Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:51 AM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

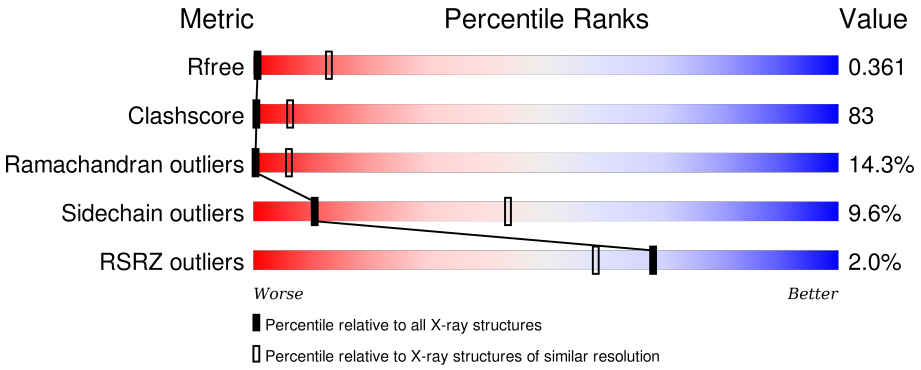
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	1067 (5.20-3.60)
Clashscore	102246	1175 (5.20-3.60)
Ramachandran outliers	100387	1114 (5.20-3.60)
Sidechain outliers	100360	1096 (5.20-3.60)
RSRZ outliers	91569	1071 (5.20-3.60)

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. 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 <=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	2% 16% 59% 15% • 8%
1	B	1284	2% 16% 59% 16% • 8%

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.

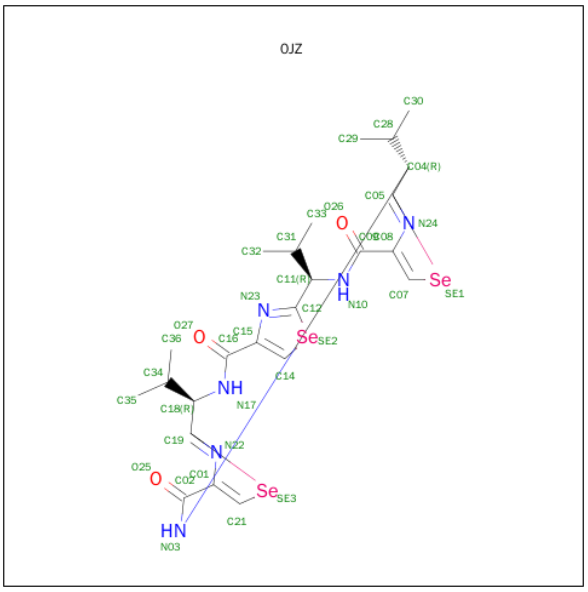
- Molecule 1 is a protein called Multidrug resistance protein 1a.

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-TRISELENA-3,10,17,22,23,24-HEXAAZATETRACYCLO[17.2.1.1 5,8 .1 12,15]TETRACOSA-1(21),5(24),7,12(23),14,19(22)-HEXAENE-2,9,16-TRIONE (three-letter code: 0JZ) (formula: $C_{24}H_{30}N_6O_3Se_3$).



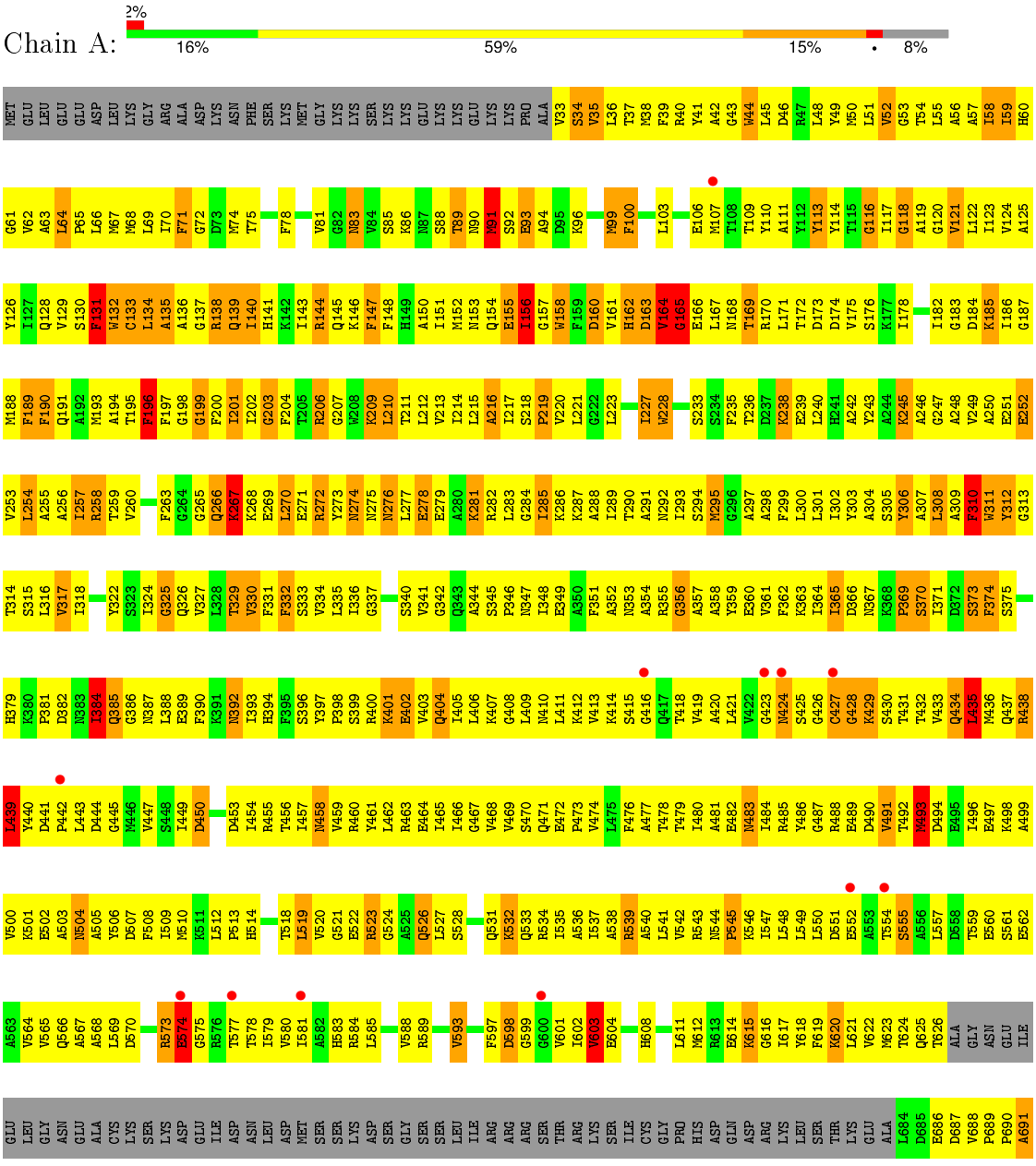
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	Se	0	0
			36	24	6	3	3		
2	B	1	Total	C	N	O	Se	0	0
			36	24	6	3	3		

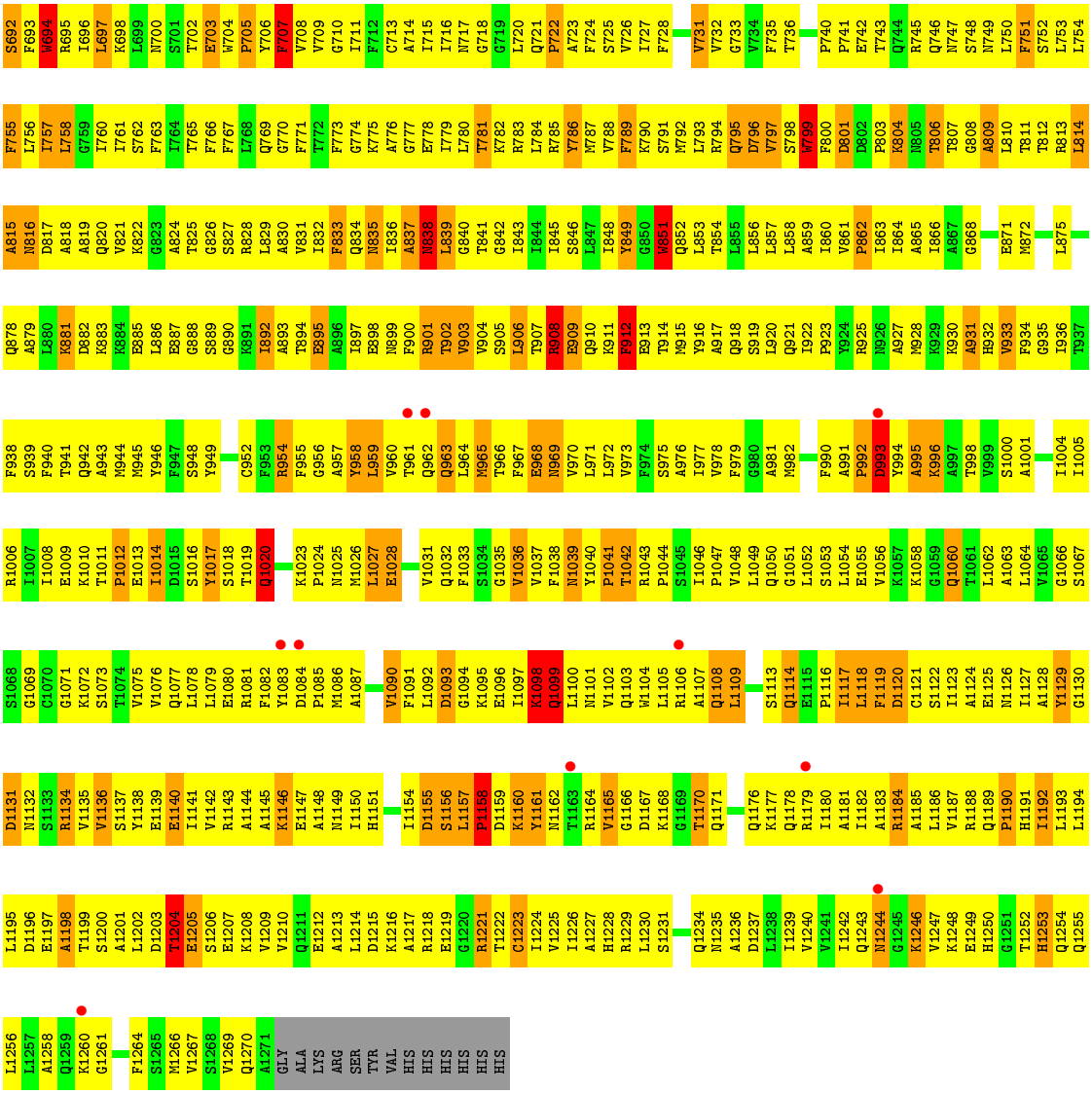
3 Residue-property plots (i)

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: Multidrug resistance protein 1a

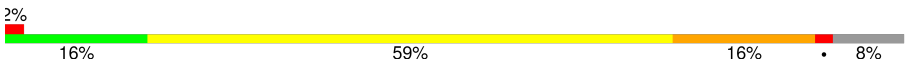
Chain A:

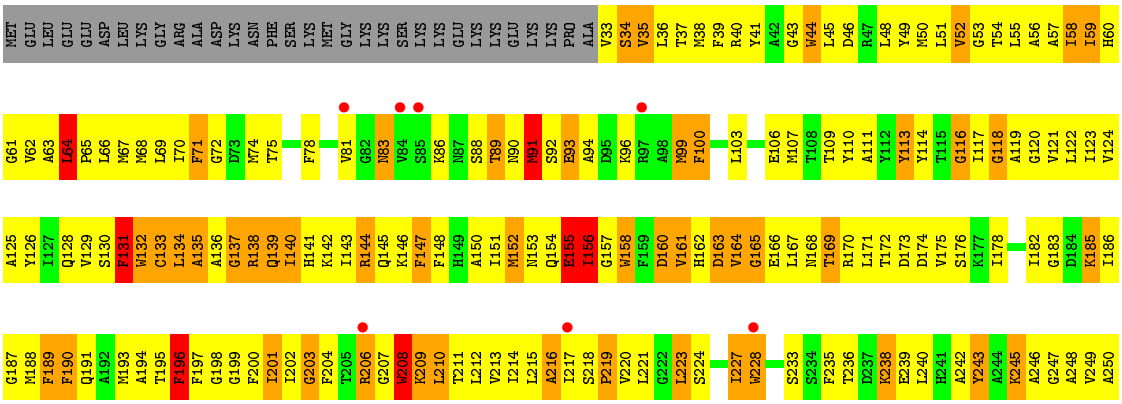


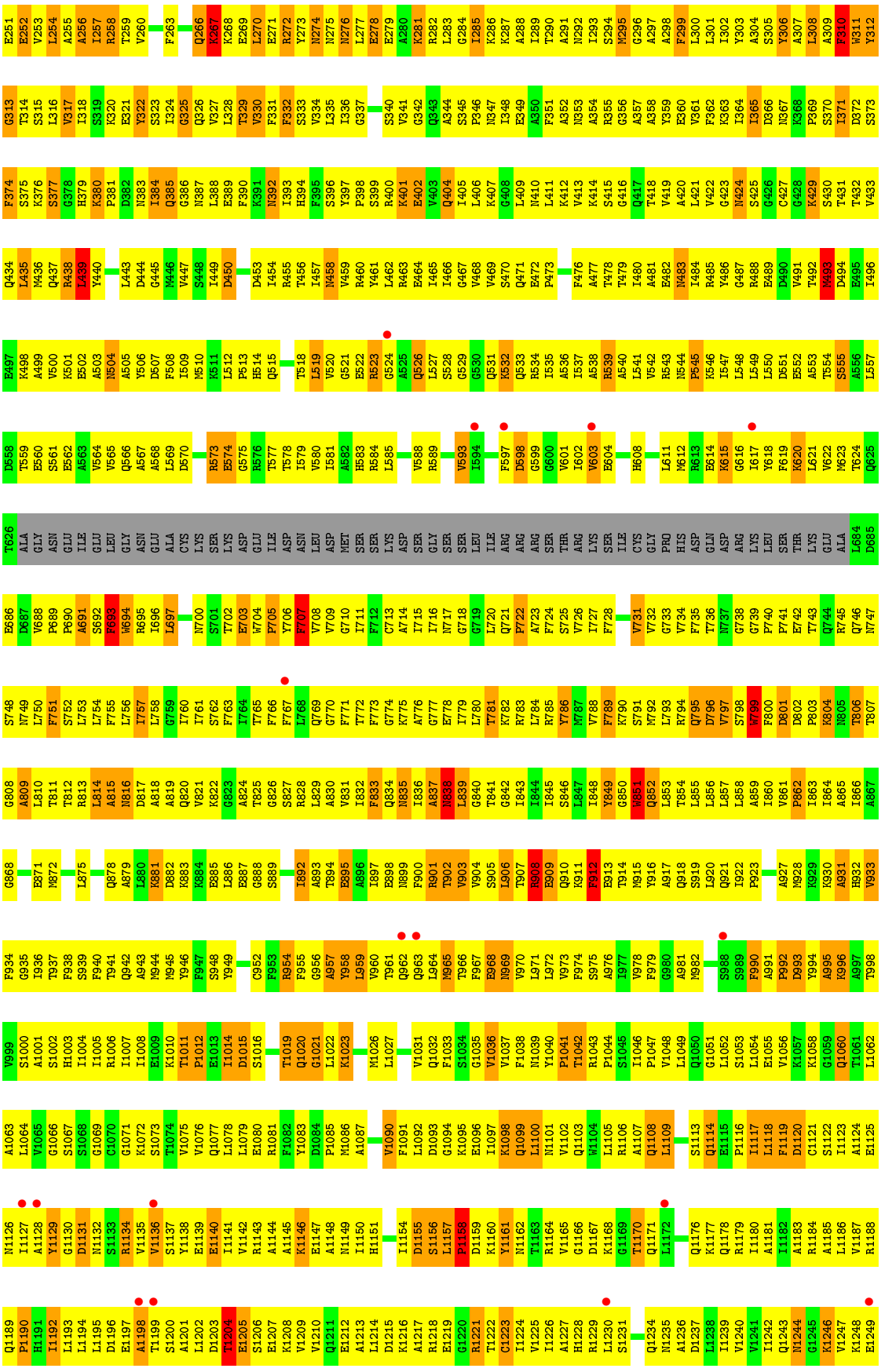


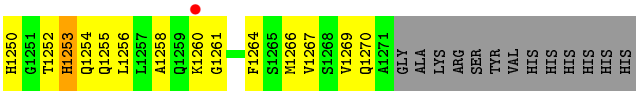
• Molecule 1: Multidrug resistance protein 1a

Chain B:








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

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	5.10 (at 4.29Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.314 , 0.365 0.316 , 0.361	Depositor DCC
R_{free} test set	2562 reflections (10.02%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 28597 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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:B:270:LEU:H	1:B:270:LEU:HD23	1.18	1.00
1:A:267:LYS:N	1:A:270:LEU:HD21	1.76	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:6001:0JZ: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:A:853:LEU:HG	1:A:973:VAL:HG21	1.48	0.94
1:B:58:ILE:HG13	1:B:193:MET:HG3	1.49	0.94
1:B:288:ALA:HA	1:B:291:ALA:HB3	1.48	0.94
1:A:718:GLY:O	1:A:722:PRO:HD2	1.68	0.93
1:A:58:ILE:HG13	1:A:193:MET:HG3	1.50	0.93
1:A:155:GLU:HB3	1:A:156:ILE:HD12	1.48	0.93
1:A:1014:ILE:HD12	1:A:1106:ARG:HH12	1.34	0.93
1:B:978:VAL:HG13	2:B:6002:0JZ: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:B:956:GLY:O	1:B:966:THR:HB	1.72	0.89
1:A:278:GLU:O	1:A:282:ARG:HG2	1.71	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:HD3	1:B:996:LYS:H	1.37	0.89
1:B:387:ASN:HD22	1:B:414:LYS:HA	1.36	0.89
1:A:267:LYS:HB3	1:A:790:LYS:HE2	1.54	0.89
1:B:693:PHE:O	1:B:696:ILE:HG12	1.72	0.89
1:A:927:ALA:HA	1:A:930:LYS:HE3	1.54	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: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:849:TYR:OH	1:A:976:ALA:HB2	1.73	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:158:TRP:HE1	1:A:900:PHE:HB3	1.36	0.88
1:A:136:ALA:HB2	1:A:182:ILE:HB	1.56	0.88
1:A:573:ARG:HD2	1:A:578:THR:HG21	1.54	0.87
1:B:849:TYR:OH	1:B:976:ALA:HB2	1.74	0.87
1:B:690:PRO:HG2	1:B:1006:ARG:NH2	1.90	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:B:314:THR:CG2	1:B:327:VAL:HG21	2.05	0.85
1:A:172:THR:O	1:A:175:VAL:HG12	1.76	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:B:976:ALA:HA	1:B:979:PHE:CD2	2.11	0.85
1:A:964:LEU:HD13	1:A:965:MET:H	1.41	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:B:1014:ILE:HA	1:B:1102:VAL:HG11	1.59	0.84
1:A:976:ALA:HA	1:A:979:PHE:CD2	2.12	0.84
1:B:401:LYS:H	1:B:401:LYS:HD2	1.42	0.84
1:A:1037:VAL:HG12	1:A:1051:GLY: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:379:HIS:O	1:B:381:PRO:HD3	1.77	0.83
1:B:118:GLY:O	1:B:121:VAL:HG22	1.77	0.83
1:B:1079:LEU:HD23	1:B:1194:LEU:HD21	1.60	0.83
1:A:725:SER:HA	2:A:6001:0JZ:H36	1.59	0.83
1:A:1091:PHE:HE1	1:A:1096:GLU:HG2	1.41	0.83
1:A:429:LYS:H	1:A:429:LYS:HD3	1.39	0.83
1:B:1037:VAL:HG12	1:B:1051:GLY:H	1.42	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:1039:ASN:HB2	1:A:1047:PRO:HA	1.60	0.83
1:B:72:GLY:HA2	1:B:326:GLN:NE2	1.93	0.83
1:A:118:GLY:O	1:A:121:VAL:HG22	1.78	0.83
1:B:59:ILE:HD11	1:B:124:VAL:HG11	1.61	0.83
1:A:202:ILE:HD12	1:A:203:GLY:N	1.93	0.82
1:A:853:LEU:HB3	1:A:973:VAL:CG1	2.08	0.82
1:A:1179:ARG:NH2	1:A:1209:VAL:HG11	1.94	0.82
1:A:564:VAL:O	1:A:567:ALA:HB3	1.79	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:358:ALA:O	1:A:362:PHE:HB2	1.79	0.82
1:A:1218:ARG:HH22	1:A:1235:ASN:HD22	1.28	0.82
1:B:1179:ARG:NH2	1:B:1209:VAL:HG11	1.95	0.82
1:B:918:GLN:O	1:B:921:GLN:HB3	1.79	0.82
1:B:694:TRP:O	1:B:697:LEU:HG	1.80	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:856:LEU:HD22	1:B:955:PHE:HD1	1.46	0.81
1:B:163:ASP:HB2	1:B:166:GLU:HB3	1.61	0.81
1:A:1121:CYS:HB2	1:A:1126:ASN:HD21	1.46	0.81
1:B:318:ILE:HD11	1:B:324:ILE:HD12	1.62	0.81
1:B:1121:CYS:HB2	1:B:1126:ASN:HD21	1.44	0.81
1:B: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:715:ILE:HG12	1:A:836:ILE:HD12	1.64	0.80
1:A:574:GLU:HG3	1:A:574:GLU:O	1.79	0.80
1:A:457:ILE:HD11	1:A:462:LEU:HD13	1.63	0.80
1:B:715:ILE:HG12	1:B:836:ILE:HD12	1.64	0.80
1:B:564:VAL:O	1:B:567:ALA:HB3	1.80	0.80
1:B:795:GLN:O	1:B:796:ASP:HB3	1.80	0.80
1:A:388:LEU:HB2	1:A:413:VAL:CG1	2.12	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:B:508:PHE:HE2	1:B:534:ARG:HD2	1.47	0.79
1:A:379:HIS:HB3	1:A:457:ILE:HA	1.64	0.79
1:A:158:TRP:HE1	1:A:900:PHE:CB	1.95	0.79
1:A:210:LEU:O	1:A:214:ILE:HG13	1.82	0.79
1:B:388:LEU:HB2	1:B:413:VAL:CG1	2.12	0.79
1:A:856:LEU:HD22	1:A:955:PHE:HD1	1.46	0.79
1:B:785:ARG:HH21	1:B:815:ALA:HA	1.46	0.79
1:A:59:ILE:HD11	1:A:124:VAL:HG11	1.62	0.79
1:A:1142:VAL:O	1:A:1146:LYS:HG2	1.82	0.79
1:A: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: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:392:ASN:O	1:A:445:GLY:HA3	1.84	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:1092:LEU:HB3	1:A:1097:ILE:HD11	1.63	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:799:TRP:O	1:A:803:PRO:HB3	1.84	0.78
1:A:797:VAL:O	1:A:801:ASP:CB	2.32	0.78
1:A:864:ILE:HD12	1:A:865:ALA:N	1.99	0.78
1:A:1260:LYS:HD2	1:A:1260:LYS:H	1.48	0.78
1:B:1092:LEU:HD22	1:B:1097:ILE:HD11	1.66	0.78
1:A:959:LEU:HD22	1:A:964:LEU:HG	1.66	0.77
1:B:897:ILE:HD12	1:B:898:GLU:N	1.99	0.77
1:B:864:ILE:HD12	1:B:865:ALA:N	1.99	0.77
1:B:163:ASP:O	1:B:165:GLY:N	2.17	0.77
1:B:1181:ALA:O	1:B:1184:ARG:HB3	1.84	0.77
1:B:379:HIS:CB	1:B:457:ILE:HA	2.15	0.77
1:B:286:LYS:O	1:B:290:THR:HG23	1.84	0.77
1:A:308:LEU:HD12	1:A:751:PHE:CE2	2.20	0.77
1:A:550:LEU:HB2	1:A:580:VAL:HG23	1.67	0.77
1:B:128:GLN:O	1:B:131:PHE:HB3	1.85	0.77
1:A:314:THR:HG23	1:A:327:VAL:HG21	1.65	0.77
1:A:857:LEU:CD1	1:A:976:ALA:HB3	2.15	0.77
1:A:91:MET:HB2	1:A:94:ALA:HB3	1.67	0.77
1:B:756:LEU:HD12	1:B:757:ILE:N	2.00	0.77
1:A:785:ARG:HH21	1:A:815:ALA:HA	1.50	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:B:550:LEU:HB2	1:B:580:VAL:HG23	1.65	0.76
1:B:285:ILE:O	1:B:289:ILE:HG12	1.84	0.76
1:A:756:LEU:HD12	1:A:757:ILE:N	1.99	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:A:1014:ILE:HB	1:A:1102:VAL:HG21	1.66	0.76
1:A:800:PHE:O	1:A:803:PRO:HD3	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:773:PHE:O	1:A:776:ALA:HB3	1.85	0.76
1:A:1038:PHE:HB2	1:A:1085:PRO:HA	1.67	0.76
1:B:1260:LYS:H	1:B:1260:LYS:HD2	1.50	0.76
1:B:91:MET:HB2	1:B:94:ALA:HB3	1.68	0.76
1:B:314:THR:HG23	1:B:327:VAL:CG2	2.11	0.76
1:A:1113:SER:HA	1:A:1196:ASP:HB3	1.67	0.76
1:B:286:LYS:HG2	1:B:778:GLU:CG	2.15	0.76
1:B:324:ILE:HD12	1:B:326:GLN:H	1.51	0.76
1:A:285:ILE:O	1:A:289:ILE:HG12	1.86	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:B:1056:VAL:HG23	1:B:1060:GLN:HE22	1.50	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:800:PHE:O	1:B:803:PRO:HD3	1.85	0.76
1:B:394:HIS:HB2	1:B:444:ASP:HB3	1.67	0.76
1:B:278:GLU:C	1:B:282:ARG:HG2	2.05	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:905:SER:C	1:B:907:THR:H	1.88	0.76
1:B:512:LEU:HD12	1:B:513:PRO:HD2	1.68	0.75
1:B:799:TRP:O	1:B:803:PRO:HB3	1.86	0.75
1:A:1020:GLN:HG3	1:A:1101:ASN:HB2	1.68	0.75
1:B:608:HIS:HD1	1:B:618:TYR:HE2	1.33	0.75
1:B:797:VAL:HG12	1:B:798:SER:N	2.01	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:35:VAL:HG12	1:B:359:TYR:CE2	2.22	0.75
1:B:270:LEU:HD23	1:B:270:LEU:N	1.98	0.75
1:B:819:ALA:O	1:B:822:LYS:HB3	1.86	0.75
1:B:843:ILE:HA	1:B:846:SER:HB3	1.68	0.75
1: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:740:PRO:HG2	1:B:741:PRO:HD3	1.68	0.75
1:A:608:HIS:HD1	1:A:618:TYR:HE2	1.33	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:B:1109:LEU:HD21	1:B:1188:ARG:HH11	1.51	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:A:218:SER:HB2	1:A:219:PRO:HD3	1.69	0.75
1:B:332:PHE:O	1:B:335:LEU:HB3	1.85	0.75
1:B:949:TYR:OH	2:B:6002:0JZ:H32	1.87	0.75
1:A:434:GLN:HE21	1:A:439:LEU:HG	1.51	0.75
1:B:407:LYS:NZ	1:B:601:VAL:HA	2.00	0.75
1:A:512:LEU:HD12	1:A:513:PRO:HD2	1.68	0.75
1:B:543:ARG:NH2	1:B:905:SER:O	2.20	0.75
1:A:265:GLY:HA2	1:A:793:LEU:HD21	1.68	0.75
1:B:1199:THR:HG23	1:B:1210:VAL:HG11	1.67	0.74
1:A:1109:LEU:HD21	1:A:1188:ARG:HH11	1.51	0.74
1:A:1033:PHE:HB3	1:A:1036:VAL:HG21	1.68	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:B:722:PRO:HB2	1:B:841:THR:HG21	1.69	0.74
1:A:306:TYR:O	1:A:310:PHE:HB2	1.87	0.74
1:B:396:SER:HA	1:B:404:GLN:HA	1.70	0.74
1:A:407:LYS:NZ	1:A:601:VAL:HA	2.01	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:B:892:ILE:HB	1:B:916:TYR:CE1	2.23	0.74
1:A:696:ILE:O	1:A:700:ASN:HB2	1.86	0.74
1:A:215:LEU:O	1:A:219:PRO:HD2	1.88	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:1063:ALA:HB2	1:A:1236:ALA:HB1	1.70	0.74
1:A:128:GLN:O	1:A:131:PHE:HB3	1.88	0.74
1:B:690:PRO:HG2	1:B:1006:ARG:HH22	1.52	0.74
1:A:1138:TYR:O	1:A:1142:VAL:HG23	1.88	0.74
1:B:557:LEU:HG	1:B:561:SER:OG	1.87	0.74
1:A:1199:THR:HG23	1:A:1210:VAL:HG11	1.69	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:B:928:MET:O	1:B:931:ALA:HB3	1.87	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:A:892:ILE:HB	1:A:916:TYR:CE1	2.23	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: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:282:ARG:O	1:B:286:LYS:HB2	1.87	0.73
1:A:703:GLU:HB3	1:A:780:LEU:HD23	1.71	0.73
1:A:36:LEU:HD12	1:A:37:THR:N	2.02	0.73
1:A:801:ASP:HB3	1:A:1083:TYR:OH	1.87	0.73
1:A:557:LEU:HG	1:A:561:SER:OG	1.88	0.73
1:B:1027:LEU:H	1:B:1027:LEU:HD23	1.53	0.73
1:B:543:ARG:HH12	1:B:905:SER:HA	1.53	0.73
1:A:722:PRO:O	1:A:725:SER:HB2	1.89	0.73
1:B:993:ASP:N	1:B:996:LYS:HZ1	1.86	0.73
1:A:394:HIS:HB2	1:A:444:ASP:HB3	1.69	0.73
1:B:722:PRO:O	1:B:725:SER:HB2	1.87	0.73
1:B:1063:ALA:HB2	1:B:1236:ALA:HB1	1.69	0.73
1:A:972:LEU:HD12	1:A:972:LEU:H	1.52	0.73
1:B:407:LYS:HZ1	1:B:601:VAL:HA	1.54	0.73
1:A:1242:ILE:HA	1:A:1247:VAL:HA	1.70	0.73
1:A:332:PHE:O	1:A:335:LEU:HB3	1.88	0.73
1:A:1013:GLU:O	1:A:1014:ILE:HG23	1.89	0.73
1:B:922:ILE:HB	1:B:923:PRO:HD3	1.70	0.73
1: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:969:ASN:HD22	1:A:970:VAL:H	1.36	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:B:1242:ILE:HA	1:B:1247:VAL:HA	1.69	0.73
1:B:1218:ARG:HH22	1:B:1235:ASN:ND2	1.87	0.72
1:A:992:PRO:HB2	1:A:996:LYS:NZ	2.04	0.72
1:B:713:CYS:SG	1:B:769:GLN:HB3	2.29	0.72
1:A:922:ILE:HB	1:A:923:PRO:HD3	1.69	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: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:204:PHE:HA	1:A:211:THR:HG21	1.71	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:B:416:GLY:N	1:B:577:THR:HG22	2.02	0.72
1:A:1014:ILE:HD12	1:A:1106:ARG:NH1	2.02	0.72
1:B:133:CYS:SG	1:B:931:ALA:HA	2.30	0.72
1:A:942:GLN:O	1:A:945:MET:HB3	1.90	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:B:132:TRP:HB2	1:B:186:ILE:HD13	1.71	0.72
1:A:303:TYR:O	1:A:306:TYR:N	2.23	0.72
1:A:214:ILE:CD1	1:A:330:VAL:HB	2.20	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:715:ILE:HG23	1:A:836:ILE:HG21	1.71	0.72
1:A:168:ASN:O	1:A:171:LEU:HB3	1.90	0.72
1:B:992:PRO:HB2	1:B:996:LYS:NZ	2.05	0.72
1:A:401:LYS:HB3	1:A:401:LYS:NZ	2.04	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:504:ASN:OD1	1:B:568:ALA:HB2	1.89	0.71
1:B:210:LEU:HD23	1:B:317:VAL:HG11	1.70	0.71
1:B:1121:CYS:HB2	1:B:1126:ASN:ND2	2.05	0.71
1:B:959:LEU:HD22	1:B:964:LEU:HB2	1.71	0.71
1:B:1150:ILE:HB	1:B:1179:ARG:HB3	1.72	0.71
1:A:267:LYS:HA	1:A:270:LEU:HD11	1.72	0.71
1:A:721:GLN:HB3	1:A:722:PRO:HD3	1.71	0.71
1:B:795:GLN:HE21	1:B:796:ASP:H	1.38	0.71
1:A:211:THR:O	1:A:215:LEU:HG	1.88	0.71
1:B:59:ILE:CD1	1:B:124:VAL:HG11	2.20	0.71
1:A:399:SER:O	1:A:402:GLU:HB2	1.90	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:725:SER:HB3	1:A:975:SER:HB3	1.71	0.71
1:B:288:ALA:HA	1:B:291:ALA:CB	2.18	0.71
1:A:187:GLY:O	1:A:190:PHE:HB3	1.89	0.71
1:A:1100:LEU:HG	1:A:1101:ASN:H	1.56	0.71
1:A:289:ILE:O	1:A:293:ILE:HG12	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ILE:HG13	1:A:187:GLY:N	2.05	0.71
1:B:942:GLN:O	1:B:945:MET:HB3	1.90	0.71
1:B:291:ALA:O	1:B:294:SER:HB2	1.90	0.71
1:A:407:LYS:HZ1	1:A:601:VAL:HA	1.56	0.71
1:B:399:SER:O	1:B:402:GLU:HB2	1.90	0.71
1:B:168:ASN:O	1:B:171:LEU:HB3	1.91	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:797:VAL:HG12	1:A:798:SER:N	2.04	0.71
1:A:384:ILE:HG22	1:A:385:GLN:H	1.56	0.71
1:A:122:LEU:HD12	1:A:939:SER:HB2	1.72	0.71
1:B:1114:GLN:NE2	1:B:1200:SER:HB3	2.03	0.71
1:B:211:THR:O	1:B:215:LEU:HG	1.91	0.70
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:A:1150:ILE:HB	1:A:1179:ARG:HB3	1.72	0.70
1:A:59:ILE:CD1	1:A:124:VAL:HG11	2.21	0.70
1:A:1248:LYS:HE3	1:A:1248:LYS:HA	1.72	0.70
1:B:239:GLU:HB3	1:B:285:ILE:HG12	1.73	0.70
1:B:1098:LYS:HG2	1:B:1098:LYS:O	1.90	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:A:157:GLY:HA2	1:A:160:ASP:HB2	1.72	0.70
1:B:109:THR:O	1:B:113:TYR:HB3	1.92	0.70
1:A:132:TRP:HB2	1:A:186:ILE:HD13	1.71	0.70
1:B:35:VAL:CG2	1:B:36:LEU:H	2.03	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: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:1019:THR:HB	1:A:1099:GLN:O	1.91	0.70
1:B:186:ILE:HG13	1:B:187:GLY:N	2.05	0.70
1:A:1121:CYS:HB2	1:A:1126:ASN:ND2	2.06	0.70
1:A:1218:ARG:NH2	1:A:1235:ASN:HD22	1.88	0.70
1:B:1218:ARG:NH2	1:B:1235:ASN:HD22	1.88	0.70
1:A:482:GLU:O	1:A:485:ARG:N	2.25	0.70
1:B:471:GLN:O	1:B:473:PRO:HD3	1.92	0.70
1:B:246:ALA:CB	1:B:277:LEU:HB3	2.22	0.70
1:A:416:GLY:N	1:A:577:THR:HG22	2.05	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:B:1031:VAL:HB	1:B:1056:VAL:HG12	1.75	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: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:781:THR:HG23	1:B:818:ALA:HB1	1.74	0.69
1:A:1193:LEU:HD11	1:A:1217:ALA:O	1.93	0.69
1:B:689:PRO:N	1:B:690:PRO:HD2	2.08	0.69
1:A:905:SER:O	1:A:907:THR:N	2.26	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:285:ILE:O	1:B:285:ILE:HD13	1.92	0.69
1:A:133:CYS:SG	1:A:931:ALA:HA	2.32	0.69
1:B:254:LEU:HD12	1:B:789:PHE:HZ	1.58	0.69
1:B:310:PHE:CZ	1:B:331:PHE:HB3	2.27	0.69
1:B:697:LEU:HA	1:B:700:ASN:HB2	1.73	0.69
1:A:1001:ALA:O	1:A:1005:ILE:HG12	1.92	0.69
1:A:697:LEU:HA	1:A:700:ASN:HB2	1.75	0.69
1:A:554:THR:OG1	1:A:562:GLU:HG3	1.93	0.69
1:B:447:VAL:HG13	1:B:454:ILE:HG21	1.75	0.69
1:B:1248:LYS:HA	1:B:1248:LYS:HE3	1.73	0.69
1:B:784:LEU:O	1:B:788:VAL:HG23	1.93	0.69
1:B:856:LEU:HD22	1:B:955:PHE:CD1	2.28	0.69
1:A: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:1106:ARG:HA	1:B:1109:LEU:HD13	1.75	0.69
1:A:826:GLY:HA2	1:A:829:LEU:HD12	1.73	0.69
1:A:795:GLN:HE21	1:A:796:ASP:H	1.40	0.69
1:B:1127:ILE:HD13	1:B:1180:ILE:HG23	1.75	0.69
1:A:1138:TYR:O	1:A:1141:ILE:HG12	1.92	0.69
1:B:552:GLU:HB3	1:B:555:SER:OG	1.92	0.69
1:B: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:B:1011:THR:N	1:B:1012:PRO:CD	2.56	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
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

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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:109:THR:O	1:A:113:TYR:HB3	1.93	0.68
1:A:762:SER:HA	1:A:765:THR:HG22	1.74	0.68
1:A:1031:VAL:HB	1:A:1056:VAL:HG12	1.75	0.68
1:A:60:HIS:O	1:A:63:ALA:HB3	1.93	0.68
1:A:394:HIS:HA	1:A:406:LEU:O	1.93	0.68
1:B:826:GLY:HA2	1:B:829:LEU:HD12	1.75	0.68
1:A:853:LEU:HB3	1:A:973:VAL:HG11	1.75	0.68
1:A:39:PHE:HE2	1:A:358:ALA:HB3	1.58	0.68
1:A:99:MET:HB3	1:A:960:VAL:O	1.93	0.68
1:A:559:THR:O	1:A:562:GLU:HB3	1.94	0.68
1: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:B:861:VAL:HB	1:B:862:PRO:HD3	1.76	0.68
1:B:267:LYS:H	1:B:270:LEU:HD21	1.57	0.68
1:B:1048:VAL:O	1:B:1049:LEU:HD22	1.94	0.68
1:A:390:PHE:HE1	1:A:432:THR:HB	1.59	0.68
1:A:1054:LEU:HD11	1:A:1240:VAL:HG11	1.75	0.68
1:A:138:ARG:HH22	1:B:515:GLN:HE21	1.40	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:164:VAL:O	1:A:164:VAL:CG2	2.32	0.68
1:B:157:GLY:HA2	1:B:160:ASP:HB2	1.74	0.68
1:A:257:ILE:HD13	1:A:257:ILE:C	2.14	0.68
1:B:559:THR:O	1:B:562:GLU:HB3	1.93	0.68
1:A:705:PRO:HG2	1:A:706:TYR:H	1.59	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:251:GLU:OE1	1:A:811:THR:HB	1.94	0.67
1:A:405:ILE:CG2	1:A:428:GLY:HA2	2.25	0.67
1:B:1054:LEU:HD11	1:B:1240:VAL:HG11	1.75	0.67
1:B:766:PHE:HA	1:B:769:GLN:HE21	1.59	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:A:1039:ASN:ND2	1:A:1047:PRO:HA	2.09	0.67
1:B:1063:ALA:HB2	1:B:1236:ALA:CB	2.24	0.67
1:B:1039:ASN:CB	1:B:1047:PRO:HA	2.24	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:202:ILE:HD12	1:A:203:GLY:H	1.56	0.67
1:A:1039:ASN:CB	1:A:1047:PRO:HA	2.24	0.67
1:A:467:GLY:HA3	1:A:545:PRO:HG3	1.77	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: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: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:B:257:ILE:O	1:B:260:VAL:HB	1.95	0.67
1:A:856:LEU:HD22	1:A:955:PHE:CD1	2.28	0.67
1:B:792:MET:HA	1:B:795:GLN:HB2	1.77	0.67
1:A:1063:ALA:HB2	1:A:1236:ALA:CB	2.25	0.67
1:A:1202:LEU:HD21	1:A:1206:SER:HB3	1.76	0.67
1:B:1266:MET:O	1:B:1269:VAL:HG12	1.94	0.67
1:A:484:ILE:HG21	1:A:496:ILE:HG23	1.75	0.67
1:B:211:THR:HA	1:B:214:ILE:HD12	1.76	0.67
1:B:195:THR:HG23	1:B:196:PHE:H	1.60	0.67
1:B:1066:GLY:H	1:B:1072:LYS:HE2	1.60	0.67
1:B:1118:LEU:HB3	1:B:1129:TYR:OH	1.95	0.66
1:B:1001:ALA:O	1:B:1005:ILE:HG12	1.94	0.66
1:B:60:HIS:O	1:B:63:ALA:HB3	1.94	0.66
1:B:467:GLY:HA3	1:B:545:PRO:HG3	1.77	0.66
1:A:178:ILE:HG12	1:A:358:ALA:CB	2.25	0.66
1:A:1218:ARG:HH12	1:A:1235:ASN:ND2	1.93	0.66
1:B:1193:LEU:HD11	1:B:1217:ALA:O	1.95	0.66
1:B:858:LEU:HD12	1:B:859:ALA:N	2.11	0.66
1:A:825:THR:O	1:A:829:LEU:HG	1.94	0.66
1:B:447:VAL:HG13	1:B:454:ILE:CG2	2.25	0.66
1:A:906:LEU:HD23	1:A:906:LEU:O	1.96	0.66
1:B:1243:GLN:O	1:B:1246:LYS:HD2	1.96	0.66
1:B:502:GLU:C	1:B:504:ASN:H	1.97	0.66
1:B:283:LEU:HD12	1:B:284:GLY:N	2.10	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

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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: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:A:447:VAL:HG13	1:A:454:ILE:HG21	1.77	0.66
1:A:1189:GLN:N	1:A:1190:PRO:HD3	2.09	0.66
1:A:96:LYS:HG2	1:A:962:GLN:HB2	1.75	0.66
1:B:692:SER:HB2	1:B:695:ARG:HB3	1.77	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:267:LYS:H	1:A:270:LEU:HD21	1.61	0.66
1:A:978:VAL:HG21	2:A:6001:0JZ:H35A	1.78	0.66
1:B:1218:ARG:HH12	1:B:1235:ASN:ND2	1.93	0.66
1:A:506:TYR:O	1:A:510:MET:HG2	1.93	0.66
1:B:218:SER:HB2	1:B:219:PRO:CD	2.26	0.66
1:A:784:LEU:HD12	1:A:1004:ILE:HD11	1.77	0.66
1:A:1150:ILE:O	1:A:1154:ILE:HD13	1.95	0.66
1:A:257:ILE:O	1:A:260:VAL:HB	1.96	0.66
1:B:603:VAL:HG23	1:B:604:GLU:H	1.61	0.66
1:B:1185:ALA:O	1:B:1190:PRO:HD3	1.96	0.66
1:B:762:SER:HA	1:B:765:THR:HG22	1.76	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:1150:ILE:O	1:B:1154:ILE:HD13	1.94	0.66
1:A:508:PHE:CE2	1:A:534:ARG:HD2	2.30	0.66
1:B:883:LYS:O	1:B:887:GLU:HB2	1.95	0.66
1:B:56:ALA:O	1:B:59:ILE:HG13	1.96	0.66
1:B:1189:GLN:N	1:B:1190:PRO:HD3	2.11	0.66
1:B:183:GLY:O	1:B:186:ILE:HG12	1.96	0.66
1:B:820:GLN:HG3	1:B:1000:SER:CB	2.26	0.66
1:B:290:THR:HG22	1:B:770:GLY:C	2.17	0.66
1:A:175:VAL:HG13	1:A:176:SER:N	2.11	0.66
1:B:39:PHE:HE2	1:B:358:ALA:HB3	1.60	0.65
1:B:384:ILE:HG22	1:B:385:GLN:H	1.60	0.65
1:B:458:ASN:HD22	1:B:459:VAL:N	1.95	0.65
1:B:506:TYR:O	1:B:510:MET:HG2	1.96	0.65
1:A:331:PHE:O	1:A:334:VAL:HG12	1.96	0.65
1:B:178:ILE:HG12	1:B:358:ALA:CB	2.26	0.65
1:B:1202:LEU:HD21	1:B:1206:SER:HB3	1.77	0.65
1:A:324:ILE:O	1:A:326:GLN:N	2.30	0.65
1:A:1039:ASN:HD22	1:A:1047:PRO:HA	1.62	0.65
1:B:386:GLY:HA3	1:B:450:ASP:HA	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ALA:CB	1:A:277:LEU:HB3	2.23	0.65
1:A:792:MET:HA	1:A:795:GLN:HB2	1.77	0.65
1:B:178:ILE:HG12	1:B:358:ALA:HB2	1.77	0.65
1:A:363:LYS:O	1:A:367:ASN:HB3	1.97	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:858:LEU:HD12	1:A:859:ALA:N	2.11	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:154:GLN:NE2	1:A:162:HIS:NE2	2.42	0.65
1:A:538:ALA:O	1:A:541:LEU:HB3	1.97	0.65
1:B:311:TRP:HA	1:B:311:TRP:HE3	1.61	0.65
1:A:185:LYS:NZ	1:A:185:LYS:HB3	2.11	0.65
1:B:1138:TYR:O	1:B:1141:ILE:HG12	1.97	0.65
1:A:163:ASP:O	1:A:164:VAL:O	2.15	0.65
1:A:1118:LEU:HB3	1:A:1129:TYR:OH	1.95	0.65
1:A:426:GLY:O	1:A:599:GLY:HA2	1.96	0.65
1:A:424:ASN:HB3	1:A:598:ASP:OD1	1.97	0.65
1:A:1243:GLN:O	1:A:1246:LYS:HD2	1.96	0.65
1:A:902:THR:HG23	1:A:903:VAL:H	1.62	0.65
1:B:465:ILE:C	1:B:466:ILE:HD12	2.17	0.65
1:A:1185:ALA:O	1:A:1190:PRO:HD3	1.97	0.65
1:B:424:ASN:HB3	1:B:598:ASP:OD1	1.97	0.65
1:B: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: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: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:1011:THR:H	1:B:1012:PRO:CD	2.10	0.65
1:B:88:SER:O	1:B:90:ASN:N	2.30	0.65
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:35:VAL:CG2	1:A:36:LEU:H	2.02	0.64
1:A:1066:GLY:H	1:A:1072:LYS:HE2	1.61	0.64
1:A:1195:LEU:HD23	1:A:1214:LEU:HD11	1.78	0.64
1:B:121:VAL:HG23	1:B:122:LEU:N	2.12	0.64
1:A:509:ILE:HD12	1:A:510:MET:N	2.13	0.64
1:B:270:LEU:CD2	1:B:270:LEU:H	2.01	0.64
1:A:270:LEU:CD2	1:A:270:LEU:H	2.02	0.64
1:A:735:PHE:HD2	1:A:747:ASN:HD21	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ILE:HD13	1:B:257:ILE:C	2.17	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:A:59:ILE:HD11	1:A:124:VAL:HG21	1.78	0.64
1:B:423:GLY:HA2	1:B:597:PHE:O	1.97	0.64
1:B:158:TRP:CZ2	1:B:900:PHE:HB2	2.33	0.64
1:B:458:ASN:HD22	1:B:459:VAL:H	1.44	0.64
1:B:1203:ASP:O	1:B:1204:THR:O	2.15	0.64
1:A: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:363:LYS:O	1:B:367:ASN:HB3	1.97	0.64
1:A:1234:GLN:HA	1:A:1253:HIS:HD2	1.62	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:B:1014:ILE:HD12	1:B:1106:ARG:HH11	1.62	0.64
1:B:1080:GLU:OE2	1:B:1109:LEU:HD12	1.97	0.64
1:A:154:GLN:HE22	1:A:162:HIS:CD2	2.16	0.64
1:A:218:SER:HB2	1:A:219:PRO:CD	2.26	0.64
1:A:883:LYS:O	1:A:887:GLU:HB2	1.98	0.64
1:A:1080:GLU:OE2	1:A:1109:LEU:HD12	1.97	0.64
1:B:881:LYS:HB2	1:B:881:LYS:NZ	2.12	0.64
1:A:502:GLU:C	1:A:504:ASN:H	2.01	0.64
1:B:879:ALA:O	1:B:883:LYS:HG2	1.97	0.64
1:B:318:ILE:CD1	1:B:324:ILE:HD12	2.27	0.64
1:A:405:ILE:HG21	1:A:428:GLY:HA2	1.79	0.64
1:A:121:VAL:HG23	1:A:122:LEU:N	2.12	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: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:972:LEU:O	1:B:975:SER:HB2	1.98	0.64
1:A:49:TYR:CE2	1:A:134:LEU:HD12	2.33	0.64
1:A:458:ASN:HD22	1:A:459:VAL:H	1.45	0.64
1:A:90:ASN:HB2	1:A:91:MET:HE2	1.80	0.64
1:A:478:THR:HG21	1:A:482:GLU:HG3	1.78	0.63
1:B:780:LEU:O	1:B:784:LEU:HD23	1.98	0.63
1:B:703:GLU:HG2	1:B:784:LEU:HD21	1.78	0.63
1:A:311:TRP:HE3	1:A:311:TRP:HA	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLY:O	1:A:186:ILE:HG12	1.97	0.63
1:A:799:TRP:HE3	1:A:799:TRP:HA	1.63	0.63
1:A:221:LEU:HD11	1:A:309:ALA:HB3	1.80	0.63
1:A:718:GLY:HA3	1:A:837:ALA:HB2	1.80	0.63
1:A:846:SER:HA	1:A:849:TYR:CD1	2.34	0.63
1:B:394:HIS:HA	1:B:406:LEU:O	1.97	0.63
1:A:881:LYS:NZ	1:A:881:LYS:HB2	2.13	0.63
1:B:569:LEU:O	1:B:573:ARG:HG3	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:A:256:ALA:O	1:A:260:VAL:HG23	1.98	0.63
1:B:1039:ASN:ND2	1:B:1047:PRO:HA	2.12	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:611:LEU:HD23	1:A:618:TYR:HB2	1.80	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:B:1179:ARG:HH21	1:B:1209:VAL:HG11	1.61	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:B:981:ALA:HB3	2:B:6002:0JZ:H35	1.78	0.63
1:A:465:ILE:C	1:A:466:ILE:HD12	2.19	0.63
1:A:1267:VAL:O	1:A:1270:GLN:HB3	1.99	0.63
1:B:1234:GLN:HA	1:B:1253:HIS:HD2	1.63	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:288:ALA:CA	1:A:291:ALA:HB3	2.26	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:311:TRP:CE3	1:A:311:TRP:HA	2.33	0.63
1:A:1095:LYS:HD2	1:A:1095:LYS:H	1.62	0.63
1:B:144:ARG:NH1	1:B:175:VAL:HG11	2.14	0.63
1:A:780:LEU:O	1:A:784:LEU:HD23	1.98	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: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:784:LEU:O	1:A:788:VAL:HG23	1.98	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: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:45:LEU:H	1:A:45:LEU:HD22	1.63	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: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:843:ILE:O	1:B:846:SER:HB3	1.99	0.62
1:A:471:GLN:HG2	1:A:472:GLU:N	2.14	0.62
1:B:696:ILE:HD13	1:B:998:THR:HG23	1.79	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:A:39:PHE:CE2	1:A:355:ARG:HA	2.34	0.62
1:B:807:THR:O	1:B:811:THR:HG23	2.00	0.62
1:A:253:VAL:HB	1:A:1119:PHE:HE1	1.63	0.62
1:B:1048:VAL:HG23	1:B:1049:LEU:CD2	2.30	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:509:ILE:HD12	1:B:510:MET:N	2.15	0.62
1:B:267:LYS:HA	1:B:270:LEU:HD11	1.81	0.62
1:B:857:LEU:HD12	1:B:973:VAL:CG1	2.29	0.62
1:B:799:TRP:HE3	1:B:799:TRP:HA	1.64	0.62
1:A:1019:THR:OG1	1:A:1101:ASN:HA	1.99	0.62
1:A:799:TRP:CE3	1:A:799:TRP:HA	2.32	0.62
1:B:1063:ALA:HB3	1:B:1239:ILE:CA	2.28	0.62
1:A:388:LEU:N	1:A:388:LEU:HD12	2.14	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:A:308:LEU:HD12	1:A:751:PHE:HE2	1.62	0.62
1:B:608:HIS:ND1	1:B:618:TYR:HE2	1.97	0.62
1:A:195:THR:HB	1:A:340:SER:OG	1.99	0.62
1:B:207:GLY:HA3	1:B:211:THR:H	1.63	0.62
1:B:211:THR:O	1:B:214:ILE:HB	1.99	0.62
1:B:287:LYS:O	1:B:291:ALA:HB2	2.00	0.62
1:B:65:PRO:O	1:B:68:MET:N	2.33	0.62
1:A:696:ILE:HD13	1:A:998:THR:HG23	1.80	0.62
1:A:1196:ASP:HA	1:A:1226:ILE:CG1	2.29	0.62
1:A:1137:SER:O	1:A:1141:ILE:HG23	2.00	0.62
1:B:195:THR:HB	1:B:340:SER:OG	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1158:PRO:O	1:B:1159:ASP:HB2	2.00	0.62
1:A:820:GLN:HG3	1:A:1000:SER:CB	2.30	0.62
1:A:144:ARG:NH1	1:A:175:VAL:HG11	2.15	0.62
1:A:1048:VAL:HG23	1:A:1049:LEU:CD2	2.29	0.62
1:A:385:GLN:NE2	1:A:386:GLY:H	1.98	0.62
1:B:158:TRP:HE1	1:B:900:PHE:HB3	1.65	0.62
1:B:846:SER:HA	1:B:849:TYR:CD1	2.35	0.62
1:A:711:ILE:O	1:A:714:ALA:HB3	2.00	0.62
1:A:1179:ARG:HH21	1:A:1209:VAL:HG11	1.60	0.62
1:B:1037:VAL:HG12	1:B:1051:GLY:N	2.14	0.62
1:A:742:GLU:O	1:A:746:GLN:HG2	2.00	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: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:A:537:ILE:O	1:A:541:LEU:HB2	1.99	0.61
1:B:39:PHE:CE2	1:B:355:ARG:HA	2.35	0.61
1:B:916:TYR:O	1:B:920:LEU:HD23	1.99	0.61
1:B:217:ILE:HD11	1:B:331:PHE:HE2	1.64	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:956:GLY:O	1:B:966:THR:CB	2.46	0.61
1:B:574:GLU:HG3	1:B:574:GLU:O	1.98	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:324:ILE:HD13	1:B:326:GLN:HB3	1.83	0.61
1:A:806:THR:O	1:A:810:LEU:HG	2.00	0.61
1:A:1037:VAL:HG12	1:A:1051:GLY:N	2.14	0.61
1:B:1095:LYS:HD2	1:B:1095:LYS:H	1.64	0.61
1:B:238:LYS:NZ	1:B:242:ALA:HB2	2.15	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:67:MET:SD	1:B:113:TYR:HE1	2.23	0.61
1:B:718:GLY:HA3	1:B:837:ALA:HB2	1.81	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:MET:SD	1:A:113:TYR:HE1	2.24	0.61
1:A:204:PHE:CA	1:A:211:THR:HG21	2.30	0.61
1: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:A:217:ILE:HD11	1:A:331:PHE:HE2	1.65	0.61
1:A:267:LYS:CA	1:A:270:LEU:HD21	2.30	0.61
1:A:286:LYS:CA	1:A:289:ILE:HB	2.26	0.61
1:A:318:ILE:HD12	1:A:322:TYR:O	2.00	0.61
1:A:1216:LYS:CE	1:A:1216:LYS:HA	2.30	0.61
1:B:969:ASN:HD22	1:B:970:VAL:N	1.98	0.61
1:B:1075:VAL:O	1:B:1076:VAL:C	2.39	0.61
1:A:268:LYS:HZ2	1:A:272:ARG:HD3	1.66	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:B:611:LEU:HD23	1:B:618:TYR:HB2	1.81	0.61
1:B:766:PHE:O	1:B:769:GLN:HG2	2.00	0.61
1:A:722:PRO:HD3	1:A:982:MET:HE1	1.81	0.61
1:B:806:THR:O	1:B:810:LEU:HG	2.01	0.61
1:B:1038:PHE:CG	1:B:1039:ASN:N	2.68	0.61
1:A:603:VAL:HG23	1:A:604:GLU:H	1.66	0.61
1:A:1148:ALA:O	1:A:1149:ASN:HB2	2.01	0.61
1:B:968:GLU:O	1:B:971:LEU:HD23	2.01	0.61
1:A:492:THR:HG22	1:A:494:ASP:H	1.66	0.61
1:A:1158:PRO:O	1:A:1159:ASP:HB2	2.01	0.61
1:B: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: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: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:373:SER:O	1:A:374:PHE:HB3	2.01	0.60
1:A:1023:LYS:O	1:A:1025:ASN:N	2.34	0.60
1:A:238:LYS:NZ	1:A:242:ALA:HB2	2.15	0.60
1:B:1079:LEU:CD2	1:B:1194:LEU:HD21	2.29	0.60
1:A:268:LYS:NZ	1:A:272:ARG:HD3	2.16	0.60
1:A:733:GLY:HA3	1:A:968:GLU:HG3	1.83	0.60
1:A:365:ILE:HG22	1:A:366:ASP:N	2.14	0.60
1:A:1144:ALA:CA	1:A:1186:LEU:HD11	2.29	0.60
1:B:1148:ALA:O	1:B:1149:ASN:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:906:LEU:O	1:B:906:LEU:HD23	2.00	0.60
1:A:731:VAL:HG22	1:A:750:LEU:HB3	1.82	0.60
1:A:766:PHE:O	1:A:769:GLN:HG2	2.01	0.60
1:B:959:LEU:O	1:B:964:LEU:HB3	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:B:1038:PHE:O	1:B:1049:LEU:HB2	2.01	0.60
1:B:288:ALA:CA	1:B:291:ALA:HB3	2.25	0.60
1:B:849:TYR:CB	1:B:854:THR:OG1	2.49	0.60
1:A:267:LYS:HB3	1:A:790:LYS:CE	2.29	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:A:1075:VAL:O	1:A:1076:VAL:C	2.40	0.60
1:B:268:LYS:NZ	1:B:272:ARG:HD3	2.17	0.60
1:B:427:CYS:O	1:B:599:GLY:HA2	2.01	0.60
1:B:256:ALA:O	1:B:260:VAL:HG23	2.02	0.60
1:B:213:VAL:O	1:B:217:ILE:HG12	2.01	0.60
1:B:64:LEU:O	1:B:67:MET:HB3	2.02	0.60
1:A:211:THR:O	1:A:214:ILE:HB	2.01	0.60
1:A:1193:LEU:HB2	1:A:1223:CYS:CB	2.32	0.60
1: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:197:PHE:O	1:A:201:ILE:HD13	2.01	0.60
1:A:886:LEU:HD12	1:A:887:GLU:N	2.17	0.60
1:A:59:ILE:CG1	1:A:124:VAL:HG11	2.31	0.60
1:A:548:LEU:HD23	1:A:549:LEU:N	2.17	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:291:ALA:HA	1:A:294:SER:HB2	1.83	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:B:197:PHE:O	1:B:201:ILE:HD13	2.01	0.60
1:A:1063:ALA:HB3	1:A:1239:ILE:CA	2.26	0.60
1:B:406:LEU:HD12	1:B:409:LEU:HB2	1.84	0.60
1:A:1038:PHE:O	1:A:1049:LEU:HB2	2.02	0.60
1:B:163:ASP:C	1:B:165:GLY:H	2.05	0.60
1:A:608:HIS:ND1	1:A:618:TYR:HE2	1.97	0.60
1:A:540:ALA:O	1:A:543:ARG:HB3	2.02	0.59
1:A:900:PHE:O	1:A:903:VAL:HG12	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:THR:O	1:A:904:VAL:N	2.35	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:731:VAL:HG22	1:B:750:LEU:HB3	1.84	0.59
1:A:235:PHE:O	1:A:239:GLU:HG2	2.02	0.59
1:A:826:GLY:O	1:A:829:LEU:HB2	2.02	0.59
1:B:1020:GLN:CD	1:B:1020:GLN:N	2.56	0.59
1:A:807:THR:O	1:A:811:THR:HG23	2.01	0.59
1:A:387:ASN:O	1:A:450:ASP:O	2.20	0.59
1:B:978:VAL:CG1	2:B:6002:0JZ:H35B	2.30	0.59
1:A:468:VAL:HG22	1:A:549:LEU:HD13	1.84	0.59
1:B:268:LYS:HZ2	1:B:272:ARG:HD3	1.67	0.59
1:A:41:TYR:HE1	1:A:143:ILE:HD11	1.67	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:1023:LYS:C	1:A:1025:ASN:H	2.06	0.59
1:A:279:GLU:HG2	1:A:782:LYS:CD	2.32	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:B:938:PHE:O	1:B:941:THR:HB	2.02	0.59
1:B:81:VAL:HG13	1:B:99:MET:HG3	1.85	0.59
1:A:207:GLY:HA3	1:A:211:THR:N	2.17	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:O	1:B:1022:LEU:HD23	2.02	0.59
1:A:585:LEU:H	1:A:585:LEU:HD22	1.68	0.59
1:B:1144:ALA:HB1	1:B:1183:ALA:HB1	1.85	0.59
1:B:528:SER:OG	1:B:531:GLN:HG3	2.02	0.59
1:B:900:PHE:O	1:B:903:VAL:HG12	2.01	0.59
1:B:235:PHE:O	1:B:239:GLU:HG2	2.02	0.59
1:A:359:TYR:O	1:A:362:PHE:HB3	2.02	0.59
1:A:254:LEU:HD23	1:A:811:THR:CG2	2.30	0.59
1:A:388:LEU:HD11	1:A:547:ILE:HD12	1.84	0.59
1:B:933:VAL:O	1:B:934:PHE:C	2.40	0.59
1:A:725:SER:HA	2:A:6001:0JZ:C36	2.32	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:A:138:ARG:NH2	1:B:515:GLN:NE2	2.50	0.59
1:A:1018:SER:O	1:A:1101:ASN:HB2	2.02	0.59
1:B:617:ILE:O	1:B:621:LEU:HD23	2.03	0.59
1:B:913:GLU:HA	1:B:913:GLU:OE2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:938:PHE:O	1:A:941:THR:HB	2.02	0.59
1:B:185:LYS:HZ3	1:B:186:ILE:N	1.99	0.59
2:A:6001:0JZ:H36B	2:A:6001:0JZ:O27	2.02	0.59
1:B:1267:VAL:O	1:B:1270:GLN:HB3	2.02	0.59
1:B:1109:LEU:HD21	1:B:1188:ARG:NH1	2.17	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:B:107:MET:HA	1:B:110:TYR:CD2	2.38	0.59
1:B:239:GLU:CB	1:B:285:ILE:HG12	2.33	0.59
1:A:1020:GLN:HB3	1:A:1100:LEU:HD12	1.85	0.59
1:B:263:PHE:CE1	1:B:1129:TYR:HB3	2.36	0.59
1:A:198:GLY:O	1:A:202:ILE:HG13	2.02	0.59
1:A:170:ARG:HB2	1:A:170:ARG:HH11	1.67	0.59
1:B:49:TYR:OH	1:B:130:SER:HB2	2.03	0.59
1:A:720:LEU:O	1:A:723:ALA:HB3	2.02	0.59
1:A:129:VAL:O	1:A:132:TRP:HB3	2.03	0.59
1:A:148:PHE:HB3	1:A:913:GLU:CD	2.24	0.59
1:A:1109:LEU:HD21	1:A:1188:ARG:NH1	2.18	0.59
1:B:1120:ASP:HA	1:B:1165:VAL:CG2	2.33	0.59
1:A:617:ILE:O	1:A:621:LEU:HD23	2.03	0.59
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:779:ILE:HG13	1:A:780:LEU:H	1.66	0.58
1:A:1016:SER:O	1:A:1017:TYR:HB2	2.02	0.58
1:A:797:VAL:O	1:A:801:ASP:CG	2.40	0.58
1:A:1071:GLY:O	1:A:1075:VAL:HG23	2.03	0.58
1:A:902:THR:OG1	1:A:908:ARG:HD3	2.03	0.58
1:B:507:ASP:OD1	1:B:508:PHE:N	2.35	0.58
1:B:199:GLY:HA2	1:B:202:ILE:HD11	1.86	0.58
1:B:1261:GLY:H	1:B:1264:PHE:HB3	1.68	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
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:A:213:VAL:O	1:A:217:ILE:HG12	2.02	0.58
1:A:993:ASP:N	1:A:996:LYS:HZ1	2.01	0.58
1:A:945:MET:O	1:A:949:TYR:HD1	1.86	0.58
1:A:81:VAL:HG13	1:A:99:MET:HG3	1.86	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:B:1199:THR:CG2	1:B:1210:VAL:HG11	2.34	0.58
1:A:64:LEU:O	1:A:67:MET:HB3	2.03	0.58
1:B:1037:VAL:HG22	1:B:1087:ALA:H	1.68	0.58
1:A:804:LYS:HD3	1:A:804:LYS:N	2.19	0.58
1:B:585:LEU:H	1:B:585:LEU:HD22	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: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:199:GLY:HA2	1:A:202:ILE:HD11	1.85	0.58
1:A:1009:GLU:O	1:A:1010:LYS:HG3	2.03	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:492:THR:HG22	1:B:494:ASP:H	1.67	0.58
1:B:500:VAL:HG23	1:B:501:LYS:N	2.19	0.58
1:B:318:ILE:HD13	1:B:327:VAL:CG1	2.23	0.58
1:B:762:SER:O	1:B:765:THR:HG22	2.04	0.58
1:A:798:SER:HB3	1:A:1041:PRO:HG2	1.85	0.58
1:B:537:ILE:O	1:B:541:LEU:HB2	2.03	0.58
1:A:257:ILE:HG13	1:A:800:PHE:CG	2.38	0.58
1:A:602:ILE:O	1:A:603:VAL:HG13	2.04	0.58
1:B:263:PHE:HE1	1:B:1129:TYR:HB3	1.67	0.58
1:A:528:SER:OG	1:A:531:GLN:HG3	2.03	0.58
1:B:468:VAL:HG22	1:B:549:LEU:HD13	1.85	0.58
1:B:429:LYS:HD3	1:B:581:ILE:HG12	1.85	0.58
1:A:993:ASP:C	1:A:995:ALA:H	2.07	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:125:ALA:O	1:A:128:GLN:HG2	2.04	0.58
1:A:1184:ARG:O	1:A:1187:VAL:HB	2.03	0.58
1:A:507:ASP:OD1	1:A:508:PHE:N	2.36	0.58
1:B:711:ILE:HG13	1:B:832:ILE:HG21	1.85	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:766:PHE:O	1:A:767:PHE:C	2.40	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:1132:ASN:OD1	1:B:1134:ARG:HG2	2.03	0.58
1:A:158:TRP:CZ2	1:A:900:PHE:HB2	2.39	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:278:GLU:OE2	1:A:785:ARG:HD2	2.03	0.57
1:A:784:LEU:HD12	1:A:1004:ILE:CD1	2.34	0.57
1:A:359:TYR:HA	1:A:362:PHE:HB3	1.86	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:993:ASP:N	1:A:996:LYS:NZ	2.52	0.57
1:A:1037:VAL:HG22	1:A:1087:ALA:H	1.68	0.57
1:B:1037:VAL:HG22	1:B:1087:ALA:N	2.19	0.57
1:A:245:LYS:HA	1:A:245:LYS:HZ1	1.68	0.57
1:B:548:LEU:HD23	1:B:549:LEU:N	2.20	0.57
1:B:212:LEU:HD12	1:B:215:LEU:HD12	1.86	0.57
1:B:850:GLY:O	1:B:852:GLN:N	2.38	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:853:LEU:CG	1:A:973:VAL:HG21	2.29	0.57
1:A:1214:LEU:HD23	1:A:1214:LEU:O	2.03	0.57
1:A:961:THR:O	1:A:962:GLN:HB3	2.04	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:908:ARG:O	1:B:909:GLU:C	2.41	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:A:1031:VAL:HB	1:A:1056:VAL:CG1	2.35	0.57
1:A:1148:ALA:HB1	1:A:1179:ARG:O	2.04	0.57
1:B:603:VAL:HG21	1:B:617:ILE:HG12	1.86	0.57
1:B:311:TRP:HZ2	1:B:728:PHE:CE2	2.22	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:A:246:ALA:HB2	1:A:281:LYS:NZ	2.19	0.57
1:A:727:ILE:HD13	1:A:754:LEU:HD23	1.85	0.57
1:A:345:SER:HB3	1:A:346:PRO:HD3	1.87	0.57
1:A:1120:ASP:HA	1:A:1165:VAL:CG2	2.34	0.57
1:B:246:ALA:HB2	1:B:281:LYS:NZ	2.20	0.57
1:A:405:ILE:HG22	1:A:406:LEU:HD22	1.87	0.57
1:A:1261:GLY:H	1:A:1264:PHE:HB3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:THR:O	1:A:482:GLU:HB2	2.04	0.57
1:B:291:ALA:HA	1:B:294:SER:HB2	1.87	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:1120:ASP:HA	1:A:1165:VAL:HG21	1.87	0.57
1:A:933:VAL:O	1:A:934:PHE:C	2.43	0.57
1:A:1132:ASN:OD1	1:A:1134:ARG:HG2	2.04	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: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:718:GLY:O	1:B:722:PRO:CD	2.47	0.57
1:B:784:LEU:HD12	1:B:1004:ILE:CD1	2.34	0.57
1:B:818:ALA:O	1:B:821:VAL:HG22	2.05	0.57
1:B:725:SER:HG	1:B:979:PHE:HE1	1.52	0.57
1:A:107:MET:HA	1:A:110:TYR:CD2	2.38	0.57
1:A:358:ALA:O	1:A:362:PHE:CB	2.52	0.57
1:B:59:ILE:HD11	1:B:124:VAL:CG1	2.34	0.57
1:A:459:VAL:O	1:A:462:LEU:HB3	2.04	0.57
1:B:618:TYR:O	1:B:622:VAL:HG23	2.03	0.57
1:A:337:GLY:O	1:A:341:VAL:HG23	2.05	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:A:233:SER:O	1:A:236:THR:HB	2.05	0.57
1:B:110:TYR:HA	1:B:113:TYR:HD2	1.70	0.57
1:B:713:CYS:O	1:B:716:ILE:HG13	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:O	1:A:465:ILE:HG22	2.05	0.57
1:B:492:THR:C	1:B:494:ASP:N	2.57	0.57
1:B:379:HIS:C	1:B:381:PRO:HD3	2.24	0.57
1:B:215:LEU:C	1:B:219:PRO:HD2	2.25	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:245:LYS:NZ	1:B:245:LYS:HA	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:207:GLY:HA3	1:A:211:THR:HB	1.87	0.57
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:A:1137:SER:CB	1:A:1140:GLU:HB2	2.35	0.57
1:A:492:THR:C	1:A:494:ASP:N	2.56	0.57
1:B:492:THR:O	1:B:494:ASP:N	2.38	0.57
1:B:186:ILE:CG1	1:B:187:GLY:N	2.68	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:A:786:TYR:HE2	1:A:790:LYS:NZ	2.03	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:B:945:MET:O	1:B:949:TYR:HD1	1.87	0.56
1:A:1037:VAL:HG22	1:A:1087:ALA:N	2.19	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:862:PRO:O	1:B:866:ILE:HG13	2.05	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: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: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: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:1212:GLU:O	1:A:1215:ASP:HB3	2.05	0.56
1:A:1252:THR:HG23	1:A:1255:GLN:HB2	1.86	0.56
1:B: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:A:166:GLU:O	1:A:169:THR:HB	2.05	0.56
1:B:543:ARG:HH21	1:B:907:THR:HG23	1.70	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
1:B:834:GLN:HG3	1:B:835:ASN:N	2.19	0.56
1:A:131:PHE:O	1:A:132:TRP:C	2.44	0.56
1:B:810:LEU:O	1:B:813:ARG:HB2	2.05	0.56
1:A:1195:LEU:O	1:A:1226:ILE:HG12	2.05	0.56
1:A:1144:ALA:HB1	1:A:1183:ALA:HB1	1.86	0.56
1:B:401:LYS:HZ2	1:B:401:LYS:HB3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LEU:HD12	1:A:409:LEU:HB2	1.87	0.56
1:A:1027:LEU:H	1:A:1027:LEU:HD12	1.70	0.56
1:B:1144:ALA:CA	1:B:1186:LEU:HD11	2.27	0.56
1:A:908:ARG:O	1:A:909:GLU:C	2.42	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:1106:ARG:O	1:A:1109:LEU:HD22	2.04	0.56
1:B:118:GLY:O	1:B:119:ALA:C	2.44	0.56
1:A:419:VAL:HG23	1:A:593:VAL:HG13	1.88	0.56
1:B:1076:VAL:HG13	1:B:1194:LEU:HD22	1.88	0.56
1:A:508:PHE:O	1:A:512:LEU:HB2	2.06	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:286:LYS:HE2	1:B:778:GLU:HG2	1.86	0.56
1:B:708:VAL:O	1:B:711:ILE:HG22	2.05	0.56
1:B:70:ILE:O	1:B:72:GLY:N	2.39	0.56
1:B:716:ILE:HD11	1:B:765:THR:OG1	2.06	0.56
1:B:795:GLN:HE21	1:B:796:ASP:N	2.03	0.56
1:A:795:GLN:O	1:A:796:ASP:CB	2.54	0.56
1:A:603:VAL:HG21	1:A:617:ILE:HG12	1.87	0.56
1:A:245:LYS:NZ	1:A:245:LYS:HA	2.20	0.56
1:B:290:THR:HG22	1:B:770:GLY:O	2.04	0.56
1:B:1166:GLY:O	1:B:1167:ASP:HB3	2.05	0.56
1:A:438:ARG:O	1:A:439:LEU:C	2.41	0.56
1:B:163:ASP:C	1:B:165:GLY:N	2.59	0.56
1:A:618:TYR:O	1:A:622:VAL:HG23	2.05	0.56
1:A:552:GLU:O	1:A:555:SER:HB2	2.06	0.56
1:A:550:LEU:N	1:A:550:LEU:HD12	2.21	0.56
1:B:549:LEU:HD12	1:B:549:LEU:N	2.20	0.56
1:A:839:LEU:O	1:A:843:ILE:HG12	2.04	0.56
1:A:722:PRO:HB2	1:A:841:THR:CG2	2.34	0.56
1:A:53:GLY:O	1:A:54:THR:C	2.42	0.56
1:A:1260:LYS:HD2	1:A:1260:LYS:N	2.20	0.56
1:A:611:LEU:HB3	1:A:618:TYR:HB3	1.86	0.56
1:B:541:LEU:O	1:B:544:ASN:N	2.37	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:A:1090:VAL:HG13	1:A:1097:ILE:CB	2.31	0.56
1:B:233:SER:O	1:B:236:THR:HB	2.06	0.56
1:B:345:SER:HB3	1:B:346:PRO:HD3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:931:ALA:O	1:B:932:HIS:C	2.43	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:A:257:ILE:HG23	1:A:258:ARG:H	1.71	0.56
1:A:405:ILE:HG23	1:A:427:CYS:O	2.05	0.56
1:A:461:TYR:O	1:A:465:ILE:HG12	2.05	0.56
1:B:733:GLY:HA3	1:B:968:GLU:HG3	1.86	0.56
1:B:1192:ILE:HA	1:B:1222:THR:O	2.06	0.56
1:A:908:ARG:HH21	1:A:908:ARG:HG3	1.71	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:A:952:CYS:SG	1:A:977:ILE:HD11	2.47	0.56
1:A:1096:GLU:HB2	1:A:1099:GLN:HE21	1.71	0.56
1:B:993:ASP:C	1:B:995:ALA:H	2.09	0.56
1:B:1255:GLN:O	1:B:1258:ALA:HB3	2.05	0.56
1:A:158:TRP:NE1	1:A:900:PHE:CB	2.66	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:A:110:TYR:HA	1:A:113:TYR:HD2	1.71	0.55
1:A:818:ALA:O	1:A:821:VAL:HG22	2.06	0.55
1:B:53:GLY:O	1:B:54:THR:C	2.45	0.55
1:B:978:VAL:HG13	2:B:6002:0JZ:C35	2.29	0.55
1:A:601:VAL:HG13	1:A:601:VAL:O	2.06	0.55
1:B:1064:LEU:HB3	1:B:1226:ILE:HG22	1.87	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:1206:SER:O	1:B:1210:VAL:HG23	2.06	0.55
1:B:111:ALA:HA	1:B:114:TYR:HE1	1.70	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
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:A:186:ILE:CG1	1:A:187:GLY:N	2.69	0.55
1:A:1196:ASP:CG	1:A:1226:ILE:HD11	2.26	0.55
1:B:1048:VAL:C	1:B:1049:LEU:HD22	2.27	0.55
1:A:1260:LYS:H	1:A:1260:LYS:CD	2.17	0.55
1:B:617:ILE:HD12	1:B:617:ILE:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:907:THR:N	1:B:908:ARG:HE	2.04	0.55
1:B:711:ILE:O	1:B:715:ILE:HG13	2.07	0.55
1:A:310:PHE:CZ	1:A:331:PHE:HB3	2.42	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:A:795:GLN:HE21	1:A:796:ASP:N	2.04	0.55
1:A:519:LEU:H	1:A:519:LEU:CD1	2.13	0.55
1:B:401:LYS:HD2	1:B:401:LYS:N	2.19	0.55
1:A:1127:ILE:CD1	1:A:1180:ILE:HG23	2.36	0.55
1:A:496:ILE:O	1:A:500:VAL:HG22	2.06	0.55
1:A:925:ARG:CZ	1:B:519:LEU:HD12	2.37	0.55
1:A:324:ILE:C	1:A:326:GLN:N	2.59	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:356:GLY:HA2	1:A:359:TYR:CE1	2.41	0.55
1:B:1011:THR:H	1:B:1012:PRO:HD3	1.70	0.55
1:B:993:ASP:N	1:B:996:LYS:NZ	2.54	0.55
1:B:1137:SER:HB3	1:B:1140:GLU:CB	2.37	0.55
1:B:804:LYS:HD3	1:B:804:LYS:N	2.21	0.55
1:B:419:VAL:HG23	1:B:593:VAL:HG13	1.88	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:302:ILE:O	1:A:305:SER:HB3	2.06	0.55
1:A:260:VAL:O	1:A:263:PHE:HB3	2.05	0.55
1:B:1037:VAL:CG2	1:B:1087:ALA:HB3	2.36	0.55
1:A:103:LEU:HD13	1:A:960:VAL:HG22	1.86	0.55
1:A:584:ARG:O	1:A:588:VAL:HG23	2.06	0.55
1:A:550:LEU:HD13	1:A:580:VAL:HB	1.89	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:1005:ILE:O	1:A:1008:ILE:HG22	2.06	0.55
1:A:721:GLN:HB3	1:A:722:PRO:CD	2.37	0.55
1:A:724:PHE:CD1	1:A:754:LEU:HD22	2.42	0.55
1:A:882:ASP:O	1:A:886:LEU:HG	2.07	0.55
1:A:1037:VAL:CG2	1:A:1087:ALA:HB3	2.37	0.55
1:A:88:SER:O	1:A:90:ASN:N	2.39	0.55
1:A:1202:LEU:HG	1:A:1206:SER:HB2	1.87	0.55
1:B:146:LYS:O	1:B:150:ALA:HB2	2.07	0.55
1:B:888:GLY:O	1:B:892:ILE:HG12	2.06	0.55
1:B:839:LEU:O	1:B:843:ILE:HG12	2.06	0.55
1:A:214:ILE:HG12	1:A:331:PHE:CZ	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PHE:CZ	1:A:967:PHE:O	2.59	0.55
1:A:810:LEU:O	1:A:811:THR:C	2.45	0.55
1:A:617:ILE:N	1:A:617:ILE:HD12	2.22	0.55
1:B:601:VAL:O	1:B:601:VAL:HG13	2.06	0.55
1:B:188:MET:O	1:B:189:PHE:C	2.44	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:A:289:ILE:O	1:A:292:ASN:HB3	2.07	0.55
1:A:713:CYS:O	1:A:716:ILE:HG13	2.07	0.55
1:A:769:GLN:HG3	1:A:770:GLY:N	2.21	0.55
1:A:1064:LEU:HB3	1:A:1226:ILE:HG22	1.89	0.55
1:A:1079:LEU:C	1:A:1081:ARG:H	2.09	0.55
1:B:1042:THR:C	1:B:1044:PRO:HD2	2.26	0.55
1:A:405:ILE:CG2	1:A:427:CYS:O	2.55	0.55
1:B:602:ILE:O	1:B:603:VAL:HG13	2.07	0.55
1:A:1203:ASP:O	1:A:1206:SER:HB2	2.07	0.55
1:A:492:THR:O	1:A:494:ASP:N	2.40	0.55
1:B:111:ALA:HA	1:B:114:TYR:CE1	2.42	0.55
1:B:209:LYS:O	1:B:213:VAL:HG23	2.07	0.55
1:A:697:LEU:HB3	1:A:828:ARG:NH2	2.22	0.55
1:A:434:GLN:O	1:A:436:MET:N	2.39	0.55
1:B:1137:SER:O	1:B:1141:ILE:HG23	2.06	0.55
1:B:1260:LYS:H	1:B:1260:LYS:CD	2.19	0.55
1:A:691:ALA:O	1:A:692:SER:HB3	2.06	0.55
1:B:1071:GLY:O	1:B:1075:VAL:HG23	2.07	0.55
1:B:255:ALA:C	1:B:257:ILE:N	2.60	0.55
1:B:210:LEU:HD13	1:B:210:LEU:C	2.26	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:210:LEU:HD23	1:A:317:VAL:CG1	2.37	0.55
1:A:860:ILE:O	1:A:864:ILE:HG13	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:B:688:VAL:O	1:B:688:VAL:HG23	2.07	0.55
1:A:433:VAL:HG13	1:A:549:LEU:HD23	1.89	0.55
1:A:401:LYS:N	1:A:401:LYS:HD2	2.20	0.55
1:B:1077:GLN:O	1:B:1080:GLU:N	2.40	0.54
1:B:1151:HIS:HA	1:B:1154:ILE:HB	1.88	0.54
1:B:1195:LEU:O	1:B:1226:ILE:HG12	2.07	0.54
1:B:708:VAL:HG13	1:B:709:VAL:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:720:LEU:HD22	1:B:761:ILE:HG22	1.90	0.54
1:A:37:THR:O	1:A:38:MET:C	2.45	0.54
1:A:888:GLY:O	1:A:892:ILE:HG12	2.07	0.54
1:A:472:GLU:OE1	1:A:473:PRO:HD2	2.07	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:209:LYS:O	1:A:213:VAL:HG23	2.06	0.54
1:A:59:ILE:HD11	1:A:124:VAL:CG1	2.34	0.54
1:A:401:LYS:HB3	1:A:401:LYS:HZ3	1.72	0.54
1:B:100:PHE:HB2	1:B:961:THR:HG23	1.88	0.54
1:B:1097:ILE:O	1:B:1098:LYS:CB	2.55	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:859:ALA:O	1:A:863:ILE:HG12	2.08	0.54
1:A:1058:LYS:HA	1:A:1222:THR:OG1	2.07	0.54
1:A:791:SER:N	1:A:794:ARG:HH21	2.05	0.54
1:A:1063:ALA:CB	1:A:1239:ILE:HG12	2.37	0.54
1:B:51:LEU:O	1:B:52:VAL:C	2.46	0.54
1:A:117:ILE:O	1:A:121:VAL:HG13	2.08	0.54
1:B:611:LEU:HB3	1:B:618:TYR:HB3	1.90	0.54
1:B:254:LEU:N	1:B:254:LEU:HD22	2.22	0.54
1:A:1255:GLN:O	1:A:1258:ALA:HB3	2.06	0.54
1:A:1011:THR:HG23	1:A:1011:THR:O	2.07	0.54
1:A:527:LEU:N	1:A:527:LEU:HD23	2.21	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:705:PRO:O	1:A:706:TYR:HB3	2.07	0.54
1:B:431:THR:O	1:B:435:LEU:HD23	2.07	0.54
1:B:370:SER:C	1:B:372:ASP:H	2.10	0.54
1:B:1090:VAL:HG13	1:B:1097:ILE:CB	2.31	0.54
1:B:536:ALA:O	1:B:537:ILE:C	2.46	0.54
1:B:324:ILE:C	1:B:326:GLN:N	2.59	0.54
1:A:336:ILE:CG1	2:A:6001:0JZ:SE1	2.99	0.54
1:A:315:SER:OG	1:A:747:ASN:HB3	2.08	0.54
1:A:311:TRP:HB2	1:A:751:PHE:HB2	1.89	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:A:136:ALA:HB2	1:A:182:ILE:CB	2.32	0.54
1:B:1011:THR:N	1:B:1012:PRO:HD2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LEU:O	1:A:52:VAL:C	2.46	0.54
1:B:1033:PHE:HB3	1:B:1036:VAL:CG2	2.36	0.54
1:A:549:LEU:HD12	1:A:549:LEU:N	2.22	0.54
1:B:419:VAL:O	1:B:579:ILE:HA	2.08	0.54
1:B:861:VAL:HB	1:B:862:PRO:CD	2.38	0.54
1:B:297:ALA:O	1:B:301:LEU:HB2	2.08	0.54
1:B:812:THR:O	1:B:813:ARG:C	2.44	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:583:HIS:O	1:B:585:LEU:HD22	2.07	0.54
1:B:247:GLY:O	1:B:250:ALA:HB3	2.06	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:812:THR:O	1:A:813:ARG:C	2.45	0.54
1:B:1108:GLN:H	1:B:1108:GLN:HE21	1.56	0.54
1:A:536:ALA:O	1:A:537:ILE:C	2.46	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:1076:VAL:HG13	1:A:1194:LEU:HD22	1.88	0.54
1:B:1143:ARG:HG2	1:B:1143:ARG:HH11	1.73	0.54
1:A:103:LEU:HB2	1:A:960:VAL:HG23	1.89	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:A:482:GLU:O	1:A:484:ILE:N	2.40	0.54
1:B:131:PHE:O	1:B:132:TRP:C	2.46	0.54
1:B:358:ALA:O	1:B:362:PHE:CB	2.53	0.54
1:B:215:LEU:O	1:B:219:PRO:CD	2.54	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:59:ILE:HD12	1:A:59:ILE:C	2.27	0.54
1:A:1137:SER:HB3	1:A:1140:GLU:CB	2.37	0.54
1:A:1140:GLU:O	1:A:1143:ARG:HB3	2.08	0.54
1:B:1053:SER:C	1:B:1054:LEU:HD22	2.28	0.54
1:A:583:HIS:O	1:A:585:LEU:HD22	2.07	0.54
1:B:185:LYS:HG3	1:B:351:PHE:CD2	2.43	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:317:VAL:HG12	1:B:317:VAL:O	2.07	0.54
1:B:697:LEU:HB3	1:B:828:ARG:NH2	2.23	0.54
1:A:111:ALA:HA	1:A:114:TYR:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:C	1:A:219:PRO:HD2	2.28	0.54
1:A:215:LEU:O	1:A:219:PRO:CD	2.56	0.54
1:A:239:GLU:HG3	1:A:288:ALA:HB2	1.90	0.54
1:A:716:ILE:HD11	1:A:765:THR:CB	2.38	0.54
1:B:117:ILE:O	1:B:121:VAL:HG13	2.07	0.54
1:B:90:ASN:HB2	1:B:91:MET:HE2	1.89	0.54
1:A:191:GLN:O	1:A:195:THR:HG22	2.08	0.54
1:A:954:ARG:HG3	1:A:954:ARG:HH11	1.73	0.54
1:B:1019:THR:HG22	1:B:1100:LEU:HD12	1.89	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:852:GLN:HB2	1:A:853:LEU:HD22	1.90	0.53
1:A:969:ASN:ND2	1:A:970:VAL:H	2.05	0.53
1:A:1048:VAL:C	1:A:1049:LEU:HD22	2.28	0.53
1:B:166:GLU:O	1:B:169:THR:HB	2.07	0.53
1:A:188:MET:HB2	1:A:347:ASN:HB3	1.89	0.53
1:A:1108:GLN:H	1:A:1108:GLN:HE21	1.56	0.53
1:A:185:LYS:HZ2	1:A:185:LYS:HB3	1.73	0.53
1:A:1221:ARG:N	1:A:1221:ARG:HD2	2.23	0.53
1:A:1033:PHE:HB3	1:A:1036:VAL:CG2	2.36	0.53
1:B:617:ILE:H	1:B:617:ILE:HD12	1.74	0.53
1:B:969:ASN:ND2	1:B:970:VAL:N	2.57	0.53
1:B:152:MET:HG3	1:B:913:GLU:OE1	2.08	0.53
1:B:245:LYS:HA	1:B:245:LYS:HZ1	1.74	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:70:ILE:C	1:A:72:GLY:N	2.59	0.53
1:A:342:GLY:O	1:A:346:PRO:CD	2.56	0.53
1:B:1063:ALA:CB	1:B:1239:ILE:HG12	2.38	0.53
1:B:1142:VAL:HA	1:B:1161:TYR:OH	2.08	0.53
1:B:337:GLY:O	1:B:341:VAL:HG23	2.08	0.53
1:B:909:GLU:O	1:B:912:PHE:HB2	2.08	0.53
1:A:284:GLY:O	1:A:287:LYS:HB3	2.08	0.53
1:A:146:LYS:O	1:A:150:ALA:HB2	2.07	0.53
1:A:1039:ASN:HB2	1:A:1047:PRO:CA	2.37	0.53
1:A:48:LEU:O	1:A:52:VAL:HG23	2.08	0.53
1:A:437:GLN:NE2	1:A:468:VAL:HG21	2.23	0.53
1:A:1124:ALA:HB2	1:A:1161:TYR:O	2.08	0.53
1:A:1206:SER:O	1:A:1210:VAL:HG23	2.09	0.53
1:B:191:GLN:O	1:B:195:THR:HG22	2.07	0.53
1:B:533:GLN:O	1:B:536:ALA:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:185:LYS:HG3	1:A:351:PHE:CD2	2.43	0.53
1:A:931:ALA:O	1:A:932:HIS:C	2.46	0.53
1:A:1144:ALA:HA	1:A:1186:LEU:CD1	2.32	0.53
1:B:1197:GLU:O	1:B:1198:ALA:C	2.46	0.53
1:A:434:GLN:NE2	1:A:439:LEU:HG	2.21	0.53
1:B:864:ILE:C	1:B:864:ILE:HD12	2.28	0.53
1:B:1005:ILE:HA	1:B:1008:ILE:HG22	1.89	0.53
1:B:853:LEU:H	1:B:853:LEU:HD22	1.73	0.53
1:A:203:GLY:C	1:A:211:THR:OG1	2.47	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:810:LEU:O	1:B:811:THR:C	2.46	0.53
1:A:1028:GLU:OE1	1:A:1058:LYS:HD2	2.08	0.53
1:A:620:LYS:HD3	1:A:624:THR:OG1	2.09	0.53
1:B:1127:ILE:CD1	1:B:1180:ILE:HG23	2.38	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: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:A:300:LEU:HA	1:A:303:TYR:HB2	1.90	0.53
1:A:1060:GLN:HB2	1:A:1237:ASP:OD1	2.09	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:405:ILE:HG22	1:B:406:LEU:HD22	1.91	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:419:VAL:O	1:A:579:ILE:HA	2.09	0.53
1:B:434:GLN:C	1:B:436:MET:H	2.13	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:279:GLU:HG2	1:A:782:LYS:HD2	1.91	0.53
1:B:620:LYS:HD3	1:B:624:THR:OG1	2.09	0.53
1:B:552:GLU:O	1:B:555:SER:HB2	2.09	0.53
1:A:483:ASN:O	1:A:486:TYR:HB2	2.08	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:68:MET:HG3	1:B:336:ILE:HD12	1.90	0.53
1:A:1092:LEU:HD22	1:A:1097:ILE:CD1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1124:ALA:HB2	1:B:1161:TYR:O	2.09	0.53
1:A:1123:ILE:O	1:A:1127:ILE:HG12	2.08	0.53
1:B:443:LEU:HD23	1:B:443:LEU:O	2.09	0.53
1:A:341:VAL:O	1:A:344:ALA:HB3	2.08	0.53
1:A:1254:GLN:N	1:A:1254:GLN:OE1	2.42	0.53
1:A:161:VAL:O	1:A:162:HIS:HB2	2.08	0.52
1:B:722:PRO:HG2	1:B:841:THR:HB	1.90	0.52
1:B:1212:GLU:O	1:B:1215:ASP:HB3	2.08	0.52
1:A:420:ALA:HA	1:A:580:VAL:O	2.09	0.52
1:B:882:ASP:O	1:B:886:LEU:HG	2.09	0.52
1:A:978:VAL:HG21	2:A:6001:0JZ:C35	2.38	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: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:1197:GLU:O	1:A:1198:ALA:C	2.47	0.52
1:B:954:ARG:HH11	1:B:954:ARG:HG3	1.74	0.52
1:B:1186:LEU:HD12	1:B:1187:VAL:N	2.24	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:318:ILE:CD1	1:B:325:GLY:N	2.67	0.52
1:B:795:GLN:O	1:B:796:ASP:CB	2.50	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:B:59:ILE:C	1:B:59:ILE:HD12	2.29	0.52
1:A:390:PHE:HB2	1:A:411:LEU:O	2.09	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:398:PRO:HD3	1:A:440:TYR:CE2	2.44	0.52
1:B:240:LEU:O	1:B:243:TYR:HB3	2.09	0.52
1:B:1144:ALA:HA	1:B:1186:LEU:CD1	2.30	0.52
1:A:907:THR:N	1:A:908:ARG:HE	2.07	0.52
1:B:420:ALA:HA	1:B:580:VAL:O	2.09	0.52
1:B:202:ILE:HG12	1:B:333:SER:OG	2.09	0.52
1:B:318:ILE:CD1	1:B:324:ILE:H	2.22	0.52
1: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:1109:LEU:O	1:A:1109:LEU:HD23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1144:ALA:HB2	1:A:1187:VAL:CG2	2.40	0.52
1:A:1143:ARG:HH11	1:A:1143:ARG:HG2	1.73	0.52
1:A:573:ARG:HD2	1:A:578:THR:CG2	2.33	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: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: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:B:188:MET:HB2	1:B:347:ASN:HB3	1.91	0.52
1:B:418:THR:HG22	1:B:578:THR:CG2	2.40	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:349:GLU:O	1:B:352:ALA:N	2.42	0.52
1:B:548:LEU:C	1:B:549:LEU:HD12	2.30	0.52
1:A:311:TRP:HD1	1:A:754:LEU:HD12	1.74	0.52
1:A:69:LEU:HA	1:A:329:THR:HG21	1.91	0.52
1:A:827:SER:O	1:A:828:ARG:C	2.48	0.52
1:A:37:THR:O	1:A:40:ARG:N	2.37	0.52
1:A:1097:ILE:O	1:A:1098:LYS:CB	2.57	0.52
1:A:254:LEU:CD2	1:A:811:THR:HG22	2.39	0.52
1:A:548:LEU:C	1:A:549:LEU:HD12	2.30	0.52
1:B:406:LEU:HD12	1:B:409:LEU:CB	2.40	0.52
1:A:1095:LYS:HD2	1:A:1095:LYS:N	2.24	0.52
1:A:170:ARG:NH1	1:A:170:ARG:HB2	2.25	0.52
1:A:1011:THR:O	1:A:1012:PRO:C	2.48	0.52
1:B:151:ILE:C	1:B:153:ASN:H	2.12	0.52
1:A:240:LEU:O	1:A:243:TYR:HB3	2.09	0.52
1:B:1092:LEU:HB3	1:B:1097:ILE:CD1	2.36	0.52
1:B:1102:VAL:HG13	1:B:1103:GLN:N	2.24	0.52
1:A:418:THR:HG22	1:A:578:THR:CG2	2.39	0.52
1:A:902:THR:O	1:A:903:VAL:C	2.47	0.52
1:B:141:HIS:O	1:B:144:ARG:HB3	2.10	0.52
1:B:460:ARG:O	1:B:461:TYR:C	2.47	0.52
1:B:859:ALA:O	1:B:863:ILE:HG12	2.10	0.52
1:B:103:LEU:HD13	1:B:960:VAL:HG22	1.91	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:A:291:ALA:HA	1:A:294:SER:CB	2.39	0.52
1:A:697:LEU:HD12	1:A:697:LEU:C	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:967:PHE:HD1	1:A:968:GLU:H	1.58	0.52
1:A:979:PHE:HA	1:A:982:MET:SD	2.50	0.52
1:A:458:ASN:ND2	1:A:459:VAL:N	2.57	0.52
1:B:584:ARG:HA	1:B:584:ARG:NE	2.24	0.52
1:A:1108:GLN:N	1:A:1108:GLN:HE21	2.07	0.52
1:A:484:ILE:O	1:A:487:GLY:N	2.43	0.52
1:A:486:TYR:O	1:A:908:ARG:NH1	2.43	0.52
1: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: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:133:CYS:CB	1:A:931:ALA:HB1	2.39	0.52
1:A:1091:PHE:CE1	1:A:1096:GLU:HG2	2.32	0.52
1:A:1202:LEU:CD2	1:A:1206:SER:HB3	2.40	0.52
1:B: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:901:ARG:HD3	1:B:901:ARG:H	1.74	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:A:138:ARG:NH2	1:B:515:GLN:HG2	2.25	0.52
1:A:806:THR:HG23	1:A:809:ALA:H	1.75	0.52
1:A:432:THR:O	1:A:433:VAL:C	2.48	0.52
1:B:1124:ALA:HB2	1:B:1161:TYR:HB3	1.91	0.52
1:A:1027:LEU:N	1:A:1027:LEU:HD12	2.25	0.52
1:A:1108:GLN:NE2	1:A:1108:GLN:N	2.58	0.52
1:B:1219:GLU:HG3	1:B:1219:GLU:O	2.09	0.51
1:B:260:VAL:O	1:B:263:PHE:HB3	2.10	0.51
1:A:158:TRP:NE1	1:A:900:PHE:HB2	2.25	0.51
1:A:534:ARG:O	1:A:537:ILE:HB	2.09	0.51
1:B:352:ALA:O	1:B:355:ARG:N	2.42	0.51
1:B:1229:ARG:C	1:B:1231:SER:H	2.13	0.51
1:B:998:THR:O	1:B:1001:ALA:HB3	2.10	0.51
1:A:206:ARG:O	1:A:330:VAL:HG11	2.10	0.51
1:A:290:THR:HG22	1:A:770:GLY:C	2.31	0.51
1:A:708:VAL:HG13	1:A:709:VAL:N	2.24	0.51
1:A:843:ILE:HA	1:A:846:SER:CB	2.40	0.51
1:A:349:GLU:O	1:A:352:ALA:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1260:LYS:HD2	1:B:1260:LYS:N	2.22	0.51
1:A:373:SER:O	1:A:374:PHE:CB	2.57	0.51
1:B:584:ARG:O	1:B:588:VAL:HG23	2.10	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: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:A:106:GLU:OE2	1:A:109:THR:HB	2.09	0.51
1:A:202:ILE:HG12	1:A:333:SER:OG	2.10	0.51
1:A:711:ILE:O	1:A:715:ILE:HG13	2.10	0.51
1:A:175:VAL:CG1	1:A:176:SER:N	2.73	0.51
1:A:354:ALA:O	1:A:358:ALA:CB	2.58	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:A:59:ILE:HG12	1:A:124:VAL:HG11	1.92	0.51
1:A:460:ARG:O	1:A:461:TYR:C	2.48	0.51
1:A:247:GLY:O	1:A:250:ALA:HB3	2.09	0.51
1:B:915:MET:O	1:B:918:GLN:HB2	2.11	0.51
1:B:106:GLU:HG3	1:B:110:TYR:CZ	2.46	0.51
1:B:724:PHE:CE1	1:B:754:LEU:HD22	2.45	0.51
1:A:981:ALA:HB3	2:A:6001:0JZ:H33	1.93	0.51
1:A:720:LEU:HD22	1:A:761:ILE:HG22	1.91	0.51
1:A:144:ARG:HH12	1:A:175:VAL:HG11	1.76	0.51
1:A:1202:LEU:HG	1:A:1203:ASP:H	1.75	0.51
1:B:427:CYS:O	1:B:599:GLY:CA	2.57	0.51
1:B:1014:ILE:HG23	1:B:1014:ILE:O	2.10	0.51
1:B:1144:ALA:HB2	1:B:1187:VAL:HG23	1.92	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:480:ILE:O	1:B:481:ALA:C	2.48	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:B:275:ASN:HA	1:B:278:GLU:HB2	1.92	0.51
1:B:757:ILE:O	1:B:761:ILE:HD13	2.09	0.51
1:A:297:ALA:O	1:A:301:LEU:HB2	2.10	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:B:802:ASP:OD2	1:B:1041:PRO:HB2	2.10	0.51
1:A:379:HIS:HB2	1:A:456:THR:O	2.10	0.51
1:B:615:LYS:HA	1:B:619:PHE:CG	2.45	0.51
1:B:1225:VAL:HG13	1:B:1225:VAL:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:THR:HG22	1:A:578:THR:HG22	1.92	0.51
1:B:697:LEU:HD12	1:B:697:LEU:C	2.31	0.51
1:A:291:ALA:O	1:A:295:MET:SD	2.68	0.51
1:A:301:LEU:O	1:A:304:ALA:HB3	2.09	0.51
1:B:1035:GLY:C	1:B:1052:LEU:O	2.49	0.51
1:A:118:GLY:HA3	1:A:946:TYR:CD2	2.45	0.51
1:B:1056:VAL:CG2	1:B:1062:LEU:HB2	2.41	0.51
1:B:421:LEU:HD23	1:B:429:LYS:HA	1.92	0.51
1:A:113:TYR:CG	1:A:114:TYR:N	2.79	0.51
1:A:318:ILE:HD13	1:A:327:VAL:CG1	2.41	0.51
1:A:1151:HIS:HA	1:A:1154:ILE:HB	1.92	0.51
1:A:1192:ILE:HA	1:A:1222:THR:O	2.10	0.51
1:A:1196:ASP:HA	1:A:1226:ILE:HD11	1.91	0.51
1:B:59:ILE:HG12	1:B:124:VAL:HG11	1.93	0.51
1:B:1123:ILE:O	1:B:1127:ILE:HG12	2.10	0.51
1:A:374:PHE:CD2	1:A:375:SER:N	2.76	0.51
1:B:1254:GLN:OE1	1:B:1254:GLN:N	2.44	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:464:GLU:HG2	1:B:543:ARG:HH21	1.75	0.51
1:A:716:ILE:HD11	1:A:765:THR:HB	1.93	0.51
1:B:800:PHE:C	1:B:803:PRO:HD3	2.31	0.51
1:A:1218:ARG:HB2	1:A:1223:CYS:SG	2.51	0.51
1:B:1120:ASP:O	1:B:1164:ARG:NE	2.43	0.51
1:A:878:GLN:NE2	1:A:881:LYS:HD3	2.26	0.51
1:B:1218:ARG:HB2	1:B:1223:CYS:SG	2.51	0.51
1:B:133:CYS:HB3	1:B:931:ALA:HB1	1.91	0.51
1:B:573:ARG:HD2	1:B:578:THR:CG2	2.33	0.51
1:B:907:THR:C	1:B:908:ARG:HE	2.15	0.51
1:B:106:GLU:OE2	1:B:109:THR:HB	2.10	0.51
1:B:203:GLY:C	1:B:211:THR:OG1	2.49	0.51
1:B:718:GLY:HA3	1:B:837:ALA:CB	2.40	0.51
1:A:857:LEU:HG	1:A:977:ILE:HG12	1.92	0.51
1:A:1144:ALA:HB2	1:A:1187:VAL:HG23	1.91	0.51
1:A:962:GLN:O	1:A:962:GLN:HG2	2.11	0.51
1:B:498:LYS:HE2	1:B:499:ALA:N	2.26	0.51
1:A:615:LYS:HA	1:A:619:PHE:CG	2.46	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:113:TYR:CG	1:B:114:TYR:N	2.78	0.51
1:B:826:GLY:O	1:B:829:LEU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1005:ILE:HA	1:A:1008:ILE:HG22	1.92	0.51
1:A:762:SER:CA	1:A:765:THR:HG22	2.40	0.51
1:A:1120:ASP:O	1:A:1164:ARG:NE	2.44	0.51
1:B:48:LEU:O	1:B:52:VAL:HG23	2.10	0.51
1:A:949:TYR:N	1:A:949:TYR:CD1	2.79	0.51
1:B:962:GLN:HG2	1:B:962:GLN:O	2.10	0.51
1:B:86:LYS:HG2	1:B:738:GLY:O	2.11	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: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:B:314:THR:O	1:B:315:SER:C	2.49	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:1109:LEU:HD23	1:B:1109:LEU:O	2.11	0.50
1:A:158:TRP:O	1:A:164:VAL:HG12	2.10	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:1202:LEU:HG	1:B:1203:ASP:H	1.76	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:788:VAL:HG21	1:B:1004:ILE:HG13	1.94	0.50
1:B:845:ILE:O	1:B:848:ILE:HG12	2.12	0.50
1:A:1020:GLN:CG	1:A:1101:ASN:HB3	2.41	0.50
1:A:1102:VAL:HG13	1:A:1103:GLN:N	2.24	0.50
1:A:801:ASP:OD2	1:A:1082:PHE:HB3	2.11	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:248:ALA:O	1:B:251:GLU:HB2	2.11	0.50
1:B:1144:ALA:HB2	1:B:1187:VAL:CG2	2.41	0.50
1:A:915:MET:O	1:A:918:GLN:HB2	2.11	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
1:B:905:SER:HB2	1:B:908:ARG:CZ	2.41	0.50
1:A:702:THR:HB	1:A:703:GLU:OE1	2.10	0.50
1:A:717:ASN:HB3	1:A:833:PHE:CE1	2.46	0.50
1:B:791:SER:N	1:B:794:ARG:HH21	2.08	0.50
1:B:121:VAL:CG2	1:B:122:LEU:N	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:PHE:C	1:A:695:ARG:H	2.14	0.50
1:A:499:ALA:CB	1:A:542:VAL:HG22	2.41	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:214:ILE:HD11	1:A:330:VAL:HB	1.92	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:A:248:ALA:O	1:A:251:GLU:HB2	2.12	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:A:314:THR:CG2	1:A:327:VAL:HG21	2.36	0.50
1:A:318:ILE:CD1	1:A:324:ILE:H	2.24	0.50
1:A:61:GLY:HA3	1:A:194:ALA:HB2	1.94	0.50
1:B:1023:LYS:HB3	1:B:1026:MET:CG	2.37	0.50
1:B:978:VAL:HG22	2:B:6002:0JZ:H35B	1.93	0.50
1:B:118:GLY:HA3	1:B:946:TYR:CD2	2.46	0.50
1:A:617:ILE:HD12	1:A:617:ILE:H	1.74	0.50
1:A:121:VAL:CG2	1:A:122:LEU:N	2.74	0.50
1:A:85:SER:HA	1:A:963:GLN:OE1	2.11	0.50
1:A:584:ARG:NE	1:A:584:ARG:HA	2.26	0.50
1:A:534:ARG:O	1:A:537:ILE:N	2.45	0.50
1:B:398:PRO:HD3	1:B:440:TYR:CE2	2.45	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: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: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:824:ALA:O	1:A:828:ARG:HG2	2.11	0.50
1:A:1186:LEU:HD12	1:A:1187:VAL:N	2.26	0.50
1:A:797:VAL:CG1	1:A:798:SER:N	2.69	0.50
1:B:1064:LEU:HD13	1:B:1064:LEU:C	2.32	0.50
1:B:1092:LEU:CD2	1:B:1097:ILE:HD11	2.40	0.50
1:A:484:ILE:O	1:A:485:ARG:C	2.50	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ALA:C	1:A:257:ILE:N	2.62	0.50
1:A:406:LEU:HD12	1:A:409:LEU:CB	2.41	0.50
1:B:170:ARG:HB2	1:B:170:ARG:NH1	2.26	0.50
1:A:691:ALA:O	1:A:692:SER:CB	2.60	0.50
1:A:531:GLN:O	1:A:534:ARG: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:267:LYS:HG2	1:A:793:LEU:HG	1.93	0.50
1:A:892:ILE:O	1:A:893:ALA:C	2.50	0.50
1:A:57:ALA:O	1:A:60:HIS:HB3	2.11	0.50
1:A:959:LEU:O	1:A:964:LEU:HB3	2.12	0.50
1:B:421:LEU:O	1:B:581:ILE:HD12	2.11	0.50
1:B:207:GLY:C	1:B:209:LYS:H	2.15	0.50
1:A:106:GLU:HG3	1:A:110:TYR:CZ	2.46	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:A:1164:ARG:C	1:A:1166:GLY:N	2.65	0.50
1:B:1037:VAL:HG21	1:B:1087:ALA:HB3	1.94	0.50
1:B:878:GLN:NE2	1:B:881:LYS:HD3	2.26	0.50
1:A:533:GLN:O	1:A:536:ALA:HB3	2.11	0.50
1:A:902:THR:HG23	1:A:903:VAL:N	2.26	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: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: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:A:35:VAL:HG21	1:A:355:ARG:HH21	1.76	0.50
1:B:991:ALA:HB1	1:B:992:PRO:HD2	1.93	0.50
1:B:1197:GLU:OE2	1:B:1228:HIS:HB2	2.12	0.50
1:A:620:LYS:O	1:A:623:MET:N	2.45	0.50
1:A:1124:ALA:HB2	1:A:1161:TYR:HB3	1.93	0.50
1:B:394:HIS:O	1:B:443:LEU:HB3	2.11	0.50
1:A:227:ILE:HG22	1:A:228:TRP:N	2.27	0.50
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:A:777:GLY:HA3	1:A:822:LYS:HG3	1.93	0.49
1:B:967:PHE:HD1	1:B:968:GLU:H	1.56	0.49
1:A:480:ILE:O	1:A:481:ALA:C	2.49	0.49
1:A:485:ARG:O	1:A:488:ARG:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:TRP:HZ2	1:B:900:PHE:HB2	1.75	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:A:311:TRP:CD1	1:A:754:LEU:HD12	2.47	0.49
1:A:1056:VAL:CG2	1:A:1062:LEU:HB2	2.41	0.49
1:A:1037:VAL:HG21	1:A:1087:ALA:HB3	1.94	0.49
1:A:466:ILE:HG22	1:A:468:VAL:HG23	1.93	0.49
1:A:120:GLY:O	1:A:121:VAL:C	2.51	0.49
1:B:425:SER:HB2	1:B:598:ASP:O	2.12	0.49
1:B:1095:LYS:N	1:B:1095:LYS:HD2	2.26	0.49
1:A:238:LYS:HZ1	1:A:242:ALA:HB2	1.76	0.49
1:B:1139:GLU:CD	1:B:1139:GLU:H	2.14	0.49
1:B:1196:ASP:HA	1:B:1226:ILE:HD11	1.93	0.49
1:B:129:VAL:HG11	1:B:935:GLY:N	2.27	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:A:307:ALA:O	1:A:308:LEU:O	2.30	0.49
1:A:136:ALA:O	1:A:139:GLN:HB2	2.12	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:A:1229:ARG:C	1:A:1231:SER:H	2.14	0.49
1:B:1056:VAL:CG2	1:B:1060:GLN:HE22	2.23	0.49
1:A:158:TRP:CE2	1:A:900:PHE:HB2	2.48	0.49
1:B:858:LEU:C	1:B:858:LEU:HD12	2.33	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:A:147:PHE:O	1:A:150:ALA:HB3	2.13	0.49
1:A:174:ASP:O	1:A:175:VAL:C	2.51	0.49
1:A:1164:ARG:O	1:A:1166:GLY:N	2.44	0.49
1:B:238:LYS:HZ1	1:B:242:ALA:HB2	1.75	0.49
1:B:499:ALA:CB	1:B:542:VAL:HG22	2.42	0.49
1:B:144:ARG:HG2	1:B:920:LEU:HD11	1.93	0.49
1:B:206:ARG:O	1:B:330:VAL:HG11	2.12	0.49
1:B:291:ALA:HA	1:B:294:SER:CB	2.42	0.49
1:B:311:TRP:CE3	1:B:311:TRP:CA	2.96	0.49
1:B:842:GLY:HA2	1:B:979:PHE:CE2	2.47	0.49
1:A:291:ALA:CA	1:A:294:SER:HB2	2.42	0.49
1:A:786:TYR:HE2	1:A:790:LYS:HZ1	1.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:VAL:HG12	1:A:359:TYR:CZ	2.47	0.49
1:A:1079:LEU:C	1:A:1081:ARG:N	2.66	0.49
1:A:620:LYS:HD2	1:A:621:LEU:HD22	1.95	0.49
1:B:620:LYS:HD2	1:B:621:LEU:HD22	1.95	0.49
1:A:1202:LEU:HG	1:A:1206:SER:CB	2.42	0.49
1:B:1178:GLN:O	1:B:1181:ALA:HB3	2.13	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: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:972:LEU:CD1	1:B:972:LEU:H	2.22	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:253:VAL:O	1:A:254:LEU:HD13	2.11	0.49
1:B:949:TYR:CD1	1:B:949:TYR:N	2.80	0.49
1:B:1166:GLY:HA3	1:B:1171:GLN:OE1	2.12	0.49
1:A:992:PRO:C	1:A:994:TYR:H	2.16	0.49
1:A:1189:GLN:N	1:A:1190:PRO:CD	2.76	0.49
1:A:1095:LYS:CD	1:A:1095:LYS:H	2.24	0.49
1:B:314:THR:CG2	1:B:327:VAL:CG2	2.81	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:795:GLN:NE2	1:B:796:ASP:H	2.08	0.49
1:A:157:GLY:HA2	1:A:160:ASP:CB	2.41	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:A:505:ALA:HB1	1:A:508:PHE:CZ	2.47	0.49
1:B:434:GLN:O	1:B:436:MET:N	2.46	0.49
1:B:907:THR:C	1:B:908:ARG:NE	2.65	0.49
1:B:843:ILE:CA	1:B:846:SER:HB3	2.39	0.49
1:A:209:LYS:HA	1:A:212:LEU:HB3	1.95	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:A:1080:GLU:OE1	1:A:1109:LEU:HD12	2.12	0.49
1:A:1147:GLU:OE1	1:A:1216:LYS:HB2	2.11	0.49
1:B:57:ALA:O	1:B:60:HIS:HB3	2.13	0.49
1:A:485:ARG:O	1:A:488:ARG:N	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:TYR:HA	1:B:113:TYR:CD2	2.47	0.49
1:B:853:LEU:HB3	1:B:973:VAL:CG2	2.43	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:816:ASN:O	1:A:819:ALA:HB3	2.13	0.49
1:A:1035:GLY:C	1:A:1052:LEU:O	2.51	0.49
1:A:1197:GLU:OE2	1:A:1228:HIS:HB2	2.12	0.49
1:A:429:LYS:O	1:A:432:THR:N	2.46	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:1205:GLU:HA	1:B:1208:LYS:HB3	1.94	0.49
1:B:1147:GLU:OE1	1:B:1216:LYS:HB2	2.12	0.49
1:B:1076:VAL:HG13	1:B:1194:LEU:HB3	1.94	0.49
1:B:255:ALA:O	1:B:257:ILE:N	2.45	0.49
1:A:901:ARG:O	1:A:902:THR:C	2.51	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: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:706:TYR:O	1:A:707:PHE:CG	2.66	0.49
1:A:498:LYS:HE2	1:A:499:ALA:N	2.28	0.49
1:B:1102:VAL:HG13	1:B:1103:GLN:H	1.77	0.48
1:B:1080:GLU:OE1	1:B:1109:LEU:HD12	2.13	0.48
1:B:342:GLY:O	1:B:345:SER:HB3	2.12	0.48
1:B:462:LEU:O	1:B:465:ILE:N	2.45	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:415:SER:HA	1:B:577:THR:CG2	2.43	0.48
1:A:394:HIS:O	1:A:443:LEU:HB3	2.12	0.48
1:A:570:ASP:HA	1:A:573:ARG:NH1	2.28	0.48
1:B:933:VAL:O	1:B:935:GLY:N	2.46	0.48
1:B:270:LEU:HG	1:B:271:GLU:H	1.78	0.48
1:A:214:ILE:HG12	1:A:331:PHE:CE2	2.48	0.48
1:A:132:TRP:CD2	1:A:183:GLY:HA3	2.47	0.48
1:A:883:LYS:HA	1:A:886:LEU:HG	1.95	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:B:281:LYS:HD2	1:B:281:LYS:N	2.28	0.48
1:A:401:LYS:HB3	1:A:401:LYS:HZ2	1.77	0.48
1:B:409:LEU:HD21	1:B:597:PHE:CE1	2.47	0.48
1:A:418:THR:HA	1:A:578:THR:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:722:PRO:HA	1:B:979:PHE:HE1	1.78	0.48
1:A:213:VAL:O	1:A:216:ALA:HB3	2.13	0.48
1:A:1043:ARG:N	1:A:1044:PRO:HD2	2.27	0.48
1:B:741:PRO:O	1:B:742:GLU:HB2	2.13	0.48
1:B:370:SER:O	1:B:372:ASP:N	2.44	0.48
1:B:167:LEU:HD23	1:B:167:LEU:C	2.34	0.48
1:B:371:ILE:HG22	1:B:371:ILE:O	2.13	0.48
1:B:1091:PHE:CE1	1:B:1096:GLU:HG2	2.32	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:132:TRP:CD2	1:B:183:GLY:HA3	2.48	0.48
1:B:147:PHE:O	1:B:150:ALA:HB3	2.14	0.48
1:B: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:A:286:LYS:HE3	1:A:822:LYS:HZ1	1.78	0.48
1:B:792:MET:HE3	1:B:810:LEU:HD22	1.95	0.48
1:A:44:TRP:CD1	1:A:45:LEU:HD22	2.48	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:846:SER:HA	1:B:849:TYR:CG	2.49	0.48
1:B:837:ALA:HB1	1:B:982:MET:CE	2.43	0.48
1:A:788:VAL:HG21	1:A:1004:ILE:HG13	1.95	0.48
1:A:837:ALA:HB1	1:A:982:MET:CE	2.44	0.48
1:A:1097:ILE:O	1:A:1098:LYS:HB3	2.13	0.48
1:A:1166:GLY:HA3	1:A:1171:GLN:OE1	2.13	0.48
1:A:795:GLN:NE2	1:A:796:ASP:H	2.10	0.48
1:A:437:GLN:HE21	1:A:468:VAL:HG21	1.79	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:1204:THR:C	1:A:1206:SER:H	2.16	0.48
1:B:881:LYS:HZ3	1:B:881:LYS:HB2	1.78	0.48
1:B:131:PHE:CD2	1:B:131:PHE:C	2.86	0.48
1:B:979:PHE:HA	1:B:982:MET:SD	2.54	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:806:THR:HG23	1:B:809:ALA:H	1.78	0.48
1:A:1090:VAL:CG1	1:A:1097:ILE:HB	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1135:VAL:O	1:B:1137:SER:N	2.47	0.48
1:B:1014:ILE:HD12	1:B:1106:ARG:NH1	2.29	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:566:GLN:HA	1:B:569:LEU:HD12	1.96	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: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:846:SER:HA	1:A:849:TYR:CG	2.48	0.48
1:A:52:VAL:O	1:A:53:GLY:C	2.52	0.48
1:B:1036:VAL:HB	1:B:1052:LEU:CB	2.35	0.48
1:A:429:LYS:N	1:A:429:LYS:HD3	2.19	0.48
1:A:583:HIS:HB2	1:A:584:ARG:HH12	1.78	0.48
1:B:1192:ILE:HD13	1:B:1193:LEU:N	2.29	0.48
1:B:1149:ASN:OD1	1:B:1213:ALA:HB2	2.14	0.48
1:A:894:THR:O	1:A:895:GLU:C	2.52	0.48
1:A:204:PHE:HA	1:A:211:THR:CG2	2.41	0.48
1:A:175:VAL:CG1	1:A:176:SER:H	2.27	0.48
1:A:1098:LYS:O	1:A:1099:GLN:HB2	2.14	0.48
1:A:1186:LEU:HD12	1:A:1186:LEU:C	2.34	0.48
1:A:1225:VAL:O	1:A:1225:VAL:HG13	2.13	0.48
1:B:335:LEU:C	1:B:335:LEU:HD23	2.35	0.48
1:A:470:SER:HB2	1:A:471:GLN:OE1	2.14	0.48
1:A:425:SER:HB2	1:A:598:ASP:O	2.14	0.48
1:B:175:VAL:HG13	1:B:176:SER:H	1.78	0.48
1:B:476:PHE:O	1:B:478:THR:N	2.41	0.48
1:B:318:ILE:CD1	1:B:325:GLY:H	2.26	0.48
1:B:779:ILE:O	1:B:780:LEU:C	2.53	0.48
1:A:221:LEU:HD13	1:A:306:TYR:HA	1.96	0.48
1:A:281:LYS:N	1:A:281:LYS:HD2	2.28	0.48
1:A:335:LEU:C	1:A:335:LEU:HD23	2.34	0.48
1:A:761:ILE:HD12	1:A:761:ILE:H	1.79	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:991:ALA:HB1	1:A:992:PRO:HD2	1.96	0.48
1:A:1137:SER:HB3	1:A:1140:GLU:HB2	1.96	0.48
1:A:43:GLY:HA3	1:A:46:ASP:HB2	1.96	0.48
1:B:1079:LEU:C	1:B:1081:ARG:N	2.68	0.47
1:A:907:THR:C	1:A:908:ARG:NE	2.68	0.47
1:B:909:GLU:OE2	1:B:909:GLU:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:930:LYS:HA	1:B:933:VAL:CG2	2.44	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:A:217:ILE:HG13	1:A:218:SER:N	2.28	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:725:SER:HG	1:A:979:PHE:HE1	1.62	0.47
1:A:1064:LEU:C	1:A:1064:LEU:HD13	2.34	0.47
1:A:1078:LEU:HD23	1:A:1083:TYR:O	2.14	0.47
1:A:1092:LEU:CD2	1:A:1097:ILE:HD11	2.40	0.47
1:A:1076:VAL:HG13	1:A:1194:LEU:HB3	1.96	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:B:1193:LEU:HD21	1:B:1221:ARG:HH11	1.78	0.47
1:A:421:LEU:O	1:A:581:ILE:HD12	2.14	0.47
1:B:453:ASP:HB3	1:B:456:THR:HG23	1.96	0.47
1:B:892:ILE:HB	1:B:916:TYR:HE1	1.75	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:A:817:ASP:OD1	1:A:1000:SER:HB3	2.14	0.47
1:A:314:THR:O	1:A:315:SER:C	2.51	0.47
1:A:278:GLU:HB3	1:A:782:LYS:HG2	1.96	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:875:LEU:HD23	1:B:875:LEU:C	2.34	0.47
1:B:1032:GLN:HE21	1:B:1055:GLU:CG	2.27	0.47
1:A:534:ARG:O	1:A:535:ILE:C	2.50	0.47
1:B:1202:LEU:HG	1:B:1206:SER:CB	2.44	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: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:1123:ILE:HG13	1:B:1124:ALA:N	2.29	0.47
1:A:1107:ALA:HB3	1:A:1108:GLN:NE2	2.29	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:A:311:TRP:CA	1:A:311:TRP:CE3	2.97	0.47
1:B:808:GLY:O	1:B:810:LEU:N	2.47	0.47
1:B:686:GLU:HB2	1:B:813:ARG:HH21	1.79	0.47
1:A:1193:LEU:HD21	1:A:1221:ARG:HH11	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1149:ASN:OD1	1:A:1213:ALA:HB2	2.14	0.47
1:A:258:ARG:O	1:A:259:THR:C	2.52	0.47
1:A:157:GLY:HA2	1:A:160:ASP:OD2	2.15	0.47
1:A:438:ARG:O	1:A:439:LEU:O	2.31	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:1208:LYS:C	1:B:1208:LYS:HD3	2.35	0.47
1:B:1031:VAL:H	1:B:1056:VAL:HG13	1.78	0.47
1:B:258:ARG:O	1:B:259:THR:C	2.51	0.47
1:B:533:GLN:O	1:B:537:ILE:HG12	2.15	0.47
1:B:295:MET:C	1:B:297:ALA:N	2.68	0.47
1:B:753:LEU:O	1:B:754:LEU:C	2.53	0.47
1:B:401:LYS:HZ3	1:B:401:LYS:HB3	1.75	0.47
1:B:959:LEU:O	1:B:964:LEU:CB	2.62	0.47
1:B:1137:SER:HB3	1:B:1140:GLU:HB2	1.95	0.47
1:B:396:SER:HB3	1:B:443:LEU:HD12	1.97	0.47
1:B:967:PHE:CD1	1:B:968:GLU:N	2.82	0.47
1:A:704:TRP:CZ2	1:A:707:PHE:N	2.82	0.47
1:B:374:PHE:HD1	1:B:375:SER:H	1.61	0.47
1:A:1139:GLU:CD	1:A:1139:GLU:H	2.17	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:724:PHE:HA	1:A:727:ILE:CG2	2.44	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:53:GLY:O	1:A:56:ALA:N	2.48	0.47
1:A:435:LEU:H	1:A:435:LEU:HD23	1.80	0.47
1:A:533:GLN:O	1:A:537:ILE:HG12	2.14	0.47
1:B:900:PHE:O	1:B:901:ARG:C	2.53	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:314:THR:HG22	1:B:315:SER:N	2.29	0.47
1:B:957:ALA:O	1:B:958:TYR:C	2.53	0.47
1:B:318:ILE:HD11	1:B:325:GLY:H	1.77	0.47
1:B:838:ASN:C	1:B:838:ASN:HD22	2.18	0.47
1:A:777:GLY:CA	1:A:822:LYS:HG3	2.43	0.47
1:A:797:VAL:HG13	1:A:1082:PHE:O	2.15	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: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:796:ASP:O	1:A:797:VAL:C	2.52	0.47
1:B:116:GLY:O	1:B:117:ILE:C	2.52	0.47
1:A:468:VAL:HG12	1:A:469:VAL:N	2.29	0.47
1:A:1204:THR:O	1:A:1206:SER:N	2.48	0.47
1:A:705:PRO:HG2	1:A:706:TYR:N	2.27	0.47
1:B:1095:LYS:CD	1:B:1095:LYS:H	2.27	0.47
1:A:188:MET:O	1:A:189:PHE:C	2.50	0.47
1:A:589:ARG:HG2	1:A:589:ARG:HH11	1.80	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:B:1203:ASP:O	1:B:1206:SER:HB2	2.13	0.47
1:A:218:SER:CB	1:A:219:PRO:HD3	2.42	0.47
1:A:727:ILE:HG21	1:A:754:LEU:HD23	1.97	0.47
1:A:125:ALA:O	1:A:126:TYR:C	2.52	0.47
1:A:415:SER:HA	1:A:577:THR:HG21	1.97	0.47
1:A:1123:ILE:HG13	1:A:1124:ALA:N	2.30	0.47
1:A:502:GLU:OE1	1:A:541:LEU:HD11	2.14	0.47
1:B:157:GLY:HA2	1:B:160:ASP:OD2	2.15	0.47
1:B:531:GLN:O	1:B:534:ARG:HB3	2.14	0.47
1:B:320:LYS:O	1:B:323:SER:OG	2.32	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:185:LYS:O	1:A:186:ILE:C	2.52	0.47
1:B:59:ILE:HD11	1:B:124:VAL:CG2	2.45	0.47
1:A:58:ILE:O	1:A:60:HIS:N	2.48	0.47
1:A:875:LEU:HD23	1:A:875:LEU:C	2.34	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:434:GLN:C	1:B:436:MET:N	2.68	0.47
1:B:249:VAL:O	1:B:273:TYR:HB3	2.14	0.47
1:B:64:LEU:O	1:B:65:PRO:C	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:B:942:GLN:O	1:B:945:MET:N	2.48	0.47
1:A:476:PHE:O	1:A:478:THR:N	2.45	0.46
1:B:468:VAL:HG22	1:B:549:LEU:HB2	1.97	0.46
1:B:933:VAL:C	1:B:935:GLY:N	2.68	0.46
1:B:291:ALA:CA	1:B:294:SER:HB2	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLY:CA	1:A:210:LEU:HB3	2.45	0.46
1:A:998:THR:O	1:A:1001:ALA:HB3	2.15	0.46
1:A:1101:ASN:OD1	1:A:1103:GLN:HB3	2.15	0.46
1:A:1135:VAL:O	1:A:1137:SER:N	2.47	0.46
1:A:868:GLY:O	1:A:871:GLU:HB3	2.14	0.46
1:B:342:GLY:O	1:B:346:PRO:HD3	2.15	0.46
1:B:536:ALA:O	1:B:539:ARG:N	2.49	0.46
1:B: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:A:274:ASN:O	1:A:278:GLU:HG3	2.15	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:A:1218:ARG:NH1	1:A:1235:ASN:HD22	2.14	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:B:1116:PRO:HB3	1:B:1178:GLN:OE1	2.15	0.46
1:A:420:ALA:C	1:A:421:LEU:HD12	2.35	0.46
1:B:383:ASN:O	1:B:384:ILE:C	2.53	0.46
1:B:902:THR:O	1:B:903:VAL:C	2.54	0.46
1:B:207:GLY:CA	1:B:210:LEU:HB3	2.45	0.46
1:B:751:PHE:CD1	1:B:752:SER:N	2.83	0.46
1:A:200:PHE:O	1:A:201:ILE:C	2.54	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:1167:ASP:O	1:B:1168:LYS:HB2	2.16	0.46
1:A:121:VAL:HG23	1:A:122:LEU:H	1.78	0.46
1:B:714:ALA:HB1	1:B:833:PHE:HB2	1.98	0.46
1:B:852:GLN:HG3	1:B:955:PHE:CZ	2.51	0.46
1:B:957:ALA:O	1:B:958:TYR:O	2.33	0.46
1:A:278:GLU:HA	1:A:282:ARG:NH1	2.31	0.46
1:A:322:TYR:CE2	1:A:324:ILE:HD11	2.50	0.46
1:A:297:ALA:HB1	1:A:763:PHE:CD2	2.51	0.46
1:A:887:GLU:O	1:A:888:GLY:C	2.53	0.46
1:A:1167:ASP:O	1:A:1168:LYS:HB2	2.15	0.46
1:A:1149:ASN:O	1:A:1179:ARG:HD3	2.15	0.46
1:B:55:LEU:C	1:B:55:LEU:HD23	2.36	0.46
1:B:1164:ARG:O	1:B:1166:GLY:N	2.49	0.46
1:B:1039:ASN:HD22	1:B:1048:VAL:N	2.14	0.46
1:B:227:ILE:HG22	1:B:228:TRP:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1157:LEU:HD22	1:B:1157:LEU:N	2.30	0.46
1:B:1032:GLN:NE2	1:B:1055:GLU:HB2	2.30	0.46
1:A:158:TRP:HA	1:A:162:HIS:CD2	2.43	0.46
1:B:550:LEU:HD23	1:B:569:LEU:HD13	1.97	0.46
1:B:470:SER:HA	1:B:551:ASP:HB3	1.97	0.46
1:B:291:ALA:C	1:B:294:SER:H	2.19	0.46
1:B:831:VAL:O	1:B:832:ILE:C	2.54	0.46
1:B:1020:GLN:O	1:B:1026:MET:CE	2.64	0.46
1:A:992:PRO:O	1:A:994:TYR:N	2.49	0.46
1:B:1243:GLN:O	1:B:1244:ASN:C	2.53	0.46
1:A:165:GLY:H	1:A:167:LEU:H	1.63	0.46
1:A:167:LEU:C	1:A:167:LEU:HD23	2.36	0.46
1:B:589:ARG:HG2	1:B:589:ARG:HH11	1.80	0.46
1:B:1170:THR:HG22	1:B:1170:THR:O	2.15	0.46
1:A:550:LEU:HD23	1:A:569:LEU:HD13	1.97	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:765:THR:HG23	1:B:766:PHE:N	2.30	0.46
1:A:210:LEU:HG	1:A:322:TYR:CD2	2.51	0.46
1:A:709:VAL:HG13	1:A:710:GLY:N	2.31	0.46
1:A:766:PHE:O	1:A:769:GLN:N	2.49	0.46
1:A:892:ILE:HB	1:A:916:TYR:HE1	1.74	0.46
1:A:1218:ARG:O	1:A:1219:GLU:HB3	2.16	0.46
1:B:52:VAL:O	1:B:53:GLY:C	2.53	0.46
1:A:462:LEU:O	1:A:465:ILE:N	2.48	0.46
1:B:969:ASN:N	1:B:969:ASN:HD22	2.12	0.46
1:A:540:ALA:O	1:A:543:ARG:CB	2.63	0.46
1:A:901:ARG:O	1:A:904:VAL:HG12	2.16	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:293:ILE:CD1	1:B:773:PHE:HZ	2.29	0.46
1:A:324:ILE:CD1	1:A:326:GLN:H	2.26	0.46
1:A:972:LEU:HD12	1:A:972:LEU:N	2.24	0.46
1:A:342:GLY:O	1:A:345:SER:HB3	2.16	0.46
1:B:940:PHE:O	1:B:944:MET:HG2	2.16	0.46
1:A:1036:VAL:HB	1:A:1052:LEU:CB	2.36	0.46
1:A:83:ASN:O	1:A:86:LYS:HB3	2.16	0.46
1:A:93:GLU:CD	1:A:93:GLU:H	2.19	0.46
1:B:1101:ASN:OD1	1:B:1103:GLN:HB3	2.16	0.46
1:A:925:ARG:HG2	1:B:514:HIS:ND1	2.31	0.46
1:B:313:GLY:O	1:B:317:VAL:HG23	2.16	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:967:PHE:CD1	1:A:968:GLU:N	2.82	0.46
1:A:722:PRO:HA	1:A:979:PHE:CE1	2.50	0.46
1:B:686:GLU:HB2	1:B:813:ARG:NH2	2.30	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:B:1145:ALA:HA	1:B:1150:ILE:HG22	1.98	0.46
1:A:536:ALA:O	1:A:539:ARG:N	2.48	0.46
1:B:383:ASN:O	1:B:384:ILE:O	2.34	0.46
1:B:894:THR:O	1:B:895:GLU:C	2.54	0.46
1:B:704:TRP:CZ2	1:B:707:PHE:HB2	2.51	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: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:1114:GLN:O	1:A:1116:PRO:HD3	2.15	0.46
1:A:449:ILE:O	1:A:450:ASP:C	2.53	0.46
1:A:55:LEU:HD23	1:A:55:LEU:C	2.35	0.46
1:A:429:LYS:H	1:A:429:LYS:CD	2.18	0.46
1:A:1026:MET:HE1	1:A:1104:TRP:CZ3	2.51	0.46
1:A:1170:THR:O	1:A:1170:THR:HG22	2.15	0.46
1:B:1078:LEU:HD23	1:B:1083:TYR:O	2.16	0.46
1:A:570:ASP:O	1:A:573:ARG:N	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: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:147:PHE:O	1:A:148:PHE:C	2.54	0.46
1:A:356:GLY:HA2	1:A:359:TYR:HE1	1.79	0.46
1:B:1128:ALA:CB	1:B:1136:VAL:HG13	2.46	0.46
1:B:620:LYS:O	1:B:623:MET:N	2.48	0.46
1:A:585:LEU:HA	1:A:588:VAL:HB	1.97	0.46
1:B:1090:VAL:CG1	1:B:1097:ILE:HB	2.35	0.45
1:A:500:VAL:HG23	1:A:501:LYS:H	1.81	0.45
1:B:901:ARG:O	1:B:902:THR:C	2.55	0.45
1:B:214:ILE:HG12	1:B:331:PHE:CZ	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:THR:HB	1:A:326:GLN:OE1	2.16	0.45
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: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:386:GLY:CA	1:A:450:ASP:HA	2.44	0.45
1:A:930:LYS:HA	1:A:933:VAL:CG2	2.46	0.45
1:B:1246:LYS:HD2	1:B:1246:LYS:H	1.81	0.45
1:B:692:SER:CB	1:B:695:ARG:HD3	2.47	0.45
1:B:1155:ASP:O	1:B:1160:LYS:HE3	2.16	0.45
1:B:1218:ARG:O	1:B:1219:GLU:HB3	2.16	0.45
1:B:817:ASP:OD1	1:B:1000:SER:HB3	2.15	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:A:1196:ASP:HA	1:A:1226:ILE:CD1	2.46	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:399:SER:O	1:B:402:GLU:N	2.46	0.45
1:A:463:ARG:HH11	1:A:463:ARG:HG3	1.82	0.45
1:B:868:GLY:O	1:B:871:GLU:HB3	2.16	0.45
1:B:157:GLY:HA2	1:B:160:ASP:CB	2.43	0.45
1:B:570:ASP:O	1:B:573:ARG:N	2.48	0.45
1:B:218:SER:CB	1:B:219:PRO:CD	2.94	0.45
1:A:282:ARG:O	1:A:286:LYS:CB	2.61	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: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:415:SER:HA	1:A:577:THR:CG2	2.46	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:B:1164:ARG:C	1:B:1166:GLY:N	2.68	0.45
1:A:1037:VAL:O	1:A:1086:MET:N	2.50	0.45
1:A:396:SER:HB3	1:A:443:LEU:HD12	1.98	0.45
1:B:134:LEU:O	1:B:138:ARG:HG3	2.16	0.45
1:B:887:GLU:O	1:B:888:GLY:C	2.55	0.45
1:B:788:VAL:CG2	1:B:1004:ILE:HG13	2.46	0.45
1:A:727:ILE:O	1:A:731:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:809:ALA:O	1:B:813:ARG:HG2	2.16	0.45
1:A:1039:ASN:HD22	1:A:1048:VAL:N	2.14	0.45
1:A:927:ALA:HA	1:A:930:LYS:CE	2.37	0.45
1:A:454:ILE:HG23	1:A:455:ARG:N	2.32	0.45
1:B:1261:GLY:H	1:B:1264:PHE:CB	2.30	0.45
1:B:528:SER:O	1:B:532:LYS:HG3	2.17	0.45
1:B:311:TRP:HZ2	1:B:728:PHE:HE2	1.62	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:68:MET:HG3	1:A:336:ILE:CD1	2.46	0.45
1:A:779:ILE:CG1	1:A:780:LEU:N	2.79	0.45
1:A:981:ALA:CB	2:A:6001:0JZ:H33	2.46	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:B:1218:ARG:CZ	1:B:1235:ASN:HD22	2.29	0.45
1:B:801:ASP:HB3	1:B:1083:TYR:CE2	2.51	0.45
1:A:154:GLN:HG2	1:A:154:GLN:O	2.17	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
1:B:901:ARG:O	1:B:904:VAL:HG12	2.16	0.45
1:B:1202:LEU:CD2	1:B:1206:SER:HB3	2.44	0.45
1:B:60:HIS:O	1:B:63:ALA:N	2.50	0.45
2:B:6002:0JZ:O25	2:B:6002:0JZ:H29B	2.16	0.45
1:B:1048:VAL:HG23	1:B:1049:LEU:HD22	1.97	0.45
1:A:942:GLN:O	1:A:945:MET:N	2.49	0.45
1:B:860:ILE:HG21	1:B:948:SER:HB3	1.97	0.45
1:A:238:LYS:HZ3	1:A:242:ALA:HB2	1.82	0.45
1:B:937:THR:O	1:B:938:PHE:C	2.54	0.45
1:B:1092:LEU:CB	1:B:1097:ILE:HD11	2.38	0.45
1:A:902:THR:C	1:A:904:VAL:N	2.68	0.45
1:B:155:GLU:O	1:B:156:ILE:C	2.55	0.45
1:B:386:GLY:CA	1:B:450:ASP:HA	2.45	0.45
1:B:470:SER:HB2	1:B:471:GLN:OE1	2.16	0.45
1:B:249:VAL:HG12	1:B:249:VAL:O	2.17	0.45
1:B:833:PHE:CG	1:B:834:GLN:N	2.83	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:860:ILE:HG21	1:A:948:SER:HB3	1.97	0.45
1:B:792:MET:CA	1:B:795:GLN:HB2	2.46	0.45
1:A:1150:ILE:HG13	1:A:1150:ILE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1048:VAL:HG23	1:B:1049:LEU:HD23	1.97	0.45
1:A:943:ALA:O	1:A:944:MET:C	2.55	0.45
1:A:740:PRO:N	1:A:741:PRO:HD2	2.32	0.45
1:B:1249:GLU:O	1:B:1250:HIS:HB3	2.16	0.45
1:B:1114:GLN:O	1:B:1116:PRO:HD3	2.17	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:883:LYS:HA	1:B:886:LEU:HG	1.99	0.45
1:B:306:TYR:CG	1:B:307:ALA:N	2.84	0.45
1:B:696:ILE:O	1:B:700:ASN:CB	2.60	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:135:ALA:O	1:A:136:ALA:C	2.54	0.45
1:A:60:HIS:O	1:A:63:ALA:N	2.50	0.45
1:A:492:THR:C	1:A:494:ASP:H	2.19	0.45
1:A:728:PHE:C	1:A:728:PHE:CD1	2.91	0.45
1:B:463:ARG:HH11	1:B:463:ARG:HG3	1.81	0.45
1:B:892:ILE:O	1:B:893:ALA:C	2.54	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: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: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:B:885:GLU:HB3	1:B:923:PRO:HG3	1.97	0.45
1:B:996:LYS:HD3	1:B:996:LYS:N	2.19	0.45
1:A:993:ASP:O	1:A:995:ALA:N	2.47	0.45
1:B:689:PRO:HG2	1:B:690:PRO:CD	2.46	0.45
1:A:1157:LEU:HD22	1:A:1157:LEU:N	2.32	0.45
1:B:1150:ILE:O	1:B:1150:ILE:HG13	2.16	0.45
1:A:908:ARG:O	1:A:911:LYS:HB3	2.17	0.45
1:B:527:LEU:HB2	1:B:531:GLN:OE1	2.17	0.45
1:B:830:ALA:O	1:B:833:PHE:HB3	2.17	0.45
1:A:304:ALA:O	1:A:307:ALA:HB3	2.17	0.45
1:A:69:LEU:O	1:A:72:GLY:N	2.49	0.45
1:B:792:MET:O	1:B:795:GLN:N	2.50	0.45
1:A:1178:GLN:HA	1:A:1178:GLN:OE1	2.17	0.45
1:A:59:ILE:HD11	1:A:124:VAL:CG2	2.45	0.45
1:B:1037:VAL:HG23	1:B:1086:MET:HB2	1.98	0.45
1:B:492:THR:C	1:B:494:ASP:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:732:VAL:O	1:B:736:THR:HG23	2.16	0.45
1:B:1056:VAL:HG21	1:B:1062:LEU:HB2	1.99	0.44
1:B:1218:ARG:NH1	1:B:1235:ASN:HD22	2.14	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: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: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:ND2	1:A:838:ASN:C	2.70	0.44
1:A:1168:LYS:HD2	1:A:1168:LYS:N	2.31	0.44
1:A:1072:LYS:HB3	1:A:1226:ILE:HD12	1.98	0.44
1:B:121:VAL:HG23	1:B:122:LEU:H	1.80	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:B:454:ILE:HG23	1:B:455:ARG:N	2.32	0.44
1:B:1189:GLN:N	1:B:1190:PRO:CD	2.78	0.44
1:A:1023:LYS:C	1:A:1025:ASN:N	2.71	0.44
1:B:612:MET:HA	1:B:619:PHE:HB2	1.99	0.44
1:A:1205:GLU:HA	1:A:1208:LYS:HB3	1.97	0.44
1:B:1097:ILE:HG23	1:B:1105:LEU:HD22	1.98	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:911:LYS:O	1:A:914:THR:HB	2.17	0.44
1:B:486:TYR:O	1:B:908:ARG:NH1	2.50	0.44
1:B:693:PHE:N	1:B:693:PHE:HD2	2.13	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:270:LEU:HB3	1:A:789:PHE:CE1	2.53	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:382:ASP:O	1:A:384:ILE:HG13	2.18	0.44
1:B:690:PRO:HG2	1:B:1006:ARG:CZ	2.47	0.44
1:B:1037:VAL:O	1:B:1086:MET:N	2.50	0.44
1:B:740:PRO:N	1:B:741:PRO:HD2	2.32	0.44
1:A:1246:LYS:H	1:A:1246:LYS:HD2	1.82	0.44
1:B:433:VAL:HG13	1:B:549:LEU:HD23	1.99	0.44
1:B:318:ILE:CG1	1:B:325:GLY:N	2.80	0.44
1:A:269:GLU:O	1:A:270:LEU:C	2.54	0.44
1:A:1032:GLN:NE2	1:A:1055:GLU:HB2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1145:ALA:HA	1:A:1150:ILE:HG22	1.99	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:A:1037:VAL:HG23	1:A:1086:MET:HB2	1.98	0.44
1:A:467:GLY:H	1:A:545:PRO:CB	2.31	0.44
1:A:44:TRP:C	1:A:46:ASP:N	2.71	0.44
1:A:732:VAL:O	1:A:736:THR:HG23	2.18	0.44
1:A:393:ILE:O	1:A:393:ILE:HG13	2.17	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: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:716:ILE:HD12	1:A:717:ASN:N	2.32	0.44
1:A:757:ILE:HA	1:A:761:ILE:HD13	1.98	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:B:120:GLY:O	1:B:121:VAL:C	2.55	0.44
1:A:940:PHE:O	1:A:944:MET:HG2	2.16	0.44
1:A:88:SER:OG	1:A:89:THR:N	2.51	0.44
1:A:740:PRO:HG2	1:A:741:PRO:CD	2.44	0.44
1:A:407:LYS:HG3	1:A:407:LYS:O	2.18	0.44
1:A:1267:VAL:HG13	1:A:1270:GLN:OE1	2.17	0.44
1:A:1027:LEU:CD1	1:A:1027:LEU:H	2.29	0.44
1:A:508:PHE:CE1	1:A:509:ILE:HG23	2.53	0.44
1:B:147:PHE:O	1:B:148:PHE:C	2.54	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: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: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: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:1125:GLU:O	1:A:1126:ASN:C	2.56	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:151:ILE:HD12	1:B:167:LEU:HD11	2.00	0.44
1:B:1090:VAL:CG2	1:B:1091:PHE:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1178:GLN:OE1	1:B:1178:GLN:HA	2.18	0.44
1:B:1196:ASP:HA	1:B:1226:ILE:CD1	2.48	0.44
1:B:539:ARG:O	1:B:540:ALA:C	2.54	0.44
1:B:916:TYR:O	1:B:920:LEU:HB2	2.17	0.44
1:B:723:ALA:O	1:B:727:ILE:HG22	2.17	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: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:788:VAL:CG2	1:A:1004:ILE:HG13	2.47	0.44
1:A:837:ALA:HB1	1:A:982:MET:HE1	2.00	0.44
1:A:1090:VAL:CG2	1:A:1091:PHE:N	2.80	0.44
1:A:384:ILE:HG23	1:A:546:LYS:HE2	2.00	0.44
1:A:411:LEU:C	1:A:411:LEU:HD23	2.38	0.44
1:A:690:PRO:O	1:A:1006:ARG:NH2	2.50	0.44
1:B:88:SER:OG	1:B:89:THR:N	2.51	0.44
1:A:1261:GLY:H	1:A:1264:PHE:CB	2.30	0.44
1:B:393:ILE:HG13	1:B:393:ILE:O	2.17	0.44
1:B:93:GLU:H	1:B:93:GLU:CD	2.21	0.44
1:A:527:LEU:HB2	1:A:531:GLN:OE1	2.18	0.44
1:B:508:PHE:CE1	1:B:509:ILE:HG23	2.53	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:A:207:GLY:C	1:A:209:LYS:H	2.21	0.44
1:A:1041:PRO:O	1:A:1042:THR:HB	2.18	0.44
1:A:58:ILE:HG22	1:A:59:ILE:N	2.33	0.44
1:B:91:MET:HE3	1:B:91:MET:N	2.32	0.44
1:B:363:LYS:O	1:B:367:ASN:CB	2.66	0.44
1:B:615:LYS:HA	1:B:619:PHE:CD2	2.53	0.44
1:A:364:ILE:O	1:A:364:ILE:HG22	2.17	0.44
1:A:541:LEU:C	1:A:543:ARG:N	2.71	0.44
1:B:129:VAL:HG11	1:B:935:GLY:CA	2.48	0.44
1:B:855:LEU:HA	1:B:858:LEU:HG	2.00	0.44
1:A:313:GLY:O	1:A:317:VAL:HG23	2.18	0.44
2:A:6001:0JZ:SE3	2:A:6001:0JZ:H35B	2.68	0.44
1:A:708:VAL:HA	1:A:711:ILE:HG22	2.00	0.44
1:B:996:LYS:H	1:B:996:LYS:CD	2.16	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:A:466:ILE:O	1:A:466:ILE:HG22	2.17	0.44
1:A:602:ILE:HG12	1:A:603:VAL:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:VAL:CG2	1:A:122:LEU:H	2.31	0.44
1:A:1159:ASP:HB3	1:A:1162:ASN:HB2	2.00	0.44
1:B:793:LEU:C	1:B:793:LEU:HD13	2.37	0.44
1:B:1193:LEU:HD21	1:B:1221:ARG:NH1	2.33	0.44
1:A:573:ARG:O	1:A:575:GLY:N	2.46	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:911:LYS:C	1:B:911:LYS:HD3	2.38	0.44
1:B:781:THR:O	1:B:782:LYS:C	2.56	0.44
1:A:306:TYR:HE1	1:A:310:PHE:CE1	2.36	0.44
1:A:778:GLU:C	1:A:782:LYS:HE2	2.39	0.44
1:A:781:THR:O	1:A:782:LYS:C	2.56	0.44
1:B:810:LEU:O	1:B:813:ARG:N	2.51	0.44
1:A:798:SER:CB	1:A:1041:PRO:HG2	2.47	0.44
1:B:1037:VAL:HG22	1:B:1087:ALA:HB3	2.00	0.44
1:B:560:GLU:O	1:B:561:SER:C	2.56	0.44
1:A:704:TRP:CZ2	1:A:707:PHE:HB2	2.53	0.44
1:A:900:PHE:O	1:A:901:ARG:C	2.56	0.43
1:B:129:VAL:CG1	1:B:935:GLY:HA2	2.48	0.43
1:B:547:ILE:HG22	1:B:549:LEU:HD11	1.99	0.43
1:B:267:LYS:HA	1:B:790:LYS:HE2	2.00	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:75:THR:HB	1:B:326:GLN:OE1	2.17	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
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:748:SER:HA	1:A:751:PHE:CD1	2.53	0.43
1:A:144:ARG:CZ	1:A:175:VAL:HG21	2.48	0.43
1:A:1131:ASP:OD2	1:A:1188:ARG:NE	2.51	0.43
1:B:55:LEU:O	1:B:58:ILE:HB	2.17	0.43
1:A:429:LYS:C	1:A:431:THR:N	2.69	0.43
1:A:945:MET:O	1:A:949:TYR:CD1	2.68	0.43
1:A:689:PRO:HB2	1:A:690:PRO:CD	2.43	0.43
1:A:470:SER:HA	1:A:551:ASP:HB3	1.98	0.43
1:A:195:THR:HA	1:A:337:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ASP:C	1:A:164:VAL:HG22	2.38	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:716:ILE:HD12	1:B:717:ASN:N	2.32	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:B:791:SER:O	1:B:795:GLN:HB2	2.18	0.43
1:A:1097:ILE:HG23	1:A:1105:LEU:HD22	2.00	0.43
1:B:51:LEU:O	1:B:54:THR:HB	2.18	0.43
1:A:1036:VAL:O	1:A:1052:LEU:HB3	2.17	0.43
1:A:363:LYS:O	1:A:367:ASN:CB	2.66	0.43
1:B:552:GLU:O	1:B:553:ALA:C	2.57	0.43
1:B:195:THR:HA	1:B:337:GLY:HA2	1.99	0.43
1:A:96:LYS:O	1:A:100:PHE:HB2	2.18	0.43
1:A:612:MET:HA	1:A:619:PHE:HB2	2.00	0.43
1:A:912:PHE:O	1:A:915:MET:N	2.51	0.43
1:B:44:TRP:CD1	1:B:45:LEU:N	2.86	0.43
1:B:384:ILE:HG23	1:B:546:LYS:HE2	1.98	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:62:VAL:O	1:B:65:PRO:HG2	2.18	0.43
1:B:65:PRO:HG3	1:B:198:GLY:CA	2.48	0.43
1:A:266:GLN:HB2	1:A:270:LEU:CD2	2.49	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:1077:GLN:O	1:A:1078:LEU:C	2.56	0.43
1:A:434:GLN:C	1:A:436:MET:H	2.20	0.43
1:A:960:VAL:CG1	1:A:966:THR:OG1	2.67	0.43
1:B:419:VAL:CG2	1:B:593:VAL:HG13	2.48	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
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:359:TYR:HA	1:A:362:PHE:CB	2.46	0.43
1:A:1009:GLU:O	1:A:1010:LYS:CG	2.65	0.43
1:A:796:ASP:HA	1:A:800:PHE:CD2	2.54	0.43
1:A:957:ALA:O	1:A:960:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1144:ALA:O	1:B:1148:ALA:CB	2.65	0.43
1:B:1147:GLU:HB3	1:B:1186:LEU:HD22	2.00	0.43
1:A:478:THR:HG22	1:A:479:THR:N	2.20	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: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:833:PHE:O	1:B:834:GLN:C	2.56	0.43
1:A:273:TYR:O	1:A:274:ASN:O	2.36	0.43
1:A:773:PHE:CD1	1:A:774:GLY:N	2.87	0.43
1:A:1101:ASN:O	1:A:1102:VAL:C	2.57	0.43
1:A:796:ASP:O	1:A:797:VAL:O	2.35	0.43
1:A:59:ILE:O	1:A:63:ALA:HB2	2.19	0.43
1:B:1039:ASN:HB2	1:B:1047:PRO:CA	2.37	0.43
1:A:91:MET:HG3	1:A:91:MET:H	1.61	0.43
1:B:561:SER:O	1:B:562:GLU:C	2.56	0.43
1:A:615:LYS:HA	1:A:619:PHE:CD2	2.53	0.43
1:B:83:ASN:O	1:B:86:LYS:HB3	2.19	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: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: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:308:LEU:HD12	1:B:751:PHE:CE2	2.54	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:58:ILE:HG22	1:B:59:ILE:N	2.33	0.43
1:A:1252:THR:CG2	1:A:1255:GLN:HB2	2.49	0.43
1:B:1176:GLN:O	1:B:1177:LYS:C	2.56	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: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: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:765:THR:HG23	1:A:766:PHE:HD1	1.84	0.43
1:A:833:PHE:O	1:A:834:GLN:C	2.57	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:A:1031:VAL:H	1:A:1056:VAL:HG13	1.83	0.43
1:A:808:GLY:O	1:A:810:LEU:N	2.52	0.43
1:B:992:PRO:C	1:B:994:TYR:H	2.21	0.43
1:A:388:LEU:N	1:A:388:LEU:CD1	2.81	0.43
1:A:949:TYR:H	1:A:949:TYR:HD1	1.67	0.43
1:A:618:TYR:CE2	1:A:622:VAL:HG21	2.53	0.43
1:B:1076:VAL:CG1	1:B:1194:LEU:HD13	2.49	0.43
1:B:171:LEU:HD13	1:B:172:THR:N	2.34	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:312:TYR:O	1:B:314:THR:N	2.52	0.43
2:A:6001:0JZ:H29B	2:A:6001:0JZ:O25	2.19	0.43
1:A:796:ASP:OD2	1:A:1014:ILE:HD11	2.19	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:257:ILE:HG13	1:A:800:PHE:CD2	2.54	0.43
1:B:58:ILE:O	1:B:60:HIS:N	2.51	0.43
1:B:993:ASP:O	1:B:995:ALA:N	2.52	0.43
1:B:1040:TYR:O	1:B:1042:THR:HG22	2.19	0.43
1:A:943:ALA:C	1:A:945:MET:N	2.71	0.43
1:B:959:LEU:C	1:B:959:LEU:HD23	2.39	0.43
1:B:407:LYS:HG3	1:B:407:LYS:O	2.18	0.43
1:B:272:ARG:O	1:B:276:ASN:HB2	2.19	0.43
1:B:1252:THR:CG2	1:B:1255:GLN:HB2	2.49	0.43
1:B:431:THR:HG22	1:B:435:LEU:HD23	2.00	0.43
1:B:936:ILE:O	1:B:939:SER:OG	2.37	0.43
1:A:389:GLU:OE1	1:A:412:LYS:HB2	2.17	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
1:B:449:ILE:O	1:B:450:ASP:C	2.57	0.43
1:B:908:ARG:O	1:B:911:LYS:HB3	2.19	0.43
1:B:324:ILE:CD1	1:B:326:GLN:H	2.24	0.43
1:A:307:ALA:O	1:A:308:LEU:C	2.55	0.43
1:A:78:PHE:HZ	1:A:967:PHE:O	1.99	0.43
1:A:362:PHE:HA	1:A:365:ILE:HD12	2.01	0.43
1:A:1014:ILE:CD1	1:A:1106:ARG:HH22	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:ALA:O	1:A:813:ARG:HG2	2.19	0.43
1:A:116:GLY:O	1:A:117:ILE:C	2.56	0.43
1:B:740:PRO:O	1:B:743:THR:HG23	2.19	0.43
1:A:492:THR:O	1:A:493:MET:C	2.57	0.43
1:B:519:LEU:HD22	1:B:526:GLN:HE22	1.84	0.43
1:B:209:LYS:C	1:B:212:LEU:HB3	2.38	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:A:203:GLY:HA2	1:A:211:THR:OG1	2.17	0.43
1:A:315:SER:C	1:A:318:ILE:HG22	2.39	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: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:B:943:ALA:O	1:B:945:MET:N	2.52	0.43
1:A:103:LEU:HD22	1:A:960:VAL:HG22	2.01	0.43
1:A:560:GLU:O	1:A:561:SER:C	2.56	0.43
1:B:875:LEU:HD23	1:B:875:LEU:O	2.19	0.43
1:A:252:GLU:OE1	1:A:252:GLU:N	2.52	0.43
1:B:1131:ASP:OD2	1:B:1188:ARG:NE	2.52	0.42
1:A:909:GLU:OE2	1:A:909:GLU:N	2.45	0.42
1:B:158:TRP:HA	1:B:162:HIS:CD2	2.45	0.42
1:B:348:ILE:O	1:B:351:PHE:HB3	2.19	0.42
1:B:362:PHE:HA	1:B:365:ILE:HD12	2.01	0.42
1:B:540:ALA:O	1:B:543:ARG:CB	2.65	0.42
1:B:820:GLN:CB	1:B:1000:SER:HB2	2.49	0.42
1:B:696:ILE:O	1:B:700:ASN:N	2.52	0.42
1:B:705:PRO:CG	1:B:706:TYR:H	2.30	0.42
1:B:821:VAL:HG23	1:B:822:LYS: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: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:171:LEU:HD13	1:A:172:THR:N	2.34	0.42
1:B:53:GLY:O	1:B:56:ALA:N	2.52	0.42
1:A:59:ILE:HD12	1:A:59:ILE:O	2.19	0.42
1:B:1041:PRO:O	1:B:1042:THR:HB	2.19	0.42
1:A:561:SER:O	1:A:562:GLU:C	2.56	0.42
1:B:1267:VAL:HG13	1:B:1270:GLN:OE1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ILE:O	1:A:153:ASN:N	2.51	0.42
1:B:151:ILE:O	1:B:153:ASN:N	2.52	0.42
1:B:252:GLU:N	1:B:252:GLU:OE1	2.52	0.42
1:B:1176:GLN:OE1	1:B:1176:GLN:N	2.52	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:B:299:PHE:O	1:B:303:TYR:N	2.51	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:352:ALA:O	1:A:353:ASN:C	2.57	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:942:GLN:O	1:A:945:MET:CB	2.64	0.42
1:A:401:LYS:H	1:A:401:LYS:CD	2.24	0.42
1:B:1159:ASP:HB3	1:B:1162:ASN:HB2	2.00	0.42
1:B:1195:LEU:HB2	1:B:1225:VAL:HA	2.01	0.42
1:A:513:PRO:O	1:A:514:HIS:HB2	2.18	0.42
1:B:185:LYS:O	1:B:186:ILE:C	2.58	0.42
1:B:352:ALA:O	1:B:353:ASN:C	2.57	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:324:ILE:O	1:B:326:GLN:HB2	2.19	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:ND2	1:B:838:ASN:C	2.71	0.42
1:A:793:LEU:HD13	1:A:793:LEU:C	2.39	0.42
1:A:182:ILE:O	1:A:186:ILE:HG23	2.20	0.42
1:A:883:LYS:HA	1:A:886:LEU:CG	2.49	0.42
1:A:1179:ARG:CZ	1:A:1209:VAL:HG11	2.49	0.42
1:B:121:VAL:CG2	1:B:122:LEU:H	2.32	0.42
1:A:519:LEU:HD22	1:A:526:GLN:HE22	1.84	0.42
1:A:1076:VAL:CG1	1:A:1194:LEU:HD13	2.50	0.42
1:A:460:ARG:O	1:A:462:LEU:N	2.52	0.42
1:B:692:SER:HB2	1:B:695:ARG:HD3	2.01	0.42
1:A:1182:ILE:N	1:A:1182:ILE:HD12	2.34	0.42
1:B:389:GLU:OE1	1:B:412:LYS:HB2	2.19	0.42
1:B:154:GLN:O	1:B:154:GLN:HG2	2.19	0.42
1:B:432:THR:O	1:B:433:VAL:C	2.56	0.42
1:B:1229:ARG:C	1:B:1231:SER:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1207:GLU:OE2	1:B:1229:ARG:NH2	2.52	0.42
1:B:315:SER:C	1:B:318:ILE:HG22	2.40	0.42
1:A:981:ALA:HB1	2:A:6001:0JZ:H32	2.02	0.42
1:A:144:ARG:HG2	1:A:920:LEU:CD1	2.49	0.42
1:A:348:ILE:O	1:A:349:GLU:C	2.57	0.42
1:A:792:MET:O	1:A:795:GLN:N	2.53	0.42
1:A:1063:ALA:HB3	1:A:1239:ILE:HG12	2.01	0.42
1:A:60:HIS:O	1:A:63:ALA:CB	2.65	0.42
1:B:974:PHE:HB3	2:B:6002:0JZ:C30	2.49	0.42
1:A:1037:VAL:HG22	1:A:1087:ALA:HB3	2.00	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: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:1129:TYR:CD2	1:B:1184:ARG:HG3	2.54	0.42
1:A:474:VAL:HG11	1:A:901:ARG:CB	2.48	0.42
1:A:900:PHE:O	1:A:903:VAL:N	2.51	0.42
1:B:136:ALA:O	1:B:137:GLY:C	2.57	0.42
1:B:548:LEU:HD22	1:B:550:LEU:HD11	2.02	0.42
1:B:286:LYS:O	1:B:290:THR:CG2	2.63	0.42
1:B:727:ILE:HD12	1:B:753:LEU:HD23	1.99	0.42
1:A:209:LYS:CA	1:A:212:LEU:HB3	2.49	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:B:54:THR:O	1:B:58:ILE:HD13	2.19	0.42
1:B:1119:PHE:HD2	1:B:1121:CYS:SG	2.42	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:238:LYS:HZ3	1:B:242:ALA:HB2	1.83	0.42
1:B:1090:VAL:HG22	1:B:1097:ILE:HG13	2.01	0.42
1:A:506:TYR:CD1	1:A:509:ILE:HD11	2.54	0.42
1:B:178:ILE:HG12	1:B:358:ALA:HB1	2.00	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
1:B:905:SER:HB3	1:B:907:THR:OG1	2.18	0.42
1:B:278:GLU:HA	1:B:282:ARG:NH1	2.34	0.42
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:A:64:LEU:O	1:A:65:PRO:C	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LEU:O	1:A:56:ALA:C	2.58	0.42
1:A:471:GLN:HG2	1:A:472:GLU:H	1.80	0.42
1:A:188:MET:C	1:A:188:MET:SD	2.97	0.42
1:A:1207:GLU:OE2	1:A:1229:ARG:NH2	2.52	0.42
1:A:532:LYS:O	1:A:535:ILE:N	2.53	0.42
1:B:135:ALA:O	1:B:136:ALA:C	2.57	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: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:A:406:LEU:O	1:A:408:GLY:N	2.47	0.42
1:B:618:TYR:CE2	1:B:622:VAL:HG21	2.54	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:541:LEU:C	1:B:543:ARG:N	2.73	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:278:GLU:OE2	1:B:785:ARG:HD2	2.20	0.42
1:A:308:LEU:O	1:A:309:ALA:C	2.55	0.42
1:A:970:VAL:HG23	1:A:971:LEU:HD22	2.02	0.42
1:A:1020:GLN:CG	1:A:1101:ASN:CB	2.92	0.42
1:A:922:ILE:HB	1:A:923:PRO:CD	2.46	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:419:VAL:CG2	1:A:593:VAL:HG13	2.48	0.42
1:B:691:ALA:HA	1:B:1002:SER:HB3	2.01	0.42
1:A:1249:GLU:O	1:A:1250:HIS:HB3	2.20	0.42
1:B:1032:GLN:HB3	1:B:1091:PHE:HD2	1.85	0.42
1:B:266:GLN:HB2	1:B:270:LEU:HD22	2.01	0.42
1:B:328:LEU:HD11	1:B:728:PHE:HZ	1.84	0.42
1:B:765:THR:HG23	1:B:766:PHE:HD1	1.84	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:B:1125:GLU:O	1:B:1126:ASN:C	2.58	0.42
1:A:945:MET:SD	1:A:946:TYR:N	2.93	0.42
1:B:447:VAL:HG13	1:B:454:ILE:HG22	2.00	0.42
1:B:1185:ALA:O	1:B:1190:PRO:CD	2.67	0.42
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:LEU:HA	1:B:588:VAL:HB	2.02	0.42
1:B:492:THR:O	1:B:493:MET:C	2.58	0.42
1:A:692:SER:HB2	1:A:695:ARG:HB3	2.02	0.42
1:A:625:GLN:O	1:A:626:THR:HB	2.20	0.42
1:B:797:VAL:O	1:B:801:ASP:OD1	2.38	0.41
1:A:538:ALA:O	1:A:539:ARG:C	2.58	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:529:GLY:HA2	1:B:532:LYS:HD3	2.01	0.41
1:B:212:LEU:CD1	1:B:215:LEU:HD12	2.49	0.41
1:B:721:GLN:HG2	1:B:982:MET:HE3	2.02	0.41
1:A:820:GLN:CB	1:A:1000:SER:HB2	2.50	0.41
1:A:281:LYS:O	1:A:285:ILE:HG22	2.21	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: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:1092:LEU:HD22	1:A:1100:LEU:HD22	2.01	0.41
1:A:1129:TYR:CD2	1:A:1184:ARG:HG3	2.54	0.41
1:B:59:ILE:O	1:B:59:ILE:HD12	2.20	0.41
1:A:54:THR:O	1:A:58:ILE:HD13	2.20	0.41
1:A:99:MET:N	1:A:99:MET:SD	2.93	0.41
1:A:1229:ARG:C	1:A:1231:SER:N	2.74	0.41
1:A:1156:SER:OG	1:A:1157:LEU:HD22	2.20	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:A:697:LEU:CA	1:A:700:ASN:HB2	2.47	0.41
1:A:718:GLY:CA	1:A:837:ALA:HB2	2.50	0.41
1:A: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:741:PRO:O	1:A:742:GLU:HB2	2.20	0.41
1:B:96:LYS:O	1:B:100:PHE:HB2	2.20	0.41
1:B:1076:VAL:O	1:B:1079:LEU:HB3	2.19	0.41
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:215:LEU:HA	1:B:219:PRO:HD2	2.01	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:887:GLU:O	1:A:890:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:GLU:HB3	1:A:923:PRO:HG3	2.02	0.41
1:B:945:MET:SD	1:B:946:TYR:N	2.93	0.41
1:A:1076:VAL:O	1:A:1079:LEU:HB3	2.20	0.41
1:B:970:VAL:HG23	1:B:971:LEU:HD22	2.02	0.41
1:A:513:PRO:O	1:A:518:THR:OG1	2.39	0.41
1:A:905:SER:HB3	1:A:907:THR:OG1	2.21	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:34:SER:O	1:B:35:VAL:C	2.59	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:1229:ARG:O	1:B:1231:SER:N	2.53	0.41
1:B:286:LYS:HG2	1:B:778:GLU:CD	2.41	0.41
1:B:702:THR:C	1:B:704:TRP:H	2.23	0.41
1:A:756:LEU:HD12	1:A:757:ILE:H	1.79	0.41
1:A:144:ARG:O	1:A:145:GLN:C	2.59	0.41
1:A:39:PHE:CD2	1:A:355:ARG:HA	2.54	0.41
1:A:1164:ARG:O	1:A:1165:VAL:C	2.57	0.41
1:A:889:SER:OG	1:A:919:SER:HB2	2.20	0.41
1:B:59:ILE:O	1:B:63:ALA:HB2	2.21	0.41
1:A:155:GLU:O	1:A:156:ILE:C	2.58	0.41
1:A:1076:VAL:HG13	1:A:1194:LEU:HD13	2.01	0.41
1:A:388:LEU:H	1:A:388:LEU:HD12	1.83	0.41
1:B:617:ILE:H	1:B:617:ILE:CD1	2.33	0.41
1:A:740:PRO:O	1:A:743:THR:HG23	2.20	0.41
1:B:740:PRO:HG2	1:B:741:PRO:CD	2.45	0.41
1:A:1234:GLN:HA	1:A:1253:HIS:CD2	2.50	0.41
1:B:152:MET:CG	1:B:913:GLU:OE1	2.69	0.41
1:A:151:ILE:C	1:A:153:ASN:N	2.72	0.41
1:B:1250:HIS:C	1:B:1256:LEU:HD21	2.40	0.41
1:A:1050:GLN:O	1:A:1050:GLN:HG3	2.21	0.41
1:B:1129:TYR:O	1:B:1131:ASP:N	2.52	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:322:TYR:CZ	1:B:324:ILE:HG12	2.55	0.41
1:B:773:PHE:CD1	1:B:773:PHE:C	2.93	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:710:GLY:O	1:A:711:ILE:C	2.57	0.41
1:A:345:SER:O	1:A:346:PRO:C	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:VAL:HG22	1:A:1097:ILE:HG13	2.03	0.41
1:A:1176:GLN:O	1:A:1177:LYS:C	2.59	0.41
1:A:1176:GLN:N	1:A:1176:GLN:OE1	2.53	0.41
1:A:705:PRO:CG	1:A:706:TYR:H	2.31	0.41
1:A:1189:GLN:O	1:A:1190:PRO:O	2.39	0.41
1:A:583:HIS:HB2	1:A:584:ARG:NH1	2.35	0.41
1:B:583:HIS:HB2	1:B:584:ARG:NH1	2.35	0.41
1:A:245:LYS:NZ	1:A:245:LYS:CA	2.83	0.41
1:B:86:LYS:HE2	1:B:739:GLY:N	2.35	0.41
1:B:1079:LEU:O	1:B:1105:LEU:HD21	2.21	0.41
1:B:345:SER:O	1:B:346:PRO:C	2.57	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:848:ILE:HG13	1:B:848:ILE:O	2.21	0.41
1:B:808:GLY:O	1:B:809:ALA:C	2.58	0.41
1:A:1176:GLN:O	1:A:1179:ARG:HB2	2.20	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:617:ILE:CD1	1:A:617:ILE:H	2.33	0.41
1:B:409:LEU:HD21	1:B:597:PHE:CZ	2.56	0.41
1:A:740:PRO:N	1:A:741:PRO:CD	2.84	0.41
1:A:92:SER:OG	1:A:962:GLN:NE2	2.51	0.41
1:A:881:LYS:HZ2	1:A:881:LYS:HB2	1.81	0.41
1:B:188:MET:SD	1:B:188:MET:C	2.98	0.41
1:A:1250:HIS:C	1:A:1256:LEU:HD21	2.40	0.41
1:A:745:ARG:O	1:A:749:ASN:HB2	2.21	0.41
1:B:223:LEU:O	1:B:224:SER:C	2.59	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:900:PHE:O	1:B:902:THR:N	2.53	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:A:731:VAL:HA	1:A:750:LEU:CD1	2.50	0.41
1:A:147:PHE:CE2	1:A:365:ILE:HG12	2.56	0.41
1:A:1031:VAL:O	1:A:1055:GLU:HA	2.21	0.41
1:B:990:PHE:O	1:B:991:ALA:C	2.58	0.41
1:A:443:LEU:HD23	1:A:443:LEU:C	2.41	0.41
1:B:733:GLY:CA	1:B:968:GLU:HG3	2.51	0.41
1:A:494:ASP:O	1:A:497:GLU:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:PHE:CG	1:A:375:SER:N	2.89	0.41
1:B:151:ILE:C	1:B:153:ASN:N	2.73	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:906:LEU:HA	1:B:909:GLU:OE2	2.21	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:779:ILE:HA	1:B:782:LYS:HE3	2.03	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: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: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:B:922:ILE:HB	1:B:923:PRO:CD	2.45	0.41
1:A:459:VAL:O	1:A:460:ARG:C	2.56	0.41
1:B:422:VAL:O	1:B:597:PHE:O	2.39	0.41
1:B:255:ALA:O	1:B:256:ALA:C	2.59	0.41
1:B:1107:ALA:O	1:B:1188:ARG:HD3	2.21	0.41
1:A:503:ALA:O	1:A:504:ASN:C	2.58	0.41
1:A:568:ALA:O	1:A:569:LEU:C	2.57	0.41
1:B:551:ASP:HA	1:B:581:ILE:HG23	2.03	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:388:LEU:H	1:B:388:LEU:HD12	1.83	0.41
1:B:449:ILE:O	1:B:450:ASP:HB3	2.21	0.41
1:B:129:VAL:HG11	1:B:934:PHE:C	2.41	0.41
1:B:1203:ASP:O	1:B:1207:GLU:HG3	2.21	0.41
1:B:693:PHE:H	1:B:693:PHE:HD2	1.65	0.41
1:B:300:LEU:O	1:B:303:TYR:CB	2.68	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:342:GLY:O	1:A:346:PRO:HD2	2.20	0.41
1:A:883:LYS:HD3	1:A:886:LEU:HD21	2.02	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: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: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:B:54:THR:O	1:B:57:ALA:HB3	2.20	0.41
1:B:974:PHE:CD1	2:B:6002:0JZ:H30B	2.56	0.41
1:A:933:VAL:O	1:A:936:ILE:HG22	2.21	0.41
1:B:689:PRO:CD	1:B:690:PRO:HD2	2.51	0.41
1:A:942:GLN:O	1:A:943:ALA:C	2.58	0.41
1:B:948:SER:O	1:B:952:CYS:SG	2.76	0.41
1:A:91:MET:HE3	1:A:91:MET:N	2.36	0.41
1:A:1252:THR:O	1:A:1255:GLN:HB3	2.21	0.41
1:B:614:GLU:O	1:B:615:LYS:C	2.59	0.41
1:B:1156:SER:OG	1:B:1157:LEU:HD22	2.20	0.41
1:A:441:ASP:OD1	1:A:442:PRO:HD2	2.21	0.41
1:B:1213:ALA:O	1:B:1217:ALA:HB2	2.21	0.41
1:A:899:ASN:OD1	1:A:901:ARG:NH2	2.54	0.41
1:B:140:ILE:O	1:B:143:ILE:N	2.53	0.41
1:B: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: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: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:B:796:ASP:HA	1:B:800:PHE:CD2	2.56	0.41
1:A:471:GLN:N	1:A:471:GLN:OE1	2.52	0.41
1:B:1067:SER:OG	1:B:1244:ASN:ND2	2.54	0.41
1:B:1003:HIS:O	1:B:1007:ILE:HG13	2.21	0.41
1:A:901:ARG:O	1:A:904:VAL:N	2.44	0.40
1:B:147:PHE:CE2	1:B:365:ILE:HG12	2.56	0.40
1:B:381:PRO:CG	1:B:457:ILE:HB	2.50	0.40
1:B:534:ARG:O	1:B:537:ILE:CB	2.68	0.40
1:B: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:VAL:O	1:A:331:PHE:HD1	2.04	0.40
1:A:703:GLU:HA	1:A:783:ARG:HH12	1.86	0.40
1:A:853:LEU:HD11	1:A:956:GLY:HA2	2.03	0.40
1:A:346:PRO:O	1:A:349:GLU:HB3	2.21	0.40
1:A:892:ILE:HG12	1:A:892:ILE:H	1.49	0.40
1:A:928:MET:O	1:A:931:ALA:CB	2.65	0.40
1:A:1067:SER:OG	1:A:1244:ASN:ND2	2.54	0.40
1:A:1255:GLN:O	1:A:1258:ALA:N	2.54	0.40
1:A:1107:ALA:HB3	1:A:1108:GLN:HE22	1.86	0.40
1:B:471:GLN:OE1	1:B:471:GLN:N	2.49	0.40
1:B:500:VAL:CG2	1:B:501:LYS:N	2.84	0.40
1:B:310:PHE:CE2	1:B:331:PHE:HB3	2.55	0.40
1:B:279:GLU:HG2	1:B:782:LYS:NZ	2.35	0.40
1:A:212:LEU:CD1	1:A:215:LEU:HD12	2.50	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:183:GLY:O	1:A:184:ASP:C	2.60	0.40
1:A:1039:ASN:O	1:A:1040:TYR:C	2.59	0.40
1:A:810:LEU:O	1:A:813:ARG:N	2.54	0.40
1:A:58:ILE:C	1:A:60:HIS:N	2.72	0.40
1:B:1038:PHE:CZ	1:B:1040:TYR:N	2.89	0.40
1:A:462:LEU:HD12	1:A:466:ILE:CD1	2.51	0.40
1:A:1155:ASP:O	1:A:1160:LYS:HE3	2.21	0.40
1:B:745:ARG:O	1:B:749:ASN:HB2	2.21	0.40
1:A:925:ARG:NE	1:B:519:LEU:HD12	2.36	0.40
1:B:342:GLY:O	1:B:346:PRO:HD2	2.21	0.40
1:B:358:ALA:O	1:B:362:PHE:N	2.53	0.40
1:B:519:LEU:N	1:B:519:LEU:HD13	2.19	0.40
1:B:899:ASN:OD1	1:B:901:ARG:NH2	2.54	0.40
1:B:206:ARG:O	1:B:211:THR:HB	2.21	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:714:ALA:O	1:A:717:ASN:HB3	2.22	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:791:SER:O	1:A:795:GLN:HB2	2.21	0.40
1:A:387:ASN:ND2	1:A:415:SER:H	2.20	0.40
1:A:449:ILE:O	1:A:450:ASP:HB3	2.21	0.40
1:B:58:ILE:C	1:B:60:HIS:N	2.72	0.40
1:B:332:PHE:HE1	2:B:6002:0JZ:N24	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:VAL:O	1:A:405:ILE:HD12	2.21	0.40
1:B:1243:GLN:HG3	1:B:1246:LYS:HZ2	1.85	0.40
1:B:1132:ASN:C	1:B:1134:ARG:H	2.25	0.40
1:B:364:ILE:HG22	1:B:364:ILE:O	2.21	0.40
1:A:901:ARG:N	1:A:901:ARG:HD3	2.36	0.40
1:B:140:ILE:O	1:B:141:HIS:C	2.60	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:302:ILE:O	1:B:303:TYR:C	2.59	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:A:110:TYR:CA	1:A:113:TYR:HD2	2.34	0.40
1:A:770:GLY:HA2	1:A:773:PHE:CZ	2.56	0.40
1:A:1191:HIS:HA	1:A:1221:ARG:HB2	2.02	0.40
1:B:688:VAL:HB	1:B:1006:ARG:HH12	1.87	0.40
1:A:409:LEU:HD21	1:A:597:PHE:CZ	2.56	0.40
1:A:961:THR:O	1:A:962:GLN:CB	2.69	0.40
1:B:92:SER:O	1:B:96:LYS:HG3	2.21	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:479:THR:HA	1:A:518:THR:O	2.21	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: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:N	1:B:901:ARG:HD3	2.35	0.40
1:B:902:THR:C	1:B:904:VAL:N	2.75	0.40
1:B:327:VAL:O	1:B:331:PHE:HD1	2.04	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: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:971:LEU:O	1:A:972:LEU:C	2.60	0.40
1:A:382:ASP:C	1:A:384:ILE:N	2.75	0.40
1:B:990:PHE:O	1:B:991:ALA:O	2.40	0.40
1:A:92:SER:O	1:A:96:LYS:HG3	2.22	0.40
1:A:1159:ASP:O	1:A:1160:LYS:C	2.60	0.40
1:A:693:PHE:O	1:A:695:ARG:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:GLU:O	1:A:615:LYS:C	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1178/1284 (92%)	704 (60%)	302 (26%)	172 (15%)	0 6
1	B	1178/1284 (92%)	707 (60%)	305 (26%)	166 (14%)	0 6
All	All	2356/2568 (92%)	1411 (60%)	607 (26%)	338 (14%)	0 6

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 (i)

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%)	11 45
1	B	976/1065 (92%)	880 (90%)	96 (10%)	10 42
All	All	1952/2130 (92%)	1764 (90%)	188 (10%)	10 43

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	A	6001	-	27,39,39	1.87	6 (22%)	24,57,57	2.48	9 (37%)
2	0JZ	B	6002	-	27,39,39	1.54	4 (14%)	24,57,57	1.89	6 (25%)

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6002	0JZ	C15-C16	-2.62	1.44	1.50
2	A	6001	0JZ	C34-C18	2.03	1.60	1.54
2	B	6002	0JZ	C16-N17	2.44	1.39	1.34
2	A	6001	0JZ	C18-N17	2.85	1.52	1.46
2	A	6001	0JZ	C19-C18	2.97	1.54	1.51
2	B	6002	0JZ	C02-N03	3.56	1.42	1.34
2	A	6001	0JZ	C09-N10	3.73	1.42	1.34
2	A	6001	0JZ	C02-N03	4.22	1.43	1.34
2	B	6002	0JZ	C09-N10	4.27	1.43	1.34
2	A	6001	0JZ	C16-N17	5.27	1.46	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	6001	0JZ	C29-C28-C04	2.06	113.18	111.30
2	A	6001	0JZ	C15-C16-N17	2.18	119.96	115.10
2	B	6002	0JZ	C01-C02-N03	2.33	120.29	115.10
2	B	6002	0JZ	C18-N17-C16	2.71	126.58	122.02
2	A	6001	0JZ	C33-C31-C11	2.91	113.96	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	6002	0JZ	C11-N10-C09	2.98	127.04	122.02
2	A	6001	0JZ	C36-C34-C18	3.06	114.09	111.30
2	B	6002	0JZ	C04-N03-C02	3.45	127.82	122.02
2	A	6001	0JZ	C11-N10-C09	3.58	128.04	122.02
2	A	6001	0JZ	C30-C28-C04	3.87	114.84	111.30
2	B	6002	0JZ	C29-C28-C04	3.88	114.85	111.30
2	B	6002	0JZ	C33-C31-C11	3.91	114.87	111.30
2	A	6001	0JZ	C35-C34-C18	4.46	115.38	111.30
2	A	6001	0JZ	C18-N17-C16	5.13	130.66	122.02
2	A	6001	0JZ	C04-N03-C02	5.38	131.07	122.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 22 short contacts:

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

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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%)	-0.07	22 (1%)	70	61	118, 194, 243, 306	0
1	B	1182/1284 (92%)	-0.09	25 (2%)	67	57	123, 200, 243, 301	0
All	All	2364/2568 (92%)	-0.08	47 (1%)	68	58	118, 197, 244, 306	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	963	GLN	5.1
1	B	1199	THR	4.8
1	A	1084	ASP	4.2
1	B	228	TRP	4.1
1	A	574	GLU	4.0
1	A	577	THR	3.5
1	B	1136	VAL	3.3
1	B	1249	GLU	3.3
1	A	1179	ARG	3.1
1	B	85	SER	3.0
1	A	993	ASP	3.0
1	B	1128	ALA	2.9
1	B	1260	LYS	2.9
1	A	554	THR	2.8
1	B	603	VAL	2.8
1	A	961	THR	2.8
1	A	1260	LYS	2.7
1	B	988	SER	2.6
1	A	427	CYS	2.6
1	B	594	ILE	2.5
1	B	597	PHE	2.5
1	B	84	VAL	2.5
1	A	962	GLN	2.5
1	A	1163	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	600	GLY	2.5
1	B	97	ARG	2.5
1	A	424	ASN	2.4
1	B	767	PHE	2.4
1	A	1244	ASN	2.4
1	B	1172	LEU	2.4
1	B	217	ILE	2.3
1	B	1230	LEU	2.3
1	B	524	GLY	2.3
1	A	581	ILE	2.2
1	B	1127	ILE	2.2
1	A	442	PRO	2.2
1	A	107	MET	2.2
1	B	81	VAL	2.2
1	A	423	GLY	2.2
1	A	416	GLY	2.2
1	B	617	ILE	2.1
1	A	1106	ARG	2.1
1	B	1198	ALA	2.1
1	A	1083	TYR	2.1
1	B	962	GLN	2.1
1	B	206	ARG	2.0
1	A	552	GLU	2.0

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

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^{th} 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(Å^2)	Q<0.9
2	0JZ	A	6001	36/36	0.64	0.43	2.00	196,196,196,196	0
2	0JZ	B	6002	36/36	0.63	0.41	0.80	196,196,196,196	0

6.5 Other polymers (i)

There are no such residues in this entry.