235:ASN:ND2	2.65	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:449:ILE:O	1:B:450:ASP:C	2.57	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:A:103:LEU:HD22	1:A:960:VAL:HG22	2.01	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: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:315:SER:C	1:A:318:ILE:HG22	2.39	0.43
1:A:560:GLU:O	1:A:561:SER:C	2.56	0.43
1:A:723:ALA:O	1:A:724:PHE:C	2.57	0.43
1:A:861:VAL:CB	1:A:862:PRO:HD3	2.48	0.43
1:B:209:LYS:C	1:B:212:LEU:HB3	2.38	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: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:561:SER:O	1:A:562:GLU:C	2.56	0.42
1:A:59:ILE:HD12	1:A:59:ILE:O	2.19	0.42
1:A:697:LEU:HD12	1:A:698:LYS:N	2.34	0.42
1:A:74:MET:HG3	1:A:75:THR:N	2.34	0.42
1:A:909:GLU:N	1:A:909:GLU:OE2	2.45	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: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:53:GLY:O	1:B:56:ALA:N	2.52	0.42
1:B:540:ALA:O	1:B:543:ARG:CB	2.65	0.42
1:B:696:ILE:O	1:B:700:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1084:ASP:HA	1:A:1085:PRO:HD2	1.89	0.42
1:A:1144:ALA:O	1:A:1148:ALA:HB3	2.19	0.42
1:A:1121:CYS:O	1:A:1165:VAL:HG13	2.19	0.42
1:A:352:ALA:O	1:A:353:ASN:C	2.57	0.42
1:A:401:LYS:CD	1:A:401:LYS:H	2.24	0.42
1:A:779:ILE:HA	1:A:782:LYS:HE3	2.01	0.42
1:A:711:ILE:HD11	1:A:832:ILE:HG21	2.01	0.42
1:A:942:GLN:O	1:A:945:MET:CB	2.64	0.42
1:B:1159:ASP:HB3	1:B:1162:ASN:HB2	2.00	0.42
1:B:1176:GLN:N	1:B:1176:GLN:OE1	2.52	0.42
1:B:299:PHE:O	1:B:303:TYR:N	2.51	0.42
1:B:436:MET:HE1	1:B:449:ILE:HD13	2.01	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:A:1076:VAL:CG1	1:A:1194:LEU:HD13	2.50	0.42
1:A:1182:ILE:N	1:A:1182:ILE:HD12	2.34	0.42
1:A:1179:ARG:CZ	1:A:1209:VAL:HG11	2.49	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:793:LEU:HD13	1:A:793:LEU:C	2.39	0.42
1:A:883:LYS:HA	1:A:886:LEU:CG	2.49	0.42
1:B:1195:LEU:HB2	1:B:1225:VAL:HA	2.01	0.42
1:B:121:VAL:CG2	1:B:122:LEU:H	2.32	0.42
1:B:185:LYS:O	1:B:186:ILE:C	2.58	0.42
1:B:324:ILE:O	1:B:326:GLN:HB2	2.19	0.42
1:B:352:ALA:O	1:B:353:ASN:C	2.57	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:74:MET:HG3	1:B:75:THR:N	2.33	0.42
1:B:827:SER:O	1:B:830:ALA:N	2.53	0.42
1:B:838:ASN:C	1:B:838:ASN:ND2	2.71	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:A:144:ARG:HG2	1:A:920:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ILE:O	1:A:349:GLU:C	2.57	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:981:ALA:HB1	2:A:6001:OJZ:H32	2.02	0.42
1:A:60:HIS:O	1:A:63:ALA:CB	2.65	0.42
1:A:792:MET:O	1:A:795:GLN:N	2.53	0.42
1:B:1229:ARG:C	1:B:1231:SER:N	2.73	0.42
1:B:1207:GLU:OE2	1:B:1229:ARG:NH2	2.52	0.42
1:B:154:GLN:O	1:B:154:GLN:HG2	2.19	0.42
1:B:315:SER:C	1:B:318:ILE:HG22	2.40	0.42
1:B:432:THR:O	1:B:433:VAL:C	2.56	0.42
1:B:974:PHE:HB3	2:B:6002:OJZ:C30	2.49	0.42
1:A:209:LYS:CA	1:A:212:LEU:HB3	2.49	0.42
1:A:474:VAL:HG11	1:A:901:ARG:CB	2.48	0.42
1:A:293:ILE:CG2	1:A:766:PHE:HB3	2.31	0.42
1:A:785:ARG:O	1:A:786:TYR:C	2.57	0.42
1:A:900:PHE:O	1:A:903:VAL:N	2.51	0.42
1:A:957:ALA:O	1:A:958:TYR:C	2.58	0.42
1:A:962:GLN:O	1:A:963:GLN:HB2	2.19	0.42
1:B:1031:VAL:O	1:B:1055:GLU:HA	2.19	0.42
1:B:1077:GLN:O	1:B:1078:LEU:C	2.58	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:B:136:ALA:O	1:B:137:GLY:C	2.57	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:54:THR:O	1:B:58:ILE:HD13	2.19	0.42
1:B:727:ILE:HD12	1:B:753:LEU:HD23	1.99	0.42
1:A:1207:GLU:OE2	1:A:1229:ARG:NH2	2.52	0.42
1:A:188:MET:C	1:A:188:MET:SD	2.97	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:55:LEU:O	1:A:56:ALA:C	2.58	0.42
1:A:64:LEU:O	1:A:65:PRO:C	2.52	0.42
1:B:1090:VAL:HG22	1:B:1097:ILE:HG13	2.01	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:348:ILE:O	1:B:349:GLU:C	2.57	0.42
1:B:39:PHE:CD2	1:B:355:ARG:HA	2.55	0.42
1:B:467:GLY:H	1:B:545:PRO:CB	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:703:GLU:HA	1:B:783:ARG:HH12	1.84	0.42
1:B:778:GLU:C	1:B:782:LYS:HE2	2.40	0.42
1:B:278:GLU:CB	1:B:782:LYS:HG2	2.43	0.42
1:B:905:SER:HB3	1:B:907:THR:OG1	2.18	0.42
1:A:279:GLU:O	1:A:282:ARG:HB2	2.19	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: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:279:GLU:CG	1:A:782:LYS:HD2	2.49	0.42
1:B:135:ALA:O	1:B:136:ALA:C	2.57	0.42
1:B:618:TYR:CE2	1:B:622:VAL:HG21	2.54	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:A:308:LEU:O	1:A:309:ALA:C	2.55	0.42
1:A:419:VAL:CG2	1:A:593:VAL:HG13	2.48	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: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:B:278:GLU:OE2	1:B:785:ARG:HD2	2.20	0.42
1:B:541:LEU:C	1:B:543:ARG:N	2.73	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:943:ALA:C	1:B:945:MET:N	2.73	0.42
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:1032:GLN:HB3	1:B:1091:PHE:HD2	1.85	0.42
1:B:1125:GLU:O	1:B:1126:ASN:C	2.58	0.42
1:B:1185:ALA:O	1:B:1190:PRO:CD	2.67	0.42
1:B:266:GLN:HB2	1:B:270:LEU:HD22	2.01	0.42
1:B:447:VAL:HG13	1:B:454:ILE:HG22	2.00	0.42
1:B:328:LEU:HD11	1:B:728:PHE:HZ	1.84	0.42
1:B:765:THR:HG23	1:B:766:PHE:HD1	1.84	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1179:ARG:CZ	1:B:1209:VAL:HG11	2.50	0.42
1:B:257:ILE:CG2	1:B:258:ARG:N	2.82	0.42
1:B:492:THR:O	1:B:493:MET:C	2.58	0.42
1:B:585:LEU:HA	1:B:588:VAL:HB	2.02	0.42
1:A:1092:LEU:HD22	1:A:1100:LEU:HD22	2.01	0.41
1:A:1156:SER:OG	1:A:1157:LEU:HD22	2.20	0.41
1:A:1129:TYR:CD2	1:A:1184:ARG:HG3	2.54	0.41
1:A:1229:ARG:C	1:A:1231:SER:N	2.74	0.41
1:A:281:LYS:O	1:A:285:ILE:HG22	2.21	0.41
1:A:538:ALA:O	1:A:539:ARG:C	2.58	0.41
1:A:54:THR:O	1:A:58:ILE:HD13	2.20	0.41
1:A:762:SER:O	1:A:763:PHE:C	2.57	0.41
1:A:779:ILE:O	1:A:780:LEU:C	2.58	0.41
1:A:820:GLN:CB	1:A:1000:SER:HB2	2.50	0.41
1:A:773:PHE:CB	1:A:829:LEU:HD13	2.50	0.41
1:A:948:SER:O	1:A:952:CYS:SG	2.75	0.41
1:A:99:MET:N	1:A:99:MET:SD	2.93	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
1:B:529:GLY:HA2	1:B:532:LYS:HD3	2.01	0.41
1:B:59:ILE:O	1:B:59:ILE:HD12	2.20	0.41
1:B:721:GLN:HG2	1:B:982:MET:HE3	2.02	0.41
1:B:797:VAL:O	1:B:801:ASP:OD1	2.38	0.41
1:A:178:ILE:HG12	1:A:358:ALA:HB1	2.00	0.41
1:A:434:GLN:C	1:A:436:MET:N	2.74	0.41
1:A:697:LEU:CA	1:A:700:ASN:HB2	2.47	0.41
1:A:741:PRO:O	1:A:742:GLU:HB2	2.20	0.41
1:A:718:GLY:CA	1:A:837:ALA:HB2	2.50	0.41
1:A:900:PHE:C	1:A:902:THR:N	2.73	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:B:96:LYS:O	1:B:100:PHE:HB2	2.20	0.41
1:A:1076:VAL:O	1:A:1079:LEU:HB3	2.20	0.41
1:A:312:TYR:O	1:A:314:THR:N	2.53	0.41
1:A:856:LEU:O	1:A:860:ILE:HG12	2.20	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:B:1076:VAL:O	1:B:1079:LEU:HB3	2.19	0.41
1:B:215:LEU:HA	1:B:219:PRO:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:LEU:HB3	1:B:440:TYR:H	1.74	0.41
1:B:466:ILE:O	1:B:466:ILE:HG22	2.20	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:A:1050:GLN:O	1:A:1050:GLN:HG3	2.21	0.41
1:A:1164:ARG:O	1:A:1165:VAL:C	2.57	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:A:144:ARG:O	1:A:145:GLN:C	2.59	0.41
1:A:151:ILE:C	1:A:153:ASN:N	2.72	0.41
1:A:155:GLU:O	1:A:156:ILE:C	2.58	0.41
1:A:39:PHE:CD2	1:A:355:ARG:HA	2.54	0.41
1:A:388:LEU:H	1:A:388:LEU:HD12	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:905:SER:HB3	1:A:907:THR:OG1	2.21	0.41
1:A:889:SER:OG	1:A:919:SER:HB2	2.20	0.41
1:B:1229:ARG:O	1:B:1231:SER:N	2.53	0.41
1:B:1250:HIS:C	1:B:1256:LEU:HD21	2.40	0.41
1:B:138:ARG:O	1:B:139:GLN:C	2.58	0.41
1:B:144:ARG:O	1:B:145:GLN:C	2.57	0.41
1:B:286:LYS:HG2	1:B:778:GLU:CD	2.41	0.41
1:B:34:SER:O	1:B:35:VAL:C	2.59	0.41
1:B:59:ILE:O	1:B:63:ALA:HB2	2.21	0.41
1:B:617:ILE:H	1:B:617:ILE:CD1	2.33	0.41
1:B:702:THR:C	1:B:704:TRP:H	2.23	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:152:MET:CG	1:B:913:GLU:OE1	2.69	0.41
1:A:1090:VAL:HG22	1:A:1097:ILE:HG13	2.03	0.41
1:A:1176:GLN:OE1	1:A:1176:GLN:N	2.53	0.41
1:A:1176:GLN:O	1:A:1177:LYS:C	2.59	0.41
1:A:1189:GLN:O	1:A:1190:PRO:O	2.39	0.41
1:A:245:LYS:CA	1:A:245:LYS:NZ	2.83	0.41
1:A:268:LYS:O	1:A:269:GLU:C	2.59	0.41
1:A:324:ILE:O	1:A:326:GLN:HB2	2.20	0.41
1:A:345:SER:O	1:A:346:PRO:C	2.56	0.41
1:A:583:HIS:HB2	1:A:584:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:PRO:CG	1:A:706:TYR:H	2.31	0.41
1:A:710:GLY:O	1:A:711:ILE:C	2.57	0.41
1:B:1129:TYR:O	1:B:1131:ASP:N	2.52	0.41
1:B:322:TYR:CZ	1:B:324:ILE:HG12	2.55	0.41
1:B:156:ILE:HG23	1:B:439:LEU:HD12	2.02	0.41
1:B:476:PHE:CE2	1:B:912:PHE:HZ	2.38	0.41
1:B:583:HIS:HB2	1:B:584:ARG:NH1	2.35	0.41
1:B:86:LYS:HE2	1:B:739:GLY:N	2.35	0.41
1:B:773:PHE:CD1	1:B:773:PHE:C	2.93	0.41
1:A:1176:GLN:O	1:A:1179:ARG:HB2	2.20	0.41
1:A:1250:HIS:C	1:A:1256:LEU:HD21	2.40	0.41
1:A:617:ILE:CD1	1:A:617:ILE:H	2.33	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:881:LYS:HZ2	1:A:881:LYS:HB2	1.81	0.41
1:A:92:SER:OG	1:A:962:GLN:NE2	2.51	0.41
1:B:1079:LEU:O	1:B:1105:LEU:HD21	2.21	0.41
1:B:188:MET:SD	1:B:188:MET:C	2.98	0.41
1:B:223:LEU:O	1:B:224:SER:C	2.59	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
1:B:345:SER:O	1:B:346:PRO:C	2.57	0.41
1:B:409:LEU:HD21	1:B:597:PHE:CZ	2.56	0.41
1:B:808:GLY:O	1:B:809:ALA:C	2.58	0.41
1:B:848:ILE:HG13	1:B:848:ILE:O	2.21	0.41
1:B:889:SER:OG	1:B:919:SER:HB2	2.21	0.41
1:B:943:ALA:O	1:B:944:MET:C	2.56	0.41
1:A:1031:VAL:O	1:A:1055:GLU:HA	2.21	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:443:LEU:HD23	1:A:443:LEU:C	2.41	0.41
1:A:494:ASP:O	1:A:497:GLU:HB3	2.21	0.41
1:A:731:VAL:HA	1:A:750:LEU:CD1	2.50	0.41
1:B:151:ILE:C	1:B:153:ASN:N	2.73	0.41
1:B:258:ARG:C	1:B:260:VAL:N	2.74	0.41
1:B:43:GLY:CA	1:B:46:ASP:HB2	2.50	0.41
1:B:710:GLY:O	1:B:711:ILE:C	2.57	0.41
1:B:716:ILE:HD12	1:B:716:ILE:C	2.41	0.41
1:B:727:ILE:HD13	1:B:754:LEU:CD2	2.50	0.41
1:B:711:ILE:HD11	1:B:832:ILE:HG21	2.02	0.41
1:B:900:PHE:O	1:B:902:THR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:GLY:CA	1:B:968:GLU:HG3	2.51	0.41
1:B:990:PHE:O	1:B:991:ALA:C	2.58	0.41
1:A:1039:ASN:CG	1:A:1047:PRO:HA	2.41	0.41
1:A:1178:GLN:O	1:A:1181:ALA:N	2.54	0.41
1:A:211:THR:HA	1:A:214:ILE:CD1	2.44	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:334:VAL:O	1:A:335:LEU:C	2.59	0.41
1:A:459:VAL:O	1:A:460:ARG:C	2.56	0.41
1:A:816:ASN:O	1:A:820:GLN:HG2	2.21	0.41
1:A:721:GLN:HG2	1:A:982:MET:HE3	2.02	0.41
1:B:274:ASN:O	1:B:275:ASN:C	2.59	0.41
1:B:296:GLY:O	1:B:300:LEU:HG	2.20	0.41
1:B:307:ALA:O	1:B:308:LEU:C	2.58	0.41
1:B:422:VAL:O	1:B:597:PHE:O	2.39	0.41
1:B:459:VAL:O	1:B:460:ARG:C	2.57	0.41
1:B:46:ASP:O	1:B:49:TYR:N	2.54	0.41
1:B:779:ILE:HA	1:B:782:LYS:HE3	2.03	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: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:1252:THR:O	1:A:1255:GLN:HB3	2.21	0.41
1:A:209:LYS:HA	1:A:212:LEU:CB	2.51	0.41
1:A:215:LEU:HA	1:A:219:PRO:HD2	2.03	0.41
1:A:286:LYS:HA	1:A:289:ILE:CB	2.31	0.41
1:A:309:ALA:O	1:A:310:PHE:C	2.59	0.41
1:A:342:GLY:O	1:A:346:PRO:HD2	2.20	0.41
1:A:441:ASP:OD1	1:A:442:PRO:HD2	2.21	0.41
1:A:503:ALA:O	1:A:504:ASN:C	2.58	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:808:GLY:O	1:A:809:ALA:C	2.59	0.41
1:A:883:LYS:HD3	1:A:886:LEU:HD21	2.02	0.41
1:B:1156:SER:OG	1:B:1157:LEU:HD22	2.20	0.41
1:B:255:ALA:O	1:B:256:ALA:C	2.59	0.41
1:B:54:THR:O	1:B:57:ALA:HB3	2.20	0.41
1:B:551:ASP:HA	1:B:581:ILE:HG23	2.03	0.41
1:B:974:PHE:CD1	2:B:6002:0JZ:H30B	2.56	0.41
1:B:614:GLU:O	1:B:615:LYS:C	2.59	0.41
1:B:689:PRO:CD	1:B:690:PRO:HD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:693:PHE:H	1:B:693:PHE:HD2	1.65	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:A:1038:PHE:CD2	1:A:1078:LEU:HD21	2.56	0.41
1:A:1147:GLU:HB3	1:A:1186:LEU:HD22	2.02	0.41
1:A:266:GLN:HB2	1:A:270:LEU:HD22	2.03	0.41
1:A:312:TYR:O	1:A:313:GLY:C	2.59	0.41
1:A:568:ALA:O	1:A:569:LEU:C	2.57	0.41
1:A:787:MET:SD	1:A:1008:ILE:HD11	2.61	0.41
1:A:845:ILE:O	1:A:849:TYR:CD2	2.74	0.41
1:A:91:MET:HE3	1:A:91:MET:N	2.36	0.41
1:A:933:VAL:O	1:A:936:ILE:HG22	2.21	0.41
1:A:942:GLN:O	1:A:943:ALA:C	2.58	0.41
1:B:1107:ALA:O	1:B:1188:ARG:HD3	2.21	0.41
1:B:1203:ASP:O	1:B:1207:GLU:HG3	2.21	0.41
1:B:129:VAL:HG11	1:B:934:PHE:C	2.41	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: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: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:N	1:A:471:GLN:OE1	2.52	0.41
1:A:899:ASN:OD1	1:A:901:ARG:NH2	2.54	0.41
1:B:1003:HIS:O	1:B:1007:ILE:HG13	2.21	0.41
1:B:1213:ALA:O	1:B:1217:ALA:HB2	2.21	0.41
1:B:1067:SER:OG	1:B:1244:ASN:ND2	2.54	0.41
1:B:140:ILE:O	1:B:143:ILE:N	2.53	0.41
1:B:142:LYS:O	1:B:143:ILE:C	2.60	0.41
1:B:480:ILE:O	1:B:482:GLU:N	2.54	0.41
1:B:796:ASP:HA	1:B:800:PHE:CD2	2.56	0.41
1:B:900:PHE:C	1:B:902:THR:N	2.73	0.41
1:B:973:VAL:O	1:B:976:ALA:N	2.51	0.41
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:1255:GLN:O	1:A:1258:ALA:N	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:853:LEU:HD11	1:A:956:GLY:HA2	2.03	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:A:1039:ASN:O	1:A:1040:TYR:C	2.59	0.40
1:A:1155:ASP:O	1:A:1160:LYS:HE3	2.21	0.40
1:A:183:GLY:O	1:A:184:ASP:C	2.60	0.40
1:A:212:LEU:CD1	1:A:215:LEU:HD12	2.50	0.40
1:A:462:LEU:HD12	1:A:466:ILE:CD1	2.51	0.40
1:A:58:ILE:C	1:A:60:HIS:N	2.72	0.40
1:A:727:ILE:HD13	1:A:754:LEU:CD2	2.50	0.40
1:A:761:ILE:CD1	1:A:761:ILE:H	2.34	0.40
1:A:810:LEU:O	1:A:813:ARG:N	2.54	0.40
1:B:1038:PHE:CZ	1:B:1040:TYR:N	2.89	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:N	1:B:471:GLN:OE1	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: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:A:253:VAL:HB	1:A:1119:PHE:CE1	2.52	0.40
1:A:282:ARG:HD3	1:A:282:ARG:HA	1.83	0.40
1:A:316:LEU:C	1:A:318:ILE:H	2.24	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: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:925:ARG:NE	1:B:519:LEU:HD12	2.36	0.40
1:B:1132:ASN:C	1:B:1134:ARG:H	2.25	0.40
1:B:1243:GLN:HG3	1:B:1246:LYS:HZ2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ILE:HG22	1:B:364:ILE:O	2.21	0.40
1:B:519:LEU:N	1:B:519:LEU:HD13	2.19	0.40
1:B:58:ILE:C	1:B:60:HIS:N	2.72	0.40
1:B:899:ASN:OD1	1:B:901:ARG:NH2	2.54	0.40
1:A:110:TYR:CA	1:A:113:TYR:HD2	2.34	0.40
1:A:1191:HIS:HA	1:A:1221:ARG:HB2	2.02	0.40
1:A:1208:LYS:HD3	1:A:1208:LYS:C	2.41	0.40
1:A:369:PRO:O	1:A:370:SER:C	2.60	0.40
1:A:409:LEU:HD21	1:A:597:PHE:CZ	2.56	0.40
1:A:770:GLY:HA2	1:A:773:PHE:CZ	2.56	0.40
1:A:901:ARG:N	1:A:901:ARG:HD3	2.36	0.40
1:A:961:THR:O	1:A:962:GLN:CB	2.69	0.40
1:B:688:VAL:HB	1:B:1006:ARG:HH12	1.87	0.40
1:B:140:ILE:O	1:B:141:HIS:C	2.60	0.40
1:B:302:ILE:O	1:B:303:TYR:C	2.59	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: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:838:ASN:O	1:B:839:LEU:O	2.38	0.40
1:B:92:SER:O	1:B:96:LYS:HG3	2.21	0.40
1:A:1159:ASP:O	1:A:1160:LYS:C	2.60	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:302:ILE:O	1:A:303:TYR:C	2.57	0.40
1:A:382:ASP:C	1:A:384:ILE:N	2.75	0.40
1:A:479:THR:HA	1:A:518:THR:O	2.21	0.40
1:A:614:GLU:O	1:A:615:LYS:C	2.60	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:835:ASN:O	1:A:836:ILE:C	2.57	0.40
1:A:92:SER:O	1:A:96:LYS:HG3	2.22	0.40
1:A:971:LEU:O	1:A:972:LEU:C	2.60	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:327:VAL:O	1:B:331:PHE:HD1	2.04	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:902:THR:C	1:B:904:VAL:N	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:990:PHE:O	1:B:991:ALA:O	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1178/1284 (92%)	704 (60%)	302 (26%)	172 (15%)	0	4
1	B	1178/1284 (92%)	707 (60%)	305 (26%)	166 (14%)	0	4
All	All	2356/2568 (92%)	1411 (60%)	607 (26%)	338 (14%)	0	4

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	884 (91%)	92 (9%)	8	30
1	B	976/1065 (92%)	880 (90%)	96 (10%)	8	29
All	All	1952/2130 (92%)	1764 (90%)	188 (10%)	8	29

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ILE
1	A	83	ASN
1	A	91	MET
1	A	93	GLU
1	A	99	MET
1	A	100	PHE
1	A	113	TYR
1	A	131	PHE
1	A	138	ARG
1	A	147	PHE
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	189	PHE
1	A	196	PHE
1	A	206	ARG
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	281	LYS
1	A	285	ILE
1	A	295	MET
1	A	306	TYR
1	A	310	PHE
1	A	311	TRP
1	A	330	VAL
1	A	332	PHE
1	A	397	TYR
1	A	401	LYS
1	A	402	GLU
1	A	404	GLN
1	A	435	LEU
1	A	438	ARG

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Mol	Chain	Res	Type
1	A	439	LEU
1	A	458	ASN
1	A	493	MET
1	A	519	LEU
1	A	694	TRP
1	A	697	LEU
1	A	703	GLU
1	A	707	PHE
1	A	722	PRO
1	A	751	PHE
1	A	755	PHE
1	A	771	PHE
1	A	786	TYR
1	A	789	PHE
1	A	795	GLN
1	A	799	TRP
1	A	801	ASP
1	A	804	LYS
1	A	816	ASN
1	A	838	ASN
1	A	851	TRP
1	A	862	PRO
1	A	872	MET
1	A	881	LYS
1	A	892	ILE
1	A	901	ARG
1	A	902	THR
1	A	908	ARG
1	A	912	PHE
1	A	954	ARG
1	A	968	GLU
1	A	969	ASN
1	A	990	PHE
1	A	993	ASP
1	A	996	LYS
1	A	1020	GLN
1	A	1060	GLN
1	A	1090	VAL
1	A	1099	GLN
1	A	1108	GLN
1	A	1109	LEU
1	A	1118	LEU

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Mol	Chain	Res	Type
1	A	1131	ASP
1	A	1140	GLU
1	A	1158	PRO
1	A	1192	ILE
1	A	1204	THR
1	A	1221	ARG
1	A	1223	CYS
1	A	1246	LYS
1	B	59	ILE
1	B	64	LEU
1	B	83	ASN
1	B	91	MET
1	B	93	GLU
1	B	99	MET
1	B	100	PHE
1	B	113	TYR
1	B	131	PHE
1	B	138	ARG
1	B	147	PHE
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	189	PHE
1	B	196	PHE
1	B	206	ARG
1	B	210	LEU
1	B	219	PRO
1	B	228	TRP
1	B	238	LYS
1	B	243	TYR
1	B	245	LYS
1	B	252	GLU
1	B	254	LEU
1	B	257	ILE
1	B	270	LEU
1	B	281	LYS
1	B	285	ILE
1	B	295	MET
1	B	299	PHE

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Mol	Chain	Res	Type
1	B	306	TYR
1	B	310	PHE
1	B	311	TRP
1	B	330	VAL
1	B	332	PHE
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	458	ASN
1	B	493	MET
1	B	519	LEU
1	B	693	PHE
1	B	694	TRP
1	B	697	LEU
1	B	703	GLU
1	B	707	PHE
1	B	722	PRO
1	B	751	PHE
1	B	755	PHE
1	B	771	PHE
1	B	786	TYR
1	B	789	PHE
1	B	795	GLN
1	B	799	TRP
1	B	801	ASP
1	B	804	LYS
1	B	816	ASN
1	B	838	ASN
1	B	851	TRP
1	B	862	PRO
1	B	872	MET
1	B	881	LYS
1	B	892	ILE
1	B	901	ARG
1	B	902	THR
1	B	908	ARG
1	B	912	PHE

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Mol	Chain	Res	Type
1	B	954	ARG
1	B	968	GLU
1	B	969	ASN
1	B	990	PHE
1	B	996	LYS
1	B	1010	LYS
1	B	1060	GLN
1	B	1090	VAL
1	B	1099	GLN
1	B	1108	GLN
1	B	1109	LEU
1	B	1118	LEU
1	B	1131	ASP
1	B	1140	GLU
1	B	1158	PRO
1	B	1192	ILE
1	B	1204	THR
1	B	1221	ARG
1	B	1223	CYS
1	B	1246	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) 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	153	ASN
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	392	ASN
1	A	394	HIS
1	A	404	GLN
1	A	434	GLN
1	A	437	GLN
1	A	458	ASN

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Mol	Chain	Res	Type
1	A	515	GLN
1	A	605	GLN
1	A	625	GLN
1	A	721	GLN
1	A	769	GLN
1	A	795	GLN
1	A	805	ASN
1	A	834	GLN
1	A	838	ASN
1	A	878	GLN
1	A	932	HIS
1	A	962	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
1	B	60	HIS
1	B	83	ASN
1	B	87	ASN
1	B	128	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	392	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

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Mol	Chain	Res	Type
1	B	605	GLN
1	B	625	GLN
1	B	721	GLN
1	B	769	GLN
1	B	795	GLN
1	B	805	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	1149	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 carbohydrates 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	0JZ	B	6002	-	21,39,39	1.74	4 (19%)	24,57,57	1.91	7 (29%)
2	0JZ	A	6001	-	21,39,39	2.04	5 (23%)	24,57,57	2.49	9 (37%)

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	0JZ	B	6002	-	-	4/24/48/48	0/3/4/4
2	0JZ	A	6001	-	-	4/24/48/48	0/3/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6001	0JZ	C16-N17	5.48	1.46	1.34
2	B	6002	0JZ	C09-N10	4.44	1.43	1.34
2	A	6001	0JZ	C02-N03	4.39	1.43	1.34
2	A	6001	0JZ	C09-N10	3.88	1.42	1.34
2	B	6002	0JZ	C02-N03	3.70	1.42	1.34
2	A	6001	0JZ	C18-N17	3.41	1.52	1.46
2	B	6002	0JZ	C16-N17	2.55	1.39	1.34
2	B	6002	0JZ	C15-C16	-2.51	1.44	1.50
2	A	6001	0JZ	C04-N03	2.38	1.50	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6001	0JZ	C04-N03-C02	5.49	131.07	122.28
2	A	6001	0JZ	C18-N17-C16	5.23	130.66	122.28
2	A	6001	0JZ	C35-C34-C18	4.30	115.38	111.24
2	B	6002	0JZ	C33-C31-C11	3.77	114.87	111.24
2	B	6002	0JZ	C29-C28-C04	3.75	114.85	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6001	0JZ	C30-C28-C04	3.74	114.84	111.24
2	A	6001	0JZ	C11-N10-C09	3.59	128.04	122.28
2	B	6002	0JZ	C04-N03-C02	3.46	127.82	122.28
2	A	6001	0JZ	C36-C34-C18	2.97	114.09	111.24
2	B	6002	0JZ	C11-N10-C09	2.97	127.04	122.28
2	A	6001	0JZ	C33-C31-C11	2.83	113.96	111.24
2	B	6002	0JZ	C01-C02-N03	2.74	120.29	115.20
2	B	6002	0JZ	C18-N17-C16	2.68	126.58	122.28
2	A	6001	0JZ	C15-C16-N17	2.56	119.96	115.20
2	B	6002	0JZ	C08-C09-N10	2.13	119.16	115.20
2	A	6001	0JZ	C29-C28-C04	2.02	113.18	111.24

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	6002	0JZ	C05-C04-N03-C02
2	B	6002	0JZ	C28-C04-N03-C02
2	A	6001	0JZ	C05-C04-N03-C02
2	A	6001	0JZ	C28-C04-N03-C02
2	A	6001	0JZ	C19-C18-N17-C16
2	A	6001	0JZ	C34-C18-N17-C16
2	B	6002	0JZ	C12-C11-N10-C09
2	B	6002	0JZ	C31-C11-N10-C09

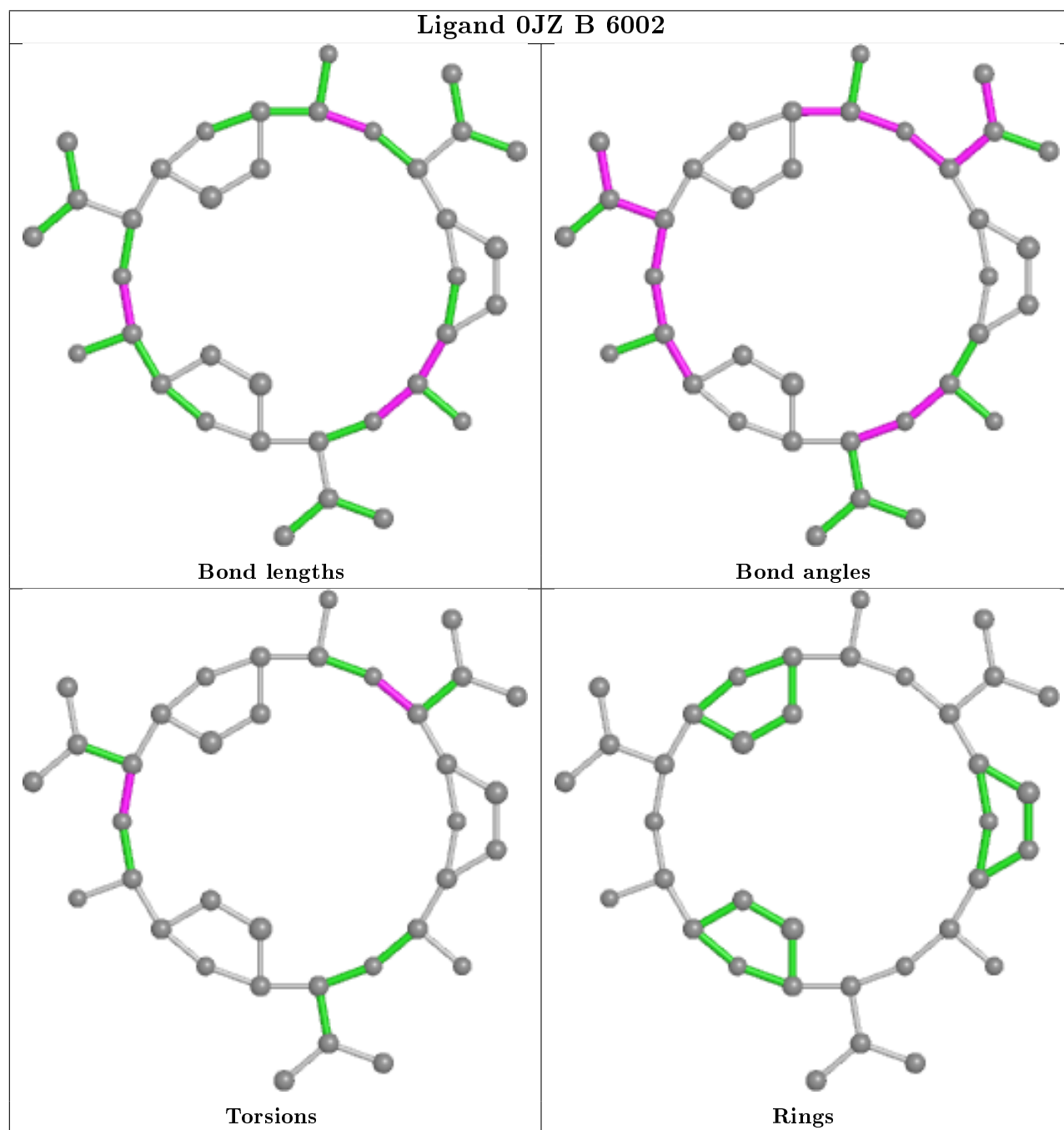
There are no ring outliers.

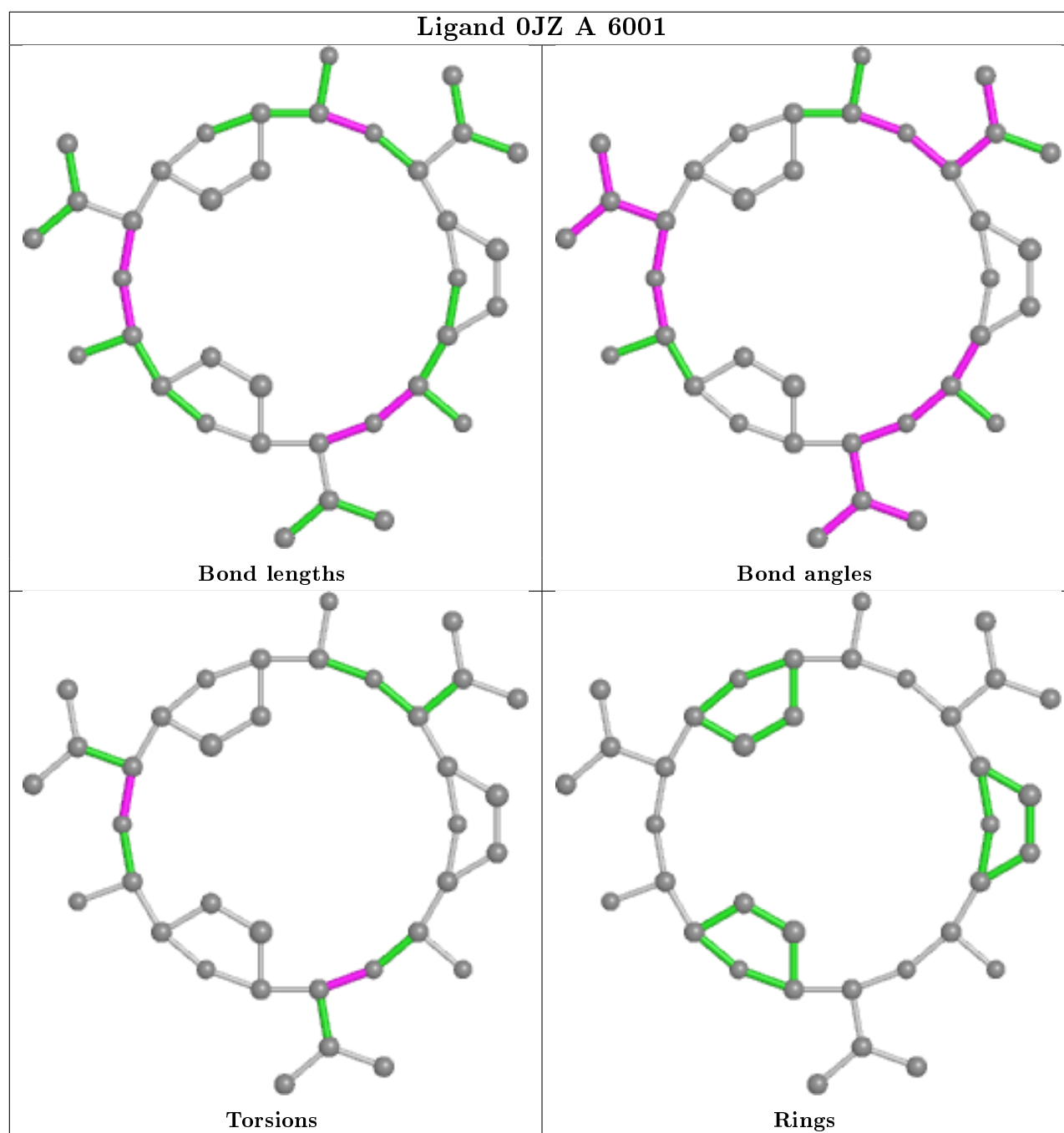
2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	6002	0JZ	10	0
2	A	6001	0JZ	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.





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%)	-0.12	20 (1%) 70 61	118, 194, 243, 306	0
1	B	1182/1284 (92%)	-0.13	21 (1%) 68 59	123, 200, 243, 301	0
All	All	2364/2568 (92%)	-0.12	41 (1%) 70 61	118, 197, 244, 306	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	963	GLN	4.9
1	B	1199	THR	4.5
1	A	1084	ASP	4.0
1	A	574	GLU	3.9
1	B	228	TRP	3.7
1	A	577	THR	3.3
1	B	1136	VAL	3.1
1	B	1249	GLU	3.1
1	A	1179	ARG	3.0
1	B	85	SER	2.9
1	A	993	ASP	2.9
1	B	1260	LYS	2.8
1	A	1260	LYS	2.6
1	A	554	THR	2.6
1	B	603	VAL	2.6
1	B	1128	ALA	2.6
1	A	961	THR	2.6
1	A	427	CYS	2.5
1	B	988	SER	2.5
1	B	97	ARG	2.4
1	A	962	GLN	2.4
1	B	84	VAL	2.4
1	B	597	PHE	2.4
1	B	594	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	600	GLY	2.3
1	A	424	ASN	2.3
1	A	1163	THR	2.3
1	A	1244	ASN	2.3
1	B	767	PHE	2.2
1	B	1172	LEU	2.2
1	A	442	PRO	2.2
1	B	217	ILE	2.1
1	B	524	GLY	2.1
1	B	1230	LEU	2.1
1	A	107	MET	2.1
1	A	581	ILE	2.1
1	B	1127	ILE	2.1
1	B	81	VAL	2.0
1	A	423	GLY	2.0
1	A	416	GLY	2.0
1	A	1106	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

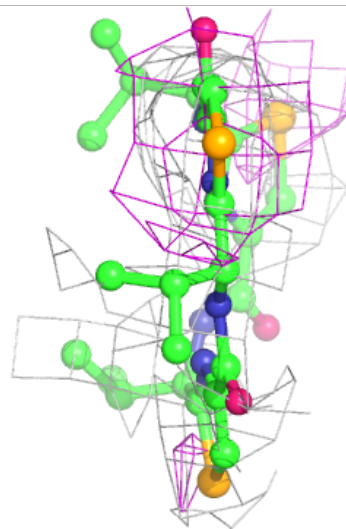
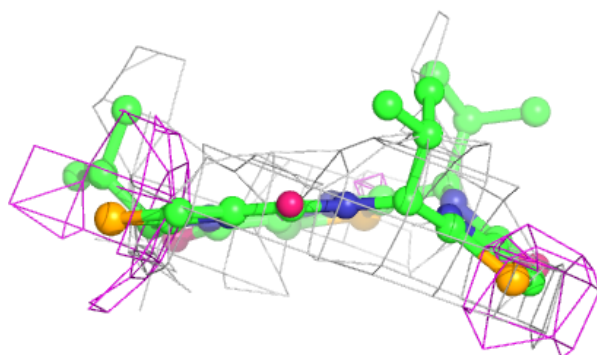
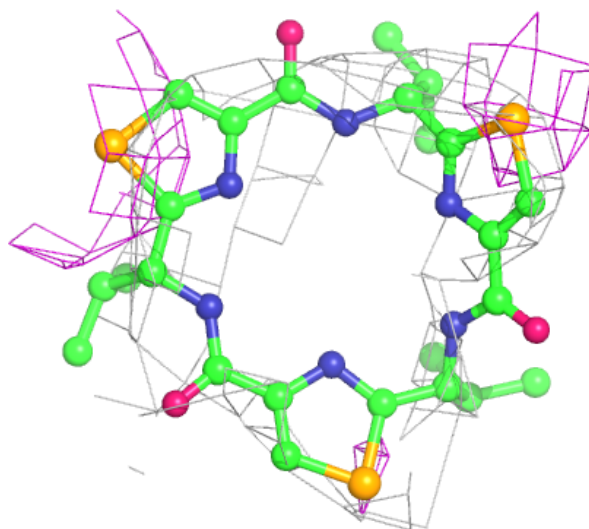
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	0JZ	B	6002	36/36	0.63	0.41	196,196,196,196	0
2	0JZ	A	6001	36/36	0.64	0.43	196,196,196,196	0

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.

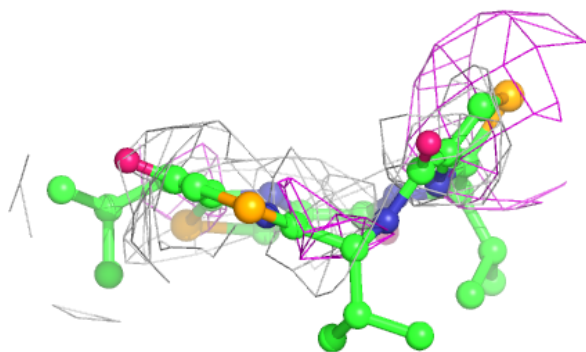
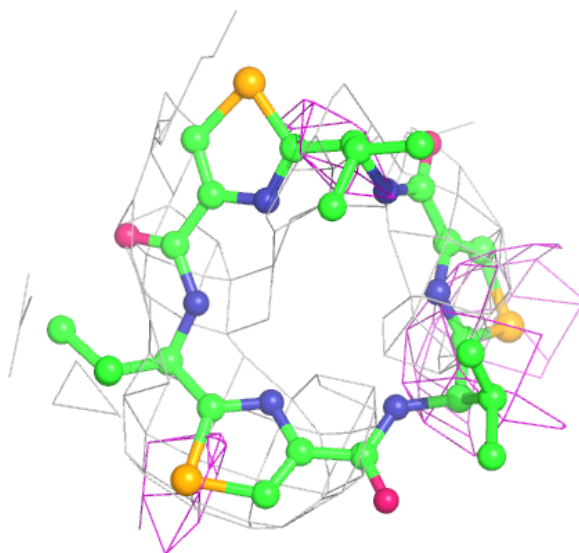
Electron density around 0JZ B 6002:

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



Electron density around 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.