



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:33 PM GMT

PDB ID : 1U6G  
Title : Crystal Structure of The Cand1-Cul1-Roc1 Complex  
Authors : Goldenberg, S.J.; Shumway, S.D.; Cascio, T.C.; Garbutt, K.C.; Liu, J.; Xiong, Y.; Zheng, N.  
Deposited on : 2004-07-29  
Resolution : 3.10 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

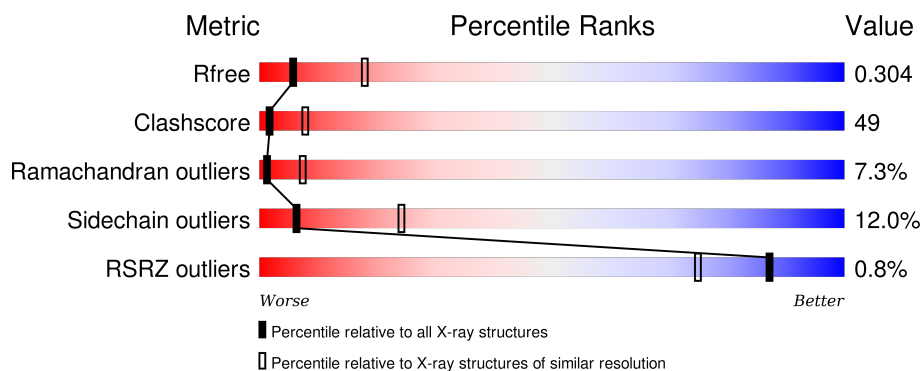
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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

Mol	Chain	Length	Quality of chain
1	A	776	<div> <div>41%</div> <div>40%</div> <div>10%</div> <div>8%</div> </div>
2	B	108	<div>2%</div> <div>31%</div> <div>38%</div> <div>11%</div> <div>19%</div>
3	C	1230	<div>30%</div> <div>50%</div> <div>11%</div> <div>7%</div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15511 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 Cullin homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	0	0	0
			5855	3719	998	1109	29			

- Molecule 2 is a protein called RING-box protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	88	Total	C	N	O	S	0	0	0
			731	464	133	125	9			

- Molecule 3 is a protein called TIP120 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	1146	Total	C	N	O	S	0	0	0
			8904	5667	1509	1672	56			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Zn	0	0
			3	3		

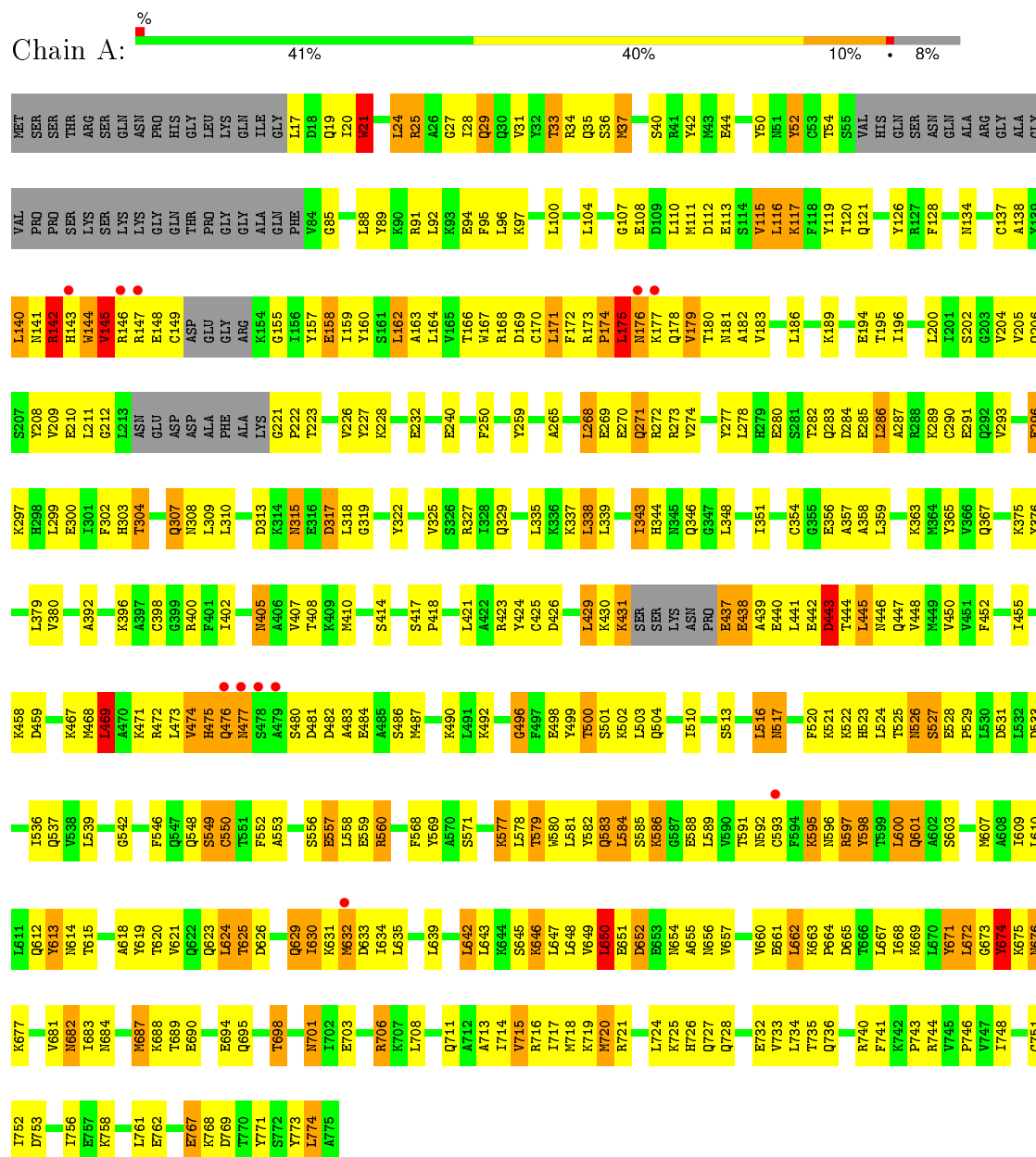
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	O	0	0
			10	10		
5	B	3	Total	O	0	0
			3	3		
5	C	5	Total	O	0	0
			5	5		

### 3 Residue-property plots

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

#### • Molecule 1: Cullin homolog 1





GLU SER MET ASP THR SER	Q1164	D1098	D1019	C954	I883
	E1165	R1099	L1020	L958	S884
	F1166	L1100	M1021	T959	
	E1167	D1101	V1022	T959	M887
	K1168	T1102	R1023	L960	L888
	Q1169	F1103	R1024	I961	P889
	D1170	E1104	V1025	D962	F890
	E1171		A1026	P963	T891
		M1107	L1027	E964	L892
	R1174	H1108	V1028	T965	F893
	S1175	V1109	T1029	L966	F894
	A1176	E1110	F1030	L967	V895
	M1177	D1111	M1031	P868	L896
	R1178	G1112	S1032	R969	Q897
	A1179	L1113	A1033	L970	E898
	V1180		A1034	R971	L899
	A1181	Y1117	N1035	G972	T900
	A1182		H1036	V973	S901
	L1183	K1120	K1037	L974	Q902
	L1184	H1121	P1038	T975	P903
	T1185	L1122	S1039	S976	R904
	I1186	T1123	L1040	G977	R905
	P1187		I1041	S978	Q906
	E1188	M1126		S979	
	A1189	L1127	L1044	V980	L913
	E1190	H1128		L981	K914
	K1191	R1129	T1047	R982	E915
	P1193	L1130	V1048		I916
	L1194	S1131	L1049	V985	I917
	M1195	T1132	P1050	V986	S918
	S1196	L1133	H1051	T987	S919
	E1197	C1134	L1052	L988	L920
	F1198	P1135	Y1053	V989	S921
	Q1199		M1054	R990	R922
	S1200	V1138	E1055	F991	V923
	Q1201	L1139	T1056	T992	G924
	T1202	Q1140		T993	L925
	S1203	R1141	R1064	S994	K926
	S1204	L1142	E1065	D995	P927
	N1205	D1143	V1066	H996	Y928
	P1206	R1144	E1067		
	E1207	L1145	M1068	P999	I932
	L1208	V1146		I1000	V933
	A1209	E1147	H1073	D1001	L934
	I1210	P1148	L1079	P1002	L935
	PHE	R1150	D1080	L1003	L936
	GLU	A1151	I1081	K1005	L937
	SER	T1152	R1082		
	C1153	C1153	K1083	I1008	E941
	I1154	T1154		G1009	C942
	T1155	T1155	C1088	L1010	A943
	LYS	K1156	M1089	F1011	E944
	ASP	V1157	Y1090	L1012	E945
	SER	K1158		K1013	G946
	SER	A1159	L1093	T1014	T947
	SER	M1160	D1094	L1015	R948
	THR	S1161	S1095	L1016	
	ASN	V1162	C1096	D1017	V951
	LEU	K1163	L1097	P1018	E953

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.47Å 151.33Å 215.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 49.68 – 2.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.10) 73.1 (49.68-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.84 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.243 , 0.317 0.236 , 0.304	Depositor DCC
$R_{free}$ test set	3108 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.5	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 53.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 105510 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	15511	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

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

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.49	3/5949 (0.1%)	1.14	14/8007 (0.2%)
2	B	0.51	0/752	0.86	1/1020 (0.1%)
3	C	0.45	1/9041 (0.0%)	0.86	31/12243 (0.3%)
All	All	0.47	4/15742 (0.0%)	0.97	46/21270 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	C	0	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	437	GLU	C-N	-8.90	1.13	1.34
1	A	443	ASP	C-N	7.93	1.52	1.34
3	C	601	GLY	C-N	-6.35	1.19	1.34
1	A	630	ILE	CG1-CD1	5.03	1.85	1.50

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	GLU	O-C-N	-72.37	6.91	122.70
3	C	117	LEU	C-N-CD	-20.01	76.58	120.60
3	C	117	LEU	C-N-CA	13.74	179.69	122.00
3	C	487	LYS	CB-CA-C	12.45	135.31	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	377	PRO	CA-N-CD	-10.61	96.64	111.50
1	A	476	GLN	N-CA-C	9.83	137.54	111.00
1	A	630	ILE	CB-CG1-CD1	-9.22	88.08	113.90
1	A	721	ARG	N-CA-C	-8.50	88.06	111.00
1	A	33	THR	N-CA-C	-8.21	88.82	111.00
1	A	175	LEU	CA-CB-CG	8.21	134.18	115.30
1	A	584	LEU	CA-CB-CG	8.01	133.72	115.30
3	C	1195	MET	N-CA-C	7.95	132.45	111.00
3	C	375	VAL	CB-CA-C	-7.63	96.91	111.40
3	C	488	SER	CA-C-N	-7.58	100.51	117.20
1	A	630	ILE	CB-CA-C	-7.42	96.77	111.60
2	B	45	CYS	N-CA-C	-7.29	91.32	111.00
1	A	111	MET	N-CA-C	7.01	129.92	111.00
3	C	1198	PHE	CB-CA-C	-6.92	96.56	110.40
3	C	487	LYS	N-CA-C	-6.81	92.60	111.00
3	C	489	SER	CA-C-N	-6.79	102.25	117.20
3	C	99	LYS	N-CA-C	-6.71	92.90	111.00
3	C	601	GLY	O-C-N	-6.67	112.03	122.70
1	A	142	ARG	N-CA-C	6.60	128.83	111.00
3	C	921	SER	N-CA-C	-6.56	93.29	111.00
3	C	941	GLU	N-CA-C	-6.56	93.29	111.00
3	C	147	ASP	N-CA-C	-6.42	93.67	111.00
3	C	488	SER	C-N-CA	6.18	137.15	121.70
3	C	118	PRO	CA-N-CD	-5.96	103.15	111.50
3	C	42	ASP	N-CA-C	-5.87	95.14	111.00
1	A	687	MET	N-CA-C	-5.86	95.17	111.00
3	C	814	GLY	N-CA-C	-5.85	98.48	113.10
3	C	974	LEU	CB-CG-CD2	-5.78	101.18	111.00
3	C	285	GLU	N-CA-C	5.61	126.15	111.00
3	C	188	ARG	N-CA-C	-5.57	95.96	111.00
3	C	488	SER	N-CA-C	5.54	125.96	111.00
3	C	485	ASN	C-N-CA	-5.54	107.86	121.70
1	A	469	LEU	CA-CB-CG	5.50	127.95	115.30
3	C	1194	LEU	N-CA-C	-5.46	96.27	111.00
3	C	977	GLY	N-CA-C	5.44	126.70	113.10
3	C	921	SER	CB-CA-C	5.41	120.37	110.10
3	C	599	ASN	N-CA-C	5.34	125.41	111.00
3	C	1198	PHE	CA-CB-CG	-5.23	101.36	113.90
1	A	650	LEU	CA-CB-CG	-5.15	103.45	115.30
3	C	490	SER	N-CA-C	-5.11	97.21	111.00
1	A	175	LEU	N-CA-C	5.08	124.71	111.00
3	C	488	SER	O-C-N	5.08	130.82	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	437	GLU	Mainchain
3	C	599	ASN	Mainchain
3	C	601	GLY	Mainchain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5855	0	5900	502	0
2	B	731	0	689	76	0
3	C	8904	0	9248	998	0
4	B	3	0	0	0	0
5	A	10	0	0	0	0
5	B	3	0	0	0	0
5	C	5	0	0	0	0
All	All	15511	0	15837	1525	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 49.

All (1525) 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)
3:C:373:LYS:CE	3:C:427:MET:HE1	1.31	1.56
3:C:373:LYS:HE3	3:C:427:MET:CE	1.36	1.54
1:A:630:ILE:CD1	1:A:630:ILE:CG1	1.85	1.51
3:C:373:LYS:CE	3:C:427:MET:CE	1.84	1.48
3:C:373:LYS:CD	3:C:427:MET:HE1	1.53	1.37
3:C:373:LYS:CG	3:C:427:MET:HE1	1.63	1.27
2:B:97:ASP:OD1	2:B:97:ASP:O	1.55	1.25
3:C:373:LYS:CG	3:C:427:MET:CE	2.19	1.18
3:C:600:LEU:O	3:C:602:ASP:N	1.81	1.14
3:C:373:LYS:CE	3:C:427:MET:HE3	1.74	1.13
3:C:375:VAL:HG13	3:C:379:LEU:HB2	1.19	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:SER:HB3	3:C:78:LYS:HD2	1.25	1.12
2:B:52:LEU:HD12	2:B:52:LEU:H	1.09	1.11
1:A:630:ILE:HD13	1:A:630:ILE:HG21	1.34	1.10
3:C:829:ARG:HB2	3:C:829:ARG:HH11	1.18	1.07
1:A:597:ARG:HH11	1:A:597:ARG:HB2	1.14	1.06
3:C:377:PRO:HB3	3:C:431:GLN:OE1	1.54	1.05
3:C:1013:LYS:HE2	3:C:1047:THR:HG21	1.38	1.05
3:C:373:LYS:HE2	3:C:427:MET:HE3	1.29	1.04
1:A:630:ILE:CB	1:A:630:ILE:CD1	2.35	1.04
1:A:625:THR:OG1	1:A:632:MET:HG2	1.58	1.02
3:C:211:ILE:O	3:C:215:LEU:HG	1.60	1.01
1:A:440:GLU:O	1:A:444:THR:N	1.94	0.99
3:C:1194:LEU:O	3:C:1194:LEU:HD12	1.63	0.99
3:C:1015:LEU:HD13	3:C:1018:PRO:HG3	1.41	0.99
3:C:1190:GLU:OE2	3:C:1191:LYS:HG2	1.63	0.98
1:A:441:LEU:O	1:A:445:LEU:HB2	1.63	0.97
3:C:982:ARG:NH2	3:C:1018:PRO:HB2	1.79	0.97
3:C:373:LYS:HG3	3:C:427:MET:CE	1.93	0.96
3:C:287:TYR:HB2	3:C:288:PRO:HD3	1.43	0.96
3:C:85:GLU:HG3	3:C:133:LYS:HE2	1.46	0.96
3:C:294:ILE:HG21	3:C:357:LEU:HG	1.44	0.96
3:C:375:VAL:CG1	3:C:379:LEU:HB2	1.95	0.95
1:A:625:THR:HG21	1:A:632:MET:HG3	1.44	0.95
3:C:1081:ILE:HG13	3:C:1082:ARG:N	1.78	0.95
3:C:192:ARG:HH21	3:C:227:THR:HG21	1.33	0.94
1:A:600:LEU:H	1:A:600:LEU:HD23	1.32	0.93
3:C:373:LYS:HE3	3:C:427:MET:SD	2.09	0.93
3:C:1011:PHE:O	3:C:1015:LEU:HB2	1.66	0.93
3:C:385:GLU:HA	3:C:391:LYS:HE2	1.51	0.92
1:A:175:LEU:HD11	1:A:208:TYR:CE1	2.04	0.92
3:C:481:ILE:HD11	3:C:520:LEU:HD23	1.51	0.92
3:C:375:VAL:HG13	3:C:379:LEU:CB	1.99	0.91
1:A:592:ASN:HD21	2:B:21:ARG:HE	1.14	0.91
3:C:231:ILE:HG23	3:C:273:GLN:NE2	1.84	0.91
1:A:600:LEU:N	1:A:600:LEU:HD23	1.84	0.91
1:A:116:LEU:O	1:A:120:THR:HG23	1.71	0.91
3:C:551:ARG:NH1	3:C:553:LEU:HB2	1.85	0.91
3:C:432:VAL:HG13	3:C:435:ILE:HB	1.53	0.90
1:A:542:GLY:H	2:B:76:ASN:HD21	1.20	0.90
1:A:625:THR:OG1	1:A:632:MET:CG	2.19	0.90
3:C:270:TYR:H	3:C:270:TYR:HD1	1.19	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:187:PRO:HB2	3:C:188:ARG:HH11	1.36	0.90
1:A:175:LEU:HG	1:A:208:TYR:OH	1.73	0.89
3:C:373:LYS:HE2	3:C:427:MET:CE	1.84	0.89
3:C:1147:GLU:HB3	3:C:1148:PRO:HD3	1.54	0.89
3:C:975:ILE:HG23	3:C:976:SER:H	1.37	0.88
1:A:672:LEU:N	1:A:672:LEU:HD12	1.87	0.88
1:A:173:ARG:HB2	1:A:174:PRO:HD3	1.53	0.88
3:C:349:VAL:HG23	3:C:350:ARG:H	1.37	0.88
3:C:285:GLU:HA	3:C:287:TYR:CE2	2.09	0.88
3:C:485:ASN:O	3:C:486:ASP:HB3	1.72	0.88
3:C:249:LEU:HA	3:C:252:ILE:HG13	1.55	0.88
3:C:298:LEU:O	3:C:298:LEU:HD22	1.72	0.88
1:A:592:ASN:HA	1:A:597:ARG:HH12	1.38	0.87
3:C:211:ILE:HG12	3:C:244:ARG:HE	1.39	0.87
1:A:642:LEU:HB3	1:A:648:LEU:HD12	1.54	0.87
1:A:592:ASN:CA	1:A:597:ARG:HH12	1.87	0.87
1:A:630:ILE:CD1	1:A:630:ILE:HG21	2.04	0.87
1:A:631:LYS:O	1:A:635:LEU:N	2.06	0.87
3:C:432:VAL:HG12	3:C:436:VAL:HG23	1.57	0.87
3:C:548:LYS:HA	3:C:551:ARG:HG3	1.54	0.87
3:C:373:LYS:CG	3:C:427:MET:HE2	2.02	0.87
3:C:211:ILE:HG12	3:C:244:ARG:NE	1.89	0.87
3:C:270:TYR:HA	3:C:273:GLN:OE1	1.75	0.87
1:A:144:TRP:O	1:A:145:VAL:HG13	1.74	0.87
3:C:92:CYS:HB3	3:C:137:ARG:HG2	1.56	0.86
3:C:373:LYS:HG3	3:C:427:MET:HE1	1.51	0.86
1:A:167:TRP:O	1:A:170:CYS:HB3	1.75	0.86
1:A:440:GLU:O	1:A:444:THR:OG1	1.91	0.86
2:B:49:ILE:HD13	2:B:50:MET:HG2	1.54	0.86
3:C:999:PRO:O	3:C:1002:PRO:HD2	1.76	0.86
3:C:1199:GLN:HB3	3:C:1202:ILE:HB	1.59	0.85
3:C:1037:LYS:HD2	3:C:1040:LEU:HD11	1.56	0.85
3:C:373:LYS:HG2	3:C:427:MET:CE	2.06	0.85
3:C:379:LEU:HA	3:C:382:ARG:HB2	1.56	0.84
3:C:812:LYS:HG3	3:C:812:LYS:O	1.76	0.84
3:C:269:GLU:O	3:C:273:GLN:HG3	1.77	0.84
1:A:287:ALA:O	1:A:291:GLU:HG3	1.76	0.84
1:A:300:GLU:O	1:A:304:THR:HG22	1.77	0.83
1:A:474:VAL:HG12	1:A:475:HIS:N	1.93	0.83
3:C:551:ARG:N	3:C:552:PRO:HD2	1.94	0.83
3:C:206:CYS:O	3:C:210:LEU:HB2	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:377:PRO:CB	3:C:431:GLN:OE1	2.27	0.83
3:C:473:ILE:O	3:C:477:VAL:HG23	1.79	0.83
3:C:590:ILE:HG21	3:C:628:THR:HG22	1.60	0.82
3:C:650:GLU:O	3:C:654:ILE:HG13	1.80	0.82
1:A:630:ILE:CG2	1:A:630:ILE:CD1	2.57	0.82
3:C:982:ARG:O	3:C:986:VAL:HG12	1.77	0.82
3:C:821:PHE:C	3:C:823:GLN:H	1.80	0.82
3:C:548:LYS:HA	3:C:551:ARG:CG	2.09	0.82
3:C:625:ARG:O	3:C:629:VAL:HG23	1.79	0.82
1:A:597:ARG:NH1	1:A:597:ARG:HB2	1.93	0.82
3:C:301:LEU:HD12	3:C:302:THR:H	1.44	0.82
3:C:386:ARG:HB2	3:C:386:ARG:CZ	2.09	0.82
3:C:673:ALA:HA	3:C:676:ILE:HD11	1.61	0.82
1:A:95:PHE:HD2	1:A:96:LEU:HD12	1.44	0.82
3:C:249:LEU:HA	3:C:252:ILE:CG1	2.09	0.82
3:C:1194:LEU:O	3:C:1195:MET:HB2	1.78	0.81
3:C:1012:LEU:O	3:C:1014:THR:N	2.14	0.81
1:A:171:LEU:HG	1:A:175:LEU:HD22	1.60	0.81
3:C:375:VAL:O	3:C:379:LEU:N	2.13	0.81
2:B:52:LEU:HD12	2:B:52:LEU:N	1.93	0.81
1:A:592:ASN:HD21	2:B:21:ARG:NE	1.78	0.81
3:C:1139:LEU:HA	3:C:1142:LEU:HB2	1.63	0.80
2:B:97:ASP:CG	2:B:97:ASP:O	2.18	0.80
3:C:181:LEU:HD13	3:C:217:GLU:HG3	1.60	0.80
1:A:27:GLY:O	1:A:31:VAL:HG23	1.81	0.80
3:C:967:LEU:N	3:C:968:PRO:HD2	1.97	0.80
3:C:566:LYS:HB2	3:C:566:LYS:HZ3	1.47	0.80
3:C:566:LYS:HD3	3:C:566:LYS:H	1.45	0.80
3:C:187:PRO:HB2	3:C:188:ARG:NH1	1.96	0.80
3:C:601:GLY:O	3:C:604:LEU:N	2.15	0.79
3:C:1142:LEU:O	3:C:1146:VAL:HG23	1.82	0.79
1:A:145:VAL:O	1:A:146:ARG:HG3	1.82	0.79
3:C:373:LYS:HG2	3:C:427:MET:HE2	1.63	0.79
3:C:1190:GLU:O	3:C:1193:PRO:HD2	1.79	0.79
1:A:672:LEU:HD12	1:A:672:LEU:H	1.45	0.79
3:C:1176:ALA:O	3:C:1180:VAL:HG23	1.82	0.79
3:C:1199:GLN:O	3:C:1203:SER:HB3	1.82	0.79
3:C:1169:GLN:HA	3:C:1169:GLN:OE1	1.82	0.79
3:C:970:LEU:HD22	3:C:985:VAL:HG23	1.64	0.79
1:A:614:ASN:ND2	2:B:21:ARG:HA	1.98	0.78
3:C:831:THR:HG22	3:C:833:SER:H	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ASN:ND2	1:A:407:VAL:H	1.81	0.78
3:C:267:LEU:HA	3:C:270:TYR:CE1	2.17	0.78
1:A:142:ARG:CZ	1:A:147:ARG:HG2	2.13	0.78
2:B:52:LEU:H	2:B:52:LEU:CD1	1.90	0.78
3:C:551:ARG:HH11	3:C:553:LEU:HB2	1.44	0.78
3:C:1052:LEU:HD11	3:C:1088:CYS:HB3	1.65	0.78
1:A:297:LYS:HD3	1:A:297:LYS:O	1.84	0.78
3:C:375:VAL:O	3:C:379:LEU:HB2	1.84	0.78
3:C:423:THR:O	3:C:427:MET:HG3	1.83	0.77
3:C:349:VAL:HG23	3:C:350:ARG:N	1.99	0.77
3:C:372:TYR:HA	3:C:377:PRO:HG2	1.64	0.77
3:C:1187:PRO:O	3:C:1189:ALA:N	2.17	0.77
3:C:110:LEU:HD23	3:C:157:ILE:HD13	1.67	0.77
3:C:432:VAL:CG1	3:C:436:VAL:HG23	2.13	0.77
3:C:170:VAL:HA	3:C:173:HIS:CD2	2.18	0.77
1:A:577:LYS:HB2	2:B:36:ASP:HB3	1.65	0.77
3:C:1081:ILE:HG13	3:C:1082:ARG:H	1.48	0.77
1:A:528:GLU:HG2	1:A:528:GLU:O	1.84	0.77
1:A:618:ALA:HB2	1:A:669:LYS:HG2	1.66	0.77
3:C:982:ARG:HH21	3:C:1018:PRO:HB2	1.48	0.77
1:A:577:LYS:NZ	1:A:578:LEU:H	1.82	0.77
3:C:77:SER:O	3:C:78:LYS:HD3	1.82	0.77
1:A:621:VAL:HG23	1:A:668:ILE:HD11	1.65	0.76
3:C:723:TYR:H	3:C:724:PRO:HD3	1.51	0.76
3:C:1055:GLU:HG3	3:C:1081:ILE:HD12	1.66	0.76
3:C:1204:SER:O	3:C:1208:LEU:HD23	1.85	0.76
3:C:686:THR:OG1	3:C:689:MET:HG3	1.86	0.76
1:A:142:ARG:HB3	1:A:142:ARG:HH11	1.48	0.76
3:C:373:LYS:HE3	3:C:427:MET:HE1	1.06	0.76
3:C:1012:LEU:C	3:C:1014:THR:H	1.89	0.76
3:C:660:ARG:HD2	3:C:696:GLU:OE2	1.85	0.76
3:C:942:CYS:HA	3:C:948:ARG:HD2	1.67	0.76
1:A:614:ASN:HD21	2:B:22:PHE:H	1.34	0.76
3:C:481:ILE:HD12	3:C:523:PRO:HG3	1.67	0.76
1:A:630:ILE:CG2	1:A:630:ILE:HD13	2.12	0.75
3:C:1015:LEU:HD12	3:C:1022:VAL:HG12	1.68	0.75
3:C:1199:GLN:HG2	3:C:1202:ILE:HG12	1.68	0.75
2:B:81:PHE:O	2:B:85:SER:HB2	1.86	0.75
3:C:299:LYS:NZ	3:C:379:LEU:HD22	2.02	0.75
1:A:651:GLU:HA	1:A:669:LYS:HZ2	1.49	0.75
3:C:820:GLN:HB3	3:C:842:LEU:HD21	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:SER:O	1:A:646:LYS:HB3	1.87	0.75
1:A:134:ASN:HA	1:A:159:ILE:HG21	1.69	0.75
1:A:134:ASN:HA	1:A:159:ILE:CG2	2.17	0.75
3:C:611:THR:HA	3:C:614:ILE:HG12	1.69	0.75
1:A:438:GLU:OE1	1:A:438:GLU:HA	1.86	0.75
1:A:614:ASN:HD21	2:B:22:PHE:N	1.85	0.74
3:C:618:ARG:HB3	3:C:624:THR:HG21	1.68	0.74
3:C:135:THR:CG2	3:C:176:ILE:HD11	2.18	0.74
3:C:738:LEU:O	3:C:742:VAL:HG23	1.87	0.74
2:B:62:SER:O	2:B:66:GLU:HG3	1.88	0.74
3:C:827:ASN:O	3:C:829:ARG:N	2.20	0.74
1:A:676:ASN:HD22	1:A:677:LYS:N	1.86	0.74
1:A:173:ARG:CB	1:A:174:PRO:HD3	2.18	0.74
1:A:315:ASN:HB3	1:A:379:LEU:HD21	1.69	0.74
1:A:720:MET:O	1:A:720:MET:HE3	1.87	0.74
1:A:117:LYS:NZ	1:A:121:GLN:HE21	1.85	0.74
3:C:268:ARG:HE	3:C:348:LYS:HB3	1.52	0.73
3:C:143:ALA:O	3:C:145:GLN:N	2.20	0.73
3:C:640:LEU:O	3:C:642:ILE:N	2.20	0.73
1:A:625:THR:CG2	1:A:632:MET:HG3	2.18	0.73
3:C:211:ILE:CG1	3:C:244:ARG:HE	2.00	0.73
1:A:592:ASN:ND2	2:B:21:ARG:HE	1.86	0.73
3:C:231:ILE:HG23	3:C:273:GLN:CD	2.09	0.73
3:C:618:ARG:CB	3:C:624:THR:HG21	2.19	0.73
3:C:36:LYS:HG3	3:C:37:ASP:OD2	1.89	0.73
3:C:94:ASN:HB3	3:C:102:LEU:HG	1.70	0.73
3:C:616:LEU:HD23	3:C:647:VAL:HG12	1.69	0.73
3:C:42:ASP:HB2	3:C:45:SER:HB2	1.71	0.73
3:C:249:LEU:HD22	3:C:250:GLU:OE1	1.89	0.73
3:C:226:THR:CG2	3:C:227:THR:N	2.52	0.72
3:C:226:THR:HG22	3:C:227:THR:N	2.05	0.72
3:C:974:LEU:HD21	3:C:1011:PHE:CD2	2.24	0.72
1:A:37:MET:HE2	1:A:42:TYR:HA	1.72	0.72
3:C:1151:ALA:O	3:C:1155:THR:HG23	1.88	0.72
3:C:1188:GLU:HA	3:C:1190:GLU:OE1	1.89	0.72
1:A:107:GLY:HA2	1:A:110:LEU:HD12	1.71	0.72
3:C:633:THR:HA	3:C:676:ILE:HD13	1.71	0.72
3:C:899:ILE:HG21	3:C:935:LEU:HD11	1.72	0.72
3:C:829:ARG:HH11	3:C:829:ARG:CB	2.00	0.72
3:C:814:GLY:N	3:C:815:PRO:HD2	2.05	0.72
1:A:603:SER:HB3	1:A:684:ASN:OD1	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:825:VAL:CG2	3:C:860:VAL:HG22	2.20	0.72
3:C:262:VAL:O	3:C:267:LEU:HD11	1.89	0.72
1:A:339:LEU:O	1:A:343:ILE:HG22	1.90	0.72
3:C:600:LEU:O	3:C:601:GLY:C	2.28	0.71
3:C:375:VAL:O	3:C:375:VAL:HG12	1.90	0.71
1:A:33:THR:O	1:A:34:ARG:HD3	1.91	0.71
1:A:134:ASN:HD22	1:A:159:ILE:HG22	1.54	0.71
3:C:735:LEU:HD11	3:C:778:MET:SD	2.30	0.71
3:C:495:ILE:HD11	3:C:534:LYS:HB3	1.73	0.71
3:C:366:GLU:OE2	3:C:367:MET:HG3	1.91	0.71
1:A:175:LEU:HD23	1:A:176:ASN:N	2.06	0.71
3:C:857:LEU:HD23	3:C:858:LYS:N	2.05	0.71
1:A:438:GLU:OE1	1:A:438:GLU:CA	2.37	0.71
1:A:186:LEU:HD11	1:A:196:ILE:HB	1.72	0.71
1:A:228:LYS:HA	1:A:232:GLU:HB3	1.72	0.71
1:A:232:GLU:OE1	1:A:282:THR:HG22	1.89	0.71
1:A:475:HIS:CE1	1:A:586:LYS:HD3	2.26	0.70
3:C:601:GLY:O	3:C:604:LEU:CB	2.39	0.70
1:A:405:ASN:HD22	1:A:407:VAL:H	1.37	0.70
3:C:375:VAL:HG22	3:C:379:LEU:HD12	1.74	0.70
1:A:533:ASP:OD2	2:B:26:LYS:HE3	1.92	0.70
3:C:287:TYR:HB2	3:C:288:PRO:CD	2.21	0.70
3:C:270:TYR:N	3:C:270:TYR:CD1	2.58	0.70
3:C:375:VAL:O	3:C:375:VAL:CG1	2.37	0.70
1:A:446:ASN:OD1	1:A:490:LYS:HE2	1.92	0.69
1:A:717:ILE:HA	3:C:25:MET:CE	2.22	0.69
1:A:592:ASN:HB3	1:A:597:ARG:HH22	1.54	0.69
3:C:1049:LEU:HD11	3:C:1100:LEU:HD23	1.74	0.69
3:C:218:LEU:HD13	3:C:234:ILE:HD13	1.75	0.69
1:A:676:ASN:HD22	1:A:677:LYS:H	1.38	0.69
3:C:820:GLN:HA	3:C:823:GLN:HG3	1.73	0.69
3:C:233:CYS:O	3:C:237:ILE:HG13	1.92	0.69
3:C:532:PHE:CZ	3:C:534:LYS:HB2	2.28	0.69
3:C:818:VAL:HG22	3:C:854:GLN:OE1	1.92	0.69
3:C:239:ARG:CZ	3:C:276:GLU:HG2	2.23	0.69
3:C:1141:ARG:O	3:C:1145:LEU:HG	1.93	0.69
3:C:244:ARG:HH11	3:C:244:ARG:HG2	1.56	0.69
3:C:855:LEU:HD11	3:C:858:LYS:HD2	1.75	0.69
1:A:344:HIS:NE2	1:A:348:LEU:HD11	2.08	0.69
3:C:211:ILE:HD13	3:C:244:ARG:HH21	1.57	0.69
3:C:914:LYS:HD3	3:C:953:GLU:HG2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:690:ILE:HG13	3:C:719:LEU:HD11	1.74	0.68
1:A:29:GLN:O	1:A:33:THR:HG23	1.93	0.68
3:C:38:SER:CB	3:C:78:LYS:HD2	2.15	0.68
1:A:174:PRO:O	1:A:178:GLN:HB3	1.93	0.68
1:A:517:ASN:HD21	1:A:536:ILE:H	1.41	0.68
1:A:660:VAL:HG12	1:A:661:GLU:N	2.08	0.68
3:C:601:GLY:O	3:C:604:LEU:HB2	1.92	0.68
1:A:718:MET:CE	1:A:771:TYR:HB2	2.23	0.68
3:C:905:ARG:CG	3:C:905:ARG:HH11	2.05	0.68
1:A:639:LEU:O	1:A:643:LEU:HG	1.94	0.68
3:C:551:ARG:HD2	3:C:551:ARG:C	2.14	0.68
3:C:551:ARG:HD2	3:C:551:ARG:O	1.94	0.68
3:C:209:ASP:O	3:C:213:HIS:NE2	2.27	0.68
3:C:633:THR:HG23	3:C:676:ILE:HG12	1.74	0.68
1:A:536:ILE:HG12	1:A:537:GLN:H	1.58	0.68
3:C:4:ALA:O	3:C:40:LYS:HG3	1.94	0.68
3:C:212:GLU:HB3	3:C:248:TYR:OH	1.93	0.68
1:A:577:LYS:HZ2	1:A:578:LEU:H	1.41	0.68
3:C:905:ARG:HG3	3:C:905:ARG:HH11	1.58	0.68
3:C:8:ILE:HD12	3:C:8:ILE:H	1.57	0.68
1:A:405:ASN:HD22	1:A:405:ASN:C	1.97	0.68
1:A:24:LEU:O	1:A:28:ILE:HG12	1.93	0.68
3:C:551:ARG:N	3:C:552:PRO:CD	2.57	0.67
3:C:701:ILE:HG21	3:C:738:LEU:HD23	1.75	0.67
3:C:283:PRO:C	3:C:284:LYS:HD3	2.15	0.67
3:C:1097:LEU:HA	3:C:1100:LEU:HD12	1.76	0.67
3:C:1008:ILE:HG23	3:C:1009:GLY:N	2.10	0.67
3:C:813:GLU:CD	3:C:814:GLY:H	1.97	0.67
3:C:825:VAL:C	3:C:827:ASN:H	1.98	0.67
3:C:826:LYS:HE2	3:C:826:LYS:HA	1.77	0.67
3:C:206:CYS:CB	3:C:207:PHE:HA	2.24	0.67
3:C:350:ARG:HH21	3:C:386:ARG:HH12	1.41	0.67
3:C:38:SER:HB3	3:C:78:LYS:CD	2.13	0.67
1:A:134:ASN:HD21	1:A:157:TYR:CB	2.08	0.67
1:A:357:ALA:H	3:C:489:SER:HB2	1.59	0.67
3:C:550:ILE:HD12	3:C:561:ALA:HB1	1.77	0.67
3:C:76:VAL:HG21	3:C:113:VAL:HG13	1.77	0.67
3:C:282:CYS:HB2	3:C:283:PRO:HD3	1.77	0.67
2:B:49:ILE:HD12	2:B:50:MET:H	1.60	0.67
3:C:253:ILE:O	3:C:257:VAL:HG23	1.94	0.67
3:C:385:GLU:CA	3:C:391:LYS:HE2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:913:LEU:O	3:C:913:LEU:HD23	1.95	0.67
3:C:295:ASN:OD1	3:C:357:LEU:HD21	1.94	0.67
3:C:1015:LEU:CD1	3:C:1018:PRO:HG3	2.19	0.66
3:C:481:ILE:CD1	3:C:520:LEU:HD23	2.25	0.66
3:C:829:ARG:HB2	3:C:829:ARG:NH1	2.03	0.66
1:A:186:LEU:HG	1:A:196:ILE:HD12	1.77	0.66
1:A:583:GLN:HE21	1:A:583:GLN:H	1.43	0.66
2:B:19:LYS:HB3	2:B:19:LYS:NZ	2.10	0.66
1:A:682:ASN:HD22	1:A:682:ASN:C	1.98	0.66
1:A:467:LYS:NZ	1:A:698:THR:HB	2.10	0.66
3:C:1188:GLU:HA	3:C:1190:GLU:CD	2.15	0.66
3:C:92:CYS:CB	3:C:137:ARG:HG2	2.26	0.66
3:C:724:PRO:O	3:C:726:SER:N	2.28	0.66
3:C:825:VAL:O	3:C:827:ASN:N	2.26	0.66
3:C:148:VAL:O	3:C:151:GLN:N	2.28	0.66
1:A:719:LYS:HA	1:A:773:TYR:CD1	2.31	0.66
3:C:168:LEU:N	3:C:168:LEU:HD23	2.10	0.66
3:C:881:GLY:O	3:C:884:SER:HB2	1.95	0.66
3:C:822:ILE:C	3:C:826:LYS:HB2	2.16	0.65
3:C:1036:ASN:O	3:C:1037:LYS:HB2	1.95	0.65
3:C:723:TYR:H	3:C:724:PRO:CD	2.08	0.65
1:A:286:LEU:HD22	1:A:290:CYS:HG	1.61	0.65
1:A:557:GLU:H	1:A:557:GLU:CD	1.98	0.65
1:A:662:LEU:HD12	1:A:662:LEU:H	1.61	0.65
3:C:618:ARG:HB3	3:C:624:THR:CG2	2.26	0.65
1:A:630:ILE:HG22	1:A:635:LEU:HB2	1.78	0.65
3:C:1055:GLU:OE1	3:C:1055:GLU:HA	1.95	0.65
3:C:407:PRO:HG2	3:C:408:VAL:H	1.60	0.65
1:A:492:LYS:HD3	3:C:108:ILE:HD11	1.78	0.65
1:A:475:HIS:NE2	1:A:584:LEU:C	2.50	0.65
3:C:1079:LEU:O	3:C:1079:LEU:HD22	1.97	0.65
3:C:390:VAL:O	3:C:394:VAL:HG23	1.96	0.65
1:A:104:LEU:HD23	1:A:173:ARG:HH11	1.61	0.65
3:C:822:ILE:HG22	3:C:826:LYS:HD2	1.78	0.65
3:C:655:LEU:HA	3:C:658:PHE:CD2	2.32	0.65
3:C:566:LYS:HB2	3:C:566:LYS:NZ	2.11	0.65
3:C:148:VAL:HA	3:C:151:GLN:HE21	1.62	0.65
3:C:989:VAL:O	3:C:992:THR:HB	1.96	0.65
1:A:591:THR:HG22	2:B:22:PHE:HE2	1.61	0.65
1:A:591:THR:HG22	2:B:22:PHE:CE2	2.31	0.64
3:C:905:ARG:NH1	3:C:905:ARG:HG3	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:550:ILE:C	3:C:552:PRO:HD2	2.16	0.64
1:A:134:ASN:HD21	1:A:157:TYR:HB2	1.63	0.64
3:C:631:ALA:O	3:C:635:ILE:HG13	1.97	0.64
1:A:527:SER:O	1:A:529:PRO:HD3	1.97	0.64
3:C:701:ILE:HD13	3:C:738:LEU:CD2	2.27	0.64
1:A:717:ILE:HA	3:C:25:MET:HE2	1.80	0.64
3:C:722:VAL:O	3:C:723:TYR:HB2	1.97	0.64
1:A:498:GLU:O	1:A:502:LYS:HG3	1.97	0.64
3:C:206:CYS:HB3	3:C:207:PHE:HA	1.80	0.64
1:A:682:ASN:HD22	1:A:684:ASN:H	1.45	0.64
3:C:1008:ILE:HG23	3:C:1009:GLY:H	1.63	0.64
3:C:129:ASN:HA	3:C:132:LYS:CB	2.27	0.64
3:C:862:LEU:O	3:C:865:PHE:HB2	1.98	0.64
3:C:573:ILE:HD12	3:C:574:LYS:N	2.13	0.64
1:A:549:SER:O	1:A:550:CYS:C	2.34	0.63
3:C:760:GLN:HG2	3:C:809:ALA:HB2	1.78	0.63
3:C:551:ARG:HD3	3:C:599:ASN:OD1	1.98	0.63
3:C:655:LEU:HA	3:C:658:PHE:HD2	1.62	0.63
1:A:147:ARG:O	1:A:148:GLU:HB2	1.97	0.63
1:A:467:LYS:HZ2	1:A:698:THR:HB	1.62	0.63
3:C:364:ARG:NE	3:C:364:ARG:HA	2.11	0.63
3:C:210:LEU:HD23	3:C:213:HIS:ND1	2.14	0.63
3:C:1164:GLN:HA	3:C:1167:GLU:HG3	1.78	0.63
2:B:97:ASP:OD1	2:B:99:ARG:HB2	1.98	0.63
3:C:551:ARG:HG2	3:C:599:ASN:ND2	2.14	0.63
1:A:273:ARG:HG2	1:A:277:TYR:OH	1.99	0.63
3:C:936:LEU:HD22	3:C:951:VAL:HG13	1.80	0.63
3:C:129:ASN:HA	3:C:132:LYS:HB2	1.81	0.63
1:A:417:SER:N	1:A:418:PRO:HD2	2.14	0.63
2:B:53:CYS:HB2	2:B:83:CYS:SG	2.38	0.63
1:A:175:LEU:CD1	1:A:208:TYR:CE1	2.81	0.63
3:C:183:GLN:C	3:C:185:THR:H	2.02	0.63
3:C:823:GLN:HA	3:C:823:GLN:HE21	1.63	0.62
1:A:592:ASN:HA	1:A:597:ARG:NH1	2.10	0.62
3:C:301:LEU:HD12	3:C:302:THR:N	2.11	0.62
3:C:385:GLU:O	3:C:386:ARG:HB3	1.99	0.62
3:C:1135:PRO:O	3:C:1138:VAL:HB	1.99	0.62
3:C:349:VAL:CG2	3:C:350:ARG:H	2.09	0.62
3:C:96:LEU:N	3:C:96:LEU:HD12	2.14	0.62
1:A:92:LEU:O	1:A:96:LEU:HD13	1.98	0.62
3:C:548:LYS:HG2	3:C:599:ASN:HD21	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:974:LEU:HD21	3:C:1011:PHE:CE2	2.34	0.62
3:C:294:ILE:CG2	3:C:357:LEU:HG	2.25	0.62
2:B:48:HIS:ND1	2:B:49:ILE:HD12	2.15	0.62
2:B:48:HIS:CE1	2:B:50:MET:HB2	2.34	0.62
3:C:158:MET:O	3:C:162:LEU:HB2	1.98	0.62
3:C:825:VAL:HG23	3:C:860:VAL:HG13	1.82	0.62
3:C:212:GLU:OE1	3:C:212:GLU:N	2.19	0.62
3:C:253:ILE:HD11	3:C:281:ARG:HH22	1.65	0.62
3:C:33:GLU:C	3:C:35:GLN:H	2.01	0.62
1:A:632:MET:HA	1:A:635:LEU:HB3	1.80	0.62
3:C:831:THR:HG22	3:C:833:SER:HB3	1.80	0.62
3:C:1177:MET:HG3	3:C:1205:ASN:HB3	1.82	0.62
3:C:810:CYS:O	3:C:812:LYS:N	2.31	0.62
1:A:734:LEU:CD2	1:A:743:PRO:HD2	2.30	0.62
1:A:344:HIS:CE1	1:A:348:LEU:HD11	2.34	0.62
3:C:153:GLU:O	3:C:157:ILE:HG13	2.00	0.62
1:A:711:GLN:HE22	1:A:758:LYS:NZ	1.97	0.62
3:C:207:PHE:C	3:C:209:ASP:N	2.51	0.62
3:C:294:ILE:HG23	3:C:353:ALA:HA	1.82	0.62
1:A:585:SER:HB2	2:B:29:ALA:HA	1.82	0.62
1:A:577:LYS:HA	1:A:577:LYS:HE2	1.81	0.62
3:C:942:CYS:CA	3:C:948:ARG:HD2	2.28	0.61
3:C:578:ALA:O	3:C:579:ALA:HB3	2.00	0.61
3:C:723:TYR:O	3:C:724:PRO:C	2.39	0.61
3:C:902:GLN:HE22	3:C:905:ARG:HH12	1.48	0.61
1:A:600:LEU:N	1:A:600:LEU:CD2	2.58	0.61
1:A:104:LEU:HD12	1:A:104:LEU:O	2.00	0.61
3:C:652:VAL:N	3:C:653:PRO:HD2	2.15	0.61
1:A:682:ASN:ND2	1:A:684:ASN:H	1.98	0.61
1:A:620:THR:OG1	1:A:623:GLN:HG3	1.99	0.61
3:C:570:THR:O	3:C:572:THR:N	2.34	0.61
3:C:821:PHE:HE2	3:C:842:LEU:HD22	1.65	0.61
1:A:210:GLU:HB2	3:C:1164:GLN:HG3	1.83	0.61
1:A:363:LYS:O	1:A:367:GLN:HB2	2.00	0.61
3:C:804:ALA:HA	3:C:845:VAL:HG22	1.82	0.61
3:C:218:LEU:HD23	3:C:230:TYR:HD1	1.66	0.61
3:C:192:ARG:HH21	3:C:227:THR:CG2	2.11	0.61
3:C:689:MET:O	3:C:692:ALA:HB3	2.01	0.61
3:C:573:ILE:HD12	3:C:574:LYS:H	1.66	0.61
3:C:423:THR:HG22	3:C:426:THR:H	1.64	0.61
3:C:54:LEU:HD13	3:C:90:THR:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:294:ILE:HD11	3:C:356:CYS:SG	2.41	0.60
3:C:42:ASP:HB2	3:C:45:SER:H	1.65	0.60
1:A:405:ASN:ND2	1:A:408:THR:H	1.99	0.60
1:A:603:SER:O	1:A:607:MET:HG3	2.01	0.60
3:C:710:GLN:HB3	3:C:751:ALA:HA	1.82	0.60
3:C:249:LEU:HD13	3:C:249:LEU:N	2.15	0.60
3:C:1107:ASN:CG	3:C:1141:ARG:HH12	2.04	0.60
3:C:821:PHE:HE2	3:C:842:LEU:CD2	2.14	0.60
3:C:281:ARG:HH21	3:C:284:LYS:HB3	1.66	0.60
1:A:676:ASN:ND2	1:A:677:LYS:N	2.49	0.60
2:B:49:ILE:HD12	2:B:50:MET:N	2.15	0.60
3:C:625:ARG:HG3	3:C:658:PHE:CE1	2.36	0.60
3:C:959:THR:HA	3:C:966:LEU:HD13	1.83	0.60
3:C:902:GLN:NE2	3:C:905:ARG:NH1	2.50	0.60
1:A:744:ARG:HG2	1:A:746:PRO:HD2	1.83	0.60
3:C:270:TYR:O	3:C:273:GLN:HB2	2.02	0.60
3:C:33:GLU:O	3:C:35:GLN:N	2.33	0.60
3:C:460:GLU:O	3:C:464:VAL:HG23	2.01	0.60
1:A:459:ASP:OD2	1:A:706:ARG:NE	2.23	0.60
1:A:452:PHE:HA	1:A:455:ILE:HD13	1.83	0.60
3:C:265:ASP:HB3	3:C:345:MET:SD	2.42	0.60
3:C:451:ARG:HD2	3:C:483:SER:OG	2.02	0.60
3:C:284:LYS:N	3:C:284:LYS:HD3	2.16	0.60
1:A:717:ILE:HG12	3:C:25:MET:CE	2.32	0.60
3:C:469:LEU:H	3:C:508:HIS:CE1	2.20	0.60
3:C:469:LEU:H	3:C:508:HIS:HE1	1.47	0.60
3:C:521:VAL:HB	3:C:522:PRO:HD3	1.84	0.60
1:A:592:ASN:CB	1:A:597:ARG:HH12	2.15	0.60
1:A:475:HIS:NE2	1:A:584:LEU:O	2.35	0.60
1:A:717:ILE:HD13	1:A:732:GLU:HB3	1.84	0.60
1:A:52:TYR:O	1:A:52:TYR:HD2	1.84	0.60
3:C:376:SER:OG	3:C:377:PRO:HD2	2.02	0.60
3:C:1194:LEU:HD12	3:C:1194:LEU:C	2.21	0.60
3:C:481:ILE:CD1	3:C:523:PRO:HG3	2.30	0.60
3:C:959:THR:HG21	3:C:967:LEU:HD23	1.82	0.60
3:C:294:ILE:HG23	3:C:353:ALA:CA	2.31	0.60
3:C:818:VAL:C	3:C:820:GLN:H	2.05	0.60
3:C:701:ILE:HG22	3:C:701:ILE:O	2.02	0.60
3:C:917:ILE:HD13	3:C:958:LEU:HG	1.84	0.60
3:C:971:LYS:HA	3:C:974:LEU:HD23	1.83	0.59
3:C:41:LEU:HD22	3:C:46:GLU:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ARG:HG3	1:A:148:GLU:N	2.16	0.59
3:C:135:THR:HG22	3:C:176:ILE:HD11	1.83	0.59
3:C:350:ARG:NE	3:C:386:ARG:NH2	2.51	0.59
3:C:246:GLY:O	3:C:249:LEU:HD11	2.03	0.59
3:C:376:SER:O	3:C:380:ILE:HB	2.03	0.59
1:A:405:ASN:HD22	1:A:407:VAL:N	1.99	0.59
2:B:42:CYS:O	2:B:45:CYS:O	2.20	0.59
3:C:965:THR:O	3:C:965:THR:HG22	2.01	0.59
3:C:551:ARG:NH1	3:C:553:LEU:H	2.00	0.59
3:C:431:GLN:O	3:C:434:ASN:HB2	2.02	0.59
3:C:365:HIS:C	3:C:367:MET:H	2.04	0.59
1:A:325:VAL:C	1:A:327:ARG:H	2.05	0.59
3:C:131:CYS:HB3	3:C:161:MET:SD	2.42	0.59
3:C:370:GLU:O	3:C:374:THR:HG22	2.03	0.59
1:A:88:LEU:HD23	1:A:140:LEU:HD23	1.84	0.59
3:C:698:PRO:HB2	3:C:699:PRO:HD3	1.85	0.59
3:C:1093:LEU:HD11	3:C:1130:LEU:HD21	1.85	0.59
1:A:629:GLN:OE1	1:A:629:GLN:HA	2.03	0.59
3:C:652:VAL:O	3:C:655:LEU:HB2	2.02	0.59
3:C:346:SER:O	3:C:349:VAL:HG22	2.02	0.59
1:A:85:GLY:HA3	1:A:144:TRP:CE3	2.38	0.59
3:C:42:ASP:C	3:C:44:ASP:H	2.05	0.59
3:C:211:ILE:CD1	3:C:244:ARG:HE	2.16	0.59
3:C:1184:LEU:HD23	3:C:1190:GLU:HG3	1.84	0.59
1:A:499:TYR:CZ	1:A:503:LEU:HD21	2.38	0.59
3:C:894:PHE:O	3:C:897:GLN:HB3	2.02	0.58
3:C:928:TYR:O	3:C:932:ILE:HG12	2.03	0.58
3:C:207:PHE:C	3:C:209:ASP:H	2.05	0.58
2:B:62:SER:H	2:B:65:SER:HB3	1.68	0.58
3:C:168:LEU:HG	3:C:169:LEU:HD12	1.86	0.58
1:A:542:GLY:H	2:B:76:ASN:ND2	1.95	0.58
3:C:562:THR:OG1	3:C:563:PRO:HD3	2.02	0.58
3:C:268:ARG:CD	3:C:348:LYS:HE3	2.33	0.58
1:A:430:LYS:HA	1:A:477:ASN:O	2.04	0.58
3:C:459:THR:HG23	3:C:503:VAL:HG21	1.84	0.58
3:C:192:ARG:NH2	3:C:227:THR:HG21	2.14	0.58
3:C:1139:LEU:HD11	3:C:1189:ALA:HB3	1.86	0.58
3:C:611:THR:HA	3:C:614:ILE:CG1	2.33	0.58
3:C:226:THR:CG2	3:C:227:THR:H	2.15	0.58
3:C:188:ARG:HD2	3:C:188:ARG:N	2.18	0.58
3:C:608:LEU:HB3	3:C:609:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:192:ARG:O	3:C:196:ILE:HG13	2.03	0.58
3:C:1185:THR:O	3:C:1185:THR:HG22	2.04	0.58
1:A:577:LYS:HA	1:A:577:LYS:CE	2.34	0.58
1:A:634:ILE:HD11	1:A:687:MET:SD	2.44	0.58
1:A:317:ASP:OD2	1:A:317:ASP:N	2.35	0.58
1:A:37:MET:HB3	3:C:1068:MET:HA	1.84	0.58
3:C:7:HIS:HB3	3:C:8:ILE:HD12	1.84	0.58
3:C:722:VAL:O	3:C:722:VAL:HG23	2.02	0.57
3:C:597:ILE:HG21	3:C:635:ILE:HD13	1.86	0.57
3:C:1117:TYR:C	3:C:1117:TYR:CD2	2.77	0.57
1:A:177:LYS:O	1:A:177:LYS:HG3	2.04	0.57
3:C:82:TYR:O	3:C:85:GLU:HB3	2.04	0.57
1:A:40:SER:O	1:A:44:GLU:HG3	2.04	0.57
1:A:579:THR:HG23	2:B:32:LEU:HB2	1.85	0.57
3:C:15:MET:CG	3:C:56:LEU:HD11	2.34	0.57
3:C:1188:GLU:HA	3:C:1190:GLU:OE2	2.04	0.57
3:C:586:LYS:O	3:C:590:ILE:HG13	2.04	0.57
3:C:1052:LEU:HD21	3:C:1089:MET:HG2	1.87	0.57
3:C:441:LYS:HB2	3:C:441:LYS:NZ	2.19	0.57
3:C:249:LEU:HD22	3:C:250:GLU:H	1.69	0.57
1:A:134:ASN:ND2	1:A:159:ILE:HG22	2.19	0.57
3:C:1037:LYS:CD	3:C:1040:LEU:HD11	2.32	0.57
3:C:275:PHE:CE2	3:C:359:ALA:HB2	2.39	0.57
1:A:635:LEU:O	1:A:635:LEU:HD13	2.04	0.57
1:A:756:ILE:HD13	1:A:761:LEU:HB2	1.86	0.57
3:C:551:ARG:HH11	3:C:553:LEU:CB	2.16	0.57
1:A:650:LEU:O	1:A:669:LYS:HD2	2.04	0.57
3:C:673:ALA:HA	3:C:676:ILE:CD1	2.34	0.57
1:A:155:GLY:HA3	3:C:1163:LYS:N	2.20	0.57
3:C:1113:LEU:O	3:C:1120:LYS:HD3	2.04	0.57
3:C:822:ILE:O	3:C:826:LYS:HB2	2.05	0.57
3:C:206:CYS:HA	3:C:211:ILE:HD11	1.87	0.57
3:C:210:LEU:HD23	3:C:213:HIS:CE1	2.39	0.57
3:C:982:ARG:O	3:C:985:VAL:HG12	2.05	0.57
1:A:441:LEU:HD21	1:A:483:ALA:CB	2.35	0.57
1:A:357:ALA:H	3:C:489:SER:CB	2.17	0.57
1:A:539:LEU:O	2:B:32:LEU:HA	2.04	0.57
3:C:553:LEU:HD13	3:C:639:PRO:HD2	1.87	0.57
3:C:831:THR:CG2	3:C:833:SER:HB3	2.34	0.57
1:A:221:GLY:HA3	3:C:1167:GLU:CD	2.26	0.57
3:C:465:LEU:O	3:C:467:GLY:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:205:SER:O	3:C:206:CYS:HB2	2.04	0.56
3:C:207:PHE:O	3:C:210:LEU:N	2.36	0.56
3:C:138:LEU:O	3:C:141:ALA:HB3	2.05	0.56
3:C:42:ASP:O	3:C:46:GLU:HG3	2.04	0.56
3:C:967:LEU:N	3:C:968:PRO:CD	2.67	0.56
3:C:8:ILE:CD1	3:C:8:ILE:H	2.17	0.56
3:C:780:THR:HG22	3:C:837:LEU:HD21	1.87	0.56
3:C:379:LEU:HD23	3:C:382:ARG:HG3	1.87	0.56
3:C:299:LYS:HZ2	3:C:379:LEU:HD22	1.69	0.56
3:C:442:GLN:O	3:C:444:LYS:N	2.39	0.56
3:C:1143:ASP:OD1	3:C:1193:PRO:HB3	2.04	0.56
3:C:1207:GLU:HG3	3:C:1208:LEU:HD22	1.88	0.56
3:C:36:LYS:NZ	3:C:36:LYS:HB3	2.20	0.56
1:A:354:CYS:HB3	1:A:358:ALA:HB2	1.87	0.56
1:A:473:LEU:HB3	1:A:510:ILE:HG13	1.87	0.56
3:C:289:HIS:O	3:C:293:ILE:HG13	2.05	0.56
3:C:17:SER:O	3:C:19:ASP:N	2.36	0.56
3:C:645:ARG:HD2	3:C:684:SER:HB2	1.88	0.56
3:C:735:LEU:HD13	3:C:735:LEU:C	2.25	0.56
1:A:762:GLU:HB3	1:A:774:LEU:HD12	1.88	0.56
3:C:216:SER:O	3:C:220:LYS:HG3	2.05	0.56
1:A:513:SER:OG	1:A:537:GLN:HA	2.06	0.56
3:C:717:THR:O	3:C:721:LYS:HB2	2.06	0.56
3:C:1199:GLN:HB3	3:C:1202:ILE:CB	2.35	0.56
1:A:718:MET:HE1	1:A:771:TYR:HB2	1.87	0.56
1:A:286:LEU:HD22	1:A:290:CYS:SG	2.46	0.56
1:A:143:HIS:O	1:A:145:VAL:N	2.37	0.56
3:C:933:TRP:CH2	3:C:966:LEU:HD22	2.41	0.56
1:A:296:GLU:HA	1:A:299:LEU:HG	1.85	0.56
2:B:87:TRP:CE2	2:B:91:ARG:HG3	2.41	0.56
1:A:625:THR:CG2	1:A:632:MET:CG	2.84	0.56
3:C:375:VAL:O	3:C:379:LEU:CB	2.53	0.56
3:C:46:GLU:OE2	3:C:79:VAL:HA	2.06	0.56
1:A:117:LYS:HZ1	1:A:121:GLN:HE21	1.52	0.56
3:C:1015:LEU:HD12	3:C:1022:VAL:CG1	2.36	0.56
3:C:495:ILE:HG23	3:C:538:GLU:HG3	1.86	0.56
1:A:660:VAL:HG12	1:A:661:GLU:H	1.70	0.56
1:A:117:LYS:HZ2	1:A:121:GLN:HE21	1.54	0.55
3:C:1015:LEU:O	3:C:1018:PRO:HD2	2.07	0.55
3:C:979:SER:HB3	3:C:1020:LEU:HD11	1.89	0.55
3:C:350:ARG:CZ	3:C:386:ARG:HH22	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:LEU:HD23	1:A:648:LEU:HB2	1.86	0.55
1:A:142:ARG:NH2	1:A:147:ARG:HG2	2.20	0.55
3:C:551:ARG:O	3:C:552:PRO:C	2.45	0.55
3:C:1047:THR:O	3:C:1050:PRO:HD2	2.06	0.55
3:C:79:VAL:HG22	3:C:83:GLN:HB2	1.87	0.55
3:C:799:ILE:HG22	3:C:837:LEU:HD11	1.88	0.55
1:A:748:ILE:O	1:A:752:ILE:HG13	2.06	0.55
1:A:621:VAL:HG11	1:A:632:MET:HE1	1.88	0.55
3:C:1037:LYS:H	3:C:1038:PRO:HD3	1.71	0.55
3:C:942:CYS:O	3:C:943:ALA:C	2.45	0.55
3:C:35:GLN:O	3:C:36:LYS:HB3	2.06	0.55
3:C:8:ILE:HD12	3:C:8:ILE:N	2.22	0.55
1:A:688:LYS:HD3	1:A:689:THR:N	2.21	0.55
1:A:595:LYS:HB3	1:A:595:LYS:NZ	2.21	0.55
3:C:285:GLU:C	3:C:285:GLU:OE2	2.45	0.55
3:C:601:GLY:HA2	3:C:604:LEU:HB2	1.89	0.55
3:C:268:ARG:HD2	3:C:348:LYS:HE3	1.87	0.55
3:C:383:PHE:HE2	3:C:386:ARG:HH21	1.54	0.55
1:A:171:LEU:HD12	1:A:175:LEU:HD13	1.88	0.55
3:C:144:LYS:O	3:C:145:GLN:C	2.45	0.55
3:C:804:ALA:HA	3:C:845:VAL:CG2	2.37	0.55
1:A:601:GLN:O	1:A:683:ILE:HG12	2.07	0.55
3:C:1012:LEU:O	3:C:1015:LEU:N	2.37	0.55
3:C:1143:ASP:CG	3:C:1193:PRO:HB3	2.28	0.55
3:C:486:ASP:O	3:C:487:LYS:CB	2.55	0.55
3:C:858:LYS:HE2	3:C:891:TYR:CD2	2.41	0.55
3:C:551:ARG:CB	3:C:599:ASN:HB3	2.37	0.55
3:C:259:PHE:HB3	3:C:270:TYR:HE2	1.71	0.55
3:C:282:CYS:O	3:C:284:LYS:N	2.40	0.55
3:C:827:ASN:O	3:C:828:SER:C	2.45	0.54
3:C:253:ILE:HG12	3:C:286:VAL:HG21	1.87	0.54
1:A:307:GLN:O	1:A:310:LEU:N	2.40	0.54
3:C:75:LEU:O	3:C:78:LYS:N	2.39	0.54
1:A:651:GLU:CA	1:A:669:LYS:HZ2	2.20	0.54
1:A:646:LYS:C	1:A:647:LEU:HD12	2.28	0.54
3:C:183:GLN:C	3:C:185:THR:N	2.61	0.54
3:C:15:MET:HG2	3:C:56:LEU:HD11	1.89	0.54
2:B:73:GLY:HA2	2:B:102:GLU:O	2.07	0.54
3:C:254:PRO:O	3:C:258:LYS:HG3	2.07	0.54
3:C:361:VAL:HA	3:C:371:PHE:CE1	2.42	0.54
1:A:631:LYS:O	1:A:635:LEU:CB	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:346:SER:C	3:C:349:VAL:HG22	2.27	0.54
3:C:405:THR:O	3:C:407:PRO:HD3	2.07	0.54
3:C:271:CYS:HB2	3:C:352:ALA:HB1	1.89	0.54
3:C:551:ARG:HG2	3:C:599:ASN:CG	2.28	0.54
3:C:970:LEU:HB3	3:C:985:VAL:CG2	2.38	0.54
3:C:658:PHE:O	3:C:660:ARG:N	2.39	0.54
1:A:21:TRP:CZ2	1:A:91:ARG:HB3	2.42	0.54
1:A:597:ARG:HH11	1:A:597:ARG:CB	2.04	0.54
3:C:372:TYR:HA	3:C:377:PRO:CG	2.37	0.54
3:C:1184:LEU:HD23	3:C:1190:GLU:CG	2.38	0.54
3:C:465:LEU:HB2	3:C:468:ALA:HB2	1.90	0.54
1:A:614:ASN:ND2	2:B:22:PHE:H	2.02	0.54
3:C:386:ARG:HG3	3:C:387:GLU:H	1.73	0.54
1:A:439:ALA:O	1:A:443:ASP:HB2	2.07	0.54
3:C:134:ILE:HG22	3:C:138:LEU:HD11	1.89	0.54
3:C:566:LYS:CD	3:C:566:LYS:H	2.16	0.54
3:C:936:LEU:HD11	3:C:954:CYS:HB3	1.90	0.54
1:A:718:MET:HE2	1:A:771:TYR:HB2	1.89	0.54
3:C:469:LEU:N	3:C:508:HIS:HE1	2.05	0.54
3:C:398:TYR:O	3:C:401:LEU:HB3	2.07	0.54
3:C:126:LEU:O	3:C:128:ALA:N	2.41	0.54
3:C:600:LEU:C	3:C:602:ASP:N	2.57	0.54
3:C:975:ILE:HG23	3:C:976:SER:N	2.17	0.54
1:A:426:ASP:OD2	1:A:430:LYS:HE3	2.08	0.54
3:C:723:TYR:N	3:C:724:PRO:CD	2.70	0.54
3:C:1012:LEU:C	3:C:1014:THR:N	2.58	0.54
3:C:88:VAL:CG1	3:C:134:ILE:HG12	2.38	0.54
1:A:137:CYS:CB	1:A:159:ILE:HG12	2.38	0.54
1:A:713:ALA:O	1:A:717:ILE:HG13	2.08	0.54
1:A:651:GLU:O	1:A:652:ASP:O	2.26	0.53
3:C:301:LEU:HD13	3:C:350:ARG:HH12	1.71	0.53
1:A:443:ASP:O	1:A:446:ASN:N	2.40	0.53
3:C:188:ARG:CD	3:C:188:ARG:N	2.71	0.53
2:B:64:THR:O	2:B:67:GLU:HB3	2.08	0.53
3:C:616:LEU:HD23	3:C:647:VAL:CG1	2.38	0.53
3:C:230:TYR:O	3:C:234:ILE:HG12	2.08	0.53
1:A:631:LYS:O	1:A:635:LEU:HB2	2.08	0.53
1:A:621:VAL:CG1	1:A:632:MET:HE1	2.39	0.53
3:C:386:ARG:HD3	3:C:390:VAL:HG12	1.89	0.53
3:C:1142:LEU:HD22	3:C:1193:PRO:HG2	1.90	0.53
3:C:41:LEU:HD22	3:C:46:GLU:CG	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:933:TRP:NE1	3:C:937:LEU:HD11	2.23	0.53
3:C:690:ILE:HG12	3:C:723:TYR:CE2	2.43	0.53
1:A:363:LYS:HA	1:A:424:TYR:CD2	2.44	0.53
2:B:77:HIS:CE1	2:B:97:ASP:HB3	2.44	0.53
1:A:423:ARG:O	1:A:426:ASP:HB3	2.07	0.53
3:C:365:HIS:O	3:C:367:MET:N	2.42	0.53
1:A:536:ILE:HG12	1:A:537:GLN:N	2.21	0.53
3:C:300:TYR:CD2	3:C:300:TYR:O	2.61	0.53
3:C:208:VAL:HA	3:C:244:ARG:NH2	2.22	0.53
3:C:285:GLU:C	3:C:287:TYR:H	2.12	0.53
1:A:270:GLU:O	1:A:274:VAL:HG23	2.07	0.53
1:A:630:ILE:HG22	1:A:630:ILE:O	2.04	0.53
3:C:294:ILE:HD13	3:C:356:CYS:HB3	1.90	0.53
3:C:83:GLN:HA	3:C:86:THR:OG1	2.08	0.53
1:A:52:TYR:CD2	1:A:52:TYR:O	2.61	0.53
3:C:1159:ALA:HA	3:C:1166:PHE:HZ	1.72	0.53
3:C:543:THR:O	3:C:547:VAL:HG23	2.09	0.53
3:C:1149:LEU:HD13	3:C:1180:VAL:HG22	1.88	0.53
1:A:619:TYR:HD2	1:A:623:GLN:HE21	1.57	0.53
3:C:206:CYS:HB3	3:C:207:PHE:CA	2.37	0.53
3:C:269:GLU:O	3:C:272:ILE:HB	2.09	0.53
3:C:982:ARG:HH22	3:C:1019:ASP:H	1.55	0.53
3:C:1023:ARG:O	3:C:1026:ALA:HB3	2.09	0.53
1:A:100:LEU:HD21	1:A:126:TYR:CE1	2.44	0.53
3:C:933:TRP:CZ3	3:C:966:LEU:HD22	2.44	0.53
3:C:133:LYS:NZ	3:C:133:LYS:HB2	2.24	0.53
3:C:85:GLU:CG	3:C:133:LYS:HE2	2.30	0.53
3:C:365:HIS:C	3:C:367:MET:N	2.62	0.53
1:A:662:LEU:HD12	1:A:662:LEU:N	2.22	0.53
1:A:221:GLY:HA3	3:C:1167:GLU:OE1	2.09	0.53
1:A:112:ASP:O	1:A:182:ALA:HB1	2.08	0.53
3:C:299:LYS:HZ1	3:C:379:LEU:HD22	1.73	0.53
3:C:1015:LEU:CD1	3:C:1022:VAL:CG1	2.87	0.53
3:C:33:GLU:HA	3:C:36:LYS:HE2	1.90	0.53
3:C:896:LEU:HD11	3:C:932:ILE:HD13	1.90	0.53
3:C:502:TYR:CE1	3:C:541:LEU:HD22	2.44	0.53
1:A:592:ASN:HB3	1:A:597:ARG:HH12	1.73	0.53
3:C:945:GLU:HA	3:C:948:ARG:HD3	1.90	0.53
1:A:719:LYS:HG3	1:A:773:TYR:HE1	1.72	0.53
3:C:208:VAL:O	3:C:212:GLU:OE2	2.27	0.52
3:C:813:GLU:OE1	3:C:814:GLY:N	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ASN:ND2	1:A:160:TYR:HB2	2.25	0.52
1:A:734:LEU:HD23	1:A:743:PRO:HD2	1.91	0.52
1:A:767:GLU:OE1	1:A:767:GLU:HA	2.09	0.52
3:C:856:GLU:O	3:C:860:VAL:HG23	2.10	0.52
3:C:227:THR:HG22	3:C:229:THR:OG1	2.09	0.52
1:A:21:TRP:CD1	1:A:91:ARG:HD3	2.44	0.52
3:C:870:GLU:H	3:C:870:GLU:CD	2.12	0.52
1:A:440:GLU:C	1:A:444:THR:HG1	2.08	0.52
1:A:719:LYS:HG3	1:A:773:TYR:CE1	2.44	0.52
3:C:926:LYS:HB3	3:C:927:PRO:HD3	1.91	0.52
1:A:630:ILE:O	1:A:635:LEU:HB2	2.09	0.52
1:A:592:ASN:HB3	1:A:597:ARG:NH2	2.23	0.52
3:C:253:ILE:CD1	3:C:281:ARG:HH22	2.21	0.52
3:C:701:ILE:HD13	3:C:738:LEU:HD21	1.89	0.52
1:A:117:LYS:O	1:A:117:LYS:HD3	2.09	0.52
1:A:186:LEU:O	1:A:189:LYS:HB2	2.10	0.52
3:C:168:LEU:C	3:C:169:LEU:HD12	2.30	0.52
1:A:472:ARG:NH1	1:A:484:GLU:OE1	2.43	0.52
3:C:19:ASP:OD1	3:C:21:ASP:HB2	2.10	0.52
3:C:727:LEU:HD13	3:C:767:THR:OG1	2.10	0.52
1:A:660:VAL:HB	1:A:662:LEU:CD1	2.39	0.52
1:A:719:LYS:HE2	1:A:773:TYR:OH	2.10	0.52
2:B:37:ILE:HG23	2:B:38:VAL:HG13	1.91	0.52
3:C:1194:LEU:O	3:C:1195:MET:CB	2.44	0.52
2:B:39:VAL:O	2:B:40:ASP:C	2.47	0.52
1:A:25:ARG:HD3	1:A:95:PHE:CD1	2.44	0.52
3:C:458:LEU:O	3:C:462:VAL:HG23	2.09	0.52
3:C:548:LYS:CA	3:C:551:ARG:HG3	2.33	0.52
3:C:971:LYS:O	3:C:971:LYS:HG2	2.08	0.52
1:A:175:LEU:CG	1:A:208:TYR:OH	2.52	0.52
3:C:821:PHE:C	3:C:823:GLN:N	2.51	0.52
1:A:107:GLY:HA2	1:A:110:LEU:CD1	2.37	0.52
3:C:239:ARG:NE	3:C:276:GLU:HG2	2.24	0.52
1:A:492:LYS:HB3	3:C:108:ILE:CD1	2.39	0.52
3:C:213:HIS:O	3:C:217:GLU:HB2	2.10	0.52
3:C:87:ILE:O	3:C:88:VAL:C	2.47	0.52
1:A:717:ILE:HA	3:C:25:MET:HE3	1.89	0.52
3:C:626:LEU:HD23	3:C:666:LEU:HD12	1.91	0.52
3:C:826:LYS:NZ	3:C:828:SER:HB2	2.23	0.52
1:A:667:LEU:HB3	1:A:669:LYS:HE3	1.91	0.52
1:A:21:TRP:NE1	1:A:91:ARG:HD3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:37:ASP:OD2	3:C:39:ILE:HG12	2.10	0.52
3:C:771:GLY:H	3:C:774:ASP:HB2	1.75	0.52
1:A:50:TYR:CE1	1:A:54:THR:HG21	2.45	0.52
3:C:903:PRO:HA	3:C:906:GLN:HG3	1.91	0.52
1:A:597:ARG:O	1:A:597:ARG:HG3	2.09	0.52
1:A:178:GLN:O	1:A:181:ASN:N	2.43	0.52
3:C:1038:PRO:C	3:C:1040:LEU:H	2.13	0.52
3:C:942:CYS:HB3	3:C:980:TYR:CD2	2.45	0.52
1:A:645:SER:O	1:A:646:LYS:CB	2.57	0.52
3:C:168:LEU:HG	3:C:169:LEU:CD1	2.39	0.52
2:B:86:ARG:O	2:B:89:LYS:HB2	2.09	0.52
1:A:614:ASN:HA	2:B:20:LYS:O	2.10	0.51
3:C:225:SER:O	3:C:226:THR:O	2.28	0.51
3:C:385:GLU:HB3	3:C:442:GLN:OE1	2.10	0.51
2:B:49:ILE:CD1	2:B:50:MET:HG2	2.34	0.51
1:A:714:ILE:HD13	1:A:733:VAL:HG21	1.93	0.51
1:A:733:VAL:HG11	1:A:748:ILE:HD13	1.91	0.51
1:A:286:LEU:O	1:A:290:CYS:SG	2.64	0.51
1:A:158:GLU:O	1:A:162:LEU:N	2.44	0.51
1:A:405:ASN:ND2	1:A:405:ASN:C	2.64	0.51
3:C:701:ILE:HD13	3:C:738:LEU:HD23	1.92	0.51
3:C:947:THR:O	3:C:951:VAL:HG23	2.10	0.51
3:C:913:LEU:CD2	3:C:917:ILE:HG13	2.40	0.51
1:A:649:VAL:HG23	1:A:671:TYR:HB2	1.92	0.51
1:A:654:ASN:HD22	1:A:656:ASN:ND2	2.09	0.51
3:C:1104:GLU:OE1	3:C:1104:GLU:HA	2.11	0.51
1:A:542:GLY:N	2:B:76:ASN:HD21	1.99	0.51
1:A:144:TRP:C	1:A:145:VAL:HG22	2.30	0.51
1:A:227:TYR:HE1	1:A:282:THR:HG23	1.75	0.51
1:A:17:LEU:N	1:A:19:GLN:HG2	2.25	0.51
3:C:543:THR:HG23	3:C:568:LEU:HD22	1.93	0.51
3:C:41:LEU:HD22	3:C:46:GLU:OE2	2.09	0.51
3:C:994:SER:O	3:C:1037:LYS:HE2	2.11	0.51
3:C:610:ASN:O	3:C:614:ILE:HG12	2.11	0.51
1:A:376:TYR:O	1:A:380:VAL:HG23	2.09	0.51
1:A:117:LYS:HZ2	1:A:121:GLN:NE2	2.08	0.51
1:A:595:LYS:HG3	1:A:596:ASN:N	2.25	0.51
3:C:961:ILE:O	3:C:962:ASP:HB3	2.10	0.51
3:C:473:ILE:N	3:C:474:PRO:CD	2.73	0.51
1:A:720:MET:HE1	3:C:29:ASP:OD2	2.11	0.51
3:C:220:LYS:C	3:C:222:ASP:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:374:THR:O	3:C:374:THR:HG23	2.10	0.51
3:C:245:ILE:O	3:C:245:ILE:HG12	2.11	0.51
1:A:612:GLN:C	1:A:614:ASN:H	2.14	0.51
3:C:301:LEU:HB2	3:C:350:ARG:NH1	2.25	0.51
3:C:933:TRP:CD1	3:C:937:LEU:HD11	2.46	0.51
1:A:660:VAL:CG1	1:A:661:GLU:N	2.72	0.51
3:C:887:ASN:CG	3:C:890:GLU:HB2	2.31	0.51
1:A:671:TYR:C	1:A:671:TYR:CD1	2.83	0.51
3:C:351:ARG:HD3	3:C:393:ASP:OD2	2.10	0.51
1:A:577:LYS:HZ3	1:A:578:LEU:H	1.58	0.51
3:C:495:ILE:CD1	3:C:534:LYS:HB3	2.41	0.51
3:C:236:ALA:HA	3:C:239:ARG:NH1	2.26	0.51
1:A:319:GLY:O	1:A:322:TYR:HB3	2.10	0.51
3:C:1024:ARG:O	3:C:1028:VAL:HG23	2.11	0.51
3:C:825:VAL:HG23	3:C:860:VAL:HG22	1.92	0.51
3:C:248:TYR:C	3:C:249:LEU:HD13	2.31	0.51
1:A:486:SER:O	1:A:490:LYS:HG3	2.11	0.51
1:A:365:TYR:CE2	1:A:407:VAL:HG21	2.46	0.51
3:C:129:ASN:HA	3:C:132:LYS:HB3	1.92	0.51
3:C:383:PHE:O	3:C:394:VAL:HG11	2.11	0.51
2:B:73:GLY:O	2:B:104:GLN:NE2	2.44	0.51
3:C:126:LEU:CD2	3:C:130:VAL:HG21	2.41	0.51
3:C:206:CYS:HB3	3:C:207:PHE:C	2.31	0.50
3:C:267:LEU:HA	3:C:270:TYR:CD1	2.46	0.50
3:C:1190:GLU:O	3:C:1193:PRO:CD	2.55	0.50
1:A:672:LEU:CD1	1:A:672:LEU:H	2.16	0.50
3:C:1037:LYS:O	3:C:1040:LEU:HG	2.11	0.50
1:A:21:TRP:HE3	1:A:21:TRP:HA	1.75	0.50
1:A:726:HIS:HA	1:A:771:TYR:HE1	1.77	0.50
3:C:1112:GLY:O	3:C:1123:THR:CB	2.59	0.50
1:A:717:ILE:HG12	3:C:25:MET:HE2	1.93	0.50
3:C:86:THR:O	3:C:87:ILE:C	2.49	0.50
3:C:1031:ASN:OD1	3:C:1088:CYS:HA	2.10	0.50
1:A:741:PHE:O	1:A:743:PRO:HD3	2.11	0.50
3:C:796:TYR:HD2	3:C:837:LEU:HB2	1.76	0.50
3:C:645:ARG:HD2	3:C:684:SER:CB	2.41	0.50
3:C:769:ASN:O	3:C:770:LEU:HD12	2.11	0.50
3:C:373:LYS:HG3	3:C:427:MET:HE2	1.74	0.50
3:C:206:CYS:HB2	3:C:207:PHE:HA	1.92	0.50
3:C:244:ARG:NH1	3:C:244:ARG:HG2	2.24	0.50
2:B:40:ASP:O	2:B:49:ILE:HD11	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1036:ASN:N	3:C:1036:ASN:ND2	2.60	0.50
1:A:21:TRP:CE3	1:A:21:TRP:HA	2.46	0.50
1:A:662:LEU:H	1:A:662:LEU:CD1	2.23	0.50
3:C:570:THR:O	3:C:571:CYS:C	2.50	0.50
1:A:598:TYR:N	1:A:598:TYR:CD1	2.79	0.50
3:C:857:LEU:HD11	3:C:883:ILE:HD13	1.93	0.50
3:C:673:ALA:CA	3:C:676:ILE:HD11	2.37	0.50
2:B:82:HIS:O	2:B:86:ARG:HB2	2.12	0.50
1:A:299:LEU:O	1:A:303:HIS:CG	2.64	0.50
3:C:254:PRO:HB2	3:C:258:LYS:HE3	1.92	0.50
3:C:500:CYS:O	3:C:504:ILE:HG13	2.11	0.50
1:A:440:GLU:O	1:A:444:THR:CB	2.59	0.50
3:C:1202:ILE:HA	3:C:1205:ASN:HD22	1.76	0.50
1:A:21:TRP:CE3	1:A:21:TRP:O	2.65	0.50
1:A:646:LYS:HG2	1:A:646:LYS:O	2.11	0.50
3:C:143:ALA:C	3:C:145:GLN:H	2.13	0.50
1:A:227:TYR:CE1	1:A:282:THR:HG23	2.46	0.50
3:C:428:LEU:O	3:C:429:GLN:C	2.49	0.50
1:A:309:LEU:HD13	1:A:317:ASP:HB2	1.92	0.50
3:C:209:ASP:O	3:C:213:HIS:CD2	2.65	0.50
1:A:441:LEU:HD21	1:A:483:ALA:HB2	1.93	0.50
3:C:290:VAL:O	3:C:291:SER:C	2.50	0.50
3:C:658:PHE:C	3:C:660:ARG:H	2.15	0.50
1:A:309:LEU:CD1	1:A:317:ASP:HB2	2.42	0.50
1:A:703:GLU:HA	1:A:703:GLU:OE1	2.12	0.50
3:C:814:GLY:O	3:C:818:VAL:HG23	2.12	0.49
1:A:141:ASN:HD21	1:A:159:ILE:H	1.58	0.49
3:C:219:SER:O	3:C:222:ASP:HB2	2.12	0.49
1:A:274:VAL:HA	1:A:278:LEU:HB2	1.93	0.49
1:A:522:LYS:O	1:A:525:THR:N	2.45	0.49
1:A:521:LYS:NZ	1:A:521:LYS:HB3	2.27	0.49
2:B:97:ASP:O	2:B:99:ARG:N	2.45	0.49
3:C:223:SER:O	3:C:225:SER:N	2.45	0.49
3:C:368:LEU:O	3:C:369:PRO:C	2.50	0.49
3:C:350:ARG:NH2	3:C:386:ARG:HH22	2.10	0.49
1:A:175:LEU:O	1:A:176:ASN:C	2.48	0.49
3:C:151:GLN:O	3:C:154:ALA:N	2.44	0.49
1:A:144:TRP:O	1:A:145:VAL:CG1	2.53	0.49
1:A:660:VAL:HB	1:A:662:LEU:HD11	1.94	0.49
3:C:887:ASN:OD1	3:C:889:PRO:HD2	2.11	0.49
3:C:1109:VAL:HG13	3:C:1123:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ASN:CG	1:A:490:LYS:HE2	2.33	0.49
3:C:821:PHE:CE1	3:C:857:LEU:HB2	2.46	0.49
3:C:697:LEU:CD1	3:C:716:LEU:HD21	2.42	0.49
3:C:697:LEU:O	3:C:700:LEU:N	2.38	0.49
3:C:902:GLN:HE22	3:C:905:ARG:NH1	2.11	0.49
3:C:509:SER:O	3:C:512:VAL:HG23	2.11	0.49
1:A:624:LEU:C	1:A:626:ASP:N	2.66	0.49
1:A:175:LEU:HG	1:A:208:TYR:CZ	2.48	0.49
3:C:1205:ASN:C	3:C:1207:GLU:H	2.15	0.49
1:A:430:LYS:HG2	1:A:477:ASN:O	2.12	0.49
3:C:75:LEU:O	3:C:76:VAL:C	2.51	0.49
3:C:249:LEU:CB	3:C:281:ARG:NH2	2.75	0.49
3:C:1001:ASP:HB2	3:C:1002:PRO:HD3	1.93	0.49
3:C:660:ARG:HD2	3:C:696:GLU:CD	2.32	0.49
3:C:663:GLN:O	3:C:664:ARG:C	2.50	0.49
3:C:267:LEU:HD23	3:C:270:TYR:CZ	2.47	0.49
3:C:301:LEU:HB2	3:C:350:ARG:CZ	2.42	0.49
1:A:175:LEU:HG	1:A:208:TYR:HH	1.77	0.49
1:A:725:LYS:O	1:A:726:HIS:C	2.51	0.49
3:C:763:VAL:HG13	3:C:775:LEU:HD12	1.93	0.49
1:A:598:TYR:CZ	1:A:675:LYS:HB3	2.48	0.49
3:C:851:LEU:C	3:C:853:GLY:H	2.16	0.49
3:C:42:ASP:HB2	3:C:45:SER:CB	2.42	0.49
2:B:48:HIS:O	2:B:50:MET:N	2.45	0.49
3:C:405:THR:O	3:C:407:PRO:N	2.46	0.49
1:A:609:ILE:HD11	1:A:635:LEU:CD2	2.42	0.49
1:A:615:THR:OG1	1:A:619:TYR:OH	2.31	0.49
1:A:618:ALA:CB	1:A:669:LYS:HG2	2.39	0.49
1:A:593:CYS:HB2	2:B:20:LYS:H	1.78	0.49
3:C:349:VAL:CG2	3:C:350:ARG:N	2.69	0.49
3:C:633:THR:HG23	3:C:676:ILE:CG1	2.41	0.49
3:C:4:ALA:HB3	3:C:7:HIS:HB2	1.95	0.49
1:A:492:LYS:HB3	3:C:108:ILE:HD11	1.95	0.49
1:A:452:PHE:O	1:A:458:LYS:NZ	2.46	0.49
3:C:386:ARG:HH11	3:C:386:ARG:HG3	1.77	0.49
1:A:134:ASN:ND2	1:A:157:TYR:HB2	2.27	0.49
3:C:17:SER:C	3:C:19:ASP:H	2.15	0.49
3:C:808:ARG:HE	3:C:848:HIS:CG	2.31	0.49
3:C:1205:ASN:C	3:C:1207:GLU:N	2.66	0.48
3:C:1079:LEU:O	3:C:1079:LEU:CD2	2.60	0.48
3:C:374:THR:CG2	3:C:374:THR:O	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:547:VAL:HG12	3:C:599:ASN:HD22	1.77	0.48
3:C:825:VAL:C	3:C:827:ASN:N	2.64	0.48
3:C:229:THR:C	3:C:231:ILE:N	2.65	0.48
1:A:170:CYS:O	1:A:174:PRO:HD2	2.12	0.48
1:A:643:LEU:HD23	1:A:648:LEU:CB	2.42	0.48
1:A:325:VAL:C	1:A:327:ARG:N	2.67	0.48
2:B:87:TRP:CZ2	2:B:95:PRO:HB3	2.48	0.48
3:C:1016:GLU:HA	3:C:1016:GLU:OE2	2.13	0.48
1:A:100:LEU:HD13	1:A:167:TRP:HA	1.96	0.48
1:A:556:SER:O	1:A:558:LEU:N	2.46	0.48
3:C:299:LYS:HZ3	3:C:382:ARG:HD3	1.79	0.48
1:A:619:TYR:HD2	1:A:623:GLN:NE2	2.11	0.48
3:C:249:LEU:HB3	3:C:281:ARG:CZ	2.43	0.48
3:C:386:ARG:CZ	3:C:386:ARG:CB	2.80	0.48
1:A:178:GLN:O	1:A:180:THR:N	2.46	0.48
1:A:475:HIS:CE1	1:A:585:SER:HA	2.47	0.48
3:C:578:ALA:O	3:C:579:ALA:CB	2.62	0.48
1:A:647:LEU:N	1:A:647:LEU:HD12	2.28	0.48
1:A:660:VAL:CG1	1:A:661:GLU:H	2.26	0.48
3:C:600:LEU:HD23	3:C:600:LEU:N	2.27	0.48
3:C:601:GLY:CA	3:C:604:LEU:HB2	2.44	0.48
3:C:1013:LYS:HB2	3:C:1047:THR:HG21	1.95	0.48
1:A:170:CYS:O	1:A:174:PRO:CD	2.61	0.48
1:A:186:LEU:HA	1:A:189:LYS:HG3	1.94	0.48
1:A:713:ALA:O	1:A:714:ILE:C	2.52	0.48
3:C:249:LEU:HD22	3:C:250:GLU:N	2.27	0.48
2:B:64:THR:O	2:B:65:SER:C	2.52	0.48
1:A:520:PHE:HD1	1:A:568:PHE:CG	2.30	0.48
3:C:1199:GLN:CG	3:C:1202:ILE:HG12	2.42	0.48
3:C:282:CYS:C	3:C:284:LYS:H	2.17	0.48
3:C:975:ILE:CG2	3:C:976:SER:H	2.19	0.48
1:A:475:HIS:O	1:A:476:GLN:HG3	2.14	0.48
3:C:633:THR:HG23	3:C:676:ILE:CD1	2.44	0.48
1:A:727:GLN:O	1:A:728:GLN:C	2.51	0.48
3:C:507:ASN:O	3:C:508:HIS:CG	2.66	0.48
3:C:61:ASN:OD1	3:C:63:GLU:HB2	2.13	0.48
3:C:590:ILE:CD1	3:C:624:THR:HG23	2.44	0.48
3:C:821:PHE:CD2	3:C:821:PHE:N	2.79	0.48
3:C:117:LEU:HD11	3:C:130:VAL:HG11	1.94	0.48
1:A:624:LEU:C	1:A:626:ASP:H	2.17	0.48
1:A:202:SER:O	1:A:206:GLN:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ASP:O	1:A:284:ASP:OD1	2.31	0.48
3:C:448:VAL:HG13	3:C:493:LEU:HD22	1.96	0.48
2:B:19:LYS:HB3	2:B:19:LYS:HZ3	1.76	0.48
3:C:181:LEU:HB3	3:C:217:GLU:OE1	2.14	0.48
3:C:226:THR:HG23	3:C:227:THR:H	1.79	0.48
3:C:1100:LEU:O	3:C:1102:ILE:HD13	2.14	0.48
3:C:294:ILE:HG23	3:C:353:ALA:HB1	1.96	0.48
3:C:134:ILE:O	3:C:137:ARG:N	2.46	0.48
3:C:633:THR:HA	3:C:676:ILE:CD1	2.42	0.48
3:C:521:VAL:HG13	3:C:525:VAL:HG23	1.94	0.48
1:A:250:PHE:CE2	1:A:259:TYR:HA	2.48	0.48
3:C:551:ARG:HD3	3:C:599:ASN:CG	2.34	0.47
2:B:19:LYS:O	2:B:20:LYS:HB2	2.14	0.47
1:A:104:LEU:O	1:A:108:GLU:HG3	2.14	0.47
3:C:46:GLU:O	3:C:47:ARG:C	2.52	0.47
3:C:79:VAL:CG2	3:C:83:GLN:HB2	2.44	0.47
3:C:166:GLY:O	3:C:168:LEU:N	2.47	0.47
1:A:734:LEU:HD23	1:A:734:LEU:HA	1.70	0.47
1:A:711:GLN:HE22	1:A:758:LYS:HZ2	1.62	0.47
3:C:462:VAL:O	3:C:462:VAL:HG12	2.14	0.47
3:C:771:GLY:O	3:C:775:LEU:HG	2.13	0.47
3:C:598:CYS:SG	3:C:638:SER:HB2	2.53	0.47
1:A:630:ILE:CD1	1:A:630:ILE:HB	2.38	0.47
3:C:380:ILE:HG23	3:C:394:VAL:HG12	1.96	0.47
3:C:897:GLN:HA	3:C:897:GLN:HE21	1.79	0.47
3:C:690:ILE:HG23	3:C:719:LEU:HD21	1.95	0.47
3:C:592:CYS:O	3:C:596:ILE:HG13	2.14	0.47
1:A:289:LYS:O	1:A:293:VAL:HG12	2.14	0.47
3:C:823:GLN:HA	3:C:823:GLN:NE2	2.29	0.47
1:A:405:ASN:ND2	1:A:408:THR:HG23	2.29	0.47
3:C:698:PRO:CG	3:C:733:SER:HB2	2.43	0.47
2:B:87:TRP:CE2	2:B:95:PRO:HB3	2.48	0.47
3:C:514:HIS:CD2	3:C:559:PHE:HB2	2.49	0.47
3:C:1017:ASP:N	3:C:1018:PRO:CD	2.78	0.47
1:A:315:ASN:HB3	1:A:318:LEU:HD12	1.96	0.47
3:C:1094:ASP:CG	3:C:1129:ARG:HH22	2.17	0.47
3:C:195:THR:O	3:C:198:ALA:HB3	2.15	0.47
1:A:115:VAL:O	1:A:119:TYR:N	2.42	0.47
1:A:504:GLN:NE2	1:A:504:GLN:HA	2.29	0.47
3:C:540:LEU:HD22	3:C:589:ALA:HA	1.96	0.47
1:A:635:LEU:HD13	1:A:635:LEU:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:371:PHE:O	3:C:376:SER:OG	2.32	0.47
3:C:386:ARG:HB2	3:C:386:ARG:NH1	2.29	0.47
3:C:383:PHE:HD2	3:C:386:ARG:HE	1.55	0.47
3:C:428:LEU:O	3:C:431:GLN:HB2	2.15	0.47
3:C:1019:ASP:O	3:C:1020:LEU:HG	2.15	0.47
3:C:891:TYR:O	3:C:894:PHE:HB3	2.14	0.47
1:A:405:ASN:ND2	1:A:407:VAL:N	2.53	0.47
3:C:734:ILE:HG22	3:C:735:LEU:N	2.28	0.47
1:A:392:ALA:O	1:A:396:LYS:HG3	2.14	0.47
1:A:205:VAL:O	1:A:209:VAL:HG23	2.15	0.47
3:C:824:ASP:O	3:C:825:VAL:C	2.53	0.47
3:C:257:VAL:O	3:C:260:CYS:N	2.47	0.47
1:A:143:HIS:C	1:A:145:VAL:H	2.18	0.47
3:C:621:ASN:HB2	3:C:624:THR:HB	1.96	0.47
3:C:724:PRO:O	3:C:727:LEU:HG	2.15	0.47
3:C:861:ILE:HG21	3:C:880:LEU:HB2	1.96	0.47
3:C:375:VAL:O	3:C:379:LEU:CA	2.61	0.47
3:C:38:SER:H	3:C:78:LYS:NZ	2.12	0.47
3:C:385:GLU:HA	3:C:391:LYS:CE	2.34	0.47
3:C:211:ILE:N	3:C:211:ILE:HD12	2.29	0.47
3:C:281:ARG:HE	3:C:284:LYS:HG2	1.79	0.47
3:C:285:GLU:O	3:C:287:TYR:N	2.47	0.47
1:A:365:TYR:CD2	1:A:407:VAL:HG21	2.49	0.47
3:C:1127:LEU:HD21	3:C:1145:LEU:HD13	1.96	0.47
3:C:148:VAL:O	3:C:149:SER:C	2.53	0.47
3:C:465:LEU:CB	3:C:468:ALA:HB2	2.44	0.47
1:A:548:GLN:HA	1:A:581:LEU:HD22	1.96	0.47
3:C:375:VAL:HG13	3:C:379:LEU:HD12	1.96	0.47
1:A:445:LEU:HG	1:A:487:MET:SD	2.55	0.47
1:A:672:LEU:N	1:A:672:LEU:CD1	2.60	0.47
3:C:590:ILE:HD11	3:C:624:THR:HG23	1.97	0.47
1:A:708:LEU:HD12	2:B:106:TYR:CD1	2.49	0.47
3:C:218:LEU:HD13	3:C:234:ILE:CD1	2.44	0.47
1:A:221:GLY:N	3:C:1171:GLU:OE2	2.48	0.47
3:C:925:LEU:O	3:C:926:LYS:C	2.53	0.47
3:C:235:ALA:O	3:C:238:SER:HB2	2.14	0.47
3:C:199:LEU:O	3:C:202:LEU:HB3	2.15	0.47
1:A:560:ARG:HG2	1:A:560:ARG:HH11	1.80	0.47
3:C:1179:ALA:O	3:C:1180:VAL:C	2.52	0.47
3:C:819:GLY:O	3:C:823:GLN:HG3	2.15	0.47
3:C:667:LYS:HE3	3:C:700:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:532:PHE:CE2	3:C:534:LYS:HB2	2.50	0.47
3:C:126:LEU:C	3:C:128:ALA:H	2.18	0.47
3:C:769:ASN:O	3:C:770:LEU:CD1	2.62	0.47
3:C:825:VAL:HG23	3:C:860:VAL:CG1	2.44	0.47
3:C:287:TYR:CB	3:C:288:PRO:HD3	2.28	0.47
3:C:1199:GLN:HG3	3:C:1201:GLN:N	2.31	0.47
1:A:694:GLU:O	1:A:698:THR:HG23	2.15	0.47
3:C:1157:VAL:HB	3:C:1166:PHE:HE2	1.79	0.47
3:C:1196:SER:O	3:C:1198:PHE:N	2.48	0.47
3:C:1158:LYS:C	3:C:1160:ASN:H	2.17	0.47
3:C:982:ARG:HH21	3:C:1018:PRO:CB	2.23	0.46
3:C:95:MET:HB2	3:C:96:LEU:HD12	1.97	0.46
3:C:590:ILE:HD13	3:C:628:THR:CG2	2.45	0.46
3:C:618:ARG:CG	3:C:624:THR:HG21	2.45	0.46
3:C:405:THR:O	3:C:407:PRO:CD	2.63	0.46
3:C:1157:VAL:HB	3:C:1166:PHE:CE2	2.50	0.46
3:C:1152:THR:C	3:C:1154:THR:H	2.18	0.46
3:C:200:GLY:O	3:C:203:VAL:HG22	2.15	0.46
3:C:253:ILE:HG21	3:C:286:VAL:HG11	1.96	0.46
1:A:171:LEU:CD1	1:A:175:LEU:HD13	2.46	0.46
3:C:432:VAL:HG11	3:C:436:VAL:HG23	1.97	0.46
1:A:167:TRP:O	1:A:170:CYS:N	2.48	0.46
1:A:408:THR:HB	1:A:414:SER:HA	1.96	0.46
1:A:159:ILE:HA	1:A:159:ILE:HD12	1.78	0.46
3:C:576:LEU:HD22	3:C:593:MET:HG2	1.98	0.46
3:C:560:ASP:OD1	3:C:562:THR:HG23	2.15	0.46
3:C:562:THR:N	3:C:563:PRO:HD2	2.30	0.46
1:A:612:GLN:HB3	1:A:619:TYR:CE1	2.51	0.46
3:C:1138:VAL:O	3:C:1142:LEU:N	2.48	0.46
1:A:613:TYR:CE2	1:A:648:LEU:HD21	2.51	0.46
1:A:142:ARG:HH22	1:A:148:GLU:HG2	1.80	0.46
3:C:384:LYS:C	3:C:385:GLU:HG3	2.36	0.46
3:C:970:LEU:C	3:C:972:GLY:H	2.18	0.46
3:C:654:ILE:O	3:C:657:SER:HB3	2.16	0.46
3:C:6:TYR:N	3:C:6:TYR:CD2	2.81	0.46
3:C:1205:ASN:HB2	3:C:1206:PRO:CD	2.46	0.46
3:C:1036:ASN:ND2	3:C:1036:ASN:H	2.14	0.46
3:C:821:PHE:O	3:C:823:GLN:N	2.44	0.46
3:C:1008:ILE:CG2	3:C:1009:GLY:N	2.78	0.46
1:A:35:GLN:O	1:A:36:SER:C	2.53	0.46
1:A:104:LEU:HD21	1:A:173:ARG:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1202:ILE:O	3:C:1206:PRO:HD2	2.16	0.46
3:C:172:PHE:O	3:C:176:ILE:HG12	2.15	0.46
3:C:469:LEU:HD13	3:C:476:LEU:HD13	1.96	0.46
3:C:206:CYS:CB	3:C:207:PHE:CA	2.94	0.46
3:C:261:ASN:O	3:C:262:VAL:C	2.53	0.46
3:C:1183:LEU:O	3:C:1186:ILE:CG2	2.63	0.46
3:C:131:CYS:O	3:C:134:ILE:HB	2.16	0.46
3:C:1117:TYR:C	3:C:1117:TYR:HD2	2.18	0.46
3:C:1123:THR:HA	3:C:1126:MET:HB2	1.97	0.46
1:A:268:LEU:O	1:A:271:GLN:HB2	2.16	0.46
3:C:186:SER:O	3:C:192:ARG:HD2	2.16	0.46
1:A:438:GLU:O	1:A:438:GLU:OE1	2.33	0.46
1:A:309:LEU:HB3	1:A:318:LEU:HD21	1.98	0.46
3:C:218:LEU:HD23	3:C:230:TYR:CD1	2.47	0.46
1:A:308:ASN:C	1:A:310:LEU:H	2.18	0.46
3:C:1051:HIS:O	3:C:1054:ASN:N	2.49	0.46
3:C:171:ASN:OD1	3:C:171:ASN:N	2.49	0.46
1:A:398:CYS:O	1:A:402:ILE:HG13	2.15	0.46
3:C:1015:LEU:CD1	3:C:1022:VAL:HG12	2.41	0.46
3:C:1036:ASN:HD22	3:C:1036:ASN:H	1.62	0.46
3:C:676:ILE:H	3:C:676:ILE:HG13	1.36	0.46
3:C:852:SER:HB2	3:C:887:ASN:HD22	1.81	0.46
1:A:553:ALA:HB2	1:A:629:GLN:HB2	1.97	0.46
2:B:74:VAL:HA	2:B:104:GLN:NE2	2.30	0.46
3:C:442:GLN:O	3:C:445:GLU:HB2	2.15	0.46
3:C:1181:ALA:O	3:C:1183:LEU:N	2.49	0.46
1:A:171:LEU:CG	1:A:175:LEU:HD13	2.46	0.46
3:C:813:GLU:HA	3:C:813:GLU:OE2	2.16	0.46
1:A:533:ASP:HB3	2:B:26:LYS:HG2	1.97	0.46
3:C:505:LEU:HD23	3:C:513:PHE:CE2	2.51	0.46
3:C:247:GLU:HG3	3:C:248:TYR:CD1	2.51	0.45
3:C:1023:ARG:HD3	3:C:1055:GLU:OE2	2.15	0.45
2:B:40:ASP:HB3	2:B:49:ILE:HD11	1.98	0.45
1:A:582:TYR:HA	1:A:585:SER:HG	1.80	0.45
3:C:35:GLN:O	3:C:36:LYS:CB	2.65	0.45
3:C:601:GLY:HA2	3:C:604:LEU:HD22	1.97	0.45
3:C:173:HIS:HB3	3:C:210:LEU:HD13	1.98	0.45
3:C:208:VAL:HA	3:C:244:ARG:HH22	1.81	0.45
3:C:1147:GLU:HB3	3:C:1148:PRO:CD	2.38	0.45
3:C:686:THR:O	3:C:689:MET:N	2.35	0.45
1:A:624:LEU:O	1:A:626:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:189:LEU:HD13	3:C:192:ARG:CZ	2.47	0.45
3:C:205:SER:O	3:C:206:CYS:CB	2.63	0.45
3:C:249:LEU:HB2	3:C:281:ARG:NH2	2.31	0.45
3:C:579:ALA:HA	3:C:586:LYS:HE2	1.99	0.45
1:A:21:TRP:O	1:A:21:TRP:CD2	2.69	0.45
1:A:655:ALA:C	1:A:657:VAL:H	2.20	0.45
3:C:168:LEU:O	3:C:169:LEU:HB2	2.16	0.45
1:A:400:ARG:HH11	1:A:400:ARG:HG2	1.81	0.45
3:C:985:VAL:HG13	3:C:986:VAL:N	2.31	0.45
3:C:1037:LYS:N	3:C:1038:PRO:HD3	2.31	0.45
3:C:933:TRP:HE1	3:C:937:LEU:HD11	1.81	0.45
1:A:145:VAL:O	1:A:146:ARG:CG	2.59	0.45
3:C:1199:GLN:HG3	3:C:1201:GLN:H	1.81	0.45
3:C:1208:LEU:HD22	3:C:1208:LEU:N	2.31	0.45
3:C:813:GLU:OE2	3:C:815:PRO:HG2	2.16	0.45
3:C:218:LEU:O	3:C:222:ASP:OD2	2.35	0.45
1:A:431:LYS:C	1:A:431:LYS:HD2	2.37	0.45
1:A:145:VAL:C	1:A:146:ARG:HG3	2.34	0.45
3:C:1034:ALA:O	3:C:1038:PRO:HG3	2.17	0.45
3:C:562:THR:OG1	3:C:563:PRO:CD	2.65	0.45
3:C:545:GLN:O	3:C:549:VAL:HG23	2.17	0.45
3:C:1199:GLN:CG	3:C:1202:ILE:H	2.29	0.45
1:A:682:ASN:HD21	1:A:684:ASN:HB3	1.82	0.45
3:C:576:LEU:CD2	3:C:593:MET:HG2	2.47	0.45
3:C:851:LEU:C	3:C:853:GLY:N	2.68	0.45
3:C:1132:THR:HG22	3:C:1133:LEU:N	2.32	0.45
3:C:433:PRO:HB2	3:C:437:LYS:HE3	1.99	0.45
2:B:70:VAL:HG12	2:B:71:ALA:N	2.32	0.45
3:C:186:SER:O	3:C:192:ARG:NH1	2.27	0.45
1:A:171:LEU:HD12	1:A:175:LEU:CD1	2.47	0.45
3:C:485:ASN:O	3:C:486:ASP:CB	2.34	0.45
1:A:682:ASN:ND2	1:A:682:ASN:C	2.69	0.45
1:A:226:VAL:HG23	1:A:227:TYR:H	1.81	0.45
3:C:958:LEU:HD23	3:C:958:LEU:HA	1.72	0.45
3:C:169:LEU:N	3:C:169:LEU:HD12	2.32	0.45
3:C:514:HIS:HE1	3:C:549:VAL:O	2.00	0.45
1:A:168:ARG:O	1:A:172:PHE:HD1	2.00	0.45
1:A:200:LEU:O	1:A:204:VAL:HG23	2.17	0.45
2:B:79:PHE:HE1	2:B:101:TRP:CZ3	2.35	0.45
1:A:632:MET:C	1:A:634:ILE:N	2.69	0.45
3:C:604:LEU:O	3:C:605:GLY:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:PHE:CD2	1:A:584:LEU:HD11	2.52	0.45
1:A:585:SER:CB	2:B:29:ALA:HA	2.47	0.45
1:A:89:TYR:CZ	1:A:162:LEU:HG	2.52	0.45
3:C:616:LEU:HD23	3:C:647:VAL:CB	2.46	0.45
1:A:706:ARG:HG2	1:A:741:PHE:CE1	2.52	0.45
3:C:588:ARG:HG3	3:C:588:ARG:HH11	1.81	0.45
3:C:982:ARG:HH22	3:C:1018:PRO:HB2	1.75	0.44
1:A:600:LEU:HA	1:A:681:VAL:O	2.17	0.44
3:C:1199:GLN:HG3	3:C:1202:ILE:H	1.83	0.44
3:C:932:ILE:HB	3:C:958:LEU:HD11	1.99	0.44
1:A:595:LYS:HG3	1:A:596:ASN:H	1.82	0.44
3:C:920:ALA:O	3:C:921:SER:OG	2.35	0.44
3:C:248:TYR:N	3:C:249:LEU:HD13	2.32	0.44
3:C:253:ILE:H	3:C:253:ILE:HD12	1.83	0.44
3:C:439:LEU:O	3:C:442:GLN:N	2.50	0.44
1:A:582:TYR:HA	1:A:585:SER:OG	2.18	0.44
3:C:818:VAL:C	3:C:820:GLN:N	2.70	0.44
3:C:858:LYS:HD3	3:C:894:PHE:CE2	2.52	0.44
3:C:177:LEU:HD11	3:C:181:LEU:HD21	1.98	0.44
1:A:171:LEU:HG	1:A:175:LEU:HD13	1.99	0.44
1:A:89:TYR:O	1:A:92:LEU:N	2.49	0.44
1:A:351:ILE:CG2	1:A:407:VAL:HG23	2.48	0.44
1:A:147:ARG:HG3	1:A:148:GLU:H	1.79	0.44
3:C:33:GLU:C	3:C:35:GLN:N	2.67	0.44
1:A:657:VAL:HA	1:A:660:VAL:CG2	2.47	0.44
3:C:799:ILE:CG2	3:C:837:LEU:HD11	2.47	0.44
1:A:472:ARG:NH1	1:A:484:GLU:OE2	2.49	0.44
3:C:555:GLN:HE21	3:C:555:GLN:HB2	1.61	0.44
1:A:500:THR:HG22	1:A:501:SER:N	2.32	0.44
2:B:21:ARG:HG3	2:B:21:ARG:HH11	1.82	0.44
3:C:1049:LEU:O	3:C:1050:PRO:C	2.55	0.44
1:A:676:ASN:HB3	1:A:681:VAL:CG2	2.47	0.44
3:C:616:LEU:O	3:C:619:LEU:HB3	2.16	0.44
1:A:717:ILE:HG12	3:C:25:MET:HE1	2.00	0.44
3:C:1008:ILE:HG23	3:C:1044:LEU:HD11	1.99	0.44
3:C:405:THR:O	3:C:406:ARG:C	2.55	0.44
3:C:1083:LYS:HD3	3:C:1083:LYS:O	2.17	0.44
3:C:251:LYS:O	3:C:254:PRO:HG2	2.18	0.44
1:A:649:VAL:CG2	1:A:671:TYR:HB2	2.48	0.44
3:C:1197:GLU:O	3:C:1198:PHE:C	2.54	0.44
3:C:31:MET:HB2	3:C:71:CYS:SG	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:MET:O	3:C:55:LYS:HB3	2.18	0.44
3:C:225:SER:O	3:C:226:THR:C	2.56	0.44
1:A:175:LEU:CG	1:A:208:TYR:CZ	3.01	0.44
1:A:173:ARG:CB	1:A:174:PRO:CD	2.90	0.44
1:A:138:ALA:O	1:A:141:ASN:HB2	2.17	0.44
1:A:588:GLU:OE2	2:B:26:LYS:HD3	2.17	0.44
1:A:724:LEU:HD22	1:A:728:GLN:HB3	1.99	0.44
3:C:1013:LYS:HB2	3:C:1047:THR:CG2	2.48	0.44
1:A:21:TRP:O	1:A:25:ARG:HB2	2.18	0.44
3:C:615:PHE:O	3:C:616:LEU:C	2.55	0.44
3:C:573:ILE:HG23	3:C:593:MET:HE3	2.00	0.44
3:C:786:GLN:HE21	3:C:786:GLN:HB2	1.63	0.44
1:A:687:MET:HB2	1:A:690:GLU:HB2	1.98	0.44
3:C:253:ILE:HD11	3:C:281:ARG:NH2	2.32	0.44
3:C:283:PRO:HD2	3:C:284:LYS:NZ	2.33	0.44
1:A:178:GLN:O	1:A:179:VAL:C	2.56	0.44
3:C:899:ILE:CG2	3:C:935:LEU:HD11	2.44	0.44
3:C:1159:ALA:C	3:C:1161:SER:H	2.20	0.44
1:A:338:LEU:HD12	1:A:338:LEU:HA	1.83	0.44
3:C:601:GLY:HA2	3:C:604:LEU:CD2	2.48	0.44
3:C:830:SER:O	3:C:831:THR:C	2.54	0.44
3:C:350:ARG:HE	3:C:386:ARG:NH2	2.15	0.44
3:C:385:GLU:HA	3:C:391:LYS:HG3	2.00	0.44
3:C:429:GLN:O	3:C:431:GLN:N	2.51	0.44
3:C:294:ILE:HG23	3:C:353:ALA:CB	2.48	0.44
3:C:406:ARG:NH1	3:C:460:GLU:OE2	2.50	0.44
1:A:166:THR:O	1:A:169:ASP:HB2	2.17	0.44
3:C:824:ASP:C	3:C:826:LYS:N	2.70	0.44
3:C:181:LEU:N	3:C:182:PRO:HD2	2.32	0.44
1:A:442:GLU:O	1:A:446:ASN:ND2	2.51	0.44
3:C:1015:LEU:C	3:C:1018:PRO:HD2	2.39	0.44
3:C:85:GLU:HG3	3:C:133:LYS:CE	2.33	0.44
3:C:686:THR:O	3:C:688:ALA:N	2.51	0.44
3:C:697:LEU:HB2	3:C:698:PRO:HD3	2.00	0.44
1:A:715:VAL:HG12	1:A:716:ARG:N	2.32	0.44
1:A:517:ASN:ND2	1:A:536:ILE:O	2.51	0.44
1:A:526:ASN:O	1:A:527:SER:HB3	2.17	0.44
2:B:83:CYS:HA	2:B:86:ARG:NH1	2.33	0.44
3:C:1198:PHE:C	3:C:1198:PHE:CD1	2.62	0.44
3:C:636:ALA:O	3:C:637:GLY:C	2.55	0.44
1:A:625:THR:HG22	1:A:625:THR:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ASP:O	1:A:444:THR:C	2.56	0.43
3:C:477:VAL:HB	3:C:478:PRO:HD3	2.00	0.43
1:A:117:LYS:HD3	1:A:117:LYS:C	2.37	0.43
3:C:148:VAL:O	3:C:150:VAL:N	2.51	0.43
3:C:228:ARG:O	3:C:228:ARG:CG	2.65	0.43
3:C:227:THR:CG2	3:C:229:THR:OG1	2.66	0.43
3:C:386:ARG:HD3	3:C:390:VAL:CG1	2.48	0.43
3:C:855:LEU:CD1	3:C:858:LYS:HD2	2.46	0.43
3:C:771:GLY:N	3:C:774:ASP:HB2	2.33	0.43
3:C:785:SER:O	3:C:786:GLN:HG3	2.17	0.43
3:C:164:ARG:HG3	3:C:164:ARG:HH11	1.83	0.43
1:A:651:GLU:HA	1:A:669:LYS:NZ	2.27	0.43
3:C:170:VAL:HA	3:C:173:HIS:NE2	2.33	0.43
1:A:178:GLN:C	1:A:180:THR:N	2.72	0.43
3:C:1032:SER:O	3:C:1036:ASN:ND2	2.52	0.43
3:C:97:SER:CB	3:C:102:LEU:HD23	2.47	0.43
3:C:733:SER:O	3:C:737:GLU:HB2	2.18	0.43
3:C:630:LYS:HG3	3:C:631:ALA:N	2.33	0.43
3:C:835:ARG:HE	3:C:835:ARG:HB2	1.54	0.43
3:C:386:ARG:HH11	3:C:386:ARG:CG	2.31	0.43
3:C:976:SER:O	3:C:977:GLY:O	2.36	0.43
3:C:88:VAL:HG13	3:C:134:ILE:HG12	2.01	0.43
1:A:95:PHE:CD2	1:A:96:LEU:HD12	2.36	0.43
2:B:36:ASP:C	2:B:36:ASP:OD2	2.57	0.43
3:C:218:LEU:CD2	3:C:230:TYR:HD1	2.29	0.43
1:A:356:GLU:O	1:A:357:ALA:C	2.57	0.43
2:B:82:HIS:HB3	2:B:86:ARG:HH21	1.83	0.43
1:A:425:CYS:O	1:A:429:LEU:HD22	2.18	0.43
3:C:423:THR:HA	3:C:424:PRO:HD3	1.81	0.43
3:C:423:THR:CG2	3:C:424:PRO:N	2.82	0.43
3:C:551:ARG:NH1	3:C:553:LEU:CB	2.71	0.43
1:A:309:LEU:HB3	1:A:318:LEU:CD2	2.49	0.43
3:C:100:GLU:C	3:C:102:LEU:N	2.72	0.43
3:C:710:GLN:HB3	3:C:751:ALA:CA	2.46	0.43
1:A:510:ILE:HA	1:A:510:ILE:HD13	1.80	0.43
1:A:447:GLN:O	1:A:450:VAL:HB	2.18	0.43
3:C:103:ARG:O	3:C:107:SER:HB2	2.19	0.43
1:A:597:ARG:NH1	1:A:597:ARG:CB	2.74	0.43
3:C:979:SER:OG	3:C:1020:LEU:HD21	2.18	0.43
1:A:631:LYS:HB3	1:A:634:ILE:HG22	2.01	0.43
3:C:826:LYS:O	3:C:830:SER:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:346:SER:O	3:C:348:LYS:N	2.51	0.43
3:C:1203:SER:OG	3:C:1204:SER:N	2.51	0.43
3:C:673:ALA:C	3:C:675:ASP:N	2.72	0.43
1:A:376:TYR:HA	1:A:379:LEU:HB3	2.01	0.43
1:A:720:MET:HG2	3:C:22:PHE:CE2	2.54	0.43
1:A:107:GLY:CA	1:A:110:LEU:HD12	2.44	0.43
1:A:716:ARG:O	3:C:25:MET:HG3	2.18	0.43
1:A:140:LEU:HD22	1:A:140:LEU:HA	1.80	0.43
3:C:769:ASN:HA	3:C:774:ASP:OD2	2.19	0.43
3:C:355:LYS:O	3:C:358:ASP:HB3	2.18	0.43
1:A:768:LYS:O	1:A:769:ASP:HB2	2.18	0.43
3:C:246:GLY:O	3:C:249:LEU:CD1	2.67	0.43
3:C:727:LEU:O	3:C:730:ILE:N	2.48	0.43
3:C:37:ASP:OD1	3:C:39:ILE:HD13	2.17	0.43
3:C:659:LEU:HD13	3:C:700:LEU:HD11	2.01	0.43
3:C:1141:ARG:NH1	3:C:1144:ARG:NH2	2.67	0.43
1:A:212:GLY:C	1:A:223:THR:HG21	2.38	0.43
3:C:146:GLU:N	3:C:146:GLU:CD	2.72	0.43
3:C:551:ARG:HH12	3:C:553:LEU:HB2	1.79	0.43
3:C:1194:LEU:CD1	3:C:1194:LEU:C	2.87	0.43
1:A:179:VAL:O	1:A:183:VAL:HG23	2.19	0.43
2:B:84:ILE:HG23	2:B:85:SER:N	2.34	0.43
3:C:913:LEU:HD23	3:C:917:ILE:HG13	1.99	0.43
1:A:472:ARG:O	1:A:473:LEU:C	2.57	0.43
3:C:544:GLN:HG3	3:C:595:GLN:CB	2.49	0.43
1:A:480:SER:C	1:A:482:ASP:H	2.22	0.43
3:C:389:ASN:O	3:C:392:ALA:HB3	2.18	0.43
1:A:625:THR:CB	1:A:632:MET:CG	2.97	0.43
1:A:440:GLU:C	1:A:444:THR:OG1	2.55	0.43
3:C:481:ILE:HD11	3:C:520:LEU:CD2	2.36	0.43
1:A:708:LEU:HD22	2:B:81:PHE:CZ	2.54	0.43
1:A:734:LEU:O	1:A:735:THR:C	2.57	0.43
3:C:1030:PHE:HE1	3:C:1041:ILE:HG23	1.83	0.43
3:C:548:LYS:HA	3:C:551:ARG:HG2	1.98	0.42
3:C:547:VAL:HG13	3:C:600:LEU:HD21	2.01	0.42
1:A:593:CYS:CB	2:B:20:LYS:H	2.32	0.42
3:C:260:CYS:HA	3:C:267:LEU:HD22	2.00	0.42
3:C:268:ARG:O	3:C:272:ILE:HG12	2.18	0.42
3:C:283:PRO:HD2	3:C:284:LYS:HZ1	1.84	0.42
3:C:1183:LEU:HA	3:C:1183:LEU:HD23	1.84	0.42
1:A:162:LEU:O	1:A:162:LEU:HD22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:TYR:CD1	1:A:157:TYR:N	2.86	0.42
1:A:346:GLN:HG2	1:A:376:TYR:OH	2.19	0.42
1:A:716:ARG:NE	1:A:736:GLN:HE22	2.17	0.42
3:C:56:LEU:C	3:C:58:GLU:N	2.73	0.42
3:C:359:ALA:O	3:C:360:VAL:C	2.57	0.42
1:A:280:GLU:HA	1:A:283:GLN:HE21	1.84	0.42
3:C:274:ALA:O	3:C:278:PHE:HD1	2.02	0.42
1:A:496:GLY:H	1:A:740:ARG:NH2	2.17	0.42
1:A:516:LEU:HD11	1:A:569:TYR:HE1	1.84	0.42
1:A:445:LEU:HD12	1:A:445:LEU:HA	1.88	0.42
1:A:171:LEU:CG	1:A:175:LEU:HD22	2.41	0.42
3:C:520:LEU:O	3:C:523:PRO:HG2	2.19	0.42
3:C:508:HIS:O	3:C:509:SER:C	2.58	0.42
3:C:461:LEU:O	3:C:461:LEU:HD22	2.19	0.42
3:C:826:LYS:CE	3:C:826:LYS:HA	2.47	0.42
3:C:825:VAL:HG21	3:C:860:VAL:HG22	1.97	0.42
3:C:89:ASP:OD1	3:C:137:ARG:NH1	2.51	0.42
3:C:1008:ILE:CG2	3:C:1009:GLY:H	2.30	0.42
3:C:127:ALA:HA	3:C:130:VAL:HB	2.00	0.42
2:B:37:ILE:HG12	2:B:37:ILE:O	2.20	0.42
3:C:209:ASP:C	3:C:212:GLU:OE1	2.57	0.42
3:C:387:GLU:O	3:C:388:GLU:HG2	2.19	0.42
3:C:625:ARG:CG	3:C:625:ARG:HH11	2.32	0.42
3:C:813:GLU:CD	3:C:814:GLY:N	2.70	0.42
3:C:110:LEU:HD12	3:C:110:LEU:HA	1.80	0.42
3:C:730:ILE:O	3:C:730:ILE:HG22	2.19	0.42
3:C:686:THR:C	3:C:688:ALA:N	2.70	0.42
3:C:148:VAL:HG12	3:C:152:LEU:HG	2.01	0.42
3:C:275:PHE:HE2	3:C:279:VAL:HG21	1.85	0.42
3:C:1109:VAL:HG13	3:C:1123:THR:CG2	2.50	0.42
3:C:731:SER:O	3:C:732:GLY:O	2.36	0.42
3:C:602:ASP:HB3	3:C:640:LEU:HD13	2.01	0.42
3:C:177:LEU:HG	3:C:181:LEU:HD11	2.01	0.42
3:C:1177:MET:O	3:C:1178:ARG:C	2.57	0.42
1:A:147:ARG:C	1:A:149:CYS:H	2.21	0.42
1:A:117:LYS:NZ	1:A:121:GLN:HG3	2.35	0.42
1:A:725:LYS:O	1:A:728:GLN:HB2	2.19	0.42
1:A:270:GLU:HA	1:A:273:ARG:HB2	2.01	0.42
1:A:195:THR:HG21	3:C:1028:VAL:HG13	2.02	0.42
1:A:663:LYS:HB3	1:A:664:PRO:HD2	2.01	0.42
3:C:599:ASN:C	3:C:600:LEU:HD23	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1186:ILE:O	3:C:1187:PRO:C	2.58	0.42
3:C:1038:PRO:C	3:C:1040:LEU:N	2.72	0.42
3:C:857:LEU:O	3:C:858:LYS:C	2.57	0.42
3:C:168:LEU:CG	3:C:169:LEU:HD12	2.49	0.42
1:A:469:LEU:HA	1:A:472:ARG:CZ	2.50	0.42
1:A:556:SER:C	1:A:558:LEU:H	2.23	0.42
1:A:667:LEU:CB	1:A:669:LYS:HE3	2.48	0.42
3:C:174:PRO:HB3	3:C:210:LEU:HD21	2.00	0.42
3:C:252:ILE:H	3:C:252:ILE:HG12	1.73	0.42
3:C:347:TRP:C	3:C:349:VAL:N	2.73	0.42
3:C:45:SER:O	3:C:49:VAL:HG23	2.20	0.42
1:A:475:HIS:HE1	1:A:585:SER:HA	1.83	0.42
3:C:814:GLY:N	3:C:815:PRO:CD	2.72	0.42
1:A:25:ARG:HD3	1:A:95:PHE:HD1	1.84	0.42
3:C:275:PHE:C	3:C:275:PHE:CD2	2.93	0.42
1:A:522:LYS:O	1:A:524:LEU:N	2.53	0.42
3:C:637:GLY:H	3:C:680:ASN:HD22	1.67	0.42
1:A:651:GLU:CB	1:A:669:LYS:HZ2	2.33	0.42
1:A:475:HIS:ND1	1:A:586:LYS:HD3	2.34	0.42
3:C:104:ASP:O	3:C:108:ILE:HG12	2.20	0.42
3:C:441:LYS:HB2	3:C:441:LYS:HZ3	1.85	0.42
3:C:781:GLY:O	3:C:783:VAL:N	2.52	0.42
1:A:646:LYS:CG	1:A:646:LYS:O	2.67	0.42
3:C:914:LYS:HE2	3:C:914:LYS:HB3	1.90	0.42
1:A:583:GLN:NE2	1:A:583:GLN:H	2.12	0.42
3:C:987:THR:O	3:C:990:LYS:HB3	2.19	0.42
1:A:195:THR:CG2	3:C:1028:VAL:HG13	2.49	0.42
3:C:536:THR:O	3:C:540:LEU:HD12	2.20	0.42
3:C:1160:ASN:O	3:C:1160:ASN:CG	2.58	0.42
1:A:128:PHE:CE1	3:C:1073:HIS:HB2	2.55	0.42
3:C:388:GLU:HA	3:C:388:GLU:OE2	2.18	0.42
3:C:391:LYS:HG2	3:C:395:PHE:HE1	1.84	0.42
3:C:432:VAL:CG1	3:C:435:ILE:HB	2.36	0.42
3:C:92:CYS:HA	3:C:95:MET:HG3	2.02	0.42
3:C:1127:LEU:HD23	3:C:1127:LEU:HA	1.89	0.42
3:C:1079:LEU:O	3:C:1083:LYS:HB2	2.20	0.42
1:A:671:TYR:OH	1:A:674:TYR:HB2	2.19	0.42
3:C:173:HIS:N	3:C:174:PRO:HD2	2.35	0.41
3:C:1015:LEU:C	3:C:1018:PRO:CD	2.88	0.41
3:C:611:THR:CA	3:C:614:ILE:HG12	2.45	0.41
3:C:115:GLY:HA2	3:C:164:ARG:HD3	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:GLU:OE1	3:C:1174:ARG:HD2	2.19	0.41
3:C:515:PRO:HG2	3:C:516:HIS:CD2	2.55	0.41
3:C:64:VAL:O	3:C:65:GLN:C	2.58	0.41
3:C:551:ARG:CD	3:C:551:ARG:C	2.84	0.41
3:C:368:LEU:O	3:C:371:PHE:HB2	2.20	0.41
3:C:581:ILE:CD1	3:C:586:LYS:HE3	2.49	0.41
3:C:540:LEU:CD2	3:C:589:ALA:HA	2.51	0.41
3:C:115:GLY:HA2	3:C:164:ARG:CD	2.50	0.41
3:C:399:LEU:O	3:C:403:LYS:HG3	2.20	0.41
3:C:1205:ASN:O	3:C:1207:GLU:N	2.53	0.41
1:A:476:GLN:O	1:A:477:ASN:HB2	2.20	0.41
1:A:160:TYR:O	1:A:163:ALA:N	2.53	0.41
1:A:375:LYS:HD3	1:A:376:TYR:CE1	2.55	0.41
3:C:237:ILE:HG13	3:C:237:ILE:H	1.72	0.41
3:C:914:LYS:HG2	3:C:954:CYS:SG	2.59	0.41
3:C:1161:SER:HB3	3:C:1165:GLU:HB3	2.02	0.41
3:C:1053:TYR:O	3:C:1056:THR:HB	2.20	0.41
3:C:1000:ILE:N	3:C:1000:ILE:HD13	2.36	0.41
1:A:468:MET:HB3	1:A:468:MET:HE2	1.94	0.41
3:C:1186:ILE:O	3:C:1190:GLU:OE1	2.39	0.41
3:C:942:CYS:CB	3:C:948:ARG:HD2	2.50	0.41
1:A:673:GLY:O	1:A:674:TYR:O	2.39	0.41
1:A:621:VAL:CG2	1:A:668:ILE:HD11	2.45	0.41
3:C:302:THR:O	3:C:303:TYR:CB	2.69	0.41
3:C:1184:LEU:HA	3:C:1190:GLU:HG3	2.03	0.41
3:C:967:LEU:HD22	3:C:967:LEU:HA	1.79	0.41
3:C:895:VAL:O	3:C:896:LEU:C	2.58	0.41
1:A:417:SER:N	1:A:418:PRO:CD	2.83	0.41
2:B:73:GLY:C	2:B:75:CYS:N	2.74	0.41
3:C:926:LYS:N	3:C:927:PRO:CD	2.83	0.41
3:C:693:VAL:O	3:C:694:LEU:C	2.59	0.41
1:A:265:ALA:O	1:A:269:GLU:HG3	2.20	0.41
1:A:632:MET:O	1:A:633:ASP:C	2.59	0.41
3:C:281:ARG:HH21	3:C:284:LYS:CB	2.33	0.41
3:C:1017:ASP:N	3:C:1018:PRO:HD2	2.34	0.41
3:C:480:ILE:HG22	3:C:481:ILE:N	2.34	0.41
1:A:344:HIS:CD2	1:A:348:LEU:HD11	2.55	0.41
3:C:936:LEU:CD1	3:C:954:CYS:HB3	2.50	0.41
3:C:469:LEU:HD13	3:C:476:LEU:CD1	2.50	0.41
1:A:354:CYS:CB	1:A:358:ALA:HB2	2.51	0.41
2:B:92:GLN:HG2	3:C:19:ASP:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:433:PRO:O	3:C:437:LYS:HG3	2.20	0.41
3:C:706:MET:O	3:C:709:SER:HB2	2.20	0.41
1:A:97:LYS:NZ	1:A:97:LYS:HB2	2.36	0.41
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.85	0.41
2:B:49:ILE:CD1	2:B:50:MET:N	2.82	0.41
1:A:474:VAL:HG12	1:A:475:HIS:H	1.77	0.41
3:C:889:PRO:HB3	3:C:928:TYR:OH	2.21	0.41
3:C:743:ARG:CZ	3:C:782:PRO:HG2	2.51	0.41
1:A:337:LYS:HB3	1:A:337:LYS:HE2	1.89	0.41
2:B:28:ASN:HD22	2:B:28:ASN:N	2.17	0.41
3:C:661:LYS:O	3:C:662:ASN:C	2.58	0.41
2:B:77:HIS:CD2	2:B:96:LEU:HD23	2.56	0.41
3:C:650:GLU:O	3:C:653:PRO:HG2	2.20	0.41
1:A:29:GLN:HB2	1:A:29:GLN:HE21	1.61	0.41
1:A:657:VAL:HA	1:A:660:VAL:HG23	2.03	0.41
1:A:694:GLU:O	1:A:698:THR:CG2	2.68	0.41
3:C:990:LYS:C	3:C:992:THR:H	2.24	0.41
3:C:1090:TYR:O	3:C:1093:LEU:HB2	2.21	0.41
3:C:65:GLN:O	3:C:69:VAL:HG23	2.20	0.41
1:A:589:LEU:HD23	1:A:610:LEU:HD12	2.03	0.41
3:C:268:ARG:HG3	3:C:269:GLU:N	2.35	0.41
3:C:267:LEU:HD23	3:C:270:TYR:CE1	2.56	0.41
3:C:386:ARG:CG	3:C:386:ARG:NH1	2.82	0.41
3:C:1020:LEU:HB2	3:C:1021:ASN:H	1.66	0.41
3:C:1183:LEU:O	3:C:1186:ILE:HG22	2.19	0.41
3:C:1143:ASP:OD2	3:C:1193:PRO:HB3	2.21	0.41
1:A:445:LEU:O	1:A:448:VAL:HB	2.21	0.41
1:A:714:ILE:HD13	1:A:733:VAL:CG2	2.51	0.41
3:C:1141:ARG:HH11	3:C:1144:ARG:NH2	2.18	0.41
3:C:1079:LEU:C	3:C:1079:LEU:CD2	2.89	0.41
3:C:710:GLN:CB	3:C:751:ALA:HA	2.47	0.41
3:C:126:LEU:C	3:C:128:ALA:N	2.74	0.41
1:A:580:TRP:N	1:A:580:TRP:CD1	2.88	0.41
3:C:602:ASP:OD1	3:C:603:ASN:N	2.53	0.41
1:A:618:ALA:HA	1:A:669:LYS:HA	2.02	0.41
3:C:1026:ALA:O	3:C:1027:LEU:C	2.57	0.41
3:C:966:LEU:C	3:C:968:PRO:HD2	2.41	0.41
3:C:723:TYR:N	3:C:724:PRO:HD3	2.26	0.41
1:A:137:CYS:HB3	1:A:159:ILE:HG12	2.02	0.41
3:C:644:LEU:O	3:C:647:VAL:HG23	2.21	0.41
3:C:667:LYS:HE3	3:C:700:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:VAL:HG23	1:A:227:TYR:N	2.35	0.41
3:C:1066:VAL:HB	3:C:1073:HIS:HB3	2.03	0.41
3:C:373:LYS:CD	3:C:427:MET:CE	2.42	0.40
1:A:609:ILE:O	1:A:610:LEU:C	2.59	0.40
3:C:1146:VAL:O	3:C:1147:GLU:C	2.59	0.40
1:A:648:LEU:HD23	1:A:648:LEU:HA	1.91	0.40
3:C:858:LYS:HE2	3:C:891:TYR:HD2	1.82	0.40
1:A:711:GLN:HE22	1:A:758:LYS:HZ3	1.65	0.40
3:C:892:LEU:O	3:C:892:LEU:HD23	2.21	0.40
3:C:639:PRO:O	3:C:641:LYS:N	2.54	0.40
3:C:294:ILE:O	3:C:298:LEU:N	2.54	0.40
3:C:220:LYS:O	3:C:222:ASP:N	2.55	0.40
3:C:1152:THR:O	3:C:1154:THR:N	2.55	0.40
1:A:701:ASN:C	1:A:701:ASN:ND2	2.73	0.40
3:C:209:ASP:O	3:C:212:GLU:CD	2.60	0.40
3:C:88:VAL:HG11	3:C:134:ILE:HG12	2.04	0.40
1:A:475:HIS:CE1	1:A:584:LEU:O	2.73	0.40
3:C:652:VAL:N	3:C:653:PRO:CD	2.83	0.40
3:C:735:LEU:C	3:C:737:GLU:H	2.24	0.40
1:A:299:LEU:HA	1:A:302:PHE:HB2	2.03	0.40
3:C:202:LEU:HD12	3:C:202:LEU:O	2.21	0.40
3:C:960:LEU:O	3:C:963:PRO:HD3	2.21	0.40
1:A:359:LEU:HD22	1:A:410:MET:SD	2.60	0.40
3:C:452:GLN:NE2	3:C:492:ASN:HB3	2.36	0.40
1:A:552:PHE:CD1	1:A:630:ILE:HG13	2.57	0.40
3:C:74:PRO:O	3:C:78:LYS:HG2	2.21	0.40
1:A:620:THR:HG22	1:A:667:LEU:CD2	2.52	0.40
3:C:1177:MET:O	3:C:1179:ALA:N	2.54	0.40
1:A:558:LEU:HD13	2:B:27:TRP:CE2	2.57	0.40
1:A:240:GLU:CD	1:A:289:LYS:NZ	2.74	0.40
1:A:560:ARG:HG2	1:A:560:ARG:NH1	2.37	0.40
3:C:456:ASN:HD22	3:C:456:ASN:HA	1.63	0.40
3:C:287:TYR:O	3:C:290:VAL:HB	2.22	0.40
3:C:696:GLU:OE1	3:C:696:GLU:HA	2.22	0.40
3:C:862:LEU:HA	3:C:862:LEU:HD23	1.91	0.40
1:A:753:ASP:O	1:A:756:ILE:N	2.48	0.40
3:C:682:SER:O	3:C:685:LEU:HG	2.22	0.40
3:C:66:ASN:HA	3:C:66:ASN:HD22	1.67	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	705/776 (91%)	584 (83%)	91 (13%)	30 (4%)	3	19
2	B	86/108 (80%)	68 (79%)	13 (15%)	5 (6%)	2	12
3	C	1134/1230 (92%)	793 (70%)	236 (21%)	105 (9%)	1	4
All	All	1925/2114 (91%)	1445 (75%)	340 (18%)	140 (7%)	1	7

All (140) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	TRP
1	A	145	VAL
1	A	646	LYS
1	A	652	ASP
1	A	674	TYR
2	B	98	ASN
3	C	34	LEU
3	C	36	LYS
3	C	87	ILE
3	C	128	ALA
3	C	144	LYS
3	C	224	MET
3	C	226	THR
3	C	252	ILE
3	C	347	TRP
3	C	375	VAL
3	C	443	MET
3	C	487	LYS
3	C	552	PRO
3	C	601	GLY
3	C	619	LEU
3	C	641	LYS
3	C	659	LEU
3	C	723	TYR

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Mol	Chain	Res	Type
3	C	724	PRO
3	C	725	SER
3	C	828	SER
3	C	901	SER
3	C	943	ALA
3	C	976	SER
3	C	977	GLY
3	C	1013	LYS
3	C	1037	LYS
3	C	1187	PRO
3	C	1188	GLU
3	C	1195	MET
1	A	285	GLU
1	A	313	ASP
1	A	475	HIS
1	A	477	ASN
1	A	527	SER
1	A	550	CYS
1	A	557	GLU
2	B	20	LYS
2	B	67	GLU
3	C	76	VAL
3	C	88	VAL
3	C	127	ALA
3	C	146	GLU
3	C	149	SER
3	C	221	ASN
3	C	228	ARG
3	C	262	VAL
3	C	285	GLU
3	C	286	VAL
3	C	345	MET
3	C	346	SER
3	C	360	VAL
3	C	386	ARG
3	C	388	GLU
3	C	430	SER
3	C	489	SER
3	C	570	THR
3	C	571	CYS
3	C	605	GLY
3	C	664	ARG

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Mol	Chain	Res	Type
3	C	732	GLY
3	C	734	ILE
3	C	750	GLY
3	C	766	GLY
3	C	772	TYR
3	C	822	ILE
3	C	826	LYS
3	C	918	SER
3	C	975	ILE
3	C	1012	LEU
3	C	1018	PRO
3	C	1096	CYS
3	C	1197	GLU
1	A	174	PRO
1	A	175	LEU
1	A	559	GLU
1	A	767	GLU
3	C	7	HIS
3	C	167	GLY
3	C	283	PRO
3	C	366	GLU
3	C	407	PRO
3	C	466	PRO
3	C	566	LYS
3	C	649	GLY
3	C	684	SER
3	C	785	SER
3	C	811	PRO
3	C	853	GLY
3	C	1153	CYS
3	C	1181	ALA
3	C	1182	ALA
3	C	1204	SER
1	A	21	TRP
1	A	176	ASN
1	A	474	VAL
1	A	549	SER
1	A	625	THR
1	A	650	LEU
1	A	662	LEU
2	B	49	ILE
3	C	18	SER

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Mol	Chain	Res	Type
3	C	151	GLN
3	C	152	LEU
3	C	579	ALA
3	C	687	ALA
3	C	731	SER
3	C	960	LEU
3	C	1132	THR
1	A	523	HIS
1	A	695	GLN
3	C	385	GLU
3	C	637	GLY
3	C	677	LEU
3	C	1134	CYS
3	C	1194	LEU
1	A	222	PRO
1	A	613	TYR
3	C	646	PRO
3	C	694	LEU
3	C	782	PRO
3	C	1039	SER
3	C	1193	PRO
2	B	38	VAL
1	A	496	GLY
3	C	73	GLY
3	C	701	ILE
3	C	1017	ASP
1	A	179	VAL
1	A	715	VAL
3	C	551	ARG
3	C	749	GLY
3	C	916	ILE
3	C	927	PRO

### 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	650/698 (93%)	575 (88%)	75 (12%)	7	27
2	B	78/90 (87%)	65 (83%)	13 (17%)	3	11
3	C	1022/1098 (93%)	900 (88%)	122 (12%)	6	25
All	All	1750/1886 (93%)	1540 (88%)	210 (12%)	6	24

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	21	TRP
1	A	24	LEU
1	A	25	ARG
1	A	29	GLN
1	A	37	MET
1	A	52	TYR
1	A	94	GLU
1	A	113	GLU
1	A	115	VAL
1	A	116	LEU
1	A	117	LYS
1	A	140	LEU
1	A	142	ARG
1	A	145	VAL
1	A	158	GLU
1	A	162	LEU
1	A	171	LEU
1	A	194	GLU
1	A	211	LEU
1	A	268	LEU
1	A	271	GLN
1	A	272	ARG
1	A	286	LEU
1	A	296	GLU
1	A	304	THR
1	A	307	GLN
1	A	315	ASN
1	A	317	ASP
1	A	329	GLN
1	A	335	LEU
1	A	338	LEU
1	A	343	ILE
1	A	405	ASN

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Mol	Chain	Res	Type
1	A	421	LEU
1	A	429	LEU
1	A	431	LYS
1	A	438	GLU
1	A	443	ASP
1	A	445	LEU
1	A	469	LEU
1	A	471	LYS
1	A	481	ASP
1	A	500	THR
1	A	516	LEU
1	A	517	ASN
1	A	526	ASN
1	A	531	ASP
1	A	560	ARG
1	A	571	SER
1	A	577	LYS
1	A	579	THR
1	A	583	GLN
1	A	586	LYS
1	A	595	LYS
1	A	597	ARG
1	A	598	TYR
1	A	600	LEU
1	A	601	GLN
1	A	624	LEU
1	A	629	GLN
1	A	632	MET
1	A	642	LEU
1	A	665	ASP
1	A	671	TYR
1	A	672	LEU
1	A	674	TYR
1	A	676	ASN
1	A	682	ASN
1	A	698	THR
1	A	701	ASN
1	A	706	ARG
1	A	720	MET
1	A	751	CYS
1	A	774	LEU
2	B	42	CYS

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Mol	Chain	Res	Type
2	B	49	ILE
2	B	52	LEU
2	B	65	SER
2	B	66	GLU
2	B	67	GLU
2	B	68	CYS
2	B	69	THR
2	B	76	ASN
2	B	84	ILE
2	B	85	SER
2	B	91	ARG
2	B	97	ASP
3	C	7	HIS
3	C	36	LYS
3	C	66	ASN
3	C	71	CYS
3	C	75	LEU
3	C	86	THR
3	C	96	LEU
3	C	116	GLU
3	C	118	PRO
3	C	144	LYS
3	C	162	LEU
3	C	168	LEU
3	C	171	ASN
3	C	189	LEU
3	C	194	ARG
3	C	204	MET
3	C	214	LEU
3	C	217	GLU
3	C	228	ARG
3	C	243	HIS
3	C	249	LEU
3	C	259	PHE
3	C	264	ASP
3	C	270	TYR
3	C	275	PHE
3	C	276	GLU
3	C	279	VAL
3	C	284	LYS
3	C	286	VAL
3	C	298	LEU

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Mol	Chain	Res	Type
3	C	344	ASP
3	C	345	MET
3	C	351	ARG
3	C	363	THR
3	C	364	ARG
3	C	366	GLU
3	C	377	PRO
3	C	382	ARG
3	C	383	PHE
3	C	384	LYS
3	C	385	GLU
3	C	386	ARG
3	C	422	GLU
3	C	423	THR
3	C	424	PRO
3	C	432	VAL
3	C	456	ASN
3	C	518	GLN
3	C	540	LEU
3	C	541	LEU
3	C	555	GLN
3	C	566	LYS
3	C	573	ILE
3	C	600	LEU
3	C	603	ASN
3	C	610	ASN
3	C	616	LEU
3	C	621	ASN
3	C	625	ARG
3	C	638	SER
3	C	664	ARG
3	C	676	ILE
3	C	683	ASP
3	C	698	PRO
3	C	711	MET
3	C	724	PRO
3	C	741	LEU
3	C	748	GLN
3	C	763	VAL
3	C	773	MET
3	C	774	ASP
3	C	786	GLN

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Mol	Chain	Res	Type
3	C	813	GLU
3	C	820	GLN
3	C	826	LYS
3	C	829	ARG
3	C	832	ASP
3	C	835	ARG
3	C	856	GLU
3	C	857	LEU
3	C	870	GLU
3	C	874	SER
3	C	892	LEU
3	C	900	THR
3	C	902	GLN
3	C	905	ARG
3	C	914	LYS
3	C	918	SER
3	C	921	SER
3	C	923	VAL
3	C	967	LEU
3	C	974	LEU
3	C	996	HIS
3	C	1000	ILE
3	C	1004	LEU
3	C	1005	LYS
3	C	1020	LEU
3	C	1027	LEU
3	C	1036	ASN
3	C	1040	LEU
3	C	1055	GLU
3	C	1056	THR
3	C	1064	ARG
3	C	1079	LEU
3	C	1093	LEU
3	C	1098	ASP
3	C	1102	ILE
3	C	1104	GLU
3	C	1111	ASP
3	C	1117	TYR
3	C	1122	LEU
3	C	1123	THR
3	C	1131	SER
3	C	1157	VAL

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Mol	Chain	Res	Type
3	C	1162	VAL
3	C	1164	GLN
3	C	1167	GLU
3	C	1169	GLN
3	C	1187	PRO
3	C	1190	GLU
3	C	1194	LEU
3	C	1195	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	51	ASN
1	A	121	GLN
1	A	134	ASN
1	A	141	ASN
1	A	143	HIS
1	A	252	GLN
1	A	253	GLN
1	A	271	GLN
1	A	283	GLN
1	A	307	GLN
1	A	323	ASN
1	A	367	GLN
1	A	377	ASN
1	A	385	ASN
1	A	405	ASN
1	A	447	GLN
1	A	477	ASN
1	A	504	GLN
1	A	517	ASN
1	A	526	ASN
1	A	583	GLN
1	A	592	ASN
1	A	596	ASN
1	A	614	ASN
1	A	622	GLN
1	A	623	GLN
1	A	656	ASN
1	A	676	ASN
1	A	682	ASN

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Mol	Chain	Res	Type
1	A	701	ASN
1	A	711	GLN
1	A	736	GLN
2	B	28	ASN
2	B	76	ASN
3	C	66	ASN
3	C	101	GLN
3	C	151	GLN
3	C	442	GLN
3	C	452	GLN
3	C	456	ASN
3	C	463	ASN
3	C	472	HIS
3	C	508	HIS
3	C	511	GLN
3	C	514	HIS
3	C	544	GLN
3	C	555	GLN
3	C	595	GLN
3	C	599	ASN
3	C	603	ASN
3	C	610	ASN
3	C	663	GLN
3	C	680	ASN
3	C	710	GLN
3	C	736	ASN
3	C	897	GLN
3	C	902	GLN
3	C	906	GLN
3	C	1036	ASN
3	C	1054	ASN
3	C	1108	HIS
3	C	1164	GLN
3	C	1205	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	715/776 (92%)	-0.56	11 (1%) 76 58	13, 46, 129, 197	0
2	B	88/108 (81%)	-0.61	2 (2%) 64 40	3, 38, 76, 151	0
3	C	1146/1230 (93%)	-0.67	2 (0%) 95 91	14, 61, 122, 190	0
All	All	1949/2114 (92%)	-0.63	15 (0%) 87 75	3, 55, 124, 197	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	478	SER	16.5
1	A	477	ASN	10.9
1	A	479	ALA	4.7
1	A	176	ASN	4.1
2	B	20	LYS	3.8
1	A	476	GLN	3.6
1	A	143	HIS	3.5
3	C	278	PHE	3.2
2	B	19	LYS	2.9
1	A	593	CYS	2.7
1	A	146	ARG	2.5
1	A	632	MET	2.5
3	C	373	LYS	2.4
1	A	177	LYS	2.3
1	A	147	ARG	2.2

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	B	1230	1/1	0.93	0.14	-0.61	56,56,56,56	0
4	ZN	B	1229	1/1	0.95	0.12	-1.25	42,42,42,42	0
4	ZN	B	1231	1/1	0.97	0.10	-2.00	36,36,36,36	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.