



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 01:43 AM EDT

PDB ID : 3KM9  
Title : Structure of complement C5 in complex with the C-terminal beta-grasp domain of SSL7  
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Deposited on : unknown  
Resolution : 4.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

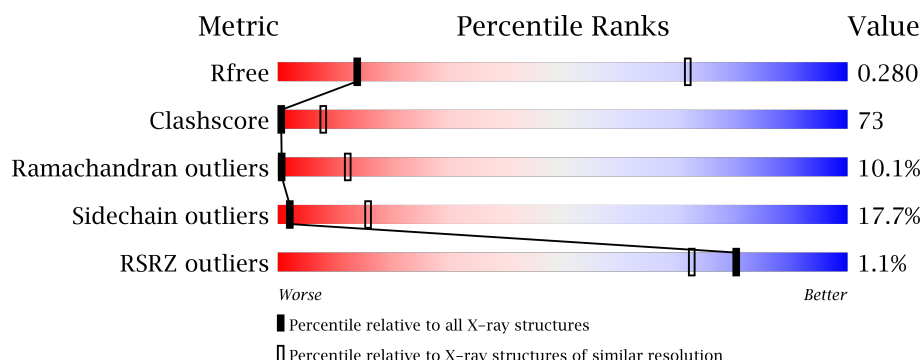
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.20 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))
$R_{free}$	100719	1177 (4.80-3.60)
Clashscore	112137	1025 (4.72-3.66)
Ramachandran outliers	110173	1024 (4.76-3.62)
Sidechain outliers	110143	1008 (4.76-3.62)
RSRZ outliers	101464	1188 (4.80-3.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1676	<div> <div>18%</div> <div>50%</div> <div>18%</div> <div>13%</div> </div>
1	B	1676	<div> <div>18%</div> <div>49%</div> <div>18%</div> <div>13%</div> </div>
2	X	103	<div> <div>9%</div> <div>37%</div> <div>52%</div> <div>10%</div> </div>
2	Y	103	<div> <div>5%</div> <div>38%</div> <div>52%</div> <div>9%</div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CD	A	1678	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 24809 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 Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1459	Total	C	N	O	S	0	0	0
			11541	7396	1903	2200	42			
1	B	1459	Total	C	N	O	S	0	0	0
			11541	7396	1903	2200	42			

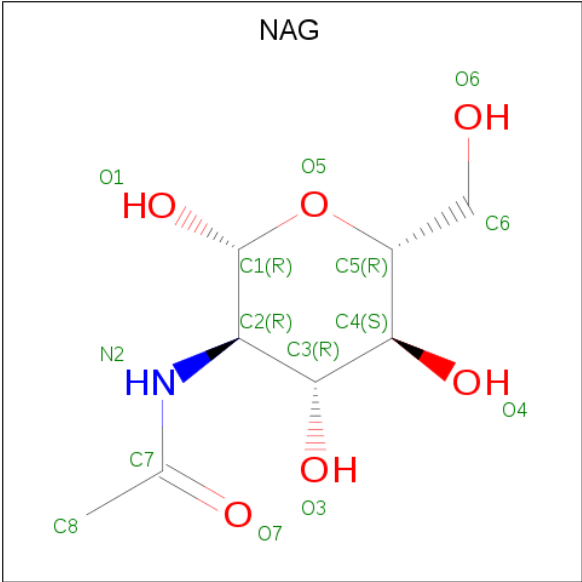
- Molecule 2 is a protein called Staphylococcal enterotoxin-like toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	102	Total	C	N	O	S	0	0	0
			819	517	138	163	1			
2	Y	102	Total	C	N	O	S	0	0	0
			819	517	138	163	1			

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cd	0	0
			2	2		
3	A	3	Total	Cd	0	0
			3	3		

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

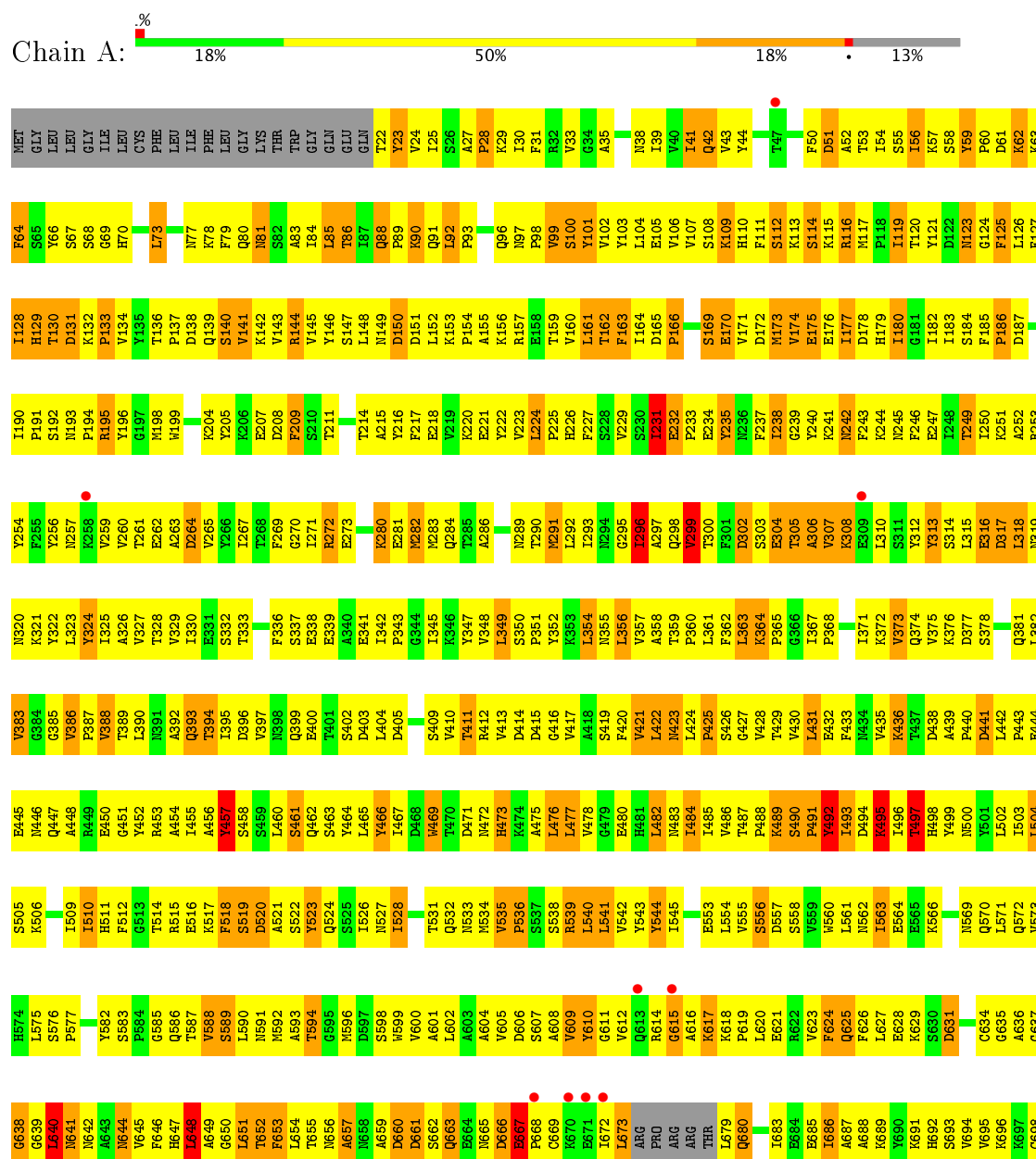


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

### 3 Residue-property plots

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

#### • Molecule 1: Complement C5



- Molecule 1: Complement C5





E200	I201	D202	L203		Q208	F209	E210	R211	M212	G213	D214		N217	S218	K219	D220	I221	N222	K223	I224	E225	V226	T227	L228	K229	Q230	ILE
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.79 Å   144.79 Å   245.28 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	49.75 – 4.20 49.75 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.75-4.20) 99.8 (49.75-4.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 4.14 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.233   ,   0.297 0.212   ,   0.280	Depositor DCC
$R_{free}$ test set	2030 reflections (4.86%)	DCC
Wilson B-factor (Å <sup>2</sup> )	115.5	Xtriage
Anisotropy	0.855	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.19   ,   90.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l 0.397 for h,-h-k,-l 0.045 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	24809	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	205.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.53	0/11793	0.77	6/16003 (0.0%)
1	B	0.53	0/11793	0.77	5/16003 (0.0%)
2	X	0.34	0/828	0.54	0/1107
2	Y	0.34	0/828	0.56	1/1107 (0.1%)
All	All	0.52	0/25242	0.75	12/34220 (0.0%)

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

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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	ASP	CB-CG-OD1	-8.57	110.58	118.30
1	B	640	LEU	CA-CB-CG	7.23	131.94	115.30
1	B	1374	VAL	CB-CA-C	-6.61	98.85	111.40
1	A	640	LEU	CA-CB-CG	6.51	130.28	115.30
1	A	1195	LEU	CA-CB-CG	-5.71	102.17	115.30
1	A	1374	VAL	CB-CA-C	-5.46	101.02	111.40
1	A	1482	LEU	CA-CB-CG	5.38	127.67	115.30
2	Y	175	LYS	CD-CE-NZ	5.25	123.78	111.70
1	B	323	LEU	CA-CB-CG	5.23	127.34	115.30
1	B	1033	ILE	CB-CA-C	-5.14	101.31	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1297	LEU	CA-CB-CG	-5.03	103.74	115.30
1	A	471	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	651	LEU	Peptide
1	B	1179	THR	Peptide
1	B	651	LEU	Peptide

## 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	11541	0	11511	1721	0
1	B	11541	0	11511	1730	0
2	X	819	0	831	85	0
2	Y	819	0	831	83	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
4	A	42	0	38	2	0
4	B	42	0	38	3	0
All	All	24809	0	24760	3610	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 73.

All (3610) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:VAL:HG23	1:A:536:PRO:HD3	1.21	1.17
1:A:698:CYS:SG	1:A:724:CYS:CB	2.33	1.16
1:A:698:CYS:SG	1:A:724:CYS:HB2	1.86	1.15
1:A:968:VAL:HG12	1:A:1368:THR:HG22	1.19	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:VAL:HG23	1:B:536:PRO:HD3	1.29	1.13
1:A:609:VAL:HG23	1:A:610:TYR:H	1.00	1.12
1:B:609:VAL:HG23	1:B:610:TYR:H	1.07	1.12
1:B:968:VAL:HG12	1:B:1368:THR:HG22	1.19	1.12
1:B:440:PRO:HD2	1:B:441:ASP:OD2	1.51	1.10
1:A:855:PHE:CZ	1:A:886:GLN:HB3	1.86	1.09
1:B:66:TYR:HD1	1:B:90:LYS:HE3	1.13	1.09
1:B:855:PHE:CZ	1:B:886:GLN:HB3	1.87	1.09
1:A:994:GLN:HE22	1:A:998:ASN:HB3	1.16	1.08
1:A:195:ARG:HD2	1:A:1058:SER:HA	1.35	1.07
1:A:1068:VAL:HG13	1:A:1069:TRP:H	1.15	1.07
1:A:617:LYS:O	1:A:618:LYS:HG2	1.55	1.07
1:A:66:TYR:HD1	1:A:90:LYS:HE3	1.14	1.06
1:B:940:SER:HB2	1:B:959:PHE:HD1	1.18	1.06
1:B:66:TYR:HE1	1:B:90:LYS:HG3	1.21	1.03
1:B:617:LYS:O	1:B:618:LYS:HG2	1.58	1.03
1:B:1068:VAL:HG13	1:B:1069:TRP:H	1.20	1.03
1:B:120:THR:HG22	1:B:121:TYR:H	1.18	1.02
1:B:38:ASN:O	1:B:39:ILE:HD13	1.60	1.01
1:B:653:PHE:CZ	1:B:660:ASP:HA	1.95	1.01
1:B:195:ARG:HD2	1:B:1058:SER:HA	1.41	1.01
1:B:133:PRO:O	1:B:134:VAL:HG23	1.58	1.01
1:A:1381:ILE:HG13	1:A:1404:ALA:HB2	1.42	1.01
1:A:984:VAL:HG11	1:A:1024:TYR:CE1	1.96	1.01
1:A:386:VAL:HG23	1:A:411:THR:HG21	1.36	1.01
1:B:541:LEU:HB2	1:B:558:SER:HB3	1.41	1.01
2:X:136:LEU:HB3	2:X:224:ILE:HB	1.43	1.01
1:A:120:THR:HG22	1:A:121:TYR:H	1.21	1.00
1:A:59:TYR:HB3	1:A:60:PRO:HD3	1.39	1.00
1:B:1255:LEU:HD21	1:B:1271:ILE:HG22	1.43	1.00
1:A:1435:ASN:HB3	1:A:1438:ASP:HB2	1.40	1.00
1:B:940:SER:HB2	1:B:959:PHE:CD1	1.95	1.00
1:A:386:VAL:H	1:A:411:THR:CG2	1.75	0.99
1:A:698:CYS:HB3	1:A:724:CYS:SG	2.01	0.99
1:B:804:ILE:HG22	1:B:809:ILE:HA	1.41	0.99
1:B:936:ARG:HB2	1:B:1364:VAL:HG22	1.44	0.99
1:A:609:VAL:HG23	1:A:610:TYR:N	1.78	0.99
1:B:840:GLN:HG2	1:B:899:THR:HG22	1.43	0.98
1:A:440:PRO:HD2	1:A:441:ASP:OD2	1.63	0.98
1:B:243:PHE:CZ	1:B:316:GLU:HG2	1.98	0.98
1:A:253:ARG:HH21	1:A:257:ASN:HA	1.29	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:922:ILE:HD12	4:B:2001:NAG:H82	1.44	0.98
1:B:59:TYR:HB3	1:B:60:PRO:HD3	1.43	0.97
1:B:982:LEU:HD23	1:B:1309:LEU:HD11	1.45	0.97
1:A:973:ILE:HG23	1:A:1365:VAL:HG23	1.46	0.97
1:A:698:CYS:CB	1:A:724:CYS:SG	2.52	0.97
1:B:973:ILE:HG23	1:B:1365:VAL:HG23	1.44	0.97
1:A:1279:ARG:HD3	1:A:1284:PHE:CG	1.99	0.97
1:A:115:LYS:HG2	1:A:117:MET:HE3	1.47	0.96
1:B:618:LYS:CB	1:B:621:GLU:HB3	1.94	0.96
1:A:922:ILE:HD12	4:A:2001:NAG:H82	1.46	0.96
1:B:994:GLN:HE22	1:B:998:ASN:HB3	1.30	0.96
1:A:618:LYS:HG3	1:A:621:GLU:CD	1.86	0.96
1:A:1244:THR:HG22	1:A:1246:ARG:H	1.31	0.95
1:B:66:TYR:CD1	1:B:90:LYS:HE3	2.00	0.95
1:B:96:GLN:O	1:B:98:PRO:HD3	1.65	0.95
1:A:133:PRO:O	1:A:134:VAL:HG23	1.66	0.95
1:A:44:TYR:HE1	1:A:497:THR:HG1	1.00	0.94
1:A:618:LYS:CB	1:A:621:GLU:HB3	1.98	0.94
1:B:635:GLY:HA2	1:B:672:ILE:HG23	1.49	0.94
1:A:984:VAL:HG11	1:A:1024:TYR:HE1	1.30	0.94
1:A:156:LYS:O	1:A:157:ARG:HG3	1.67	0.94
1:A:66:TYR:CD1	1:A:90:LYS:HE3	2.02	0.94
1:A:940:SER:HB2	1:A:959:PHE:CD1	2.03	0.94
1:A:940:SER:HB2	1:A:959:PHE:HD1	1.33	0.94
1:A:1255:LEU:HD22	1:A:1270:VAL:HG12	1.50	0.93
1:A:38:ASN:O	1:A:39:ILE:HD13	1.67	0.93
1:B:1381:ILE:HG13	1:B:1404:ALA:HB2	1.47	0.93
1:A:609:VAL:CG2	1:A:610:TYR:H	1.82	0.93
1:B:618:LYS:HG3	1:B:621:GLU:CD	1.89	0.93
1:B:115:LYS:HG2	1:B:117:MET:HE3	1.49	0.93
1:B:1244:THR:HG22	1:B:1246:ARG:H	1.34	0.93
1:B:1202:HIS:HD2	1:B:1204:GLN:H	1.14	0.93
1:A:1434:ALA:HA	1:A:1479:ILE:HG22	1.49	0.93
1:A:96:GLN:O	1:A:98:PRO:HD3	1.69	0.93
2:Y:136:LEU:HB3	2:Y:224:ILE:HB	1.50	0.93
1:A:940:SER:OG	1:A:1361:VAL:HG12	1.67	0.93
1:B:319:ASN:ND2	1:B:347:TYR:CD1	2.36	0.92
1:B:1348:VAL:HG11	1:B:1359:VAL:HG21	1.49	0.92
1:B:386:VAL:HG23	1:B:411:THR:HG21	1.50	0.92
1:B:253:ARG:HH21	1:B:257:ASN:HA	1.31	0.92
1:B:1206:ARG:HG3	1:B:1206:ARG:HH11	1.31	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:140:LYS:HG2	2:Y:228:LEU:HD12	1.50	0.92
1:B:1180:LEU:HD21	1:B:1208:ILE:HA	1.49	0.92
1:B:679:LEU:HD13	1:B:742:ILE:HG12	1.50	0.92
1:B:956:ARG:HG3	1:B:1349:SER:HB3	1.50	0.92
1:B:120:THR:CG2	1:B:121:TYR:H	1.82	0.92
1:A:1118:PHE:O	1:A:1144:LEU:HD23	1.69	0.92
1:A:653:PHE:CZ	1:A:660:ASP:HA	2.05	0.91
1:B:66:TYR:CE1	1:B:90:LYS:HG3	2.05	0.91
1:B:835:ARG:HG2	1:B:835:ARG:HH11	1.34	0.91
1:A:986:GLU:HA	1:A:986:GLU:OE2	1.66	0.91
1:A:1090:ASN:HD22	1:A:1158:ILE:HD13	1.35	0.91
1:B:359:THR:HG21	1:B:372:LYS:H	1.34	0.91
1:B:1162:VAL:HG23	1:B:1163:LYS:H	1.35	0.91
1:B:163:PHE:HD1	1:B:163:PHE:H	1.19	0.91
1:B:1217:LEU:O	1:B:1218:VAL:HG13	1.70	0.90
1:B:1251:THR:HG1	1:B:1273:TRP:HZ3	0.94	0.90
1:B:823:VAL:HG22	1:B:847:ASN:HA	1.54	0.90
1:B:1438:ASP:OD2	1:B:1478:ARG:HG3	1.72	0.90
1:B:571:LEU:HD12	1:B:572:GLN:N	1.85	0.90
1:A:1279:ARG:HD3	1:A:1284:PHE:CD2	2.07	0.89
1:B:156:LYS:O	1:B:157:ARG:HG3	1.71	0.89
1:A:1438:ASP:OD2	1:A:1478:ARG:HG3	1.72	0.89
1:B:973:ILE:HG23	1:B:1365:VAL:CG2	2.01	0.89
1:A:1180:LEU:HD21	1:A:1208:ILE:HA	1.52	0.89
1:A:66:TYR:HE1	1:A:90:LYS:HG3	1.35	0.89
1:B:386:VAL:H	1:B:411:THR:CG2	1.85	0.89
1:A:644:ASN:HD21	1:A:648:LEU:HD12	1.37	0.89
1:A:804:ILE:HG22	1:A:809:ILE:HA	1.54	0.89
1:B:1090:ASN:HD22	1:B:1158:ILE:HD13	1.35	0.89
1:B:1149:VAL:HA	1:B:1152:ILE:HD12	1.55	0.89
1:A:412:ARG:HB3	1:A:415:ASP:HB3	1.53	0.89
1:A:635:GLY:HA2	1:A:672:ILE:HG23	1.55	0.89
1:B:319:ASN:O	1:B:320:ASN:ND2	2.06	0.89
1:B:386:VAL:HG12	1:B:387:PRO:HD2	1.55	0.89
1:A:968:VAL:HG12	1:A:1368:THR:CG2	2.03	0.88
1:B:412:ARG:HD2	1:B:415:ASP:HB2	1.55	0.88
1:B:528:ILE:H	1:B:528:ILE:HD12	1.37	0.88
1:B:59:TYR:CB	1:B:60:PRO:HD3	2.03	0.88
1:A:120:THR:CG2	1:A:121:TYR:H	1.85	0.88
1:A:371:ILE:HD11	1:A:422:LEU:HD11	1.55	0.88
1:A:679:LEU:HD13	1:A:742:ILE:HG12	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:TYR:CB	1:A:60:PRO:HD3	2.01	0.88
1:B:157:ARG:H	1:B:178:ASP:HB3	1.38	0.88
1:B:249:THR:HG23	1:B:298:GLN:HE21	1.38	0.88
1:A:243:PHE:CZ	1:A:316:GLU:HG2	2.07	0.88
1:B:984:VAL:HG11	1:B:1024:TYR:CE1	2.08	0.88
1:A:1206:ARG:HH11	1:A:1206:ARG:HG3	1.38	0.88
1:A:956:ARG:HG3	1:A:1349:SER:HB3	1.55	0.87
1:A:441:ASP:HA	1:B:443:PRO:HB3	1.55	0.87
2:X:140:LYS:HG2	2:X:228:LEU:HD12	1.55	0.87
1:A:412:ARG:HD2	1:A:415:ASP:HB2	1.54	0.87
1:B:569:ASN:OD1	1:B:596:MET:HB2	1.74	0.87
1:B:120:THR:HG22	1:B:121:TYR:N	1.89	0.87
1:B:609:VAL:HG23	1:B:610:TYR:N	1.89	0.87
1:B:855:PHE:CE1	1:B:886:GLN:HB3	2.08	0.87
1:B:1193:TYR:O	1:B:1196:SER:HB3	1.73	0.87
1:B:242:ASN:HB3	1:B:245:ASN:O	1.74	0.87
1:B:944:LEU:HB2	1:B:1357:ALA:HB3	1.54	0.87
1:B:231:ILE:HG12	1:B:342:ILE:HD11	1.55	0.87
1:A:386:VAL:H	1:A:411:THR:HG23	1.39	0.86
1:A:1244:THR:HB	1:A:1247:MET:HB2	1.55	0.86
1:A:242:ASN:HB3	1:A:245:ASN:O	1.75	0.86
1:B:1318:LYS:HG2	1:B:1319:HIS:CE1	2.10	0.86
1:A:443:PRO:HB3	1:B:441:ASP:HA	1.55	0.86
1:A:936:ARG:HB3	1:A:1364:VAL:HG22	1.55	0.86
1:A:1180:LEU:HD12	1:A:1204:GLN:NE2	1.90	0.86
2:X:146:LEU:HD22	2:X:147:ASP:N	1.89	0.86
1:B:1193:TYR:CE1	1:B:1256:LEU:HB3	2.10	0.86
1:B:412:ARG:HB3	1:B:415:ASP:HB3	1.57	0.86
1:A:1255:LEU:HD21	1:A:1271:ILE:HG22	1.58	0.86
1:A:365:PRO:HD2	1:A:464:TYR:CD2	2.10	0.86
1:B:1193:TYR:HA	1:B:1257:THR:HG23	1.57	0.86
1:A:1090:ASN:HD21	1:A:1158:ILE:HG21	1.38	0.85
1:B:576:SER:OG	1:B:589:SER:HB2	1.76	0.85
1:A:577:PRO:HD2	1:A:588:VAL:HG23	1.58	0.85
1:A:976:ILE:HD12	1:A:1362:THR:HG23	1.59	0.85
1:B:984:VAL:HG11	1:B:1024:TYR:HE1	1.39	0.85
1:A:1348:VAL:HG11	1:A:1359:VAL:HG21	1.57	0.85
1:A:560:TRP:CZ3	1:A:562:ASN:HB2	2.12	0.85
1:B:602:LEU:HD12	1:B:774:LEU:HD22	1.56	0.85
1:A:1193:TYR:HA	1:A:1257:THR:HG23	1.59	0.85
1:A:936:ARG:CB	1:A:1364:VAL:HG22	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1209:VAL:O	1:B:1213:LYS:HB2	1.76	0.84
1:A:571:LEU:HD12	1:A:572:GLN:N	1.92	0.84
1:B:1304:VAL:HG12	1:B:1305:LYS:N	1.92	0.84
1:B:1381:ILE:HD13	1:B:1509:TYR:CD1	2.12	0.84
1:A:618:LYS:HG3	1:A:621:GLU:OE1	1.77	0.84
1:A:841:LEU:HD12	1:A:859:MET:HE1	1.59	0.84
1:B:617:LYS:HE3	1:B:625:GLN:HE22	1.43	0.84
1:B:733:VAL:O	1:B:737:GLN:HG2	1.76	0.84
1:B:1304:VAL:HG12	1:B:1305:LYS:H	1.38	0.84
1:B:1118:PHE:O	1:B:1144:LEU:HD23	1.76	0.84
1:B:1435:ASN:HB3	1:B:1438:ASP:HB2	1.58	0.84
1:A:639:GLY:H	1:A:645:VAL:HG22	1.41	0.84
1:B:940:SER:OG	1:B:1361:VAL:HG12	1.77	0.84
1:A:1283:GLY:HA3	1:A:1290:THR:HG23	1.59	0.84
1:B:242:ASN:H	1:B:242:ASN:HD22	1.22	0.84
1:A:1255:LEU:HB2	1:A:1270:VAL:HG11	1.58	0.83
1:B:367:ILE:HD13	1:B:466:TYR:HD2	1.43	0.83
1:B:497:THR:HG23	1:B:498:HIS:H	1.42	0.83
1:B:1132:THR:HB	1:B:1134:PRO:HD2	1.59	0.83
1:B:618:LYS:HB2	1:B:621:GLU:HB3	1.59	0.83
1:B:835:ARG:NH2	1:B:905:ILE:HD11	1.93	0.83
1:B:1255:LEU:CD2	1:B:1271:ILE:HG22	2.07	0.83
1:B:968:VAL:CG1	1:B:1368:THR:HG22	2.07	0.83
1:A:1323:LEU:HD12	1:A:1324:HIS:H	1.43	0.83
1:A:1381:ILE:HG13	1:A:1404:ALA:CB	2.08	0.83
1:A:359:THR:HG21	1:A:372:LYS:H	1.42	0.83
1:B:1255:LEU:HD22	1:B:1270:VAL:HG12	1.58	0.83
1:B:43:VAL:HG12	1:B:79:PHE:HB3	1.58	0.83
1:B:981:GLY:O	1:B:982:LEU:HB2	1.78	0.83
1:A:1304:VAL:HG12	1:A:1305:LYS:H	1.42	0.83
1:A:1068:VAL:HG13	1:A:1069:TRP:N	1.93	0.82
1:A:835:ARG:HG2	1:A:835:ARG:HH11	1.44	0.82
1:B:364:LYS:CD	1:B:364:LYS:H	1.91	0.82
1:B:534:MET:HB3	1:B:538:SER:OG	1.78	0.82
1:B:354:LEU:H	1:B:354:LEU:CD2	1.92	0.82
1:B:618:LYS:HG3	1:B:621:GLU:OE1	1.79	0.82
1:A:120:THR:HG22	1:A:121:TYR:N	1.94	0.82
1:A:386:VAL:HG23	1:A:411:THR:CG2	2.08	0.82
1:B:1279:ARG:HB2	1:B:1284:PHE:HB2	1.62	0.82
1:B:1434:ALA:HA	1:B:1479:ILE:HG22	1.59	0.82
1:A:541:LEU:HB2	1:A:558:SER:HB3	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1180:LEU:HD12	1:B:1204:GLN:NE2	1.95	0.82
1:B:834:VAL:HG21	1:B:1489:SER:OG	1.78	0.82
1:B:371:ILE:HD11	1:B:422:LEU:HD11	1.60	0.82
2:Y:146:LEU:HD22	2:Y:147:ASP:N	1.94	0.82
1:B:977:LEU:HD12	1:B:1361:VAL:HG21	1.60	0.82
1:B:160:VAL:HG22	1:B:174:VAL:O	1.80	0.82
2:Y:165:LEU:O	2:Y:169:ILE:HG12	1.80	0.82
1:A:1304:VAL:HG12	1:A:1305:LYS:N	1.93	0.82
1:B:494:ASP:O	1:B:496:ILE:HD12	1.77	0.82
1:A:618:LYS:HB2	1:A:621:GLU:HB3	1.61	0.81
1:B:42:GLN:HG3	1:B:80:GLN:HE21	1.44	0.81
1:A:569:ASN:OD1	1:A:596:MET:HB2	1.79	0.81
1:B:639:GLY:H	1:B:645:VAL:HG22	1.43	0.81
1:A:306:ALA:O	1:A:307:VAL:HG23	1.80	0.81
1:B:30:ILE:HG22	1:B:31:PHE:N	1.95	0.81
1:B:841:LEU:HD12	1:B:859:MET:HE1	1.61	0.81
1:B:936:ARG:CB	1:B:1364:VAL:HG22	2.10	0.81
1:A:617:LYS:HE3	1:A:625:GLN:HE22	1.44	0.81
1:A:1372:GLU:HG3	1:A:1373:GLU:H	1.45	0.81
1:A:157:ARG:H	1:A:178:ASP:HB3	1.45	0.81
1:A:330:ILE:HG22	1:A:337:SER:CB	2.10	0.81
1:A:371:ILE:HD12	1:A:390:LEU:HD21	1.63	0.81
1:A:361:LEU:O	1:A:454:ALA:HA	1.80	0.81
1:A:653:PHE:CD2	1:A:653:PHE:N	2.48	0.81
1:B:1244:THR:HG22	1:B:1246:ARG:N	1.95	0.81
1:B:134:VAL:HG22	1:B:218:GLU:HB3	1.63	0.81
1:A:1193:TYR:O	1:A:1196:SER:HB3	1.81	0.81
1:A:364:LYS:CD	1:A:364:LYS:H	1.93	0.81
1:A:492:TYR:HD2	1:A:493:ILE:N	1.79	0.81
1:A:576:SER:OG	1:A:589:SER:HB2	1.81	0.81
1:B:1372:GLU:HG3	1:B:1373:GLU:H	1.46	0.81
1:A:1209:VAL:O	1:A:1213:LYS:HB2	1.81	0.80
1:A:30:ILE:HG22	1:A:31:PHE:N	1.96	0.80
1:A:973:ILE:HG23	1:A:1365:VAL:CG2	2.12	0.80
1:A:115:LYS:HG2	1:A:117:MET:CE	2.11	0.80
1:B:1218:VAL:HG12	1:B:1225:TYR:O	1.81	0.80
1:A:1217:LEU:O	1:A:1218:VAL:HG13	1.82	0.80
1:A:386:VAL:O	1:A:411:THR:HG22	1.81	0.80
1:B:242:ASN:CB	1:B:245:ASN:O	2.29	0.80
1:B:977:LEU:HD12	1:B:1361:VAL:CG2	2.12	0.80
1:A:528:ILE:H	1:A:528:ILE:HD12	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1429:PRO:HG2	1:B:1511:THR:HB	1.63	0.79
1:B:977:LEU:HA	1:B:1361:VAL:HG23	1.62	0.79
1:A:134:VAL:HG22	1:A:218:GLU:HB3	1.64	0.79
1:A:934:VAL:HG22	1:A:1366:HIS:CD2	2.15	0.79
1:A:1435:ASN:HD22	1:A:1478:ARG:HB2	1.48	0.79
1:A:246:PHE:O	1:A:300:THR:HA	1.82	0.79
1:A:388:VAL:O	1:A:388:VAL:HG12	1.83	0.79
1:B:653:PHE:CD2	1:B:653:PHE:N	2.50	0.79
2:Y:219:LYS:HD2	2:Y:219:LYS:N	1.97	0.79
1:A:395:ILE:HD12	1:A:396:ASP:O	1.82	0.79
1:A:354:LEU:H	1:A:354:LEU:CD2	1.96	0.79
1:A:386:VAL:N	1:A:411:THR:CG2	2.46	0.79
1:B:253:ARG:NH2	1:B:257:ASN:HA	1.98	0.79
1:B:388:VAL:O	1:B:388:VAL:HG12	1.83	0.79
1:B:486:VAL:O	1:B:488:PRO:HD3	1.80	0.79
1:B:560:TRP:CH2	1:B:562:ASN:HB2	2.18	0.78
1:B:560:TRP:CZ3	1:B:562:ASN:HB2	2.18	0.78
1:B:896:VAL:O	1:B:897:THR:HG22	1.82	0.78
1:A:534:MET:HB3	1:A:538:SER:OG	1.84	0.78
1:B:1090:ASN:HD21	1:B:1158:ILE:HG21	1.48	0.78
2:Y:219:LYS:HD2	2:Y:219:LYS:H	1.49	0.78
1:A:535:VAL:CG2	1:A:536:PRO:HD3	2.10	0.78
1:A:824:PHE:CE1	1:A:846:TYR:HD1	2.01	0.78
1:A:160:VAL:HG22	1:A:174:VAL:O	1.84	0.78
1:A:163:PHE:H	1:A:163:PHE:HD1	1.32	0.78
1:B:1206:ARG:CG	1:B:1206:ARG:HH11	1.97	0.78
1:B:1279:ARG:HD3	1:B:1284:PHE:CD2	2.19	0.78
1:B:987:ILE:HD13	1:B:1294:ILE:HG23	1.65	0.78
1:B:1323:LEU:HD12	1:B:1324:HIS:H	1.49	0.78
1:B:92:LEU:N	1:B:93:PRO:HD3	1.99	0.78
1:A:735:ALA:HB1	1:A:754:MET:HE1	1.64	0.78
1:A:92:LEU:N	1:A:93:PRO:HD3	1.99	0.78
1:A:1283:GLY:HA3	1:A:1290:THR:CG2	2.14	0.78
1:A:386:VAL:HG12	1:A:387:PRO:HD2	1.65	0.78
1:B:31:PHE:HZ	1:B:104:LEU:HD22	1.49	0.78
1:B:360:PRO:HA	1:B:636:ALA:HB3	1.65	0.78
1:B:392:ALA:HB3	1:B:404:LEU:HD12	1.66	0.78
1:A:85:LEU:H	1:A:85:LEU:HD22	1.49	0.78
1:B:717:ARG:HD3	1:B:1449:LEU:HA	1.65	0.78
1:A:1162:VAL:HG23	1:A:1163:LYS:H	1.49	0.77
1:A:392:ALA:HB3	1:A:404:LEU:HD12	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1244:THR:HG22	1:A:1246:ARG:N	1.99	0.77
1:A:1429:PRO:HG2	1:A:1511:THR:HB	1.66	0.77
1:A:296:ILE:HG22	1:A:297:ALA:H	1.49	0.77
1:B:1248:VAL:HG21	1:B:1277:GLU:HG2	1.64	0.77
1:B:1381:ILE:HG13	1:B:1404:ALA:CB	2.14	0.77
1:B:739:ARG:HB3	1:B:754:MET:SD	2.24	0.77
1:A:1439:LEU:HA	1:A:1442:LEU:HD12	1.66	0.77
1:A:249:THR:HG23	1:A:298:GLN:HE21	1.49	0.77
1:A:253:ARG:NH2	1:A:257:ASN:HA	2.00	0.77
1:B:1090:ASN:ND2	1:B:1158:ILE:HD13	1.98	0.77
1:B:41:ILE:O	1:B:80:GLN:HA	1.84	0.77
1:B:59:TYR:CG	1:B:60:PRO:HD3	2.19	0.77
1:A:115:LYS:HG3	1:A:116:ARG:N	1.99	0.77
1:A:1193:TYR:CE1	1:A:1256:LEU:HB3	2.19	0.77
1:B:1146:ALA:HB1	1:B:1190:ILE:HG22	1.66	0.77
1:B:1229:LYS:HE3	1:B:1231:ASN:OD1	1.85	0.77
1:B:315:LEU:HB2	1:B:318:LEU:HB2	1.67	0.77
1:A:1466:SER:OG	1:A:1468:PRO:HD3	1.85	0.77
1:B:1027:THR:HG22	1:B:1302:LEU:HD21	1.66	0.77
1:A:1435:ASN:HB3	1:A:1438:ASP:CB	2.14	0.76
1:B:1430:THR:O	1:B:1485:VAL:HG11	1.83	0.76
1:B:142:LYS:HD3	1:B:775:TRP:CG	2.20	0.76
2:X:219:LYS:N	2:X:219:LYS:HD2	2.01	0.76
1:A:25:ILE:HB	1:A:654:LEU:HB3	1.68	0.76
1:B:938:SER:OG	1:B:1279:ARG:CZ	2.32	0.76
1:B:618:LYS:HB3	1:B:621:GLU:HB3	1.65	0.76
1:A:1430:THR:O	1:A:1485:VAL:HG11	1.84	0.76
1:B:968:VAL:O	1:B:971:THR:HG23	1.85	0.76
1:A:1434:ALA:HB1	1:A:1477:PHE:CD1	2.20	0.76
1:B:1255:LEU:HB2	1:B:1270:VAL:HG11	1.66	0.76
1:A:1132:THR:HB	1:A:1134:PRO:HD2	1.65	0.76
1:A:232:GLU:OE2	1:A:251:LYS:HE2	1.84	0.76
1:B:1246:ARG:O	1:B:1250:THR:HG23	1.85	0.76
1:B:232:GLU:OE2	1:B:251:LYS:HE2	1.85	0.76
1:A:739:ARG:HB3	1:A:754:MET:SD	2.26	0.76
1:A:849:ARG:HG2	1:A:853:MET:HE1	1.67	0.76
1:A:944:LEU:HB2	1:A:1357:ALA:HB3	1.66	0.76
1:B:161:LEU:HG	1:B:185:PHE:CE1	2.20	0.76
1:A:1146:ALA:HB1	1:A:1190:ILE:HG22	1.66	0.76
1:A:1230:ASP:OD2	1:A:1246:ARG:HD2	1.85	0.76
1:A:1318:LYS:HG2	1:A:1319:HIS:CE1	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ILE:HG22	1:A:31:PHE:H	1.48	0.76
1:A:29:LYS:HE2	1:A:666:ASP:HB3	1.67	0.76
1:B:115:LYS:HG2	1:B:117:MET:CE	2.15	0.76
1:B:866:CYS:O	1:B:900:VAL:HG12	1.83	0.76
1:A:1030:HIS:NE2	1:A:1306:GLN:NE2	2.34	0.76
1:A:644:ASN:ND2	1:A:648:LEU:HD12	2.00	0.76
1:B:246:PHE:O	1:B:300:THR:HA	1.85	0.76
1:B:386:VAL:HG23	1:B:411:THR:CG2	2.14	0.76
1:A:1211:ALA:O	1:A:1214:ARG:HB3	1.85	0.75
1:B:1283:GLY:HA3	1:B:1290:THR:HG23	1.68	0.75
1:B:1236:ASP:HB2	1:B:1412:ARG:HH22	1.48	0.75
1:A:317:ASP:O	1:A:319:ASN:N	2.18	0.75
1:A:977:LEU:HD12	1:A:1361:VAL:CG2	2.17	0.75
1:A:938:SER:OG	1:A:1279:ARG:CZ	2.35	0.75
1:B:429:THR:OG1	1:B:430:VAL:N	2.14	0.75
1:A:1279:ARG:CG	1:A:1284:PHE:HB2	2.16	0.75
2:X:165:LEU:O	2:X:169:ILE:HG12	1.87	0.75
1:A:820:PHE:HZ	1:A:848:TYR:HB2	1.51	0.75
1:A:85:LEU:O	1:A:86:THR:HB	1.85	0.75
1:B:1229:LYS:HD2	1:B:1239:VAL:HG12	1.67	0.75
1:B:59:TYR:HB3	1:B:60:PRO:CD	2.17	0.75
1:A:1279:ARG:HB2	1:A:1284:PHE:HB2	1.68	0.75
1:B:1205:PHE:CZ	1:B:1261:LEU:HD11	2.20	0.75
1:B:541:LEU:HD12	1:B:645:VAL:HG12	1.69	0.75
1:A:1186:PHE:HD1	1:A:1250:THR:HG22	1.52	0.74
1:B:115:LYS:HG3	1:B:116:ARG:N	2.00	0.74
1:B:1186:PHE:HD1	1:B:1250:THR:HG22	1.52	0.74
1:B:302:ASP:OD2	1:B:304:GLU:HB2	1.86	0.74
1:B:371:ILE:HD12	1:B:390:LEU:HD21	1.69	0.74
1:A:494:ASP:O	1:A:496:ILE:HD12	1.85	0.74
1:B:330:ILE:HG22	1:B:337:SER:CB	2.16	0.74
1:B:963:ILE:HG23	1:B:973:ILE:HD11	1.69	0.74
2:X:219:LYS:H	2:X:219:LYS:HD2	1.51	0.74
1:B:1271:ILE:O	1:B:1271:ILE:HD12	1.87	0.74
1:B:367:ILE:HG21	1:B:466:TYR:HD2	1.52	0.74
1:A:486:VAL:O	1:A:488:PRO:HD3	1.86	0.74
1:B:386:VAL:H	1:B:411:THR:HG23	1.51	0.74
1:A:59:TYR:CG	1:A:60:PRO:HD3	2.22	0.74
1:B:1440:LYS:HD3	1:B:1453:TYR:CE1	2.21	0.74
1:B:829:ILE:HG13	1:B:925:LYS:HG2	1.69	0.74
1:A:1108:VAL:HG13	1:A:1109:GLU:H	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:TYR:CD2	1:A:60:PRO:HD3	2.22	0.74
2:X:224:ILE:O	2:X:225:GLU:HG3	1.87	0.74
1:A:59:TYR:HB3	1:A:60:PRO:CD	2.16	0.74
1:B:365:PRO:HD2	1:B:464:TYR:CD2	2.23	0.74
1:A:1251:THR:HG1	1:A:1273:TRP:HZ3	1.34	0.73
1:A:363:LEU:O	1:A:363:LEU:HD12	1.88	0.73
1:B:1180:LEU:HD12	1:B:1204:GLN:HE22	1.52	0.73
1:A:1427:SER:HB3	1:A:1492:THR:H	1.53	0.73
1:A:497:THR:HG23	1:A:498:HIS:H	1.52	0.73
1:B:139:GLN:O	1:B:190:ILE:HG12	1.87	0.73
1:A:295:GLY:O	1:A:296:ILE:HD13	1.88	0.73
1:A:386:VAL:CG2	1:A:411:THR:HG21	2.16	0.73
1:B:1283:GLY:HA3	1:B:1290:THR:CG2	2.18	0.73
1:B:297:ALA:O	1:B:298:GLN:HG3	1.88	0.73
1:B:1068:VAL:HG13	1:B:1069:TRP:N	1.99	0.73
1:B:1503:LYS:HD2	1:B:1503:LYS:N	2.02	0.73
1:A:1205:PHE:CZ	1:A:1261:LEU:HD11	2.24	0.73
1:A:1246:ARG:O	1:A:1250:THR:HG23	1.88	0.73
1:A:618:LYS:HB3	1:A:621:GLU:HB3	1.70	0.73
1:A:66:TYR:CE1	1:A:90:LYS:HG3	2.22	0.73
1:B:718:ILE:HG12	1:B:1446:VAL:HG12	1.70	0.73
1:A:1229:LYS:HE3	1:A:1231:ASN:OD1	1.88	0.73
1:A:837:GLU:HG2	1:A:1487:PHE:O	1.88	0.73
1:B:1427:SER:HB3	1:B:1492:THR:H	1.54	0.73
1:B:515:ARG:HH12	1:B:527:ASN:H	1.37	0.73
1:B:59:TYR:CD2	1:B:60:PRO:HD3	2.23	0.73
1:A:1205:PHE:HZ	1:A:1261:LEU:HD11	1.52	0.73
1:A:1440:LYS:HD3	1:A:1453:TYR:CE1	2.23	0.73
1:A:42:GLN:HG3	1:A:80:GLN:HE21	1.53	0.73
1:A:1230:ASP:CG	1:A:1246:ARG:HD2	2.08	0.73
1:A:1236:ASP:HB2	1:A:1412:ARG:HH22	1.53	0.73
1:A:492:TYR:CD2	1:A:493:ILE:N	2.57	0.73
1:B:1193:TYR:CD1	1:B:1256:LEU:HB3	2.23	0.73
1:B:42:GLN:HB2	1:B:80:GLN:HG2	1.68	0.73
1:B:25:ILE:HB	1:B:654:LEU:HB3	1.69	0.73
1:A:43:VAL:HG12	1:A:79:PHE:HB3	1.68	0.73
1:A:913:SER:HB2	1:A:922:ILE:HG12	1.71	0.73
1:B:367:ILE:HD13	1:B:466:TYR:CD2	2.24	0.73
1:A:267:ILE:HG12	1:A:327:VAL:HG13	1.69	0.73
1:B:153:LYS:HB3	1:B:154:PRO:HD2	1.71	0.73
1:A:977:LEU:HD12	1:A:1361:VAL:HG21	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ILE:HG22	1:B:31:PHE:H	1.52	0.72
1:B:354:LEU:H	1:B:354:LEU:HD23	1.52	0.72
1:B:700:TYR:HE1	1:B:758:LEU:HB2	1.53	0.72
1:B:1113:LEU:HD12	1:B:1117:SER:OG	1.88	0.72
2:X:146:LEU:HD11	2:X:148:ALA:HB2	1.71	0.72
1:A:976:ILE:HD12	1:A:1362:THR:CG2	2.20	0.72
1:B:849:ARG:HG2	1:B:853:MET:HE1	1.72	0.72
1:A:700:TYR:HE1	1:A:758:LEU:HB2	1.54	0.72
1:B:234:GLU:HG3	1:B:247:GLU:HB3	1.70	0.72
1:B:354:LEU:HD12	1:B:435:VAL:CG1	2.20	0.72
1:A:443:PRO:HG3	1:B:441:ASP:O	1.88	0.72
2:Y:186:TYR:CD2	2:Y:229:LYS:HD3	2.24	0.72
1:A:1229:LYS:HD2	1:A:1239:VAL:HG12	1.71	0.72
1:B:306:ALA:O	1:B:307:VAL:HG23	1.88	0.72
1:B:386:VAL:N	1:B:411:THR:CG2	2.52	0.72
1:B:367:ILE:HG21	1:B:466:TYR:CD2	2.23	0.72
1:B:794:LEU:HD21	1:B:824:PHE:CZ	2.23	0.72
1:B:837:GLU:HG2	1:B:1488:LEU:HA	1.72	0.72
1:A:1334:LEU:N	1:A:1334:LEU:HD22	2.04	0.72
1:B:492:TYR:CD2	1:B:493:ILE:N	2.57	0.72
1:A:1024:TYR:CD2	1:A:1024:TYR:C	2.63	0.72
1:A:157:ARG:HD2	1:A:205:TYR:CE2	2.24	0.72
1:A:367:ILE:HD13	1:A:466:TYR:HD2	1.54	0.72
1:A:638:GLY:HA2	1:A:645:VAL:HG13	1.70	0.72
1:A:915:GLU:OE2	1:A:920:LYS:HE3	1.89	0.72
1:B:1030:HIS:O	1:B:1033:ILE:HG13	1.90	0.72
1:B:1421:HIS:CE1	1:B:1498:TYR:CD2	2.78	0.72
1:B:364:LYS:HD2	1:B:364:LYS:H	1.52	0.72
1:A:1445:GLY:O	1:A:1448:GLN:HB3	1.89	0.72
1:B:242:ASN:ND2	1:B:242:ASN:H	1.86	0.72
1:B:644:ASN:HD21	1:B:648:LEU:HD12	1.53	0.72
1:A:386:VAL:H	1:A:411:THR:HG22	1.54	0.72
1:B:1230:ASP:OD2	1:B:1246:ARG:HD2	1.90	0.72
1:B:585:GLY:HA2	1:B:790:LEU:O	1.89	0.72
1:A:1030:HIS:CE1	1:A:1306:GLN:NE2	2.58	0.72
1:A:1465:ASN:H	1:A:1465:ASN:HD22	1.37	0.72
1:A:571:LEU:HG	1:A:812:ALA:HB2	1.71	0.72
1:B:1024:TYR:CE2	1:B:1030:HIS:CD2	2.78	0.72
1:B:1274:LEU:HB3	1:B:1297:LEU:HD11	1.71	0.72
1:A:441:ASP:O	1:B:443:PRO:HG3	1.90	0.72
1:A:428:VAL:HG22	1:A:429:THR:H	1.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:ILE:HG12	1:A:1446:VAL:HG12	1.72	0.71
1:B:1205:PHE:HZ	1:B:1261:LEU:HD11	1.53	0.71
1:A:1084:ARG:HD2	1:A:1154:LYS:HG3	1.72	0.71
1:A:242:ASN:H	1:A:242:ASN:HD22	1.37	0.71
1:A:710:THR:HG23	1:A:713:GLN:CD	2.10	0.71
2:Y:189:ILE:O	2:Y:200:GLU:HA	1.89	0.71
1:A:532:GLN:O	1:A:535:VAL:HG13	1.90	0.71
1:B:1024:TYR:CD2	1:B:1024:TYR:C	2.63	0.71
1:B:363:LEU:HD12	1:B:363:LEU:O	1.91	0.71
1:B:504:LEU:HD21	1:B:651:LEU:HG	1.70	0.71
1:A:1422:ALA:O	1:A:1464:LEU:HD12	1.90	0.71
2:Y:136:LEU:HD21	2:Y:153:PHE:HB2	1.72	0.71
1:A:981:GLY:HA3	1:A:1309:LEU:HD11	1.73	0.71
1:A:499:TYR:O	1:A:514:THR:HG23	1.89	0.71
1:B:1466:SER:OG	1:B:1468:PRO:HD3	1.89	0.71
1:A:123:ASN:HD22	1:A:123:ASN:C	1.94	0.71
1:A:695:VAL:HA	1:A:698:CYS:SG	2.31	0.71
1:B:43:VAL:CG1	1:B:79:PHE:HB3	2.20	0.71
1:A:1488:LEU:O	1:A:1488:LEU:HD12	1.90	0.71
1:A:425:PRO:O	1:A:427:GLY:N	2.23	0.71
1:A:733:VAL:O	1:A:737:GLN:HG2	1.90	0.71
1:A:839:ILE:HG22	1:A:900:VAL:HG23	1.72	0.71
1:B:1053:MET:HE1	1:B:1086:LEU:HD22	1.72	0.71
1:B:1334:LEU:HD22	1:B:1334:LEU:N	2.06	0.71
2:X:140:LYS:HA	2:X:228:LEU:HB2	1.72	0.71
1:B:1239:VAL:O	1:B:1241:ASN:N	2.24	0.71
1:B:1251:THR:HG21	1:B:1273:TRP:CH2	2.25	0.71
1:B:271:ILE:HG21	1:B:313:TYR:CE1	2.25	0.71
1:B:835:ARG:CZ	1:B:905:ILE:HD11	2.20	0.71
1:A:1080:ALA:O	1:A:1083:LEU:N	2.24	0.71
1:A:1296:GLY:O	1:A:1298:THR:N	2.24	0.71
1:A:330:ILE:HG22	1:A:337:SER:OG	1.91	0.71
1:B:1449:LEU:HD12	1:B:1449:LEU:O	1.90	0.71
1:B:1449:LEU:HG	1:B:1450:PHE:CD1	2.26	0.71
1:B:1465:ASN:H	1:B:1465:ASN:HD22	1.38	0.71
1:B:386:VAL:H	1:B:411:THR:HG22	1.56	0.71
1:B:352:TYR:HA	1:B:376:LYS:O	1.91	0.71
1:A:1180:LEU:O	1:A:1182:ALA:N	2.24	0.70
1:A:1421:HIS:CE1	1:A:1498:TYR:CD2	2.79	0.70
1:A:41:ILE:O	1:A:80:GLN:HA	1.90	0.70
1:B:635:GLY:HA2	1:B:672:ILE:CG2	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1449:LEU:HG	1:A:1450:PHE:CD1	2.26	0.70
1:A:42:GLN:HB2	1:A:80:GLN:HG2	1.72	0.70
1:B:1211:ALA:O	1:B:1214:ARG:HB3	1.90	0.70
1:B:157:ARG:HD2	1:B:205:TYR:CE2	2.27	0.70
1:B:542:VAL:O	1:B:556:SER:HB2	1.91	0.70
1:A:194:PRO:O	1:A:1070:LYS:NZ	2.25	0.70
2:Y:134:THR:HG23	2:Y:153:PHE:HB3	1.73	0.70
1:A:794:LEU:HD21	1:A:824:PHE:CZ	2.26	0.70
1:B:1142:LEU:HD13	1:B:1187:THR:CG2	2.21	0.70
1:A:242:ASN:CB	1:A:245:ASN:O	2.39	0.70
1:A:367:ILE:HG21	1:A:466:TYR:CD2	2.26	0.70
1:B:1008:ALA:HB3	1:B:1078:LEU:HD11	1.71	0.70
1:B:1279:ARG:HD3	1:B:1284:PHE:CG	2.27	0.70
1:B:243:PHE:CE2	1:B:316:GLU:HG2	2.27	0.70
1:A:1202:HIS:HD2	1:A:1204:GLN:H	1.38	0.70
1:B:1377:PHE:CE1	1:B:1467:ILE:HD12	2.27	0.70
1:B:1423:VAL:HG21	1:B:1496:TYR:HE1	1.56	0.70
2:X:183:THR:O	2:X:230:GLN:HA	1.92	0.70
1:A:1449:LEU:HG	1:A:1450:PHE:CE1	2.26	0.70
1:B:1435:ASN:ND2	1:B:1478:ARG:HE	1.90	0.70
1:B:1488:LEU:O	1:B:1488:LEU:HD12	1.92	0.70
1:A:599:TRP:HB2	1:A:804:ILE:O	1.92	0.70
1:B:1219:LYS:HB2	1:B:1225:TYR:HB2	1.72	0.70
1:B:1317:TYR:HB3	1:B:1344:ASP:OD2	1.92	0.70
1:B:354:LEU:N	1:B:354:LEU:CD2	2.53	0.70
1:A:1078:LEU:O	1:A:1078:LEU:HD23	1.92	0.69
1:A:367:ILE:HG21	1:A:466:TYR:HD2	1.56	0.69
1:A:774:LEU:HD11	1:A:788:PHE:CZ	2.27	0.69
1:A:968:VAL:O	1:A:971:THR:HG23	1.92	0.69
1:B:1217:LEU:C	1:B:1218:VAL:HG22	2.11	0.69
1:B:1449:LEU:HG	1:B:1450:PHE:CE1	2.26	0.69
1:B:396:ASP:OD1	1:B:398:ASN:HB2	1.92	0.69
1:B:585:GLY:O	1:B:789:ALA:HB1	1.92	0.69
1:A:717:ARG:HD3	1:A:1449:LEU:HA	1.72	0.69
1:A:244:LYS:HE3	1:A:304:GLU:OE1	1.92	0.69
1:A:560:TRP:CH2	1:A:562:ASN:HB2	2.27	0.69
1:B:577:PRO:HD2	1:B:588:VAL:HG23	1.73	0.69
1:A:554:LEU:HB3	1:A:642:ASN:OD1	1.91	0.69
1:A:1435:ASN:ND2	1:A:1478:ARG:HE	1.90	0.69
1:A:492:TYR:HD2	1:A:493:ILE:H	1.38	0.69
1:A:719:SER:O	1:A:721:GLY:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:PHE:HA	1:A:915:GLU:O	1.91	0.69
1:B:191:PRO:HG2	1:B:194:PRO:HB3	1.75	0.69
1:B:194:PRO:O	1:B:1070:LYS:NZ	2.25	0.69
1:A:1279:ARG:HG3	1:A:1284:PHE:HB2	1.74	0.69
1:B:1069:TRP:HE1	1:B:1463:GLN:NE2	1.89	0.69
1:B:1300:TYR:CZ	1:B:1304:VAL:HG21	2.27	0.69
1:B:1421:HIS:HE1	1:B:1498:TYR:CD2	2.10	0.69
1:B:428:VAL:HG22	1:B:429:THR:H	1.57	0.69
1:B:85:LEU:HD22	1:B:85:LEU:H	1.57	0.69
1:A:1239:VAL:O	1:A:1241:ASN:N	2.26	0.69
1:B:242:ASN:ND2	1:B:242:ASN:N	2.41	0.69
1:B:994:GLN:NE2	1:B:998:ASN:HB3	2.06	0.69
1:A:1180:LEU:HD12	1:A:1204:GLN:HE22	1.55	0.69
1:A:1255:LEU:HD22	1:A:1270:VAL:CG1	2.22	0.69
1:A:180:ILE:HG21	1:A:599:TRP:CE2	2.28	0.69
1:A:1000:LEU:HD12	1:A:1017:PRO:HG3	1.75	0.69
1:B:99:VAL:HB	1:B:121:TYR:OH	1.93	0.69
1:B:1218:VAL:HG12	1:B:1226:ARG:HA	1.74	0.69
1:B:1249:GLU:HB2	1:B:1289:ASP:HB3	1.75	0.69
1:B:1348:VAL:HG21	1:B:1359:VAL:HG11	1.75	0.69
1:B:609:VAL:CG2	1:B:610:TYR:H	1.91	0.69
1:A:1027:THR:HG22	1:A:1302:LEU:HD21	1.74	0.69
1:A:1039:LEU:O	1:A:1042:LYS:HB3	1.93	0.69
1:A:1490:PRO:HB3	1:A:1509:TYR:O	1.92	0.69
1:A:625:GLN:O	1:A:629:LYS:HE2	1.93	0.69
1:A:641:ASN:H	1:A:644:ASN:HB3	1.57	0.69
1:B:1491:ALA:HB3	1:B:1509:TYR:HE2	1.56	0.69
1:B:588:VAL:HG11	1:B:790:LEU:HD11	1.75	0.69
1:B:686:ILE:O	1:B:689:LYS:HG2	1.92	0.69
1:A:1079:THR:HG21	1:A:1106:TRP:CE3	2.27	0.69
1:A:271:ILE:O	1:A:280:LYS:HB2	1.93	0.69
1:A:307:VAL:HG11	1:A:313:TYR:HB2	1.74	0.69
1:A:429:THR:OG1	1:A:430:VAL:N	2.20	0.69
1:B:199:TRP:HB2	1:B:217:PHE:O	1.93	0.69
1:B:488:PRO:O	1:B:491:PRO:HD2	1.93	0.69
1:A:1300:TYR:CZ	1:A:1304:VAL:HG21	2.28	0.68
1:A:977:LEU:HA	1:A:1361:VAL:HG23	1.75	0.68
1:A:1487:PHE:N	1:A:1487:PHE:CD2	2.60	0.68
2:Y:166:ASP:CG	2:Y:201:ILE:HD13	2.13	0.68
1:A:620:LEU:HD13	1:A:811:VAL:H	1.59	0.68
1:B:1104:LEU:HD13	1:B:1164:ILE:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1348:VAL:HG11	1:B:1359:VAL:CG2	2.22	0.68
1:B:227:PHE:HB3	1:B:254:TYR:HD2	1.57	0.68
1:B:315:LEU:CB	1:B:318:LEU:HB2	2.24	0.68
1:B:492:TYR:HD2	1:B:493:ILE:N	1.91	0.68
1:B:947:ARG:O	1:B:949:ILE:N	2.25	0.68
2:Y:140:LYS:O	2:Y:146:LEU:HD23	1.94	0.68
2:Y:142:TYR:HB2	2:Y:145:ASN:HB2	1.74	0.68
1:A:628:GLU:C	1:A:629:LYS:HD3	2.14	0.68
1:B:1487:PHE:N	1:B:1487:PHE:CD2	2.61	0.68
1:B:915:GLU:OE2	1:B:920:LYS:HE3	1.93	0.68
1:B:131:ASP:OD1	1:B:132:LYS:N	2.25	0.68
1:B:617:LYS:HE3	1:B:625:GLN:NE2	2.08	0.68
1:A:1334:LEU:HD22	1:A:1334:LEU:H	1.58	0.68
1:A:823:VAL:HG22	1:A:847:ASN:HA	1.76	0.68
1:A:1183:GLN:C	1:A:1232:LEU:HD22	2.14	0.68
1:A:1429:PRO:HB2	1:A:1432:ILE:HG13	1.75	0.68
1:A:297:ALA:O	1:A:298:GLN:HG3	1.93	0.68
1:B:1019:PHE:CE2	1:B:1020:TYR:CE1	2.82	0.68
1:B:1019:PHE:HE2	1:B:1088:GLN:HE21	1.38	0.68
1:B:478:VAL:HG11	1:B:566:LYS:HD3	1.75	0.68
1:B:151:ASP:OD2	1:B:508:LYS:NZ	2.27	0.68
1:A:498:HIS:HB3	1:A:514:THR:CG2	2.24	0.68
1:B:1271:ILE:C	1:B:1271:ILE:HD12	2.14	0.68
1:B:644:ASN:ND2	1:B:648:LEU:HD12	2.09	0.68
1:B:653:PHE:HD2	1:B:653:PHE:N	1.92	0.68
2:X:189:ILE:O	2:X:200:GLU:HA	1.93	0.68
1:A:1029:ASN:O	1:A:1029:ASN:ND2	2.27	0.68
1:A:1219:LYS:HB2	1:A:1225:TYR:HB2	1.74	0.68
1:B:44:TYR:CE1	1:B:497:THR:HG21	2.29	0.68
1:A:29:LYS:O	1:A:30:ILE:HD13	1.94	0.68
1:A:412:ARG:HD2	1:A:415:ASP:CB	2.24	0.68
1:B:820:PHE:CE2	1:B:848:TYR:HD2	2.11	0.68
1:B:986:GLU:OE2	1:B:986:GLU:HA	1.92	0.68
1:A:1132:THR:CB	1:A:1134:PRO:HD2	2.24	0.68
1:A:1378:TYR:CZ	1:A:1409:LYS:HE3	2.29	0.68
1:A:231:ILE:HD13	1:A:342:ILE:HG13	1.76	0.68
1:A:561:LEU:O	1:A:563:ILE:HG22	1.94	0.68
1:A:182:ILE:HG12	1:A:804:ILE:HD11	1.74	0.68
1:B:244:LYS:HE3	1:B:304:GLU:OE1	1.94	0.68
1:B:425:PRO:O	1:B:427:GLY:N	2.27	0.68
1:B:968:VAL:HG12	1:B:1368:THR:CG2	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:189:ILE:HD11	2:X:203:LEU:HD21	1.76	0.68
1:A:1157:ASP:O	1:A:1160:PRO:HD3	1.94	0.67
1:A:131:ASP:CG	1:A:132:LYS:N	2.48	0.67
1:A:1491:ALA:HB3	1:A:1509:TYR:HE2	1.58	0.67
1:A:488:PRO:O	1:A:491:PRO:HD2	1.94	0.67
1:A:541:LEU:HD12	1:A:645:VAL:HG12	1.76	0.67
1:A:62:LYS:HD3	1:A:105:GLU:OE2	1.92	0.67
1:B:520:ASP:CG	1:B:521:ALA:H	1.97	0.67
1:B:600:VAL:O	1:B:777:VAL:HG13	1.93	0.67
1:B:835:ARG:CG	1:B:835:ARG:HH11	2.06	0.67
1:A:1142:LEU:HD13	1:A:1187:THR:CG2	2.24	0.67
1:A:1494:THR:HB	1:A:1506:THR:HG23	1.77	0.67
1:A:302:ASP:OD2	1:A:304:GLU:HB2	1.93	0.67
1:B:532:GLN:O	1:B:535:VAL:HG13	1.94	0.67
1:A:109:LYS:HD2	1:A:110:HIS:N	2.09	0.67
1:B:1184:SER:HA	1:B:1232:LEU:HB2	1.76	0.67
1:B:249:THR:HG23	1:B:298:GLN:NE2	2.08	0.67
2:X:153:PHE:HE1	2:X:168:LYS:HB3	1.59	0.67
1:A:1150:ILE:HD11	1:A:1190:ILE:HG23	1.74	0.67
1:A:1218:VAL:HG12	1:A:1225:TYR:O	1.95	0.67
1:A:1278:GLN:NE2	1:A:1278:GLN:HA	2.09	0.67
1:A:157:ARG:O	1:A:178:ASP:HB2	1.94	0.67
1:A:316:GLU:O	1:A:317:ASP:C	2.33	0.67
1:A:354:LEU:HD22	1:A:354:LEU:N	2.10	0.67
1:A:504:LEU:HD21	1:A:651:LEU:HG	1.75	0.67
1:A:51:ASP:OD2	1:A:70:HIS:NE2	2.27	0.67
1:B:1183:GLN:C	1:B:1232:LEU:HD22	2.15	0.67
1:B:1244:THR:HB	1:B:1247:MET:CB	2.23	0.67
1:B:271:ILE:O	1:B:280:LYS:HB2	1.93	0.67
1:B:620:LEU:HD13	1:B:811:VAL:H	1.60	0.67
1:B:932:GLU:N	1:B:932:GLU:OE1	2.28	0.67
1:A:1249:GLU:HB2	1:A:1289:ASP:HB3	1.76	0.67
1:A:1323:LEU:CD1	1:A:1324:HIS:H	2.07	0.67
1:B:1111:TYR:CE1	1:B:1121:ASN:HB2	2.30	0.67
2:X:143:GLY:C	2:X:145:ASN:H	1.97	0.67
2:Y:183:THR:O	2:Y:230:GLN:HA	1.94	0.67
1:A:412:ARG:CD	1:A:415:ASP:HB2	2.23	0.67
1:A:99:VAL:HB	1:A:121:TYR:OH	1.94	0.67
1:B:1025:LEU:HD13	1:B:1031:TRP:CZ3	2.30	0.67
1:B:1296:GLY:O	1:B:1298:THR:N	2.27	0.67
1:A:292:LEU:HD13	1:A:293:ILE:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:PHE:CE2	1:A:848:TYR:HD2	2.13	0.67
1:A:859:MET:HB2	1:A:912:PHE:CE1	2.30	0.67
1:B:1019:PHE:CE2	1:B:1020:TYR:HE1	2.13	0.67
1:B:350:SER:CB	1:B:446:ASN:O	2.43	0.67
1:B:528:ILE:N	1:B:528:ILE:HD12	2.08	0.67
2:Y:189:ILE:HD11	2:Y:203:LEU:HD21	1.76	0.67
1:A:227:PHE:O	1:A:338:GLU:HG2	1.95	0.67
1:A:375:VAL:HG12	1:A:383:VAL:HG13	1.77	0.67
1:A:23:TYR:CE1	1:A:656:ASN:HB2	2.30	0.67
2:X:134:THR:HG23	2:X:153:PHE:HB3	1.76	0.67
1:A:354:LEU:CD2	1:A:354:LEU:N	2.57	0.67
1:A:947:ARG:HB2	1:A:949:ILE:HG13	1.77	0.67
1:B:1079:THR:HG21	1:B:1106:TRP:CE3	2.30	0.67
1:B:1323:LEU:CD1	1:B:1324:HIS:H	2.08	0.67
1:B:837:GLU:HG2	1:B:1487:PHE:O	1.95	0.67
1:B:386:VAL:O	1:B:411:THR:HG22	1.94	0.67
1:B:702:GLY:HA2	1:B:728:PHE:CE1	2.30	0.67
1:B:856:CYS:HB3	1:B:915:GLU:HB2	1.76	0.67
1:A:1003:LEU:HD13	1:A:1498:TYR:CE1	2.30	0.66
1:A:1090:ASN:ND2	1:A:1158:ILE:HD13	2.08	0.66
1:A:160:VAL:HG22	1:A:174:VAL:C	2.16	0.66
1:A:855:PHE:CE1	1:A:886:GLN:HB3	2.28	0.66
1:B:700:TYR:CE1	1:B:758:LEU:HB2	2.29	0.66
1:B:859:MET:HB2	1:B:912:PHE:CE1	2.31	0.66
2:X:166:ASP:CG	2:X:201:ILE:HD13	2.14	0.66
2:Y:224:ILE:O	2:Y:225:GLU:HG3	1.95	0.66
1:A:1217:LEU:C	1:A:1218:VAL:HG22	2.14	0.66
1:A:1425:ASP:HB3	1:A:1494:THR:HG23	1.77	0.66
1:A:617:LYS:HE3	1:A:625:GLN:NE2	2.10	0.66
1:A:837:GLU:OE2	1:A:1488:LEU:HB2	1.95	0.66
1:B:977:LEU:HA	1:B:1361:VAL:CG2	2.24	0.66
1:B:719:SER:O	1:B:721:GLY:N	2.28	0.66
1:A:242:ASN:H	1:A:242:ASN:ND2	1.92	0.66
1:A:520:ASP:CG	1:A:521:ALA:H	1.99	0.66
1:A:835:ARG:CZ	1:A:905:ILE:HD11	2.26	0.66
1:B:123:ASN:HD22	1:B:123:ASN:C	1.99	0.66
1:B:1244:THR:HB	1:B:1247:MET:HB2	1.77	0.66
2:Y:167:PHE:O	2:Y:171:GLN:HB2	1.95	0.66
1:A:352:TYR:HA	1:A:376:LYS:O	1.94	0.66
1:A:73:LEU:H	1:A:73:LEU:HD23	1.60	0.66
1:A:1068:VAL:CG1	1:A:1069:TRP:H	1.99	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1115:ASN:ND2	1:A:1117:SER:H	1.94	0.66
1:B:1328:MET:O	1:B:1329:THR:HG23	1.96	0.66
1:B:1334:LEU:HD22	1:B:1334:LEU:H	1.60	0.66
1:A:1054:LEU:O	1:A:1056:ILE:N	2.29	0.66
1:A:1279:ARG:CB	1:A:1284:PHE:HB2	2.25	0.66
1:A:1024:TYR:OH	1:A:1306:GLN:NE2	2.29	0.66
1:B:831:TYR:CE1	1:B:1457:ASP:HB3	2.31	0.66
1:B:1379:LEU:HD21	1:B:1495:VAL:HG11	1.75	0.66
2:Y:162:LEU:CD1	2:Y:165:LEU:HD23	2.26	0.66
1:A:1136:GLU:OE1	1:A:1415:SER:CB	2.43	0.66
1:A:837:GLU:HG2	1:A:1488:LEU:HA	1.77	0.66
1:A:77:ASN:ND2	1:A:81:ASN:ND2	2.43	0.66
1:B:1008:ALA:HB3	1:B:1078:LEU:CD1	2.26	0.66
1:B:109:LYS:HD2	1:B:110:HIS:N	2.10	0.66
1:B:291:MET:O	1:B:293:ILE:HG13	1.95	0.66
1:A:1025:LEU:HD13	1:A:1031:TRP:CZ3	2.31	0.66
1:A:113:LYS:HG3	1:A:114:SER:H	1.61	0.66
1:A:28:PRO:HB2	1:A:30:ILE:O	1.95	0.66
1:A:315:LEU:HB2	1:A:318:LEU:HB2	1.78	0.66
1:B:1144:LEU:O	1:B:1148:THR:HG22	1.96	0.66
1:B:1150:ILE:HD11	1:B:1190:ILE:HG23	1.75	0.66
1:B:415:ASP:CG	1:B:417:VAL:HB	2.16	0.66
1:A:161:LEU:HG	1:A:185:PHE:CE1	2.31	0.66
1:A:308:LYS:HG2	1:A:314:SER:HA	1.78	0.66
1:A:857:VAL:HG21	1:A:896:VAL:HG11	1.78	0.66
1:B:1245:ALA:HB2	1:B:1501:PRO:HD2	1.77	0.66
1:B:1380:LYS:HG3	1:B:1405:CYS:SG	2.36	0.66
1:B:315:LEU:HD12	1:B:318:LEU:HD12	1.76	0.66
1:B:395:ILE:O	1:B:429:THR:HG23	1.96	0.66
1:B:364:LYS:HG2	1:B:465:LEU:O	1.94	0.66
1:B:629:LYS:HD3	1:B:629:LYS:N	2.10	0.66
1:B:839:ILE:CG2	1:B:900:VAL:HG23	2.26	0.66
2:X:143:GLY:O	2:X:145:ASN:N	2.28	0.66
1:A:1104:LEU:HD13	1:A:1164:ILE:HD13	1.77	0.66
1:A:946:PRO:HB3	1:A:1352:PHE:O	1.96	0.66
1:A:1503:LYS:N	1:A:1503:LYS:HD2	2.10	0.66
1:A:317:ASP:C	1:A:319:ASN:H	1.97	0.66
1:A:350:SER:HB2	1:A:446:ASN:O	1.95	0.66
1:A:927:LEU:HD22	1:A:929:VAL:HG22	1.76	0.66
1:B:1203:PRO:O	1:B:1206:ARG:HB2	1.96	0.66
1:B:1422:ALA:O	1:B:1464:LEU:HD12	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:SER:HB2	1:B:446:ASN:O	1.95	0.66
1:B:708:ASP:OD2	1:B:1401:ARG:NH2	2.29	0.66
1:A:350:SER:CB	1:A:446:ASN:O	2.44	0.65
1:A:563:ILE:HG13	1:A:564:GLU:N	2.10	0.65
1:B:1020:TYR:HD2	1:B:1294:ILE:HG22	1.60	0.65
1:B:1024:TYR:OH	1:B:1306:GLN:NE2	2.29	0.65
1:B:182:ILE:HG12	1:B:804:ILE:HD11	1.76	0.65
1:B:249:THR:CG2	1:B:298:GLN:HE21	2.09	0.65
1:B:503:ILE:HG12	1:B:540:LEU:HB3	1.78	0.65
2:X:162:LEU:CD1	2:X:165:LEU:HD23	2.26	0.65
1:A:700:TYR:CE1	1:A:758:LEU:HB2	2.31	0.65
1:B:1202:HIS:CD2	1:B:1204:GLN:HB3	2.31	0.65
1:B:987:ILE:HD11	1:B:1294:ILE:HD13	1.77	0.65
1:B:243:PHE:CE1	1:B:316:GLU:HG2	2.31	0.65
1:B:364:LYS:HD2	1:B:364:LYS:N	2.11	0.65
1:A:1020:TYR:HD2	1:A:1294:ILE:HG22	1.61	0.65
1:A:1239:VAL:HG23	1:A:1239:VAL:O	1.95	0.65
1:A:156:LYS:O	1:A:157:ARG:CG	2.41	0.65
1:A:617:LYS:CE	1:A:625:GLN:HE22	2.09	0.65
1:B:1028:GLY:O	1:B:1029:ASN:C	2.33	0.65
1:B:1378:TYR:CZ	1:B:1409:LYS:HE3	2.31	0.65
1:B:492:TYR:HD2	1:B:493:ILE:H	1.41	0.65
2:X:189:ILE:HG23	2:X:226:VAL:HG22	1.76	0.65
1:A:952:THR:OG1	1:A:953:ILE:N	2.29	0.65
1:B:1213:LYS:HE3	1:B:1266:TYR:CE2	2.32	0.65
1:B:1320:LYS:HD2	1:B:1321:GLY:H	1.62	0.65
1:B:583:SER:OG	1:B:586:GLN:HB2	1.97	0.65
2:Y:143:GLY:C	2:Y:145:ASN:H	1.99	0.65
1:A:1221:ASN:HA	1:A:1222:PRO:C	2.17	0.65
1:A:1379:LEU:HD21	1:A:1495:VAL:HG11	1.78	0.65
1:A:394:THR:HG22	1:A:402:SER:OG	1.96	0.65
1:A:968:VAL:O	1:A:968:VAL:HG23	1.95	0.65
1:B:1263:ASP:O	1:B:1265:ASN:N	2.30	0.65
1:B:238:ILE:HG12	1:B:246:PHE:CE1	2.32	0.65
1:B:242:ASN:HB3	1:B:245:ASN:OD1	1.96	0.65
1:A:1008:ALA:HB2	1:A:1059:TYR:CD2	2.31	0.65
1:A:1076:THR:CG2	1:A:1120:GLU:HA	2.27	0.65
1:A:856:CYS:O	1:A:914:LEU:HA	1.97	0.65
1:B:1003:LEU:HD13	1:B:1498:TYR:CE1	2.31	0.65
1:B:1115:ASN:HD22	1:B:1115:ASN:C	1.99	0.65
1:B:1445:GLY:O	1:B:1448:GLN:HB3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:146:LEU:O	2:X:146:LEU:HD13	1.96	0.65
1:A:712:GLU:HA	1:A:715:ALA:HB3	1.78	0.65
1:A:43:VAL:CG1	1:A:79:PHE:HB3	2.26	0.65
1:B:227:PHE:HZ	1:B:329:VAL:O	1.80	0.65
1:B:628:GLU:C	1:B:629:LYS:HD3	2.16	0.65
1:B:683:ILE:HD13	1:B:735:ALA:HB2	1.77	0.65
1:B:934:VAL:HG22	1:B:1366:HIS:CD2	2.32	0.65
2:Y:146:LEU:HD11	2:Y:148:ALA:HB2	1.78	0.65
1:A:1227:PHE:HA	1:A:1228:TRP:CE3	2.32	0.65
1:A:987:ILE:HD13	1:A:1294:ILE:HG23	1.77	0.65
1:A:160:VAL:HG23	1:A:175:GLU:HB3	1.79	0.65
1:A:360:PRO:HA	1:A:636:ALA:HB3	1.79	0.65
1:B:160:VAL:HG22	1:B:174:VAL:C	2.17	0.65
1:B:163:PHE:CD1	1:B:163:PHE:N	2.65	0.65
1:A:1465:ASN:ND2	1:A:1465:ASN:H	1.95	0.65
1:A:157:ARG:H	1:A:178:ASP:CB	2.10	0.65
1:A:307:VAL:CG1	1:A:313:TYR:HB2	2.27	0.65
1:B:1148:THR:O	1:B:1152:ILE:HG13	1.97	0.65
1:B:1279:ARG:CB	1:B:1284:PHE:HB2	2.27	0.65
1:B:1284:PHE:HD2	1:B:1285:TYR:CE1	2.15	0.65
1:A:1342:LEU:C	1:A:1343:ASN:HD22	2.01	0.64
1:B:1007:SER:HA	1:B:1069:TRP:CD1	2.32	0.64
1:B:1047:LYS:O	1:B:1049:LEU:N	2.30	0.64
1:B:1105:LEU:HA	1:B:1108:VAL:CG1	2.27	0.64
1:B:1218:VAL:CG1	1:B:1226:ARG:HA	2.27	0.64
1:B:1239:VAL:HG23	1:B:1239:VAL:O	1.96	0.64
1:B:123:ASN:ND2	1:B:150:ASP:H	1.95	0.64
1:B:498:HIS:HD2	1:B:516:GLU:HA	1.61	0.64
1:A:536:PRO:HG3	1:A:624:PHE:HE2	1.61	0.64
1:A:982:LEU:HD23	1:A:1309:LEU:HD11	1.78	0.64
1:B:1029:ASN:ND2	1:B:1029:ASN:O	2.30	0.64
1:B:1255:LEU:HD21	1:B:1271:ILE:CG2	2.24	0.64
2:Y:140:LYS:HA	2:Y:228:LEU:HB2	1.79	0.64
2:Y:189:ILE:HG23	2:Y:226:VAL:HG22	1.78	0.64
1:A:1000:LEU:HD12	1:A:1017:PRO:CG	2.27	0.64
1:A:1274:LEU:HB3	1:A:1297:LEU:HD11	1.78	0.64
1:A:169:SER:O	1:A:170:GLU:O	2.15	0.64
1:A:835:ARG:NH2	1:A:905:ILE:HD11	2.13	0.64
1:B:975:ARG:HG3	1:B:1340:VAL:HB	1.79	0.64
1:B:976:ILE:HD12	1:B:1362:THR:CG2	2.27	0.64
1:A:1213:LYS:HE3	1:A:1266:TYR:CE2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:LYS:HD3	1:B:105:GLU:OE2	1.98	0.64
1:B:253:ARG:HB2	1:B:253:ARG:CZ	2.27	0.64
1:B:838:GLN:O	1:B:1486:GLY:N	2.30	0.64
1:B:906:GLY:O	1:B:908:HIS:CE1	2.51	0.64
1:B:1019:PHE:HE2	1:B:1020:TYR:HE1	1.46	0.64
1:B:515:ARG:HH22	1:B:527:ASN:N	1.96	0.64
1:B:554:LEU:HB3	1:B:642:ASN:OD1	1.97	0.64
1:A:1053:MET:CE	1:A:1086:LEU:HD13	2.26	0.64
1:A:1079:THR:HG21	1:A:1106:TRP:HE3	1.62	0.64
1:A:517:LYS:HA	1:A:524:GLN:HE22	1.62	0.64
1:A:598:SER:HA	1:A:805:SER:OG	1.98	0.64
1:B:1104:LEU:HD22	1:B:1152:ILE:HG23	1.79	0.64
1:B:1161:LEU:HB3	1:B:1164:ILE:HG23	1.79	0.64
1:A:1083:LEU:HD11	1:A:1107:LEU:HD11	1.80	0.64
1:B:364:LYS:CD	1:B:364:LYS:N	2.60	0.64
1:B:956:ARG:HG3	1:B:1349:SER:CB	2.27	0.64
2:X:169:ILE:HG21	2:X:189:ILE:HD13	1.79	0.64
1:A:1090:ASN:HD22	1:A:1158:ILE:CD1	2.08	0.64
1:A:1379:LEU:HD13	1:A:1493:PHE:CE2	2.33	0.64
1:A:835:ARG:HD3	1:A:903:LEU:O	1.98	0.64
1:A:839:ILE:CG2	1:A:900:VAL:HG23	2.28	0.64
1:A:906:GLY:O	1:A:908:HIS:CE1	2.50	0.64
1:B:1316:SER:O	1:B:1346:LEU:HD12	1.98	0.64
1:B:160:VAL:HG23	1:B:175:GLU:HB3	1.78	0.64
1:B:319:ASN:ND2	1:B:347:TYR:CG	2.65	0.64
1:B:653:PHE:H	1:B:653:PHE:HD2	1.43	0.64
1:B:679:LEU:HD22	1:B:738:LEU:HD11	1.80	0.64
1:A:50:PHE:CG	1:A:109:LYS:HE2	2.33	0.64
1:A:31:PHE:HB2	1:A:119:ILE:HB	1.79	0.64
1:A:686:ILE:O	1:A:689:LYS:HG2	1.97	0.64
1:B:50:PHE:CG	1:B:109:LYS:HE2	2.32	0.64
1:B:1162:VAL:HG23	1:B:1163:LYS:N	2.10	0.64
1:B:1142:LEU:HD13	1:B:1187:THR:HG22	1.79	0.64
1:B:1379:LEU:HD22	1:B:1493:PHE:CE2	2.32	0.64
1:B:31:PHE:CZ	1:B:104:LEU:HD13	2.33	0.64
1:B:835:ARG:NH1	1:B:835:ARG:HG2	2.12	0.64
1:A:1105:LEU:HA	1:A:1108:VAL:CG1	2.28	0.64
1:B:119:ILE:HG13	1:B:120:THR:N	2.13	0.64
1:B:1213:LYS:HE3	1:B:1266:TYR:CD2	2.33	0.64
1:B:363:LEU:HD23	1:B:454:ALA:HB3	1.77	0.64
1:B:412:ARG:HD2	1:B:415:ASP:CB	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:LEU:O	1:B:540:LEU:HA	1.98	0.64
1:B:641:ASN:O	1:B:644:ASN:N	2.31	0.64
1:A:159:THR:HG22	1:A:160:VAL:N	2.14	0.63
1:A:544:TYR:HD1	1:A:544:TYR:H	1.45	0.63
1:B:490:SER:O	1:B:491:PRO:C	2.34	0.63
1:B:493:ILE:HG23	1:B:494:ASP:N	2.13	0.63
1:A:1381:ILE:HD12	1:A:1493:PHE:HB2	1.81	0.63
1:B:85:LEU:O	1:B:86:THR:HB	1.97	0.63
1:A:583:SER:OG	1:A:586:GLN:HB2	1.98	0.63
1:A:856:CYS:HB3	1:A:915:GLU:HB2	1.80	0.63
1:B:1132:THR:CB	1:B:1134:PRO:HD2	2.28	0.63
1:B:717:ARG:CD	1:B:1449:LEU:HA	2.29	0.63
1:B:42:GLN:HB2	1:B:80:GLN:CG	2.28	0.63
1:A:1232:LEU:O	1:A:1233:GLN:HG2	1.99	0.63
1:A:263:ALA:HB3	1:A:292:LEU:HB3	1.81	0.63
1:B:113:LYS:HG3	1:B:114:SER:N	2.13	0.63
1:B:441:ASP:OD2	1:B:441:ASP:N	2.30	0.63
1:A:1202:HIS:O	1:A:1203:PRO:C	2.37	0.63
1:A:1255:LEU:HD21	1:A:1271:ILE:CG2	2.28	0.63
1:A:23:TYR:HE1	1:A:656:ASN:HB2	1.62	0.63
1:A:491:PRO:O	1:A:493:ILE:N	2.32	0.63
1:B:1378:TYR:O	1:B:1406:ALA:HA	1.99	0.63
1:B:180:ILE:HG21	1:B:599:TRP:CE2	2.34	0.63
1:A:1113:LEU:HD12	1:A:1117:SER:OG	1.98	0.63
1:A:386:VAL:C	1:A:410:VAL:HG13	2.19	0.63
1:A:493:ILE:HG23	1:A:494:ASP:N	2.12	0.63
1:B:491:PRO:O	1:B:493:ILE:N	2.32	0.63
1:B:653:PHE:CZ	1:B:660:ASP:CA	2.79	0.63
1:B:839:ILE:HD11	1:B:1483:PHE:CZ	2.34	0.63
1:A:1263:ASP:O	1:A:1265:ASN:N	2.31	0.63
1:A:1128:LYS:NZ	1:A:1415:SER:HB3	2.14	0.63
1:A:857:VAL:HA	1:A:913:SER:O	1.98	0.63
1:B:1143:TYR:HE1	1:B:1186:PHE:CZ	2.16	0.63
1:B:710:THR:N	1:B:713:GLN:OE1	2.29	0.63
1:B:911:ASN:CG	1:B:924:VAL:HG13	2.19	0.63
2:Y:153:PHE:HE1	2:Y:168:LYS:HB3	1.64	0.63
1:A:101:TYR:HE1	1:A:116:ARG:CZ	2.12	0.63
1:A:1380:LYS:HG3	1:A:1405:CYS:SG	2.39	0.63
1:A:451:GLY:C	1:A:452:TYR:CD2	2.73	0.63
1:A:710:THR:N	1:A:713:GLN:OE1	2.29	0.63
1:A:906:GLY:H	1:A:929:VAL:HB	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1156:PHE:CD1	1:B:1164:ILE:HD11	2.34	0.63
1:B:1429:PRO:HB2	1:B:1432:ILE:HG13	1.81	0.63
1:B:295:GLY:C	1:B:296:ILE:HG12	2.19	0.63
1:B:571:LEU:HD21	1:B:600:VAL:HG13	1.81	0.63
1:A:1050:LYS:O	1:A:1053:MET:HB3	1.98	0.63
2:X:166:ASP:OD2	2:X:201:ILE:HG21	1.99	0.63
1:A:467:ILE:HD12	1:A:484:ILE:CD1	2.29	0.62
1:B:1315:VAL:HG22	1:B:1346:LEU:HD11	1.81	0.62
1:B:267:ILE:HG12	1:B:327:VAL:HG13	1.81	0.62
1:B:679:LEU:HB3	1:B:738:LEU:HD11	1.81	0.62
1:B:905:ILE:HD13	1:B:931:PRO:HG3	1.80	0.62
2:X:142:TYR:HB2	2:X:145:ASN:HB2	1.80	0.62
1:A:1205:PHE:O	1:A:1209:VAL:HG23	1.99	0.62
1:A:1273:TRP:CE3	1:A:1274:LEU:HD23	2.34	0.62
1:A:1378:TYR:O	1:A:1406:ALA:HA	2.00	0.62
1:A:730:GLU:O	1:A:734:VAL:HG23	1.99	0.62
1:B:269:PHE:HB2	1:B:283:MET:HE3	1.81	0.62
1:B:330:ILE:HG22	1:B:337:SER:OG	1.99	0.62
1:A:1218:VAL:HG12	1:A:1226:ARG:HA	1.79	0.62
1:A:295:GLY:C	1:A:296:ILE:HG12	2.19	0.62
1:A:307:VAL:HG12	1:A:313:TYR:O	1.98	0.62
1:A:796:THR:HA	1:A:818:LYS:HA	1.81	0.62
1:A:840:GLN:HG2	1:A:899:THR:HG22	1.82	0.62
1:A:92:LEU:N	1:A:93:PRO:CD	2.62	0.62
1:B:386:VAL:N	1:B:411:THR:HG23	2.14	0.62
1:B:610:TYR:CB	1:B:614:ARG:HD2	2.30	0.62
2:Y:146:LEU:HD13	2:Y:146:LEU:O	2.00	0.62
1:A:701:ASP:O	1:A:704:CYS:HB2	2.00	0.62
1:B:835:ARG:HD3	1:B:903:LEU:O	1.99	0.62
2:X:162:LEU:HD12	2:X:165:LEU:HD23	1.80	0.62
1:A:1162:VAL:HG23	1:A:1163:LYS:N	2.13	0.62
1:A:1248:VAL:HG21	1:A:1277:GLU:HG2	1.82	0.62
1:A:315:LEU:CB	1:A:318:LEU:HB2	2.30	0.62
1:A:1003:LEU:HD22	1:A:1004:PRO:HD2	1.80	0.62
1:A:315:LEU:O	1:A:316:GLU:O	2.17	0.62
1:B:133:PRO:O	1:B:134:VAL:CG2	2.43	0.62
1:B:375:VAL:HG12	1:B:383:VAL:HG13	1.81	0.62
1:B:361:LEU:O	1:B:454:ALA:HA	1.99	0.62
1:B:942:VAL:HG21	1:B:957:LYS:HB3	1.82	0.62
1:A:367:ILE:HG23	1:A:368:PRO:HD2	1.81	0.62
1:A:717:ARG:CD	1:A:1449:LEU:HA	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:PRO:HG3	1:B:624:PHE:HE2	1.63	0.62
1:A:1081:PHE:CE1	1:A:1288:GLN:NE2	2.66	0.62
1:A:1316:SER:O	1:A:1346:LEU:HD12	1.99	0.62
1:A:640:LEU:H	1:A:644:ASN:HB3	1.65	0.62
1:A:909:ASN:H	1:A:926:THR:HG22	1.65	0.62
1:B:1097:GLN:O	1:B:1099:SER:N	2.33	0.62
1:B:1202:HIS:O	1:B:1203:PRO:C	2.37	0.62
1:B:1279:ARG:CG	1:B:1284:PHE:HB2	2.30	0.62
2:X:140:LYS:O	2:X:146:LEU:HD23	2.00	0.62
1:A:364:LYS:HD2	1:A:364:LYS:H	1.62	0.62
1:A:490:SER:O	1:A:491:PRO:C	2.36	0.62
1:A:932:GLU:N	1:A:932:GLU:OE1	2.33	0.62
1:A:1255:LEU:CD2	1:A:1271:ILE:HG22	2.29	0.62
1:A:124:GLY:O	1:A:125:PHE:CD2	2.53	0.62
1:A:354:LEU:H	1:A:354:LEU:HD23	1.64	0.62
1:A:73:LEU:N	1:A:73:LEU:HD23	2.14	0.62
1:B:1050:LYS:O	1:B:1053:MET:HB3	1.99	0.62
1:B:829:ILE:CG1	1:B:925:LYS:HG2	2.29	0.62
2:X:153:PHE:CD2	2:X:154:SER:N	2.68	0.62
1:A:1127:ILE:HD12	1:A:1127:ILE:H	1.64	0.61
1:A:119:ILE:HG13	1:A:120:THR:N	2.15	0.61
1:A:1245:ALA:HB2	1:A:1501:PRO:HD2	1.82	0.61
1:B:1076:THR:CG2	1:B:1120:GLU:HA	2.30	0.61
1:B:131:ASP:CG	1:B:132:LYS:N	2.53	0.61
1:A:1379:LEU:HD22	1:A:1493:PHE:CE2	2.35	0.61
1:A:718:ILE:HG12	1:A:1446:VAL:O	2.01	0.61
1:A:364:LYS:HG2	1:A:465:LEU:O	2.00	0.61
1:A:59:TYR:CB	1:A:60:PRO:CD	2.76	0.61
1:A:635:GLY:HA2	1:A:672:ILE:CG2	2.30	0.61
1:B:1079:THR:HG21	1:B:1106:TRP:HE3	1.64	0.61
1:B:1337:PRO:O	1:B:1338:VAL:HG23	2.00	0.61
1:B:1432:ILE:O	1:B:1432:ILE:HG22	2.00	0.61
1:B:214:THR:HG22	1:B:215:ALA:N	2.15	0.61
1:B:947:ARG:HB2	1:B:949:ILE:HG13	1.82	0.61
1:A:1313:ILE:HG22	1:A:1314:ASP:N	2.16	0.61
1:A:1434:ALA:HB1	1:A:1477:PHE:HD1	1.63	0.61
1:A:866:CYS:O	1:A:900:VAL:HG12	2.00	0.61
1:A:994:GLN:HE22	1:A:998:ASN:CB	2.02	0.61
1:B:1146:ALA:O	1:B:1150:ILE:HG13	2.00	0.61
1:B:1425:ASP:HB3	1:B:1494:THR:HG23	1.82	0.61
1:B:30:ILE:CG2	1:B:31:PHE:N	2.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:GLY:N	1:B:411:THR:HG23	2.16	0.61
1:B:563:ILE:HG13	1:B:564:GLU:N	2.14	0.61
1:B:641:ASN:H	1:B:644:ASN:HB3	1.64	0.61
2:Y:178:GLY:O	2:Y:184:THR:HG21	1.99	0.61
1:B:1080:ALA:O	1:B:1083:LEU:N	2.33	0.61
1:B:1380:LYS:HE3	1:B:1405:CYS:SG	2.41	0.61
1:B:59:TYR:CB	1:B:60:PRO:CD	2.77	0.61
1:B:628:GLU:O	1:B:628:GLU:HG3	2.01	0.61
1:B:909:ASN:HA	1:B:925:LYS:O	2.00	0.61
1:B:855:PHE:HA	1:B:915:GLU:O	1.99	0.61
1:A:1161:LEU:HD12	1:A:1162:VAL:N	2.15	0.61
1:A:1226:ARG:CZ	1:A:1266:TYR:CE1	2.84	0.61
1:A:265:VAL:HG23	1:A:292:LEU:H	1.66	0.61
1:A:362:PHE:HA	1:A:455:ILE:H	1.64	0.61
1:A:629:LYS:HD3	1:A:629:LYS:N	2.14	0.61
1:B:599:TRP:HB2	1:B:804:ILE:O	2.01	0.61
1:A:1019:PHE:HE2	1:A:1020:TYR:HE1	1.48	0.61
1:A:1161:LEU:HD12	1:A:1162:VAL:HG22	1.81	0.61
1:A:1213:LYS:HE3	1:A:1266:TYR:CD2	2.36	0.61
1:A:1290:THR:O	1:A:1294:ILE:HG12	1.99	0.61
1:A:1434:ALA:HB1	1:A:1477:PHE:CE1	2.35	0.61
1:A:153:LYS:HB3	1:A:154:PRO:HD2	1.83	0.61
1:B:101:TYR:HE1	1:B:116:ARG:NE	1.97	0.61
1:B:322:TYR:N	1:B:322:TYR:HD2	1.98	0.61
1:B:464:TYR:H	1:B:491:PRO:HD3	1.65	0.61
1:B:92:LEU:N	1:B:93:PRO:CD	2.63	0.61
2:X:146:LEU:C	2:X:146:LEU:HD22	2.18	0.61
1:A:1104:LEU:HD22	1:A:1152:ILE:HG23	1.82	0.61
1:A:1435:ASN:O	1:A:1438:ASP:N	2.30	0.61
1:A:352:TYR:O	1:A:448:ALA:HB2	2.00	0.61
1:A:85:LEU:N	1:A:85:LEU:HD22	2.16	0.61
1:B:100:SER:O	1:B:101:TYR:HB2	2.01	0.61
1:B:1157:ASP:O	1:B:1160:PRO:HD3	2.01	0.61
1:B:1423:VAL:HG21	1:B:1496:TYR:CE1	2.35	0.61
1:B:1423:VAL:CG2	1:B:1496:TYR:CE1	2.83	0.61
1:B:161:LEU:HD11	1:B:185:PHE:CD1	2.35	0.61
1:B:362:PHE:HB3	1:B:455:ILE:O	2.00	0.61
1:B:73:LEU:HD12	1:B:79:PHE:HD2	1.65	0.61
1:B:92:LEU:H	1:B:93:PRO:HD3	1.65	0.61
2:Y:166:ASP:OD2	2:Y:201:ILE:HG21	2.01	0.61
1:A:1019:PHE:CE2	1:A:1020:TYR:CE1	2.88	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LYS:N	1:A:364:LYS:CD	2.61	0.61
1:B:1279:ARG:O	1:B:1280:TYR:C	2.38	0.61
1:B:610:TYR:HB3	1:B:614:ARG:HD2	1.83	0.61
1:A:106:VAL:HG12	1:A:107:VAL:N	2.16	0.61
1:A:131:ASP:OD1	1:A:132:LYS:N	2.33	0.61
1:A:1401:ARG:HB2	1:A:1478:ARG:HG2	1.83	0.61
1:A:1496:TYR:HD1	1:A:1496:TYR:O	1.83	0.61
1:A:293:ILE:N	1:A:296:ILE:O	2.22	0.61
1:A:386:VAL:N	1:A:411:THR:HG23	2.11	0.61
1:A:946:PRO:HD2	1:A:947:ARG:H	1.66	0.61
1:B:349:LEU:HD22	1:B:349:LEU:C	2.20	0.61
1:B:535:VAL:CG2	1:B:536:PRO:HD3	2.17	0.61
1:B:820:PHE:HZ	1:B:848:TYR:HB2	1.64	0.61
2:X:179:LEU:HD12	2:X:180:TYR:H	1.66	0.61
1:A:113:LYS:HG3	1:A:114:SER:N	2.15	0.61
1:A:103:TYR:HA	1:A:115:LYS:O	2.01	0.61
1:A:271:ILE:HG21	1:A:313:TYR:CE1	2.36	0.61
1:A:73:LEU:HD12	1:A:79:PHE:HD2	1.65	0.61
1:B:352:TYR:O	1:B:448:ALA:HB2	2.01	0.61
1:B:361:LEU:HB3	1:B:453:ARG:O	2.01	0.61
1:B:730:GLU:O	1:B:734:VAL:HG23	2.00	0.61
2:X:183:THR:HB	2:X:230:GLN:HB3	1.83	0.61
1:A:976:ILE:HG21	1:A:1280:TYR:HE1	1.65	0.60
1:A:243:PHE:CE1	1:A:316:GLU:HG2	2.35	0.60
1:B:1063:ASP:O	1:B:1064:TYR:HB2	2.01	0.60
1:B:982:LEU:CD2	1:B:1309:LEU:HD11	2.26	0.60
1:B:1381:ILE:HD13	1:B:1509:TYR:CE1	2.36	0.60
1:B:321:LYS:C	1:B:322:TYR:HD2	2.05	0.60
1:B:386:VAL:C	1:B:410:VAL:HG13	2.21	0.60
2:Y:143:GLY:O	2:Y:145:ASN:N	2.33	0.60
1:B:1313:ILE:HG22	1:B:1314:ASP:N	2.16	0.60
1:B:371:ILE:HD12	1:B:390:LEU:CD2	2.31	0.60
1:A:1076:THR:HG21	1:A:1120:GLU:HA	1.83	0.60
1:A:1278:GLN:CA	1:A:1278:GLN:HE21	2.13	0.60
1:B:1202:HIS:CD2	1:B:1204:GLN:H	2.06	0.60
1:B:307:VAL:HG11	1:B:313:TYR:HB2	1.83	0.60
1:B:438:ASP:O	1:B:439:ALA:C	2.39	0.60
1:A:498:HIS:HB3	1:A:514:THR:HG21	1.83	0.60
1:A:948:GLY:HA2	1:A:952:THR:O	2.01	0.60
1:B:113:LYS:HG3	1:B:114:SER:H	1.66	0.60
1:B:29:LYS:O	1:B:30:ILE:HD13	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:GLY:C	1:B:452:TYR:CD2	2.75	0.60
1:B:835:ARG:HH21	1:B:905:ILE:HD11	1.64	0.60
2:Y:179:LEU:HD12	2:Y:180:TYR:H	1.67	0.60
1:A:250:ILE:HG13	1:A:250:ILE:O	2.01	0.60
1:A:505:SER:HB3	1:A:510:ILE:HD11	1.82	0.60
1:A:855:PHE:CZ	1:A:886:GLN:CB	2.73	0.60
1:B:243:PHE:CE2	1:B:316:GLU:CG	2.85	0.60
1:B:840:GLN:HG2	1:B:899:THR:CG2	2.25	0.60
1:A:1023:HIS:O	1:A:1027:THR:HB	2.01	0.60
1:A:1146:ALA:O	1:A:1150:ILE:HG13	2.01	0.60
1:A:242:ASN:ND2	1:A:242:ASN:N	2.49	0.60
1:A:352:TYR:HD1	1:A:375:VAL:CG1	2.14	0.60
1:A:802:ILE:HD11	1:A:804:ILE:HG23	1.84	0.60
1:A:857:VAL:HG12	1:A:914:LEU:HB3	1.84	0.60
1:B:308:LYS:HG2	1:B:314:SER:HA	1.83	0.60
1:B:354:LEU:HD12	1:B:435:VAL:HG11	1.82	0.60
1:B:735:ALA:HB1	1:B:754:MET:HE1	1.81	0.60
1:B:982:LEU:HD23	1:B:1309:LEU:CD1	2.25	0.60
2:X:178:GLY:O	2:X:184:THR:HG21	2.01	0.60
1:A:653:PHE:H	1:A:653:PHE:HD2	1.41	0.60
1:B:185:PHE:HB3	1:B:186:PRO:CD	2.31	0.60
1:B:392:ALA:CB	1:B:404:LEU:HD12	2.32	0.60
1:B:511:HIS:HE2	1:B:531:THR:HG21	1.66	0.60
1:B:605:VAL:HG12	1:B:606:ASP:N	2.16	0.60
1:B:903:LEU:N	1:B:903:LEU:HD22	2.16	0.60
1:A:1028:GLY:O	1:A:1029:ASN:C	2.40	0.60
1:A:269:PHE:HB2	1:A:283:MET:CE	2.32	0.60
1:A:394:THR:HG23	1:A:395:ILE:N	2.16	0.60
1:A:653:PHE:N	1:A:653:PHE:HD2	1.94	0.60
1:B:29:LYS:HE2	1:B:666:ASP:HB3	1.83	0.60
1:B:571:LEU:HG	1:B:812:ALA:HB2	1.84	0.60
1:A:137:PRO:O	1:A:138:ASP:HB2	2.01	0.60
1:A:362:PHE:HB3	1:A:455:ILE:O	2.02	0.60
1:A:385:GLY:N	1:A:411:THR:HG23	2.16	0.60
1:A:450:GLU:HB3	1:A:452:TYR:CE2	2.37	0.60
1:A:257:ASN:OD1	1:A:893:SER:O	2.20	0.60
1:A:927:LEU:HD22	1:A:929:VAL:CG2	2.32	0.60
1:B:157:ARG:H	1:B:178:ASP:CB	2.12	0.60
1:B:23:TYR:CE1	1:B:656:ASN:HB2	2.37	0.60
1:B:354:LEU:N	1:B:354:LEU:HD22	2.16	0.60
1:B:829:ILE:HG22	1:B:830:PRO:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:166:ASP:OD1	2:X:201:ILE:HD13	2.01	0.60
1:A:1144:LEU:O	1:A:1148:THR:HG22	2.02	0.60
1:A:249:THR:HG23	1:A:298:GLN:NE2	2.16	0.60
1:A:679:LEU:HB3	1:A:738:LEU:HD11	1.83	0.60
1:A:837:GLU:OE2	1:A:1488:LEU:HA	2.02	0.60
1:B:1250:THR:O	1:B:1253:TYR:N	2.35	0.60
1:B:961:TYR:OH	1:B:1343:ASN:ND2	2.35	0.60
1:B:349:LEU:HD22	1:B:349:LEU:O	2.02	0.60
1:B:412:ARG:HD3	1:B:414:ASP:OD1	2.02	0.60
1:A:968:VAL:CG1	1:A:1368:THR:HG22	2.12	0.59
1:A:464:TYR:H	1:A:491:PRO:HD3	1.67	0.59
1:A:936:ARG:HB2	1:A:1364:VAL:HG22	1.83	0.59
1:B:1180:LEU:O	1:B:1182:ALA:N	2.34	0.59
1:B:373:VAL:HG23	1:B:374:GLN:N	2.17	0.59
1:B:457:TYR:CD2	1:B:457:TYR:C	2.76	0.59
1:B:66:TYR:CE1	1:B:90:LYS:CG	2.84	0.59
1:B:906:GLY:H	1:B:929:VAL:HB	1.66	0.59
1:A:238:ILE:HG12	1:A:246:PHE:CE1	2.37	0.59
1:A:647:HIS:O	1:A:649:ALA:N	2.34	0.59
1:B:1232:LEU:O	1:B:1233:GLN:HG2	2.02	0.59
1:B:244:LYS:C	1:B:302:ASP:HA	2.23	0.59
1:B:322:TYR:N	1:B:322:TYR:CD2	2.70	0.59
1:A:888:VAL:HG12	1:A:894:HIS:HB2	1.84	0.59
1:B:1024:TYR:HD2	1:B:1025:LEU:N	2.01	0.59
1:B:1206:ARG:CG	1:B:1206:ARG:NH1	2.61	0.59
1:B:1465:ASN:H	1:B:1465:ASN:ND2	1.98	0.59
1:B:1434:ALA:HB1	1:B:1477:PHE:CD1	2.37	0.59
1:B:239:GLY:O	1:B:241:LYS:N	2.36	0.59
1:B:588:VAL:CG1	1:B:790:LEU:HD11	2.31	0.59
2:X:136:LEU:HD21	2:X:153:PHE:HB2	1.84	0.59
1:A:1379:LEU:HD13	1:A:1493:PHE:CD2	2.38	0.59
1:A:1421:HIS:HE1	1:A:1498:TYR:CD2	2.20	0.59
1:A:244:LYS:C	1:A:302:ASP:HA	2.23	0.59
1:B:1221:ASN:HA	1:B:1222:PRO:C	2.21	0.59
1:B:1401:ARG:HB2	1:B:1478:ARG:HG2	1.83	0.59
1:B:163:PHE:CD2	1:B:188:PHE:CD2	2.91	0.59
1:B:250:ILE:HG21	1:B:327:VAL:HG21	1.83	0.59
1:A:1093:VAL:HG12	1:A:1095:GLN:NE2	2.17	0.59
1:B:101:TYR:HE1	1:B:116:ARG:CZ	2.15	0.59
1:B:1054:LEU:O	1:B:1056:ILE:N	2.36	0.59
1:B:208:ASP:O	1:B:209:PHE:HB2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ILE:HG23	1:B:106:VAL:HG22	1.84	0.59
1:B:855:PHE:CE1	1:B:886:GLN:CB	2.84	0.59
1:B:994:GLN:HE22	1:B:998:ASN:CB	2.11	0.59
1:A:1278:GLN:HE21	1:A:1278:GLN:N	2.00	0.59
1:A:199:TRP:HB2	1:A:217:PHE:O	2.02	0.59
1:A:249:THR:CG2	1:A:298:GLN:HE21	2.15	0.59
1:A:859:MET:HB2	1:A:912:PHE:HE1	1.67	0.59
1:B:1196:SER:HB2	1:B:1257:THR:HG23	1.83	0.59
1:A:1053:MET:HE3	1:A:1086:LEU:HD13	1.85	0.59
1:A:1495:VAL:O	1:A:1495:VAL:HG13	2.03	0.59
1:A:185:PHE:HB3	1:A:186:PRO:CD	2.31	0.59
1:A:361:LEU:HB3	1:A:453:ARG:O	2.01	0.59
1:A:457:TYR:C	1:A:457:TYR:HD2	2.06	0.59
1:A:979:VAL:HG13	1:A:1359:VAL:HG22	1.84	0.59
1:B:1145:THR:O	1:B:1149:VAL:HG23	2.03	0.59
1:B:1090:ASN:ND2	1:B:1158:ILE:HG21	2.18	0.59
1:B:976:ILE:O	1:B:1361:VAL:HG22	2.02	0.59
1:A:1132:THR:CG2	1:A:1134:PRO:HD2	2.33	0.59
1:A:324:TYR:C	1:A:324:TYR:CD2	2.75	0.59
1:A:786:LEU:N	1:A:786:LEU:HD23	2.17	0.59
1:A:994:GLN:NE2	1:A:998:ASN:HB3	2.02	0.59
1:B:41:ILE:HG22	1:B:81:ASN:O	2.02	0.59
1:B:837:GLU:OE2	1:B:1488:LEU:HB2	2.02	0.59
1:A:1304:VAL:CG1	1:A:1305:LYS:N	2.66	0.59
1:A:610:TYR:CB	1:A:614:ARG:HD2	2.32	0.59
1:A:838:GLN:O	1:A:1486:GLY:N	2.34	0.59
1:B:269:PHE:HB2	1:B:283:MET:CE	2.32	0.59
1:B:271:ILE:HD11	1:B:307:VAL:HG22	1.83	0.59
1:B:639:GLY:N	1:B:645:VAL:HG22	2.16	0.59
1:B:902:PRO:C	1:B:903:LEU:HD13	2.23	0.59
1:A:30:ILE:CG2	1:A:31:PHE:N	2.65	0.59
1:A:44:TYR:CE1	1:A:497:THR:HG21	2.38	0.59
1:A:902:PRO:C	1:A:903:LEU:HD13	2.23	0.59
1:B:1255:LEU:O	1:B:1255:LEU:HD12	2.01	0.59
1:B:485:ILE:CG2	1:B:487:THR:HG23	2.33	0.59
1:B:553:GLU:OE1	1:B:555:VAL:HG23	2.03	0.59
1:B:988:LEU:HD23	1:B:1021:VAL:HG13	1.84	0.59
1:A:100:SER:O	1:A:101:TYR:HB2	2.03	0.58
1:A:1105:LEU:O	1:A:1109:GLU:HG3	2.03	0.58
1:A:1228:TRP:N	1:A:1228:TRP:CE3	2.71	0.58
1:A:348:VAL:HG12	1:A:349:LEU:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1304:VAL:CG1	1:B:1305:LYS:N	2.66	0.58
1:B:161:LEU:CG	1:B:185:PHE:CE1	2.86	0.58
1:B:227:PHE:O	1:B:338:GLU:HG2	2.03	0.58
1:B:263:ALA:HB3	1:B:292:LEU:HB3	1.84	0.58
1:B:293:ILE:N	1:B:296:ILE:O	2.28	0.58
1:B:98:PRO:HB2	1:B:99:VAL:HG23	1.85	0.58
1:A:936:ARG:NH1	1:A:1002:HIS:CE1	2.71	0.58
1:A:1226:ARG:NE	1:A:1266:TYR:CE1	2.71	0.58
1:A:1255:LEU:HD12	1:A:1255:LEU:O	2.03	0.58
1:A:975:ARG:HG3	1:A:1340:VAL:HB	1.84	0.58
1:A:1401:ARG:HB2	1:A:1478:ARG:HA	1.84	0.58
1:A:239:GLY:O	1:A:241:LYS:N	2.36	0.58
1:A:835:ARG:NE	1:A:905:ILE:HD11	2.17	0.58
1:B:947:ARG:C	1:B:949:ILE:H	2.05	0.58
1:A:571:LEU:C	1:A:571:LEU:HD12	2.22	0.58
1:B:1108:VAL:HG13	1:B:1109:GLU:H	1.68	0.58
1:B:265:VAL:HG23	1:B:292:LEU:H	1.68	0.58
1:B:491:PRO:C	1:B:493:ILE:N	2.55	0.58
1:A:1143:TYR:HE1	1:A:1186:PHE:CZ	2.20	0.58
1:A:457:TYR:C	1:A:457:TYR:CD2	2.77	0.58
1:A:52:ALA:HB2	1:A:73:LEU:HD21	1.86	0.58
1:A:594:THR:O	1:A:782:ARG:HG2	2.03	0.58
1:A:981:GLY:O	1:A:982:LEU:HB2	2.03	0.58
1:B:1008:ALA:HB2	1:B:1059:TYR:CD2	2.39	0.58
1:B:635:GLY:O	1:B:673:LEU:HB2	2.03	0.58
1:A:1432:ILE:O	1:A:1432:ILE:HG22	2.03	0.58
1:A:330:ILE:HG22	1:A:337:SER:HA	1.85	0.58
1:A:475:ALA:C	1:A:476:LEU:HD23	2.24	0.58
1:A:641:ASN:O	1:A:644:ASN:N	2.36	0.58
1:B:124:GLY:HA3	1:B:148:LEU:O	2.03	0.58
1:A:1007:SER:HA	1:A:1069:TRP:CD1	2.39	0.58
1:A:315:LEU:HD12	1:A:318:LEU:HD12	1.85	0.58
1:A:498:HIS:HD2	1:A:516:GLU:HA	1.66	0.58
1:A:758:LEU:C	1:A:760:VAL:H	2.07	0.58
1:B:1003:LEU:N	1:B:1003:LEU:HD23	2.19	0.58
1:B:1255:LEU:HD22	1:B:1270:VAL:CG1	2.30	0.58
1:B:42:GLN:CG	1:B:80:GLN:HE21	2.13	0.58
1:B:444:GLU:O	1:B:445:GLU:C	2.39	0.58
1:B:23:TYR:HE1	1:B:656:ASN:H	1.50	0.58
1:B:768:TYR:CE2	1:B:770:PRO:HA	2.38	0.58
2:Y:192:ASN:O	2:Y:221:ILE:HG23	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1228:TRP:N	1:A:1228:TRP:HE3	2.01	0.58
1:A:1279:ARG:O	1:A:1280:TYR:C	2.41	0.58
1:A:160:VAL:HG23	1:A:175:GLU:CB	2.33	0.58
1:A:290:THR:HG22	1:A:290:THR:O	2.04	0.58
1:A:505:SER:HB3	1:A:510:ILE:CD1	2.34	0.58
1:A:628:GLU:O	1:A:629:LYS:HD3	2.04	0.58
1:B:1226:ARG:CZ	1:B:1266:TYR:CE1	2.87	0.58
1:B:457:TYR:HD2	1:B:457:TYR:C	2.07	0.58
1:B:702:GLY:HA2	1:B:728:PHE:CD1	2.37	0.58
1:A:1368:THR:O	1:A:1508:PHE:HE2	1.87	0.58
1:A:161:LEU:HD11	1:A:185:PHE:CD1	2.39	0.58
1:A:576:SER:CB	1:A:577:PRO:HD3	2.33	0.58
1:A:794:LEU:O	1:A:795:THR:HG23	2.03	0.58
1:B:123:ASN:O	1:B:211:THR:HG21	2.04	0.58
1:B:940:SER:HG	1:B:1361:VAL:HG12	1.66	0.58
1:B:140:SER:OG	1:B:187:ASP:HB3	2.04	0.58
1:B:307:VAL:CG1	1:B:313:TYR:HB2	2.33	0.58
1:A:1080:ALA:HA	1:A:1083:LEU:HD12	1.86	0.58
1:A:129:HIS:HD2	1:A:130:THR:O	1.87	0.58
1:A:502:LEU:O	1:A:540:LEU:HA	2.04	0.58
1:B:1438:ASP:O	1:B:1441:ALA:HB3	2.04	0.58
1:B:1244:THR:HG23	1:B:1502:ASP:OD2	2.03	0.58
1:B:256:TYR:O	1:B:257:ASN:ND2	2.37	0.58
1:B:27:ALA:O	1:B:28:PRO:O	2.22	0.58
1:B:494:ASP:O	1:B:496:ILE:N	2.31	0.58
1:A:1255:LEU:HB2	1:A:1270:VAL:CG1	2.30	0.58
1:B:156:LYS:O	1:B:157:ARG:CG	2.48	0.58
1:B:30:ILE:CG2	1:B:31:PHE:H	2.17	0.58
2:X:153:PHE:CE1	2:X:168:LYS:HB3	2.39	0.58
1:A:31:PHE:HZ	1:A:104:LEU:HD22	1.69	0.57
1:A:363:LEU:HD21	1:A:431:LEU:HB2	1.86	0.57
1:B:141:VAL:HG23	1:B:190:ILE:HD11	1.84	0.57
1:B:952:THR:OG1	1:B:953:ILE:N	2.37	0.57
1:A:1047:LYS:O	1:A:1049:LEU:N	2.37	0.57
1:A:290:THR:CG2	1:A:290:THR:O	2.51	0.57
1:A:319:ASN:C	1:A:320:ASN:HD22	2.08	0.57
1:A:823:VAL:HG13	1:A:846:TYR:O	2.04	0.57
1:B:1019:PHE:CD2	1:B:1020:TYR:CD1	2.92	0.57
1:B:284:GLN:NE2	1:B:310:LEU:HD22	2.18	0.57
1:A:1096:ASN:C	1:A:1096:ASN:HD22	2.08	0.57
1:A:24:VAL:HG11	1:A:543:TYR:OH	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1334:LEU:CD2	1:B:1334:LEU:H	2.17	0.57
1:B:1370:THR:HG22	1:B:1370:THR:O	2.03	0.57
1:B:1408:TYR:CD1	1:B:1409:LYS:N	2.72	0.57
1:B:814:THR:OG1	1:B:815:VAL:N	2.36	0.57
1:B:86:THR:HG23	1:B:86:THR:O	2.05	0.57
1:A:1083:LEU:CD1	1:A:1107:LEU:HD11	2.34	0.57
1:A:271:ILE:HD11	1:A:307:VAL:HG22	1.85	0.57
1:A:30:ILE:CG2	1:A:31:PHE:H	2.17	0.57
1:A:443:PRO:HG2	1:A:446:ASN:OD1	2.04	0.57
1:B:1049:LEU:CD2	1:B:1089:VAL:HG13	2.35	0.57
1:B:1183:GLN:O	1:B:1232:LEU:HD22	2.04	0.57
1:B:1495:VAL:O	1:B:1495:VAL:HG13	2.05	0.57
1:B:154:PRO:HB3	1:B:180:ILE:O	2.04	0.57
1:A:1320:LYS:HD2	1:A:1321:GLY:H	1.70	0.57
1:A:388:VAL:O	1:A:420:PHE:HZ	1.88	0.57
1:A:41:ILE:HG22	1:A:81:ASN:O	2.04	0.57
1:A:528:ILE:HD12	1:A:528:ILE:N	2.15	0.57
1:A:686:ILE:CG2	1:A:689:LYS:HE3	2.35	0.57
1:B:1024:TYR:C	1:B:1024:TYR:HD2	2.08	0.57
1:B:478:VAL:CG1	1:B:566:LYS:HD3	2.35	0.57
1:B:786:LEU:N	1:B:786:LEU:HD23	2.19	0.57
1:A:1069:TRP:HE1	1:A:1463:GLN:NE2	2.03	0.57
1:A:124:GLY:C	1:A:125:PHE:CG	2.78	0.57
1:A:1323:LEU:HD12	1:A:1324:HIS:N	2.16	0.57
1:A:1423:VAL:CG2	1:A:1496:TYR:CE1	2.87	0.57
1:A:1465:ASN:ND2	1:A:1465:ASN:N	2.53	0.57
1:A:128:ILE:HG13	1:A:215:ALA:HB2	1.85	0.57
1:A:284:GLN:N	1:A:284:GLN:OE1	2.37	0.57
1:A:415:ASP:CG	1:A:417:VAL:HB	2.25	0.57
1:A:367:ILE:HD13	1:A:466:TYR:CD2	2.39	0.57
1:A:503:ILE:HG12	1:A:540:LEU:HB3	1.85	0.57
1:A:634:CYS:SG	1:A:635:GLY:N	2.78	0.57
1:B:1342:LEU:HD23	1:B:1342:LEU:N	2.19	0.57
1:B:1381:ILE:HD12	1:B:1493:PHE:HB2	1.87	0.57
1:B:412:ARG:CD	1:B:415:ASP:HB2	2.31	0.57
1:B:415:ASP:OD2	1:B:417:VAL:HB	2.03	0.57
1:B:576:SER:CB	1:B:577:PRO:HD3	2.34	0.57
1:B:589:SER:HB2	1:B:785:GLN:HE21	1.68	0.57
1:B:823:VAL:HG13	1:B:846:TYR:O	2.04	0.57
2:Y:153:PHE:CD2	2:Y:154:SER:N	2.72	0.57
1:A:1076:THR:HG22	1:A:1120:GLU:OE2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:CYS:SG	1:A:672:ILE:HG22	2.44	0.57
1:A:693:SER:O	1:A:696:LYS:HB3	2.05	0.57
1:B:1133:LEU:HD12	1:B:1133:LEU:N	2.19	0.57
1:A:1100:ILE:O	1:A:1103:SER:HB2	2.03	0.57
1:A:1279:ARG:CD	1:A:1284:PHE:CG	2.81	0.57
1:A:208:ASP:O	1:A:209:PHE:CB	2.53	0.57
1:A:364:LYS:N	1:A:364:LYS:HD2	2.17	0.57
1:A:24:VAL:HA	1:A:655:THR:OG1	2.04	0.57
1:A:719:SER:HB2	1:A:1123:GLN:NE2	2.20	0.57
1:B:1039:LEU:O	1:B:1042:LYS:HB3	2.05	0.57
1:B:1056:ILE:O	1:B:1058:SER:N	2.38	0.57
1:B:1490:PRO:HB3	1:B:1509:TYR:O	2.04	0.57
1:B:157:ARG:O	1:B:178:ASP:HB2	2.05	0.57
1:B:27:ALA:O	1:B:652:THR:O	2.23	0.57
1:B:774:LEU:HD11	1:B:788:PHE:CZ	2.40	0.57
1:B:77:ASN:ND2	1:B:81:ASN:ND2	2.52	0.57
1:A:132:LYS:NZ	1:A:139:GLN:HE22	2.03	0.57
1:A:173:MET:O	1:A:174:VAL:HB	2.05	0.57
1:A:604:ALA:O	1:A:772:SER:HB3	2.04	0.57
1:A:61:ASP:O	1:A:63:LYS:N	2.36	0.57
1:A:829:ILE:CG1	1:A:925:LYS:HG2	2.35	0.57
1:B:1435:ASN:HB3	1:B:1438:ASP:CB	2.33	0.57
1:B:1379:LEU:HD13	1:B:1493:PHE:CD2	2.39	0.57
1:B:1423:VAL:CG2	1:B:1496:TYR:HE1	2.18	0.57
1:B:386:VAL:CG2	1:B:411:THR:HG21	2.31	0.57
1:A:1008:ALA:N	1:A:1068:VAL:O	2.37	0.57
1:A:1274:LEU:O	1:A:1276:GLU:N	2.38	0.57
1:A:1370:THR:O	1:A:1370:THR:HG22	2.04	0.57
1:A:834:VAL:HG11	1:A:1489:SER:OG	2.05	0.57
1:A:222:TYR:OH	1:A:224:LEU:HD22	2.05	0.57
1:A:227:PHE:HZ	1:A:329:VAL:O	1.88	0.57
1:A:98:PRO:HB2	1:A:99:VAL:HG23	1.86	0.57
1:B:367:ILE:HG23	1:B:368:PRO:HD2	1.86	0.57
1:B:602:LEU:HB2	1:B:774:LEU:O	2.05	0.57
1:B:707:ASN:HB3	1:B:739:ARG:HH12	1.69	0.57
1:A:1156:PHE:CD1	1:A:1164:ILE:HD11	2.39	0.56
1:A:1186:PHE:CD1	1:A:1250:THR:HG22	2.37	0.56
1:A:1307:LEU:O	1:A:1308:ARG:C	2.43	0.56
1:A:298:GLN:O	1:A:299:VAL:HG13	2.04	0.56
1:A:304:GLU:O	1:A:305:THR:O	2.22	0.56
1:A:814:THR:OG1	1:A:815:VAL:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ILE:HD13	2:X:135:HIS:CD2	2.40	0.56
1:B:1027:THR:HG22	1:B:1028:GLY:N	2.20	0.56
1:B:234:GLU:HB2	1:B:247:GLU:H	1.69	0.56
1:B:303:SER:HB3	1:B:347:TYR:OH	2.05	0.56
1:B:422:LEU:H	1:B:422:LEU:HD12	1.70	0.56
1:B:451:GLY:O	1:B:452:TYR:CD2	2.58	0.56
1:B:42:GLN:CD	1:B:543:TYR:HH	2.09	0.56
1:B:758:LEU:C	1:B:760:VAL:H	2.07	0.56
1:A:1206:ARG:HG3	1:A:1206:ARG:NH1	2.15	0.56
1:A:465:LEU:HD13	1:A:544:TYR:CE1	2.40	0.56
1:A:614:ARG:NH2	1:A:798:GLU:OE2	2.38	0.56
1:A:829:ILE:HG13	1:A:925:LYS:HG2	1.87	0.56
1:B:1202:HIS:HD2	1:B:1204:GLN:N	1.93	0.56
1:B:1320:LYS:HG2	1:B:1342:LEU:HD12	1.86	0.56
1:B:1509:TYR:CD2	1:B:1509:TYR:O	2.58	0.56
1:B:169:SER:O	1:B:170:GLU:O	2.23	0.56
1:B:393:GLN:O	1:B:431:LEU:HD23	2.05	0.56
1:B:592:MET:HB3	1:B:780:VAL:HG11	1.87	0.56
1:B:835:ARG:NH1	1:B:835:ARG:CG	2.67	0.56
1:A:1080:ALA:HA	1:A:1083:LEU:HB2	1.86	0.56
1:A:123:ASN:ND2	1:A:150:ASP:H	2.02	0.56
1:A:544:TYR:HE1	1:A:555:VAL:HG12	1.70	0.56
1:B:1016:VAL:HG12	1:B:1017:PRO:N	2.20	0.56
1:B:1370:THR:HG21	1:B:1506:THR:O	2.05	0.56
1:B:153:LYS:HB3	1:B:154:PRO:CD	2.35	0.56
1:B:242:ASN:HB2	1:B:245:ASN:O	2.04	0.56
1:B:28:PRO:HB2	1:B:30:ILE:O	2.05	0.56
1:B:466:TYR:HD1	1:B:467:ILE:N	2.03	0.56
1:A:1056:ILE:O	1:A:1057:MET:C	2.43	0.56
1:A:1100:ILE:HG21	1:A:1158:ILE:HD12	1.86	0.56
1:A:1216:ALA:C	1:A:1217:LEU:HG	2.25	0.56
1:A:1193:TYR:CD1	1:A:1256:LEU:HB3	2.41	0.56
1:A:1278:GLN:CA	1:A:1278:GLN:NE2	2.68	0.56
1:A:1278:GLN:HE21	1:A:1278:GLN:HA	1.70	0.56
1:A:364:LYS:H	1:A:364:LYS:HD3	1.68	0.56
1:B:1320:LYS:HD2	1:B:1321:GLY:N	2.20	0.56
1:B:1465:ASN:ND2	1:B:1465:ASN:N	2.52	0.56
1:B:208:ASP:O	1:B:209:PHE:CB	2.53	0.56
1:B:456:ALA:O	1:B:458:SER:N	2.38	0.56
1:B:686:ILE:CG2	1:B:689:LYS:HE3	2.35	0.56
1:B:909:ASN:H	1:B:926:THR:HG22	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:158:GLU:HG3	2:Y:159:GLU:OE1	2.06	0.56
1:A:1063:ASP:O	1:A:1064:TYR:HB2	2.06	0.56
1:A:644:ASN:C	1:A:644:ASN:HD22	2.07	0.56
1:A:702:GLY:HA2	1:A:728:PHE:CE1	2.41	0.56
1:B:1323:LEU:HD12	1:B:1324:HIS:N	2.20	0.56
1:B:1401:ARG:HB2	1:B:1478:ARG:HA	1.87	0.56
1:B:394:THR:HG23	1:B:395:ILE:N	2.19	0.56
1:B:485:ILE:HG22	1:B:487:THR:HG23	1.86	0.56
1:B:641:ASN:ND2	1:B:644:ASN:HB2	2.20	0.56
2:Y:169:ILE:HG21	2:Y:189:ILE:HD13	1.88	0.56
1:A:1449:LEU:O	1:A:1449:LEU:HD12	2.06	0.56
1:A:215:ALA:C	1:A:216:TYR:CD2	2.79	0.56
1:B:103:TYR:HA	1:B:115:LYS:O	2.06	0.56
1:B:1117:SER:HA	1:B:1145:THR:HG21	1.87	0.56
1:B:348:VAL:HG12	1:B:349:LEU:N	2.21	0.56
1:B:373:VAL:HG23	1:B:374:GLN:H	1.71	0.56
1:B:240:TYR:CZ	1:B:443:PRO:CD	2.88	0.56
1:B:52:ALA:HB2	1:B:73:LEU:HD21	1.87	0.56
1:A:1024:TYR:CE2	1:A:1030:HIS:CD2	2.93	0.56
1:A:1500:ARG:C	1:A:1502:ASP:H	2.08	0.56
1:A:478:VAL:HG11	1:A:566:LYS:HD3	1.88	0.56
1:A:765:ILE:O	1:A:765:ILE:HG23	2.05	0.56
1:B:1244:THR:O	1:B:1285:TYR:HD2	1.88	0.56
1:B:165:ASP:HB3	1:B:171:VAL:HG21	1.86	0.56
1:B:42:GLN:HA	1:B:79:PHE:O	2.06	0.56
1:B:54:ILE:HG23	1:B:105:GLU:O	2.06	0.56
1:A:54:ILE:HG23	1:A:106:VAL:HG22	1.86	0.56
1:A:1090:ASN:ND2	1:A:1158:ILE:HG21	2.15	0.56
1:A:451:GLY:O	1:A:452:TYR:CD2	2.58	0.56
1:A:531:THR:HG23	1:A:533:ASN:HB2	1.87	0.56
1:A:963:ILE:HG23	1:A:973:ILE:HD11	1.88	0.56
1:A:976:ILE:HG21	1:A:1280:TYR:CE1	2.41	0.56
1:B:430:VAL:HG22	1:B:455:ILE:HG12	1.87	0.56
1:B:743:SER:OG	1:B:752:LEU:HD13	2.05	0.56
1:B:42:GLN:CB	1:B:80:GLN:HG2	2.35	0.56
1:A:1191:SER:O	1:A:1195:LEU:HG	2.05	0.56
1:A:1218:VAL:CG1	1:A:1226:ARG:HA	2.35	0.56
1:A:1317:TYR:HB3	1:A:1344:ASP:OD2	2.06	0.56
1:A:1372:GLU:HG3	1:A:1373:GLU:N	2.19	0.56
1:A:243:PHE:CE2	1:A:316:GLU:HG2	2.38	0.56
1:A:438:ASP:O	1:A:439:ALA:C	2.43	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:SER:HB2	1:A:67:SER:O	2.04	0.56
1:A:42:GLN:HB2	1:A:80:GLN:CG	2.35	0.56
1:B:1143:TYR:CE1	1:B:1186:PHE:CZ	2.94	0.56
1:B:226:HIS:CD2	1:B:336:PHE:CE2	2.93	0.56
1:B:576:SER:HG	1:B:589:SER:HB2	1.67	0.56
1:A:1023:HIS:CD2	1:A:1092:TYR:OH	2.59	0.56
1:A:1238:SER:C	1:A:1240:PRO:HD3	2.26	0.56
1:A:1250:THR:O	1:A:1253:TYR:N	2.39	0.56
1:A:1315:VAL:HG22	1:A:1346:LEU:HD11	1.88	0.56
1:A:190:ILE:HG22	1:A:194:PRO:HG3	1.88	0.56
1:A:600:VAL:O	1:A:777:VAL:HG13	2.06	0.56
1:A:24:VAL:HA	1:A:655:THR:HG1	1.71	0.56
1:A:835:ARG:HG2	1:A:835:ARG:NH1	2.19	0.56
1:A:903:LEU:N	1:A:903:LEU:HD22	2.21	0.56
1:B:123:ASN:HD22	1:B:124:GLY:N	2.03	0.56
2:Y:162:LEU:HD12	2:Y:165:LEU:HD23	1.87	0.56
1:A:1206:ARG:HH11	1:A:1206:ARG:CG	2.12	0.56
1:A:1307:LEU:HD13	1:A:1356:LEU:HD12	1.88	0.56
1:A:208:ASP:O	1:A:209:PHE:HB2	2.06	0.56
1:A:291:MET:O	1:A:293:ILE:HG13	2.06	0.56
1:A:503:ILE:HB	1:A:511:HIS:HB2	1.88	0.56
1:B:1435:ASN:O	1:B:1438:ASP:N	2.38	0.56
1:B:1496:TYR:HB3	1:B:1504:GLN:HG3	1.87	0.56
1:B:707:ASN:OD1	1:B:707:ASN:N	2.39	0.56
1:B:707:ASN:HB3	1:B:739:ARG:NH1	2.21	0.56
1:A:1008:ALA:HA	1:A:1059:TYR:CE2	2.41	0.55
1:A:1244:THR:HB	1:A:1247:MET:CB	2.30	0.55
1:A:1259:LEU:CD1	1:A:1300:TYR:HB2	2.36	0.55
1:A:1304:VAL:CG1	1:A:1305:LYS:H	2.17	0.55
1:A:833:VAL:HA	1:A:1430:THR:HG21	1.86	0.55
1:A:838:GLN:HB3	1:A:1486:GLY:HA3	1.88	0.55
1:B:1019:PHE:CD2	1:B:1020:TYR:CE1	2.95	0.55
1:B:352:TYR:HD1	1:B:375:VAL:CG1	2.18	0.55
2:X:186:TYR:CD2	2:X:229:LYS:HD3	2.41	0.55
2:Y:166:ASP:OD1	2:Y:201:ILE:HD13	2.04	0.55
1:A:1225:TYR:CE1	1:A:1272:LYS:CG	2.89	0.55
1:A:486:VAL:O	1:A:486:VAL:HG12	2.05	0.55
1:B:1304:VAL:CG1	1:B:1305:LYS:H	2.16	0.55
1:B:477:LEU:HA	1:B:564:GLU:HG2	1.88	0.55
1:B:497:THR:HG23	1:B:498:HIS:N	2.17	0.55
1:B:915:GLU:HG3	1:B:920:LYS:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:968:VAL:O	1:B:968:VAL:HG23	2.04	0.55
1:A:1020:TYR:CD2	1:A:1294:ILE:HG22	2.40	0.55
1:A:1024:TYR:HD2	1:A:1024:TYR:C	2.08	0.55
1:A:1023:HIS:HD2	1:A:1092:TYR:OH	1.89	0.55
1:A:269:PHE:HB2	1:A:283:MET:HE3	1.88	0.55
1:A:295:GLY:O	1:A:296:ILE:CD1	2.55	0.55
1:A:444:GLU:O	1:A:445:GLU:C	2.44	0.55
1:B:1491:ALA:HB3	1:B:1509:TYR:CE2	2.40	0.55
1:A:1248:VAL:CG2	1:A:1277:GLU:HG2	2.37	0.55
1:A:1502:ASP:C	1:A:1503:LYS:HD2	2.27	0.55
1:A:905:ILE:HD13	1:A:931:PRO:HG3	1.87	0.55
1:B:1290:THR:O	1:B:1294:ILE:CG1	2.54	0.55
1:B:163:PHE:CE2	1:B:188:PHE:CD2	2.95	0.55
1:B:113:LYS:NZ	1:B:656:ASN:HD21	2.05	0.55
1:B:824:PHE:CE1	1:B:846:TYR:HD1	2.25	0.55
1:A:1108:VAL:HG13	1:A:1109:GLU:N	2.21	0.55
1:A:124:GLY:HA3	1:A:148:LEU:O	2.06	0.55
1:B:1056:ILE:O	1:B:1057:MET:C	2.44	0.55
1:B:330:ILE:HG22	1:B:337:SER:HA	1.87	0.55
1:B:950:TYR:CE1	1:B:1271:ILE:HD11	2.41	0.55
1:A:330:ILE:HG22	1:A:337:SER:CA	2.35	0.55
1:A:432:GLU:OE2	1:A:453:ARG:NH2	2.40	0.55
1:A:647:HIS:O	1:A:650:GLY:N	2.38	0.55
1:A:92:LEU:H	1:A:93:PRO:HD3	1.72	0.55
1:B:106:VAL:HG12	1:B:107:VAL:N	2.22	0.55
1:B:1143:TYR:CE1	1:B:1186:PHE:CE2	2.94	0.55
1:B:1184:SER:HA	1:B:1232:LEU:CB	2.36	0.55
1:B:442:LEU:O	1:B:443:PRO:C	2.41	0.55
1:B:24:VAL:HA	1:B:655:THR:HG1	1.71	0.55
1:B:981:GLY:O	1:B:982:LEU:CB	2.49	0.55
2:Y:146:LEU:HD22	2:Y:146:LEU:C	2.27	0.55
1:A:1277:GLU:OE2	1:A:1277:GLU:HA	2.06	0.55
1:A:1259:LEU:HD11	1:A:1300:TYR:HB2	1.89	0.55
1:A:829:ILE:HG13	1:A:925:LYS:CG	2.37	0.55
1:B:1112:GLN:HB2	1:B:1118:PHE:CE1	2.42	0.55
1:B:33:VAL:HB	1:B:209:PHE:HE2	1.72	0.55
1:B:481:HIS:CE1	1:B:529:PRO:HG3	2.41	0.55
1:B:686:ILE:HG22	1:B:689:LYS:HE3	1.88	0.55
1:B:838:GLN:H	1:B:1486:GLY:HA3	1.71	0.55
1:A:1066:TYR:CD1	1:A:1066:TYR:N	2.74	0.55
1:A:1115:ASN:HD22	1:A:1115:ASN:C	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1221:ASN:ND2	1:A:1222:PRO:HA	2.22	0.55
1:A:829:ILE:HG22	1:A:830:PRO:HD2	1.89	0.55
1:A:834:VAL:HG21	1:A:1489:SER:OG	2.06	0.55
1:A:896:VAL:O	1:A:897:THR:HG22	2.06	0.55
1:A:957:LYS:HG3	1:A:958:GLU:N	2.21	0.55
1:B:1216:ALA:C	1:B:1217:LEU:HG	2.27	0.55
1:B:1272:LYS:O	1:B:1272:LYS:HG3	2.05	0.55
1:B:1279:ARG:HG3	1:B:1284:PHE:HB2	1.89	0.55
1:B:465:LEU:HD13	1:B:544:TYR:CE1	2.42	0.55
1:B:498:HIS:HB3	1:B:514:THR:CG2	2.36	0.55
1:B:606:ASP:O	1:B:608:ALA:N	2.40	0.55
1:A:1429:PRO:HB3	1:A:1488:LEU:HD22	1.88	0.55
1:A:515:ARG:HH12	1:A:527:ASN:H	1.55	0.55
1:A:561:LEU:O	1:A:563:ILE:CG2	2.55	0.55
1:B:1432:ILE:HG21	1:B:1479:ILE:HD12	1.89	0.55
1:B:1379:LEU:HD13	1:B:1493:PHE:CE2	2.41	0.55
1:B:348:VAL:CG1	1:B:349:LEU:N	2.70	0.55
1:B:50:PHE:CD1	1:B:109:LYS:HE2	2.42	0.55
1:A:768:TYR:CE2	1:A:770:PRO:HA	2.42	0.55
1:B:1012:LEU:O	1:B:1015:VAL:HG13	2.07	0.55
1:B:1024:TYR:HB2	1:B:1298:THR:CG2	2.37	0.55
1:B:1230:ASP:CG	1:B:1246:ARG:HD2	2.26	0.55
1:B:306:ALA:O	1:B:307:VAL:CG2	2.55	0.55
1:B:628:GLU:O	1:B:629:LYS:HD3	2.07	0.55
1:B:707:ASN:HB3	1:B:739:ARG:NH2	2.22	0.55
2:X:194:LYS:HG3	2:X:195:ASP:H	1.72	0.55
2:Y:208:GLN:O	2:Y:212:MET:HG3	2.07	0.55
1:A:1401:ARG:HH11	1:A:1403:VAL:CG2	2.20	0.54
1:A:395:ILE:O	1:A:429:THR:HG23	2.06	0.54
1:A:42:GLN:CB	1:A:80:GLN:HG2	2.37	0.54
1:B:1028:GLY:O	1:B:1029:ASN:O	2.25	0.54
1:B:1244:THR:HG22	1:B:1245:ALA:N	2.21	0.54
1:B:1300:TYR:C	1:B:1300:TYR:CD2	2.80	0.54
1:B:182:ILE:HD12	1:B:777:VAL:HG11	1.89	0.54
1:B:489:LYS:O	1:B:490:SER:HB2	2.08	0.54
1:B:707:ASN:HB3	1:B:739:ARG:HH22	1.71	0.54
2:Y:153:PHE:CE1	2:Y:168:LYS:HB3	2.42	0.54
1:A:123:ASN:O	1:A:211:THR:HG21	2.08	0.54
1:A:1408:TYR:O	1:A:1410:PRO:HD3	2.06	0.54
1:B:1083:LEU:CD1	1:B:1107:LEU:HD11	2.38	0.54
1:B:1196:SER:HB2	1:B:1257:THR:CG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ILE:HG22	1:B:194:PRO:HG3	1.89	0.54
1:B:235:TYR:CD2	1:B:235:TYR:N	2.74	0.54
1:A:1204:GLN:OE1	1:A:1204:GLN:HA	2.07	0.54
1:A:160:VAL:HG13	1:A:161:LEU:O	2.07	0.54
1:A:226:HIS:CD2	1:A:336:PHE:CE2	2.96	0.54
1:A:373:VAL:HG23	1:A:374:GLN:N	2.22	0.54
1:A:477:LEU:HA	1:A:564:GLU:HG2	1.89	0.54
1:A:556:SER:OG	1:A:557:ASP:N	2.40	0.54
1:A:703:ALA:HB1	1:A:735:ALA:HB3	1.90	0.54
1:B:1238:SER:C	1:B:1240:PRO:HD3	2.28	0.54
1:B:617:LYS:CE	1:B:625:GLN:HE22	2.17	0.54
1:B:700:TYR:CE1	1:B:758:LEU:HD12	2.43	0.54
1:B:765:ILE:O	1:B:765:ILE:HG23	2.07	0.54
1:A:1066:TYR:HD1	1:A:1066:TYR:N	2.06	0.54
1:A:1320:LYS:HG2	1:A:1342:LEU:HD12	1.88	0.54
1:A:1136:GLU:OE1	1:A:1415:SER:HB2	2.06	0.54
1:B:1076:THR:HG22	1:B:1120:GLU:OE2	2.08	0.54
1:B:1104:LEU:HD13	1:B:1164:ILE:CD1	2.38	0.54
1:B:1278:GLN:NE2	1:B:1278:GLN:HA	2.22	0.54
1:B:373:VAL:CG2	1:B:374:GLN:N	2.70	0.54
1:B:387:PRO:HA	1:B:410:VAL:HG22	1.90	0.54
1:B:73:LEU:N	1:B:73:LEU:HD23	2.23	0.54
1:B:796:THR:HA	1:B:818:LYS:HA	1.88	0.54
1:B:856:CYS:O	1:B:914:LEU:HA	2.08	0.54
2:X:158:GLU:HG3	2:X:159:GLU:OE1	2.07	0.54
1:A:1311:MET:HE2	1:A:1354:SER:O	2.08	0.54
1:A:489:LYS:O	1:A:490:SER:HB2	2.07	0.54
1:A:511:HIS:NE2	1:A:531:THR:HG21	2.22	0.54
1:A:831:TYR:CE1	1:A:1457:ASP:HB3	2.42	0.54
1:A:835:ARG:CG	1:A:835:ARG:HH11	2.18	0.54
1:B:292:LEU:HD22	1:B:296:ILE:O	2.08	0.54
1:B:457:TYR:CD2	1:B:457:TYR:O	2.61	0.54
1:B:541:LEU:HB2	1:B:558:SER:CB	2.26	0.54
1:B:947:ARG:HB2	1:B:949:ILE:CG1	2.37	0.54
1:A:628:GLU:HG3	1:A:628:GLU:O	2.06	0.54
1:A:915:GLU:HG3	1:A:920:LYS:HG3	1.88	0.54
1:B:1186:PHE:CD1	1:B:1250:THR:HG22	2.38	0.54
1:B:1228:TRP:HZ3	1:B:1270:VAL:HG22	1.73	0.54
1:B:1500:ARG:C	1:B:1502:ASP:H	2.11	0.54
1:B:160:VAL:HG13	1:B:161:LEU:O	2.06	0.54
1:B:394:THR:HG22	1:B:402:SER:OG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:TRP:CD1	1:B:482:LEU:HD21	2.43	0.54
1:B:640:LEU:H	1:B:644:ASN:HB3	1.73	0.54
1:B:823:VAL:HA	1:B:846:TYR:O	2.06	0.54
1:A:1290:THR:HG22	1:A:1290:THR:O	2.07	0.54
1:A:1325:ASN:O	1:A:1325:ASN:ND2	2.41	0.54
1:A:743:SER:OG	1:A:752:LEU:HD13	2.08	0.54
1:A:987:ILE:HG12	1:A:1294:ILE:HD12	1.90	0.54
1:B:1066:TYR:HD1	1:B:1066:TYR:N	2.05	0.54
1:B:544:TYR:HE1	1:B:555:VAL:HG12	1.73	0.54
1:B:739:ARG:HB2	1:B:752:LEU:HD21	1.88	0.54
1:A:1423:VAL:HG21	1:A:1496:TYR:CE1	2.43	0.54
1:A:1456:LYS:O	1:A:1457:ASP:C	2.46	0.54
1:A:491:PRO:C	1:A:493:ILE:N	2.60	0.54
1:A:56:ILE:HG13	1:A:66:TYR:HD2	1.73	0.54
1:A:142:LYS:HD3	1:A:775:TRP:CG	2.43	0.54
1:A:144:ARG:HG2	1:A:775:TRP:CZ2	2.43	0.54
1:A:961:TYR:OH	1:A:1343:ASN:ND2	2.41	0.54
1:B:1115:ASN:HD22	1:B:1117:SER:H	1.56	0.54
1:B:362:PHE:HA	1:B:455:ILE:H	1.72	0.54
1:B:509:ILE:HD11	1:B:651:LEU:HD21	1.90	0.54
1:B:839:ILE:HG22	1:B:900:VAL:HG23	1.88	0.54
1:A:1043:GLN:O	1:A:1046:LYS:HB2	2.08	0.54
1:A:1381:ILE:CG1	1:A:1404:ALA:HB2	2.28	0.54
1:A:942:VAL:HG21	1:A:957:LYS:HB3	1.89	0.54
1:B:101:TYR:CE1	1:B:116:ARG:NE	2.75	0.54
1:B:1341:LEU:HB3	1:B:1342:LEU:HD23	1.89	0.54
1:B:1236:ASP:HB2	1:B:1412:ARG:NH2	2.20	0.54
1:B:235:TYR:N	1:B:235:TYR:HD2	2.05	0.54
1:B:493:ILE:HG23	1:B:494:ASP:H	1.72	0.54
1:B:948:GLY:HA2	1:B:952:THR:O	2.08	0.54
1:A:1307:LEU:HB2	1:A:1355:GLY:HA2	1.90	0.54
1:A:235:TYR:CD2	1:A:235:TYR:N	2.76	0.54
1:A:968:VAL:HG23	1:A:971:THR:HG21	1.91	0.54
1:B:35:ALA:HA	1:B:150:ASP:OD1	2.07	0.54
1:B:647:HIS:O	1:B:650:GLY:N	2.41	0.54
1:A:1161:LEU:HB3	1:A:1164:ILE:HG23	1.90	0.53
1:A:1273:TRP:CZ3	1:A:1274:LEU:HD23	2.43	0.53
1:A:1381:ILE:HD13	1:A:1509:TYR:CD1	2.43	0.53
1:A:195:ARG:HH11	1:A:195:ARG:CG	2.22	0.53
1:A:25:ILE:O	1:A:654:LEU:N	2.38	0.53
1:A:718:ILE:HG21	1:A:725:ILE:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1082:ALA:O	1:B:1083:LEU:C	2.46	0.53
1:B:1205:PHE:HA	1:B:1208:ILE:HG13	1.90	0.53
1:B:138:ASP:H	1:B:190:ILE:HB	1.73	0.53
1:B:794:LEU:O	1:B:795:THR:HG23	2.08	0.53
2:X:167:PHE:O	2:X:171:GLN:HB2	2.09	0.53
2:Y:162:LEU:O	2:Y:166:ASP:HB2	2.08	0.53
1:A:1225:TYR:CE1	1:A:1272:LYS:HG2	2.43	0.53
1:A:161:LEU:C	1:A:162:THR:HG22	2.28	0.53
1:A:371:ILE:HD12	1:A:390:LEU:CD2	2.35	0.53
1:A:59:TYR:CD1	1:A:103:TYR:HE1	2.25	0.53
1:A:605:VAL:HG12	1:A:606:ASP:N	2.22	0.53
1:A:610:TYR:HB2	1:A:614:ARG:HD2	1.90	0.53
1:B:1334:LEU:CD2	1:B:1334:LEU:N	2.71	0.53
1:B:160:VAL:HG23	1:B:175:GLU:CB	2.38	0.53
1:B:608:ALA:O	1:B:609:VAL:C	2.47	0.53
1:B:614:ARG:NH2	1:B:798:GLU:OE2	2.39	0.53
1:B:23:TYR:HE1	1:B:656:ASN:HB2	1.72	0.53
1:B:686:ILE:C	1:B:688:ALA:N	2.58	0.53
1:A:1053:MET:O	1:A:1056:ILE:HG23	2.08	0.53
1:A:195:ARG:HG2	1:A:195:ARG:NH1	2.23	0.53
1:A:541:LEU:HB2	1:A:558:SER:CB	2.35	0.53
1:A:823:VAL:HA	1:A:846:TYR:O	2.09	0.53
1:B:1190:ILE:HG12	1:B:1253:TYR:CE1	2.44	0.53
1:B:124:GLY:C	1:B:125:PHE:CG	2.81	0.53
1:B:231:ILE:HB	1:B:250:ILE:HG22	1.89	0.53
1:B:292:LEU:HD13	1:B:293:ILE:N	2.22	0.53
1:B:718:ILE:HG21	1:B:725:ILE:HG12	1.89	0.53
1:B:781:PRO:O	1:B:782:ARG:HB2	2.08	0.53
1:B:855:PHE:CZ	1:B:886:GLN:CB	2.77	0.53
2:Y:150:ILE:O	2:Y:150:ILE:HG13	2.09	0.53
1:A:1184:SER:HA	1:A:1232:LEU:HB2	1.90	0.53
1:A:154:PRO:HB3	1:A:180:ILE:O	2.08	0.53
1:A:172:ASP:OD2	1:A:173:MET:N	2.38	0.53
1:A:493:ILE:HG23	1:A:494:ASP:H	1.72	0.53
1:A:593:ALA:HA	1:A:782:ARG:O	2.08	0.53
1:A:739:ARG:HB2	1:A:752:LEU:HD21	1.91	0.53
1:A:911:ASN:CG	1:A:924:VAL:HG13	2.29	0.53
1:A:988:LEU:HD23	1:A:1021:VAL:HG13	1.89	0.53
1:B:1008:ALA:O	1:B:1009:GLU:C	2.47	0.53
1:B:137:PRO:O	1:B:138:ASP:HB2	2.08	0.53
1:B:326:ALA:HA	1:B:341:GLU:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:VAL:HG23	1:B:610:TYR:CD2	2.43	0.53
1:A:1148:THR:OG1	1:A:1152:ILE:HD11	2.08	0.53
1:A:1020:TYR:HD2	1:A:1294:ILE:CG2	2.21	0.53
1:A:1337:PRO:O	1:A:1338:VAL:HG23	2.09	0.53
1:A:1348:VAL:HG11	1:A:1359:VAL:CG2	2.35	0.53
1:A:1377:PHE:CE1	1:A:1467:ILE:HD12	2.43	0.53
1:A:1467:ILE:N	1:A:1468:PRO:HD3	2.23	0.53
1:A:42:GLN:HA	1:A:79:PHE:O	2.08	0.53
1:A:639:GLY:N	1:A:645:VAL:HG22	2.16	0.53
1:A:85:LEU:O	1:A:86:THR:CB	2.54	0.53
1:B:1090:ASN:O	1:B:1090:ASN:OD1	2.27	0.53
1:B:635:GLY:C	1:B:673:LEU:HA	2.28	0.53
1:A:1145:THR:O	1:A:1149:VAL:HG23	2.08	0.53
1:A:1030:HIS:CE1	1:A:1306:GLN:HE22	2.25	0.53
1:A:1429:PRO:HG2	1:A:1511:THR:CB	2.36	0.53
1:A:229:VAL:HG22	1:A:252:ALA:HB2	1.90	0.53
1:A:308:LYS:HA	1:A:313:TYR:O	2.08	0.53
1:A:467:ILE:HD12	1:A:484:ILE:HD12	1.90	0.53
1:B:1080:ALA:HA	1:B:1083:LEU:HB2	1.91	0.53
1:B:1153:ARG:CZ	1:B:1168:LEU:HD22	2.39	0.53
1:B:1257:THR:O	1:B:1260:ASN:HB2	2.08	0.53
1:B:169:SER:O	1:B:171:VAL:HG23	2.08	0.53
1:B:922:ILE:CD1	4:B:2001:NAG:H82	2.28	0.53
1:B:284:GLN:OE1	1:B:284:GLN:N	2.42	0.53
1:B:290:THR:O	1:B:290:THR:CG2	2.57	0.53
1:B:598:SER:HA	1:B:805:SER:OG	2.08	0.53
1:B:625:GLN:O	1:B:629:LYS:HE2	2.08	0.53
1:A:1003:LEU:HD13	1:A:1498:TYR:CD1	2.43	0.53
1:A:141:VAL:HG23	1:A:190:ILE:HD11	1.91	0.53
1:A:456:ALA:O	1:A:458:SER:N	2.42	0.53
1:A:754:MET:O	1:A:755:LYS:HG2	2.09	0.53
1:A:841:LEU:HD12	1:A:859:MET:CE	2.36	0.53
1:A:951:GLY:HA3	1:A:1224:ILE:HG23	1.91	0.53
1:B:243:PHE:CZ	1:B:316:GLU:CG	2.85	0.53
1:B:296:ILE:HG22	1:B:297:ALA:H	1.73	0.53
1:B:56:ILE:HG13	1:B:66:TYR:HD2	1.74	0.53
1:B:710:THR:HG23	1:B:713:GLN:CD	2.29	0.53
1:B:857:VAL:HG21	1:B:896:VAL:HG11	1.90	0.53
1:B:983:LEU:HD11	1:B:1356:LEU:HD22	1.91	0.53
2:X:136:LEU:HD23	2:X:136:LEU:N	2.24	0.53
1:A:1090:ASN:O	1:A:1090:ASN:OD1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:THR:HG22	1:A:215:ALA:N	2.23	0.53
1:A:73:LEU:HB2	1:A:79:PHE:HA	1.89	0.53
1:B:1043:GLN:HA	1:B:1043:GLN:OE1	2.09	0.53
1:B:298:GLN:O	1:B:299:VAL:HG13	2.09	0.53
1:B:515:ARG:NH1	1:B:527:ASN:H	2.04	0.53
1:B:837:GLU:C	1:B:901:LEU:HD12	2.30	0.53
1:A:1142:LEU:HD13	1:A:1187:THR:HG22	1.90	0.53
1:A:240:TYR:CZ	1:A:443:PRO:CD	2.92	0.53
1:A:313:TYR:CZ	1:A:321:LYS:HD2	2.43	0.53
1:A:435:VAL:CG1	1:A:436:LYS:N	2.72	0.53
1:A:531:THR:CG2	1:A:533:ASN:HB2	2.38	0.53
1:A:707:ASN:N	1:A:707:ASN:OD1	2.41	0.53
1:A:907:LEU:HD12	1:A:908:HIS:H	1.73	0.53
1:A:979:VAL:C	1:A:980:LYS:HD2	2.29	0.53
1:B:1096:ASN:HD22	1:B:1099:SER:H	1.56	0.53
1:B:1150:ILE:HD11	1:B:1190:ILE:CG2	2.38	0.53
1:B:1290:THR:O	1:B:1294:ILE:HG12	2.09	0.53
1:B:1439:LEU:HA	1:B:1442:LEU:HD12	1.90	0.53
1:B:1475:VAL:HG22	1:B:1476:ARG:N	2.22	0.53
1:B:838:GLN:HB3	1:B:1486:GLY:HA3	1.89	0.53
1:B:27:ALA:HB2	1:B:39:ILE:HD12	1.91	0.53
1:B:430:VAL:HA	1:B:454:ALA:O	2.09	0.53
1:B:240:TYR:OH	1:B:443:PRO:HD3	2.09	0.53
1:B:606:ASP:C	1:B:608:ALA:H	2.12	0.53
1:B:653:PHE:CE1	1:B:660:ASP:HB3	2.44	0.53
1:B:700:TYR:C	1:B:702:GLY:N	2.60	0.53
1:B:835:ARG:NE	1:B:905:ILE:HD11	2.24	0.53
1:A:1115:ASN:ND2	1:A:1115:ASN:C	2.63	0.53
1:A:1257:THR:O	1:A:1260:ASN:HB2	2.09	0.53
1:A:1491:ALA:HB3	1:A:1509:TYR:CE2	2.42	0.53
1:A:284:GLN:NE2	1:A:310:LEU:HD22	2.24	0.53
1:A:306:ALA:O	1:A:307:VAL:CG2	2.56	0.53
1:B:1105:LEU:HD22	1:B:1109:GLU:OE1	2.09	0.53
1:B:1383:THR:HG22	1:B:1402:ILE:HG12	1.91	0.53
1:B:1467:ILE:N	1:B:1468:PRO:HD3	2.23	0.53
1:B:499:TYR:O	1:B:514:THR:HG23	2.09	0.53
1:B:561:LEU:O	1:B:563:ILE:CG2	2.57	0.53
1:B:61:ASP:O	1:B:63:LYS:N	2.37	0.53
1:A:319:ASN:O	1:A:320:ASN:ND2	2.43	0.52
1:A:686:ILE:C	1:A:688:ALA:H	2.12	0.52
1:B:1028:GLY:O	1:B:1030:HIS:CD2	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1053:MET:O	1:B:1056:ILE:HG23	2.08	0.52
1:B:1136:GLU:OE1	1:B:1415:SER:CB	2.57	0.52
1:B:1129:LEU:HD13	1:B:1139:GLU:HB3	1.91	0.52
1:B:177:ILE:HD11	1:B:179:HIS:HB2	1.91	0.52
1:B:50:PHE:CE2	1:B:79:PHE:CE2	2.97	0.52
1:A:1003:LEU:N	1:A:1003:LEU:HD23	2.23	0.52
1:A:1019:PHE:CD2	1:A:1020:TYR:CD1	2.98	0.52
1:A:127:PHE:CE2	1:A:809:ILE:HD12	2.44	0.52
1:A:1452:ASP:O	1:A:1462:LEU:HA	2.08	0.52
1:A:505:SER:O	1:A:506:LYS:HB2	2.10	0.52
1:A:661:ASP:OD2	1:A:663:GLN:NE2	2.43	0.52
1:A:992:LEU:HD21	1:A:1045:LEU:HD11	1.90	0.52
1:B:1105:LEU:HA	1:B:1108:VAL:HG11	1.91	0.52
1:B:1210:SER:OG	1:B:1211:ALA:N	2.40	0.52
1:B:1456:LYS:O	1:B:1457:ASP:C	2.48	0.52
1:B:328:THR:OG1	1:B:339:GLU:HG2	2.08	0.52
1:B:363:LEU:HD23	1:B:454:ALA:CB	2.40	0.52
1:B:531:THR:HG23	1:B:533:ASN:H	1.74	0.52
2:X:222:ASN:O	2:X:223:LYS:HG3	2.07	0.52
1:A:1408:TYR:HD2	1:A:1418:GLY:HA2	1.74	0.52
1:A:363:LEU:HD23	1:A:454:ALA:HB3	1.91	0.52
1:A:792:ASP:O	1:A:793:SER:HB2	2.10	0.52
1:A:957:LYS:HG3	1:A:958:GLU:H	1.73	0.52
1:B:1288:GLN:O	1:B:1292:ASN:ND2	2.43	0.52
1:B:142:LYS:HD3	1:B:775:TRP:CD2	2.43	0.52
1:B:349:LEU:HD22	1:B:446:ASN:HD22	1.75	0.52
1:B:571:LEU:CD2	1:B:600:VAL:HG13	2.39	0.52
1:B:719:SER:HB2	1:B:1123:GLN:NE2	2.25	0.52
1:A:1113:LEU:N	1:A:1117:SER:O	2.43	0.52
1:A:348:VAL:CG1	1:A:349:LEU:N	2.72	0.52
1:A:720:LEU:HD11	1:A:1446:VAL:HG22	1.91	0.52
1:A:838:GLN:HA	1:A:901:LEU:HB2	1.92	0.52
1:B:1226:ARG:NE	1:B:1266:TYR:CE1	2.77	0.52
1:B:1432:ILE:CG2	1:B:1479:ILE:HD12	2.39	0.52
1:B:27:ALA:CB	1:B:39:ILE:HD12	2.39	0.52
2:X:162:LEU:O	2:X:166:ASP:HB2	2.10	0.52
2:X:192:ASN:O	2:X:221:ILE:HG23	2.08	0.52
1:A:57:LYS:HD2	1:A:105:GLU:OE1	2.10	0.52
1:A:173:MET:O	1:A:174:VAL:CB	2.57	0.52
1:A:322:TYR:CD2	1:A:322:TYR:N	2.78	0.52
1:A:460:LEU:C	1:A:462:GLN:H	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:TYR:HD1	1:A:467:ILE:N	2.08	0.52
1:A:814:THR:O	1:A:815:VAL:HG23	2.10	0.52
1:B:1016:VAL:HG12	1:B:1017:PRO:HD3	1.92	0.52
1:B:1045:LEU:HD23	1:B:1045:LEU:N	2.25	0.52
1:B:198:MET:HE1	1:B:218:GLU:HB2	1.91	0.52
1:B:517:LYS:HA	1:B:524:GLN:HE22	1.75	0.52
1:B:362:PHE:CE1	1:B:638:GLY:O	2.62	0.52
1:B:916:THR:HG22	1:B:917:TRP:N	2.25	0.52
1:A:1128:LYS:O	1:A:1246:ARG:NH2	2.42	0.52
1:A:1236:ASP:HB2	1:A:1412:ARG:NH2	2.24	0.52
1:A:1196:SER:HB2	1:A:1257:THR:CG2	2.39	0.52
1:A:977:LEU:HA	1:A:1361:VAL:CG2	2.38	0.52
1:A:250:ILE:HG21	1:A:327:VAL:HG21	1.91	0.52
1:A:944:LEU:HD13	1:A:1350:THR:HB	1.90	0.52
1:B:386:VAL:N	1:B:410:VAL:HG13	2.25	0.52
1:A:1249:GLU:HG2	1:A:1253:TYR:HE2	1.75	0.52
1:A:1431:GLY:C	1:A:1432:ILE:HG12	2.30	0.52
1:A:1440:LYS:O	1:A:1444:GLU:HB2	2.09	0.52
1:A:196:TYR:CZ	1:A:221:GLU:HB2	2.45	0.52
1:A:267:ILE:HG23	1:A:327:VAL:HG22	1.91	0.52
1:A:431:LEU:C	1:A:431:LEU:CD2	2.78	0.52
1:A:901:LEU:HD23	1:A:901:LEU:O	2.10	0.52
1:B:1022:PHE:HD2	1:B:1092:TYR:CD2	2.27	0.52
1:B:24:VAL:HA	1:B:655:THR:OG1	2.09	0.52
1:B:987:ILE:CD1	1:B:1294:ILE:HD13	2.39	0.52
1:A:132:LYS:HZ1	1:A:139:GLN:HE22	1.58	0.52
1:A:1432:ILE:CG2	1:A:1479:ILE:HD12	2.40	0.52
1:A:244:LYS:HE3	1:A:304:GLU:CD	2.30	0.52
1:A:686:ILE:HG22	1:A:689:LYS:HE3	1.92	0.52
1:B:1066:TYR:CD1	1:B:1066:TYR:N	2.75	0.52
1:B:1115:ASN:ND2	1:B:1117:SER:H	2.07	0.52
1:B:1153:ARG:HD2	1:B:1197:LEU:O	2.10	0.52
1:B:1411:SER:O	1:B:1414:GLU:HB2	2.10	0.52
1:B:1423:VAL:HG22	1:B:1496:TYR:CD1	2.45	0.52
1:B:661:ASP:OD2	1:B:663:GLN:NE2	2.42	0.52
1:B:85:LEU:HD22	1:B:85:LEU:N	2.23	0.52
1:B:948:GLY:O	1:B:950:TYR:N	2.42	0.52
1:A:1334:LEU:N	1:A:1334:LEU:CD2	2.72	0.52
1:A:172:ASP:O	1:A:173:MET:HB2	2.09	0.52
1:A:243:PHE:CZ	1:A:316:GLU:HA	2.45	0.52
1:A:227:PHE:HB3	1:A:254:TYR:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ALA:HA	1:A:341:GLU:HA	1.90	0.52
1:A:435:VAL:HG12	1:A:436:LYS:N	2.25	0.52
1:B:1003:LEU:HD13	1:B:1498:TYR:CD1	2.45	0.52
1:B:222:TYR:OH	1:B:224:LEU:HD22	2.09	0.52
2:Y:190:THR:HG22	2:Y:200:GLU:HG2	1.92	0.52
1:A:1022:PHE:HE2	1:A:1092:TYR:CG	2.28	0.52
1:A:1421:HIS:CE1	1:A:1498:TYR:CG	2.97	0.52
1:A:1435:ASN:O	1:A:1438:ASP:HB2	2.10	0.52
1:A:1511:THR:HG23	1:A:1511:THR:O	2.10	0.52
1:A:163:PHE:N	1:A:163:PHE:CD1	2.73	0.52
1:A:362:PHE:CE1	1:A:638:GLY:O	2.63	0.52
1:A:621:GLU:O	1:A:625:GLN:HG3	2.10	0.52
1:A:680:GLN:HG2	1:A:680:GLN:O	2.10	0.52
1:A:840:GLN:HG2	1:A:899:THR:CG2	2.40	0.52
1:B:1025:LEU:HD13	1:B:1031:TRP:HZ3	1.74	0.52
1:B:1313:ILE:HG22	1:B:1314:ASP:H	1.75	0.52
1:B:138:ASP:OD1	1:B:192:SER:HA	2.10	0.52
1:B:1408:TYR:HD2	1:B:1418:GLY:HA2	1.75	0.52
1:B:169:SER:O	1:B:170:GLU:C	2.49	0.52
1:B:269:PHE:CB	1:B:283:MET:CE	2.88	0.52
1:B:44:TYR:HE1	1:B:497:THR:OG1	1.92	0.52
1:B:626:PHE:O	1:B:628:GLU:N	2.44	0.52
1:B:686:ILE:C	1:B:688:ALA:H	2.10	0.52
1:A:1016:VAL:HG12	1:A:1017:PRO:N	2.25	0.51
1:A:101:TYR:HE1	1:A:116:ARG:NE	2.08	0.51
1:A:1045:LEU:N	1:A:1045:LEU:HD23	2.24	0.51
1:A:1228:TRP:HZ3	1:A:1270:VAL:HG22	1.73	0.51
1:A:1411:SER:O	1:A:1414:GLU:HB2	2.10	0.51
1:A:328:THR:OG1	1:A:339:GLU:HG2	2.10	0.51
1:A:415:ASP:OD2	1:A:417:VAL:HB	2.09	0.51
1:B:1019:PHE:HE2	1:B:1088:GLN:NE2	2.07	0.51
1:B:1133:LEU:H	1:B:1133:LEU:HD12	1.74	0.51
1:B:128:ILE:HG23	1:B:145:VAL:CG2	2.39	0.51
1:B:1030:HIS:CE1	1:B:1306:GLN:NE2	2.78	0.51
1:B:1434:ALA:HB1	1:B:1477:PHE:CE1	2.45	0.51
1:B:1435:ASN:HD22	1:B:1478:ARG:HB2	1.74	0.51
1:B:295:GLY:O	1:B:296:ILE:HD13	2.10	0.51
2:X:183:THR:CB	2:X:230:GLN:HB3	2.40	0.51
1:A:1133:LEU:N	1:A:1134:PRO:CD	2.73	0.51
1:A:1272:LYS:HG3	1:A:1272:LYS:O	2.09	0.51
1:A:1284:PHE:HD2	1:A:1285:TYR:CE1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1320:LYS:HD2	1:A:1321:GLY:N	2.25	0.51
1:A:162:THR:OG1	1:A:162:THR:O	2.27	0.51
1:A:253:ARG:HB2	1:A:253:ARG:CZ	2.40	0.51
1:A:839:ILE:HD11	1:A:1483:PHE:CE1	2.44	0.51
1:B:100:SER:O	1:B:101:TYR:HD2	1.94	0.51
1:B:1172:ASP:O	1:B:1175:LEU:HB2	2.10	0.51
1:B:215:ALA:C	1:B:216:TYR:CD2	2.83	0.51
1:B:227:PHE:CZ	1:B:329:VAL:O	2.63	0.51
1:B:250:ILE:O	1:B:250:ILE:HG13	2.10	0.51
1:B:754:MET:O	1:B:755:LYS:HG2	2.11	0.51
1:B:594:THR:O	1:B:782:ARG:HG2	2.09	0.51
1:B:829:ILE:HG13	1:B:925:LYS:CG	2.38	0.51
1:A:106:VAL:HG12	1:A:107:VAL:H	1.74	0.51
1:A:269:PHE:CB	1:A:283:MET:CE	2.89	0.51
1:A:322:TYR:N	1:A:322:TYR:HD2	2.07	0.51
1:A:585:GLY:HA2	1:A:790:LEU:O	2.10	0.51
1:B:1018:VAL:O	1:B:1021:VAL:N	2.44	0.51
1:B:1023:HIS:O	1:B:1027:THR:HB	2.11	0.51
1:B:1076:THR:HG22	1:B:1120:GLU:HA	1.92	0.51
1:B:1193:TYR:CA	1:B:1257:THR:HG23	2.36	0.51
1:B:330:ILE:HG22	1:B:337:SER:CA	2.40	0.51
1:B:701:ASP:O	1:B:704:CYS:HB2	2.11	0.51
1:A:1401:ARG:HA	1:A:1478:ARG:HA	1.93	0.51
1:A:1429:PRO:CG	1:A:1511:THR:HB	2.39	0.51
1:A:165:ASP:HB3	1:A:171:VAL:HG21	1.91	0.51
1:B:491:PRO:O	1:B:492:TYR:C	2.49	0.51
1:B:544:TYR:H	1:B:544:TYR:HD1	1.57	0.51
1:B:647:HIS:O	1:B:649:ALA:N	2.43	0.51
1:B:712:GLU:HA	1:B:715:ALA:HB3	1.92	0.51
1:B:573:VAL:O	1:B:815:VAL:HG21	2.09	0.51
1:A:1161:LEU:HD12	1:A:1162:VAL:CG2	2.41	0.51
1:A:1210:SER:O	1:A:1214:ARG:N	2.38	0.51
1:A:1296:GLY:O	1:A:1299:GLU:N	2.42	0.51
1:A:1334:LEU:CD2	1:A:1334:LEU:H	2.21	0.51
1:B:1043:GLN:O	1:B:1046:LYS:HB2	2.10	0.51
1:B:1049:LEU:O	1:B:1050:LYS:C	2.47	0.51
1:B:1076:THR:HG21	1:B:1120:GLU:HA	1.93	0.51
1:B:1157:ASP:C	1:B:1160:PRO:HD3	2.31	0.51
1:B:1259:LEU:CD1	1:B:1300:TYR:HB2	2.40	0.51
1:B:799:ILE:O	1:B:799:ILE:HG12	2.10	0.51
1:B:849:ARG:CG	1:B:853:MET:HE1	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1080:ALA:O	1:A:1081:PHE:C	2.47	0.51
1:A:1432:ILE:O	1:A:1433:SER:C	2.49	0.51
1:A:1460:VAL:O	1:A:1460:VAL:HG12	2.10	0.51
1:A:169:SER:O	1:A:170:GLU:C	2.49	0.51
1:A:586:GLN:O	1:A:790:LEU:HD12	2.11	0.51
1:A:80:GLN:HB3	1:A:512:PHE:HE1	1.76	0.51
1:A:913:SER:HA	1:A:921:GLU:O	2.11	0.51
1:B:1008:ALA:O	1:B:1011:GLU:N	2.44	0.51
1:B:1096:ASN:ND2	1:B:1099:SER:H	2.08	0.51
1:B:1127:ILE:HD12	1:B:1127:ILE:H	1.74	0.51
1:B:1307:LEU:O	1:B:1308:ARG:C	2.48	0.51
1:B:981:GLY:HA3	1:B:1309:LEU:HD11	1.92	0.51
1:B:342:ILE:CG2	1:B:343:PRO:HD2	2.41	0.51
1:B:494:ASP:C	1:B:496:ILE:H	2.14	0.51
1:B:571:LEU:HD12	1:B:572:GLN:H	1.68	0.51
1:A:1229:LYS:HB3	1:A:1231:ASN:OD1	2.10	0.51
1:A:582:TYR:HB2	1:A:819:VAL:HG12	1.93	0.51
1:A:626:PHE:O	1:A:629:LYS:HG2	2.10	0.51
1:B:1022:PHE:CE2	1:B:1092:TYR:CG	2.99	0.51
1:B:847:ASN:O	1:B:848:TYR:CD1	2.63	0.51
1:A:1025:LEU:HD13	1:A:1031:TRP:HZ3	1.74	0.51
1:A:1290:THR:HA	1:A:1293:ALA:HB3	1.93	0.51
1:A:1311:MET:HG2	1:A:1350:THR:OG1	2.11	0.51
1:A:269:PHE:CD1	1:A:286:ALA:HB1	2.46	0.51
1:A:27:ALA:HB2	1:A:39:ILE:HD12	1.92	0.51
1:A:493:ILE:CG2	1:A:494:ASP:N	2.73	0.51
1:A:50:PHE:CD1	1:A:109:LYS:HE2	2.45	0.51
1:A:700:TYR:C	1:A:702:GLY:N	2.62	0.51
1:B:1100:ILE:HG21	1:B:1158:ILE:HD12	1.92	0.51
1:B:1251:THR:HG21	1:B:1273:TRP:HH2	1.73	0.51
1:B:269:PHE:CB	1:B:283:MET:HE3	2.41	0.51
1:B:323:LEU:HB3	1:B:345:ILE:HB	1.92	0.51
1:B:575:LEU:HG	1:B:815:VAL:HG11	1.93	0.51
1:B:592:MET:HE2	1:B:784:LYS:HB3	1.93	0.51
1:B:73:LEU:H	1:B:73:LEU:HD23	1.76	0.51
1:B:833:VAL:HA	1:B:1430:THR:HG21	1.92	0.51
1:A:1316:SER:O	1:A:1347:ILE:HG13	2.11	0.51
1:A:146:TYR:CE1	1:A:182:ILE:HG23	2.46	0.51
1:A:27:ALA:O	1:A:652:THR:O	2.29	0.51
1:A:316:GLU:O	1:A:319:ASN:N	2.43	0.51
1:A:330:ILE:HB	1:A:336:PHE:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ILE:HG13	1:A:429:THR:OG1	2.10	0.51
1:A:412:ARG:HD3	1:A:414:ASP:OD1	2.11	0.51
1:A:701:ASP:OD1	1:A:702:GLY:N	2.44	0.51
1:B:976:ILE:HG21	1:B:1280:TYR:HE1	1.76	0.51
1:B:1030:HIS:NE2	1:B:1306:GLN:NE2	2.59	0.51
1:B:961:TYR:HD2	1:B:1344:ASP:O	1.94	0.51
1:B:1372:GLU:HG3	1:B:1373:GLU:N	2.20	0.51
1:B:1440:LYS:HD3	1:B:1453:TYR:CZ	2.45	0.51
1:B:155:ALA:O	1:B:156:LYS:C	2.49	0.51
1:B:165:ASP:C	1:B:165:ASP:OD1	2.49	0.51
1:B:515:ARG:HH22	1:B:527:ASN:C	2.14	0.51
1:B:142:LYS:HD3	1:B:775:TRP:CD1	2.46	0.51
1:B:73:LEU:HB2	1:B:79:PHE:HA	1.92	0.51
2:Y:192:ASN:HB2	2:Y:223:LYS:H	1.76	0.51
1:A:296:ILE:HG22	1:A:297:ALA:N	2.23	0.51
1:A:354:LEU:HD12	1:A:435:VAL:CG1	2.41	0.51
1:B:1202:HIS:CD2	1:B:1204:GLN:CB	2.94	0.51
1:B:1346:LEU:HG	1:B:1347:ILE:N	2.26	0.51
1:B:1429:PRO:HB3	1:B:1488:LEU:CD2	2.41	0.51
1:B:272:ARG:CG	1:B:273:GLU:H	2.24	0.51
1:B:364:LYS:H	1:B:364:LYS:HD3	1.74	0.51
1:A:702:GLY:HA2	1:A:728:PHE:CD1	2.46	0.50
1:B:1432:ILE:O	1:B:1433:SER:O	2.28	0.50
1:B:173:MET:O	1:B:174:VAL:HB	2.11	0.50
1:B:30:ILE:HG22	1:B:31:PHE:O	2.11	0.50
1:B:936:ARG:NH1	1:B:1002:HIS:CE1	2.78	0.50
1:A:78:LYS:NZ	2:X:144:GLY:HA2	2.26	0.50
1:A:150:ASP:N	1:A:150:ASP:OD2	2.44	0.50
1:A:271:ILE:O	1:A:272:ARG:HB2	2.11	0.50
1:A:352:TYR:HD1	1:A:375:VAL:HG11	1.76	0.50
1:B:1431:GLY:C	1:B:1432:ILE:HG12	2.32	0.50
1:B:244:LYS:HE3	1:B:304:GLU:CD	2.31	0.50
1:B:450:GLU:HB3	1:B:452:TYR:CE2	2.47	0.50
1:B:953:ILE:O	1:B:953:ILE:HG13	2.10	0.50
1:A:1111:TYR:CE1	1:A:1121:ASN:HB2	2.47	0.50
1:A:1343:ASN:N	1:A:1343:ASN:HD22	2.08	0.50
1:A:242:ASN:HB3	1:A:245:ASN:OD1	2.10	0.50
1:A:412:ARG:HD3	1:A:414:ASP:CG	2.32	0.50
1:A:491:PRO:O	1:A:492:TYR:C	2.48	0.50
1:A:54:ILE:HG22	1:A:55:SER:N	2.27	0.50
1:A:571:LEU:HD21	1:A:600:VAL:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:LEU:HD22	1:A:738:LEU:HD11	1.94	0.50
1:A:700:TYR:CE1	1:A:758:LEU:HD12	2.46	0.50
1:A:683:ILE:HD13	1:A:735:ALA:HB2	1.93	0.50
1:A:983:LEU:HD11	1:A:1356:LEU:HD22	1.92	0.50
1:A:987:ILE:CD1	1:A:1294:ILE:HD12	2.41	0.50
1:B:1404:ALA:C	1:B:1474:CYS:SG	2.89	0.50
1:B:234:GLU:C	1:B:235:TYR:HD2	2.15	0.50
1:B:946:PRO:HD2	1:B:947:ARG:H	1.75	0.50
2:Y:193:LEU:HD23	2:Y:221:ILE:HG12	1.93	0.50
1:A:1210:SER:OG	1:A:1211:ALA:N	2.44	0.50
1:A:139:GLN:O	1:A:190:ILE:HG12	2.12	0.50
1:A:42:GLN:HG3	1:A:80:GLN:NE2	2.25	0.50
1:A:485:ILE:CG2	1:A:487:THR:HG23	2.41	0.50
1:A:905:ILE:CD1	1:A:931:PRO:HG3	2.42	0.50
1:A:950:TYR:CE2	1:A:1356:LEU:HD11	2.47	0.50
1:B:1274:LEU:CB	1:B:1297:LEU:HD11	2.38	0.50
1:B:1488:LEU:HD11	1:B:1510:SER:OG	2.12	0.50
1:B:159:THR:HG22	1:B:160:VAL:N	2.25	0.50
1:B:256:TYR:C	1:B:257:ASN:HD22	2.14	0.50
1:B:599:TRP:HE3	1:B:778:HIS:O	1.94	0.50
1:B:59:TYR:CD1	1:B:103:TYR:HE1	2.30	0.50
1:B:720:LEU:HD11	1:B:1446:VAL:HG22	1.94	0.50
1:B:902:PRO:O	1:B:903:LEU:HD13	2.11	0.50
1:A:105:GLU:HA	1:A:114:SER:HB3	1.94	0.50
1:A:161:LEU:CG	1:A:185:PHE:CE1	2.94	0.50
1:A:536:PRO:HG3	1:A:624:PHE:CE2	2.45	0.50
1:A:56:ILE:HD13	1:A:86:THR:H	1.76	0.50
1:B:1093:VAL:HG12	1:B:1095:GLN:NE2	2.27	0.50
1:B:1151:GLY:O	1:B:1152:ILE:C	2.48	0.50
1:B:1323:LEU:CG	1:B:1324:HIS:H	2.24	0.50
1:B:136:THR:HB	1:B:137:PRO:HD2	1.94	0.50
1:B:365:PRO:HD2	1:B:464:TYR:CE2	2.46	0.50
1:B:693:SER:O	1:B:696:LYS:HB3	2.11	0.50
1:B:700:TYR:C	1:B:702:GLY:H	2.14	0.50
1:B:942:VAL:HG22	1:B:957:LYS:HD3	1.94	0.50
2:X:190:THR:HG22	2:X:200:GLU:HG2	1.93	0.50
1:A:1082:ALA:O	1:A:1083:LEU:C	2.48	0.50
1:A:1049:LEU:CD2	1:A:1089:VAL:HG13	2.42	0.50
1:A:1128:LYS:HE2	1:A:1129:LEU:O	2.10	0.50
1:A:1434:ALA:CA	1:A:1479:ILE:HG22	2.34	0.50
1:A:224:LEU:HD13	1:A:225:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1016:VAL:HG12	1:B:1017:PRO:CD	2.41	0.50
1:B:1081:PHE:CE1	1:B:1288:GLN:NE2	2.77	0.50
1:B:1376:SER:O	1:B:1409:LYS:HB2	2.11	0.50
1:B:1466:SER:CB	1:B:1468:PRO:HD3	2.42	0.50
1:B:1429:PRO:HB3	1:B:1488:LEU:HD22	1.94	0.50
1:B:234:GLU:C	1:B:235:TYR:CD2	2.85	0.50
1:B:835:ARG:HH21	1:B:971:THR:HG22	1.76	0.50
1:A:1022:PHE:CE2	1:A:1092:TYR:CG	3.00	0.50
1:A:1299:GLU:O	1:A:1302:LEU:HB2	2.11	0.50
1:A:1466:SER:CB	1:A:1468:PRO:HD3	2.41	0.50
1:B:1069:TRP:HE1	1:B:1463:GLN:HE21	1.58	0.50
1:B:109:LYS:HD2	1:B:110:HIS:HB2	1.93	0.50
1:B:149:ASN:O	1:B:152:LEU:N	2.41	0.50
1:B:816:LYS:O	1:B:817:ALA:HB2	2.12	0.50
1:B:853:MET:O	1:B:888:VAL:HG22	2.11	0.50
1:B:866:CYS:HB2	1:B:901:LEU:O	2.12	0.50
1:A:1240:PRO:O	1:A:1242:THR:HG23	2.11	0.50
1:A:128:ILE:CG1	1:A:215:ALA:HB2	2.42	0.50
1:A:1423:VAL:HG21	1:A:1496:TYR:HE1	1.75	0.50
1:A:316:GLU:O	1:A:318:LEU:N	2.45	0.50
1:A:227:PHE:CE1	1:A:338:GLU:CB	2.94	0.50
1:A:478:VAL:O	1:A:478:VAL:HG13	2.12	0.50
1:A:594:THR:HB	1:A:596:MET:O	2.12	0.50
1:B:1189:ALA:O	1:B:1192:ALA:HB3	2.11	0.50
1:B:1226:ARG:N	1:B:1269:PRO:O	2.31	0.50
1:B:150:ASP:N	1:B:150:ASP:OD2	2.45	0.50
1:B:839:ILE:HG13	1:B:840:GLN:N	2.26	0.50
1:B:927:LEU:HD23	1:B:928:ARG:N	2.27	0.50
1:A:1080:ALA:O	1:A:1083:LEU:HB2	2.12	0.50
1:A:834:VAL:HG11	1:A:1489:SER:CB	2.42	0.50
1:A:260:VAL:HG12	1:A:261:THR:N	2.27	0.50
1:A:395:ILE:O	1:A:429:THR:CG2	2.60	0.50
1:A:485:ILE:HG22	1:A:487:THR:HG23	1.94	0.50
1:A:52:ALA:CB	1:A:73:LEU:HD21	2.41	0.50
1:B:1115:ASN:ND2	1:B:1115:ASN:C	2.65	0.50
1:B:1334:LEU:O	1:B:1335:GLY:O	2.29	0.50
1:B:532:GLN:O	1:B:535:VAL:HG22	2.12	0.50
1:B:592:MET:HE1	1:B:784:LYS:O	2.12	0.50
2:Y:186:TYR:O	2:Y:229:LYS:HB3	2.12	0.50
1:A:349:LEU:HD22	1:A:349:LEU:C	2.32	0.49
1:A:777:VAL:HG12	1:A:778:HIS:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:TYR:C	1:B:466:TYR:CD1	2.85	0.49
1:B:553:GLU:OE1	1:B:555:VAL:CG2	2.60	0.49
1:B:683:ILE:CD1	1:B:735:ALA:HB2	2.41	0.49
1:A:1376:SER:O	1:A:1409:LYS:HB2	2.12	0.49
1:A:149:ASN:N	1:A:155:ALA:HB2	2.27	0.49
1:A:330:ILE:HA	1:A:337:SER:HA	1.95	0.49
1:A:467:ILE:HD12	1:A:484:ILE:HD11	1.94	0.49
1:A:800:GLN:O	1:A:800:GLN:HG2	2.11	0.49
1:A:820:PHE:HE2	1:A:848:TYR:HD2	1.57	0.49
1:A:979:VAL:HB	1:A:1326:TYR:OH	2.12	0.49
1:B:1421:HIS:CE1	1:B:1498:TYR:CG	2.99	0.49
1:B:188:PHE:C	1:B:188:PHE:CD1	2.86	0.49
1:B:412:ARG:HD3	1:B:414:ASP:CG	2.33	0.49
1:A:1229:LYS:CD	1:A:1239:VAL:HG12	2.42	0.49
1:A:1245:ALA:HA	1:A:1285:TYR:HB3	1.93	0.49
1:A:1286:SER:OG	1:A:1287:THR:N	2.41	0.49
1:A:1381:ILE:HD13	1:A:1509:TYR:CE1	2.47	0.49
1:A:571:LEU:CD2	1:A:600:VAL:HG13	2.42	0.49
1:A:727:ALA:O	1:A:731:CYS:SG	2.71	0.49
1:A:85:LEU:H	1:A:85:LEU:CD2	2.20	0.49
1:B:1439:LEU:HD12	1:B:1455:ILE:HD11	1.95	0.49
1:B:493:ILE:CG2	1:B:494:ASP:N	2.75	0.49
1:B:849:ARG:CB	1:B:853:MET:HE1	2.42	0.49
2:Y:136:LEU:N	2:Y:136:LEU:HD23	2.27	0.49
1:A:1183:GLN:O	1:A:1232:LEU:HD22	2.12	0.49
1:A:1332:ASN:O	1:A:1332:ASN:CG	2.51	0.49
1:A:1496:TYR:HB3	1:A:1504:GLN:HG3	1.93	0.49
1:A:128:ILE:HG13	1:A:214:THR:O	2.11	0.49
1:A:440:PRO:HD2	1:A:441:ASP:H	1.77	0.49
1:A:700:TYR:HE1	1:A:758:LEU:CB	2.24	0.49
1:A:825:LEU:HA	1:A:845:VAL:HA	1.94	0.49
1:A:855:PHE:HD1	1:A:856:CYS:N	2.10	0.49
1:B:1221:ASN:ND2	1:B:1222:PRO:HA	2.27	0.49
1:B:1024:TYR:HB2	1:B:1298:THR:HG23	1.94	0.49
1:B:52:ALA:CB	1:B:73:LEU:HD21	2.42	0.49
1:B:534:MET:O	1:B:537:SER:O	2.30	0.49
1:B:634:CYS:SG	1:B:635:GLY:N	2.85	0.49
1:B:96:GLN:O	1:B:98:PRO:CD	2.51	0.49
1:A:558:SER:OG	1:A:638:GLY:N	2.44	0.49
1:A:765:ILE:HD11	1:A:769:PHE:HE2	1.76	0.49
1:A:906:GLY:N	1:A:929:VAL:HB	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:LEU:HD23	1:A:1309:LEU:CD1	2.42	0.49
1:B:1128:LYS:HE2	1:B:1129:LEU:O	2.12	0.49
1:B:855:PHE:CE2	1:B:888:VAL:HG13	2.47	0.49
1:A:1225:TYR:HD1	1:A:1273:TRP:HB2	1.77	0.49
1:A:1328:MET:O	1:A:1329:THR:HG23	2.11	0.49
1:A:824:PHE:HE1	1:A:846:TYR:HD1	1.59	0.49
1:B:1202:HIS:O	1:B:1204:GLN:N	2.45	0.49
1:B:161:LEU:C	1:B:162:THR:HG22	2.31	0.49
1:B:27:ALA:HB1	1:B:28:PRO:HD2	1.95	0.49
1:B:352:TYR:HD1	1:B:375:VAL:HG13	1.77	0.49
1:B:896:VAL:HG12	1:B:897:THR:N	2.27	0.49
2:X:140:LYS:HE3	2:X:228:LEU:HD12	1.93	0.49
1:A:1268:ASN:N	1:A:1269:PRO:CD	2.75	0.49
1:A:195:ARG:HH11	1:A:195:ARG:HG2	1.77	0.49
1:A:243:PHE:CE2	1:A:316:GLU:CG	2.95	0.49
1:A:394:THR:CG2	1:A:428:VAL:HG23	2.42	0.49
1:A:707:ASN:HB3	1:A:739:ARG:HH12	1.78	0.49
1:A:781:PRO:O	1:A:782:ARG:HB2	2.13	0.49
1:B:1284:PHE:HD2	1:B:1285:TYR:CD1	2.31	0.49
1:B:224:LEU:HD13	1:B:225:PRO:HD2	1.95	0.49
1:A:1308:ARG:HH11	1:A:1308:ARG:HG2	1.78	0.49
1:A:1423:VAL:HG22	1:A:1496:TYR:CD1	2.48	0.49
1:A:1439:LEU:CD1	1:A:1455:ILE:HD11	2.42	0.49
1:A:1450:PHE:CZ	1:A:1475:VAL:HB	2.48	0.49
1:A:281:GLU:O	1:A:282:MET:O	2.29	0.49
1:A:922:ILE:O	1:A:922:ILE:HG22	2.12	0.49
1:B:120:THR:CG2	1:B:121:TYR:N	2.54	0.49
1:B:982:LEU:CD2	1:B:1309:LEU:CD1	2.90	0.49
1:B:1435:ASN:O	1:B:1436:GLU:C	2.51	0.49
1:B:191:PRO:CG	1:B:194:PRO:HB3	2.41	0.49
1:B:371:ILE:CD1	1:B:390:LEU:HD21	2.42	0.49
1:B:460:LEU:C	1:B:462:GLN:H	2.16	0.49
1:B:703:ALA:HB1	1:B:735:ALA:HB3	1.95	0.49
1:B:71:VAL:HG11	1:B:82:SER:O	2.12	0.49
2:Y:166:ASP:OD2	2:Y:201:ILE:HD13	2.12	0.49
1:A:1148:THR:O	1:A:1152:ILE:HD12	2.12	0.49
1:A:123:ASN:C	1:A:211:THR:HG21	2.34	0.49
1:A:1429:PRO:O	1:A:1432:ILE:HG12	2.12	0.49
1:A:386:VAL:N	1:A:411:THR:HG22	2.23	0.49
1:A:540:LEU:O	1:A:558:SER:HB2	2.13	0.49
1:A:606:ASP:O	1:A:608:ALA:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625:GLN:O	1:A:626:PHE:C	2.51	0.49
1:B:100:SER:O	1:B:101:TYR:CD2	2.66	0.49
1:B:1432:ILE:O	1:B:1433:SER:C	2.50	0.49
1:B:173:MET:O	1:B:174:VAL:CB	2.61	0.49
1:B:395:ILE:O	1:B:429:THR:CG2	2.60	0.49
1:B:494:ASP:HA	1:B:496:ILE:HD11	1.95	0.49
1:B:51:ASP:OD2	1:B:70:HIS:NE2	2.43	0.49
1:B:58:SER:HB3	1:B:66:TYR:OH	2.12	0.49
1:A:1076:THR:O	1:A:1079:THR:HB	2.13	0.49
1:A:1132:THR:HG22	1:A:1134:PRO:HD2	1.93	0.49
1:A:1342:LEU:N	1:A:1342:LEU:HD23	2.27	0.49
1:A:1401:ARG:HB2	1:A:1478:ARG:CB	2.43	0.49
1:A:606:ASP:C	1:A:608:ALA:H	2.16	0.49
1:A:839:ILE:HD11	1:A:1483:PHE:CZ	2.48	0.49
1:B:1096:ASN:HD22	1:B:1096:ASN:C	2.15	0.49
1:B:685:GLU:HG3	1:B:686:ILE:CD1	2.42	0.49
2:Y:194:LYS:HG3	2:Y:195:ASP:H	1.78	0.49
1:A:1244:THR:HG23	1:A:1502:ASP:OD2	2.12	0.48
1:A:129:HIS:CD2	1:A:129:HIS:O	2.66	0.48
1:A:415:ASP:OD1	1:A:417:VAL:HG23	2.13	0.48
1:A:457:TYR:CD2	1:A:457:TYR:O	2.66	0.48
1:A:855:PHE:C	1:A:855:PHE:CD1	2.86	0.48
1:B:1108:VAL:HG13	1:B:1109:GLU:N	2.28	0.48
1:B:1341:LEU:CB	1:B:1342:LEU:HD23	2.43	0.48
1:B:149:ASN:N	1:B:155:ALA:HB2	2.28	0.48
1:B:438:ASP:C	1:B:439:ALA:O	2.51	0.48
1:B:838:GLN:HA	1:B:901:LEU:HB2	1.95	0.48
1:A:1184:SER:HA	1:A:1232:LEU:CB	2.43	0.48
1:A:124:GLY:O	1:A:125:PHE:CG	2.66	0.48
1:A:1439:LEU:HD12	1:A:1455:ILE:HD11	1.94	0.48
1:A:940:SER:HB2	1:A:959:PHE:CE1	2.48	0.48
1:B:1003:LEU:HD22	1:B:1004:PRO:HD2	1.94	0.48
1:B:1317:TYR:CB	1:B:1320:LYS:HB3	2.43	0.48
1:B:269:PHE:CD1	1:B:286:ALA:HB1	2.48	0.48
1:B:465:LEU:HD13	1:B:544:TYR:CD1	2.48	0.48
1:B:897:THR:C	1:B:898:PHE:CD2	2.87	0.48
1:B:907:LEU:HD12	1:B:908:HIS:H	1.77	0.48
1:A:1008:ALA:CB	1:A:1059:TYR:CD2	2.96	0.48
1:A:1249:GLU:OE2	1:A:1288:GLN:HB3	2.13	0.48
1:A:147:SER:O	1:A:148:LEU:HD12	2.14	0.48
1:A:1381:ILE:CG2	1:A:1509:TYR:CD1	2.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ALA:CB	1:A:39:ILE:HD12	2.43	0.48
1:A:735:ALA:HB1	1:A:754:MET:CE	2.40	0.48
1:A:182:ILE:HD12	1:A:777:VAL:HG11	1.96	0.48
1:B:1047:LYS:C	1:B:1049:LEU:N	2.64	0.48
1:B:229:VAL:HG22	1:B:252:ALA:HB2	1.95	0.48
1:B:281:GLU:O	1:B:282:MET:O	2.31	0.48
1:B:727:ALA:O	1:B:731:CYS:SG	2.71	0.48
1:B:733:VAL:HG13	1:B:737:GLN:NE2	2.28	0.48
1:A:1098:ASN:HA	1:A:1101:CYS:HB2	1.95	0.48
1:A:1199:ASP:OD1	1:A:1201:THR:OG1	2.29	0.48
1:A:1427:SER:HB3	1:A:1491:ALA:HB1	1.93	0.48
1:A:165:ASP:C	1:A:165:ASP:OD1	2.51	0.48
1:A:365:PRO:HG2	1:A:464:TYR:CE2	2.49	0.48
1:A:352:TYR:CD1	1:A:375:VAL:HG11	2.48	0.48
1:A:686:ILE:C	1:A:688:ALA:N	2.65	0.48
1:A:53:THR:HA	1:A:69:GLY:O	2.14	0.48
1:A:981:GLY:HA3	1:A:1309:LEU:CD1	2.42	0.48
1:B:1007:SER:OG	1:B:1008:ALA:N	2.47	0.48
1:B:102:VAL:HG13	1:B:119:ILE:HG21	1.95	0.48
1:B:1259:LEU:HD21	1:B:1267:VAL:HG11	1.95	0.48
1:B:304:GLU:O	1:B:305:THR:C	2.52	0.48
1:B:38:ASN:C	1:B:39:ILE:HD13	2.30	0.48
1:B:489:LYS:O	1:B:490:SER:CB	2.62	0.48
1:B:564:GLU:HG3	1:B:564:GLU:O	2.13	0.48
1:B:857:VAL:HG21	1:B:896:VAL:CG1	2.44	0.48
1:B:978:SER:OG	1:B:980:LYS:HD3	2.13	0.48
2:Y:179:LEU:HA	2:Y:184:THR:HB	1.95	0.48
2:Y:217:ASN:HB2	2:Y:220:ASP:CG	2.34	0.48
1:A:1408:TYR:CD1	1:A:1409:LYS:N	2.81	0.48
1:A:1509:TYR:CD2	1:A:1509:TYR:C	2.86	0.48
1:A:208:ASP:O	1:A:209:PHE:CG	2.67	0.48
1:A:357:VAL:O	1:A:359:THR:HG23	2.14	0.48
1:A:373:VAL:CG2	1:A:374:GLN:N	2.75	0.48
1:A:489:LYS:O	1:A:490:SER:CB	2.60	0.48
1:A:589:SER:HB2	1:A:785:GLN:HE21	1.77	0.48
1:A:837:GLU:OE2	1:A:1488:LEU:CA	2.61	0.48
1:B:1019:PHE:CE2	1:B:1088:GLN:HB3	2.49	0.48
1:B:1189:ALA:HB1	1:B:1253:TYR:HB2	1.94	0.48
1:B:1244:THR:HB	1:B:1247:MET:H	1.79	0.48
1:B:377:ASP:O	1:B:379:LEU:N	2.47	0.48
1:B:857:VAL:HG12	1:B:914:LEU:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:PRO:CB	1:A:1352:PHE:O	2.62	0.48
1:A:146:TYR:HE1	1:A:182:ILE:HG23	1.77	0.48
1:A:352:TYR:O	1:A:448:ALA:CB	2.61	0.48
1:A:90:LYS:O	1:A:92:LEU:HG	2.14	0.48
1:A:969:PRO:O	1:A:971:THR:HG23	2.14	0.48
1:B:1248:VAL:CG2	1:B:1277:GLU:HG2	2.38	0.48
1:B:1452:ASP:O	1:B:1462:LEU:HA	2.14	0.48
1:B:377:ASP:C	1:B:379:LEU:H	2.17	0.48
1:B:616:ALA:O	1:B:617:LYS:C	2.51	0.48
1:B:830:PRO:HG3	1:B:1483:PHE:CZ	2.48	0.48
2:X:153:PHE:CG	2:X:154:SER:N	2.81	0.48
2:Y:146:LEU:HD13	2:Y:146:LEU:C	2.34	0.48
1:A:1226:ARG:CD	1:A:1266:TYR:CE1	2.96	0.48
1:A:1262:LYS:O	1:A:1264:ILE:HG13	2.14	0.48
1:A:1509:TYR:O	1:A:1509:TYR:CD2	2.66	0.48
1:A:29:LYS:HE2	1:A:666:ASP:CB	2.38	0.48
1:A:494:ASP:C	1:A:496:ILE:H	2.17	0.48
1:A:634:CYS:HB3	1:A:648:LEU:HD23	1.95	0.48
1:A:588:VAL:CG1	1:A:790:LEU:HD11	2.44	0.48
1:B:1022:PHE:HE2	1:B:1092:TYR:CG	2.32	0.48
1:B:1205:PHE:O	1:B:1209:VAL:HG23	2.13	0.48
1:B:1215:GLU:OE2	1:B:1233:GLN:HB3	2.14	0.48
1:B:494:ASP:C	1:B:496:ILE:HD12	2.33	0.48
1:B:710:THR:HG23	1:B:713:GLN:OE1	2.14	0.48
1:B:592:MET:CE	1:B:784:LYS:HB3	2.43	0.48
1:B:837:GLU:OE2	1:B:1488:LEU:HA	2.13	0.48
1:B:946:PRO:HB3	1:B:1352:PHE:O	2.13	0.48
2:X:183:THR:HG1	2:X:230:GLN:HB3	1.78	0.48
1:A:1228:TRP:H	1:A:1251:THR:HG22	1.77	0.48
1:A:423:ASN:H	1:A:423:ASN:ND2	2.11	0.48
1:A:505:SER:CB	1:A:510:ILE:HD11	2.43	0.48
1:A:716:ALA:C	1:A:718:ILE:H	2.17	0.48
1:A:77:ASN:HD22	1:A:81:ASN:ND2	2.11	0.48
1:A:837:GLU:C	1:A:901:LEU:HD12	2.34	0.48
1:A:83:ALA:O	1:A:85:LEU:HD22	2.14	0.48
1:B:100:SER:O	1:B:101:TYR:CB	2.61	0.48
1:B:105:GLU:HA	1:B:114:SER:HB3	1.95	0.48
1:B:1189:ALA:HB1	1:B:1253:TYR:CB	2.44	0.48
1:B:1203:PRO:O	1:B:1206:ARG:CB	2.61	0.48
1:B:486:VAL:HG12	1:B:486:VAL:O	2.14	0.48
1:B:66:TYR:HD1	1:B:90:LYS:CE	2.03	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:975:ARG:O	1:B:1339:GLU:HA	2.14	0.48
1:A:1280:TYR:HD1	1:A:1362:THR:CG2	2.25	0.48
1:A:1507:MET:HG2	1:A:1508:PHE:O	2.13	0.48
1:A:159:THR:HG23	1:A:204:LYS:O	2.13	0.48
1:A:162:THR:O	1:A:164:ILE:HG13	2.13	0.48
1:A:317:ASP:C	1:A:319:ASN:N	2.64	0.48
1:A:361:LEU:N	1:A:361:LEU:HD12	2.29	0.48
1:A:409:SER:OG	1:A:410:VAL:N	2.47	0.48
1:A:707:ASN:HB3	1:A:739:ARG:HH22	1.78	0.48
1:B:1240:PRO:O	1:B:1242:THR:HG23	2.13	0.48
1:B:1296:GLY:O	1:B:1299:GLU:N	2.47	0.48
1:B:978:SER:N	1:B:1360:HIS:O	2.43	0.48
1:B:394:THR:CG2	1:B:428:VAL:HG23	2.44	0.48
1:B:349:LEU:CD2	1:B:446:ASN:HD22	2.27	0.48
1:B:825:LEU:HD11	1:B:827:MET:SD	2.54	0.48
1:A:1128:LYS:HZ1	1:A:1415:SER:HB3	1.78	0.48
1:A:393:GLN:O	1:A:431:LEU:HD23	2.13	0.48
1:A:349:LEU:CD2	1:A:446:ASN:HD22	2.27	0.48
1:A:44:TYR:HE1	1:A:497:THR:OG1	1.79	0.48
1:A:602:LEU:HD12	1:A:774:LEU:HD22	1.96	0.48
1:A:88:GLN:HB3	1:A:89:PRO:HD2	1.94	0.48
1:B:938:SER:OG	1:B:1279:ARG:NH1	2.47	0.48
1:B:1290:THR:HA	1:B:1293:ALA:HB3	1.96	0.48
1:B:1496:TYR:HD1	1:B:1496:TYR:O	1.96	0.48
1:B:304:GLU:O	1:B:305:THR:O	2.32	0.48
1:B:503:ILE:HG12	1:B:540:LEU:CB	2.42	0.48
1:B:505:SER:O	1:B:506:LYS:HB2	2.14	0.48
1:B:593:ALA:HA	1:B:782:ARG:O	2.13	0.48
1:B:833:VAL:O	1:B:929:VAL:HA	2.14	0.48
1:A:1056:ILE:O	1:A:1058:SER:N	2.47	0.47
1:A:977:LEU:HD13	1:A:1346:LEU:CD2	2.44	0.47
1:A:395:ILE:HA	1:A:400:GLU:O	2.14	0.47
1:A:637:GLY:O	1:A:638:GLY:O	2.32	0.47
1:B:1217:LEU:O	1:B:1218:VAL:CG1	2.53	0.47
1:B:292:LEU:HD22	1:B:296:ILE:C	2.34	0.47
1:B:792:ASP:O	1:B:793:SER:HB2	2.14	0.47
1:B:88:GLN:HB3	1:B:89:PRO:CD	2.43	0.47
1:A:1049:LEU:HD21	1:A:1089:VAL:HG13	1.96	0.47
1:A:1053:MET:HE1	1:A:1086:LEU:HD13	1.94	0.47
1:A:1196:SER:HB2	1:A:1257:THR:HG23	1.96	0.47
1:A:1203:PRO:O	1:A:1206:ARG:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1227:PHE:HA	1:A:1228:TRP:HE3	1.78	0.47
1:A:1284:PHE:HD2	1:A:1285:TYR:CD1	2.32	0.47
1:A:692:HIS:NE2	1:A:694:VAL:HG23	2.28	0.47
1:B:1200:LYS:HE3	1:B:1261:LEU:HD23	1.96	0.47
1:B:23:TYR:O	1:B:655:THR:HG23	2.14	0.47
1:B:515:ARG:HH22	1:B:527:ASN:H	1.60	0.47
1:B:646:PHE:O	1:B:651:LEU:HB2	2.14	0.47
1:B:942:VAL:HG23	1:B:959:PHE:HZ	1.78	0.47
1:A:1056:ILE:HD11	1:A:1066:TYR:CE2	2.49	0.47
1:A:1153:ARG:O	1:A:1154:LYS:C	2.52	0.47
1:A:1204:GLN:O	1:A:1207:SER:N	2.47	0.47
1:A:198:MET:HE1	1:A:218:GLU:HB2	1.96	0.47
1:A:61:ASP:OD1	1:A:63:LYS:HB2	2.14	0.47
1:A:647:HIS:C	1:A:649:ALA:N	2.67	0.47
1:A:41:ILE:HD13	1:A:73:LEU:HD22	1.96	0.47
1:B:1117:SER:HB3	1:B:1174:PHE:CD1	2.49	0.47
1:B:1173:ASN:O	1:B:1174:PHE:C	2.52	0.47
1:B:1244:THR:O	1:B:1285:TYR:CD2	2.67	0.47
1:B:718:ILE:HG12	1:B:1446:VAL:O	2.15	0.47
1:B:466:TYR:CD1	1:B:467:ILE:N	2.82	0.47
1:A:1157:ASP:C	1:A:1160:PRO:HD3	2.34	0.47
1:A:123:ASN:HD22	1:A:124:GLY:N	2.11	0.47
1:A:1379:LEU:HD12	1:A:1507:MET:HE2	1.96	0.47
1:A:351:PRO:O	1:A:377:ASP:HA	2.15	0.47
1:A:96:GLN:O	1:A:98:PRO:CD	2.52	0.47
1:B:1453:TYR:HA	1:B:1462:LEU:HD23	1.96	0.47
1:B:260:VAL:HG12	1:B:261:THR:N	2.29	0.47
1:B:431:LEU:CD2	1:B:431:LEU:C	2.83	0.47
1:B:520:ASP:CG	1:B:521:ALA:N	2.66	0.47
1:B:558:SER:OG	1:B:638:GLY:N	2.46	0.47
1:B:905:ILE:CD1	1:B:931:PRO:HG3	2.44	0.47
1:B:935:LYS:HA	1:B:935:LYS:HD2	1.67	0.47
1:B:938:SER:HB3	1:B:1362:THR:OG1	2.14	0.47
2:X:150:ILE:HG13	2:X:150:ILE:O	2.14	0.47
1:A:1053:MET:HE1	1:A:1086:LEU:HD22	1.96	0.47
1:A:1090:ASN:HD21	1:A:1158:ILE:CG2	2.18	0.47
1:A:1174:PHE:O	1:A:1178:ASN:HB2	2.14	0.47
1:A:1024:TYR:HB2	1:A:1298:THR:CG2	2.44	0.47
1:A:129:HIS:CD2	1:A:129:HIS:C	2.86	0.47
1:A:1346:LEU:HD12	1:A:1347:ILE:H	1.78	0.47
1:A:396:ASP:N	1:A:400:GLU:O	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:GLU:O	1:A:564:GLU:HG3	2.14	0.47
1:A:700:TYR:C	1:A:702:GLY:H	2.17	0.47
1:A:707:ASN:HB3	1:A:739:ARG:NH1	2.30	0.47
1:A:592:MET:HE2	1:A:780:VAL:HG21	1.96	0.47
1:B:1031:TRP:CE3	1:B:1031:TRP:HA	2.50	0.47
1:B:1050:LYS:O	1:B:1053:MET:CB	2.63	0.47
1:B:1439:LEU:CD1	1:B:1455:ILE:HD11	2.45	0.47
1:B:352:TYR:O	1:B:448:ALA:CB	2.61	0.47
1:B:481:HIS:HE1	1:B:529:PRO:HG3	1.79	0.47
1:B:569:ASN:ND2	1:B:598:SER:HB2	2.29	0.47
1:B:606:ASP:C	1:B:608:ALA:N	2.68	0.47
1:B:680:GLN:O	1:B:680:GLN:HG2	2.14	0.47
1:B:85:LEU:CD2	1:B:85:LEU:H	2.26	0.47
1:B:896:VAL:O	1:B:897:THR:CG2	2.60	0.47
1:A:987:ILE:HD11	1:A:1294:ILE:HD13	1.97	0.47
1:A:1401:ARG:HB2	1:A:1478:ARG:CA	2.44	0.47
1:A:1381:ILE:HG21	1:A:1509:TYR:CD1	2.49	0.47
1:A:183:ILE:CG2	1:A:185:PHE:CE2	2.97	0.47
1:A:157:ARG:NH1	1:A:209:PHE:CD1	2.82	0.47
1:A:867:THR:HG23	1:A:900:VAL:HG12	1.95	0.47
1:A:987:ILE:O	1:A:1021:VAL:HG21	2.13	0.47
1:B:1290:THR:O	1:B:1290:THR:HG22	2.14	0.47
1:B:1325:ASN:ND2	1:B:1325:ASN:O	2.48	0.47
1:B:394:THR:CG2	1:B:395:ILE:N	2.78	0.47
1:B:440:PRO:HD2	1:B:441:ASP:H	1.80	0.47
1:B:531:THR:HG23	1:B:533:ASN:HB2	1.97	0.47
1:B:653:PHE:O	1:B:660:ASP:HB2	2.14	0.47
1:A:1152:ILE:O	1:A:1156:PHE:HB2	2.14	0.47
1:A:390:LEU:O	1:A:390:LEU:HG	2.15	0.47
1:A:394:THR:CG2	1:A:395:ILE:N	2.77	0.47
1:A:430:VAL:HG22	1:A:455:ILE:HG12	1.97	0.47
1:A:430:VAL:HA	1:A:454:ALA:O	2.15	0.47
1:A:523:TYR:O	1:A:524:GLN:HB3	2.15	0.47
1:A:635:GLY:C	1:A:673:LEU:HA	2.35	0.47
1:A:602:LEU:HB2	1:A:774:LEU:O	2.15	0.47
1:B:1080:ALA:HA	1:B:1083:LEU:HD12	1.97	0.47
1:B:1155:ALA:O	1:B:1158:ILE:HG13	2.15	0.47
1:B:30:ILE:HG23	1:B:119:ILE:HA	1.96	0.47
1:B:1268:ASN:N	1:B:1269:PRO:HD3	2.29	0.47
1:B:1271:ILE:CD1	1:B:1271:ILE:O	2.61	0.47
1:B:1280:TYR:CD2	1:B:1280:TYR:C	2.86	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:TYR:HB3	1:B:556:SER:HB3	1.96	0.47
1:B:621:GLU:O	1:B:625:GLN:HG3	2.15	0.47
1:B:659:ALA:C	1:B:661:ASP:H	2.18	0.47
2:Y:159:GLU:HG2	2:Y:159:GLU:O	2.14	0.47
2:Y:179:LEU:HD12	2:Y:180:TYR:N	2.29	0.47
1:A:1019:PHE:HE2	1:A:1020:TYR:CE1	2.26	0.47
1:A:1021:VAL:O	1:A:1025:LEU:HG	2.14	0.47
1:A:975:ARG:HB3	1:A:1363:THR:HA	1.96	0.47
1:A:177:ILE:HD11	1:A:179:HIS:HB2	1.96	0.47
1:A:488:PRO:HG2	1:A:499:TYR:OH	2.15	0.47
1:A:707:ASN:HB3	1:A:739:ARG:NH2	2.29	0.47
1:B:1047:LYS:O	1:B:1048:LYS:C	2.53	0.47
1:B:1404:ALA:O	1:B:1474:CYS:SG	2.73	0.47
1:B:933:GLY:HA3	1:B:1367:LYS:O	2.14	0.47
2:X:158:GLU:HA	2:X:219:LYS:NZ	2.30	0.47
1:A:1084:ARG:O	1:A:1088:GLN:HG3	2.15	0.47
1:A:1136:GLU:O	1:A:1140:ASN:N	2.32	0.47
1:A:1378:TYR:CE1	1:A:1409:LYS:HE3	2.49	0.47
1:A:1379:LEU:HD22	1:A:1493:PHE:HE2	1.79	0.47
1:A:1507:MET:HB3	1:A:1507:MET:HE3	1.73	0.47
1:A:922:ILE:HG21	4:A:2001:NAG:C7	2.44	0.47
1:A:323:LEU:HB3	1:A:345:ILE:HB	1.97	0.47
1:A:708:ASP:OD2	1:A:1476:ARG:HD2	2.15	0.47
1:B:271:ILE:HD11	1:B:283:MET:SD	2.55	0.47
1:B:351:PRO:O	1:B:377:ASP:HA	2.14	0.47
1:B:352:TYR:HE2	1:B:442:LEU:HD11	1.80	0.47
1:B:536:PRO:HG3	1:B:624:PHE:CE2	2.48	0.47
2:X:136:LEU:HD23	2:X:136:LEU:H	1.80	0.47
2:X:226:VAL:HG12	2:X:227:THR:N	2.30	0.47
1:A:1076:THR:HG22	1:A:1120:GLU:HA	1.97	0.47
1:A:1115:ASN:HD22	1:A:1117:SER:H	1.61	0.47
1:A:1251:THR:HG21	1:A:1273:TRP:CH2	2.50	0.47
1:A:1434:ALA:CB	1:A:1477:PHE:CE1	2.98	0.47
1:A:232:GLU:HA	1:A:233:PRO:HD3	1.59	0.47
1:A:382:LEU:HD22	1:A:416:GLY:HA3	1.97	0.47
1:B:1309:LEU:O	1:B:1310:SER:HB2	2.15	0.47
1:B:214:THR:CG2	1:B:215:ALA:N	2.77	0.47
1:B:475:ALA:C	1:B:476:LEU:HD23	2.35	0.47
1:B:547:THR:O	1:B:547:THR:HG22	2.15	0.47
1:A:110:HIS:CD2	1:A:110:HIS:O	2.68	0.47
1:A:1172:ASP:O	1:A:1175:LEU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1180:LEU:HA	1:A:1180:LEU:HD23	1.53	0.47
1:A:1423:VAL:HG22	1:A:1496:TYR:CE1	2.49	0.47
1:A:304:GLU:O	1:A:305:THR:C	2.52	0.47
1:A:515:ARG:CZ	1:A:526:ILE:HG23	2.45	0.47
1:A:58:SER:HB3	1:A:66:TYR:OH	2.14	0.47
1:A:857:VAL:HG21	1:A:896:VAL:CG1	2.44	0.47
1:A:86:THR:HG23	1:A:86:THR:O	2.15	0.47
1:B:1153:ARG:O	1:B:1154:LYS:C	2.52	0.47
1:B:1174:PHE:O	1:B:1178:ASN:HB2	2.15	0.47
1:B:1229:LYS:CD	1:B:1239:VAL:HG12	2.41	0.47
1:B:1401:ARG:HA	1:B:1478:ARG:HA	1.96	0.47
1:B:431:LEU:O	1:B:453:ARG:HA	2.15	0.47
2:X:150:ILE:HD12	2:X:151:ASP:N	2.29	0.47
1:A:1153:ARG:CZ	1:A:1168:LEU:HD22	2.45	0.46
1:A:1024:TYR:HB2	1:A:1298:THR:HG23	1.98	0.46
1:A:1432:ILE:O	1:A:1433:SER:O	2.33	0.46
1:A:155:ALA:O	1:A:156:LYS:C	2.53	0.46
1:A:539:ARG:NH1	1:A:631:ASP:OD1	2.49	0.46
1:A:835:ARG:HH21	1:A:971:THR:HG22	1.79	0.46
1:A:838:GLN:H	1:A:1486:GLY:HA3	1.80	0.46
1:B:1105:LEU:O	1:B:1109:GLU:HG3	2.15	0.46
1:B:1113:LEU:N	1:B:1117:SER:O	2.46	0.46
1:B:1278:GLN:O	1:B:1360:HIS:NE2	2.48	0.46
1:B:1370:THR:CG2	1:B:1370:THR:O	2.63	0.46
1:B:175:GLU:O	1:B:176:GLU:HB2	2.15	0.46
1:B:307:VAL:HG12	1:B:313:TYR:O	2.15	0.46
1:B:542:VAL:C	1:B:556:SER:HB2	2.35	0.46
1:B:692:HIS:NE2	1:B:694:VAL:HG23	2.30	0.46
1:B:886:GLN:HG3	1:B:887:LYS:H	1.80	0.46
2:X:208:GLN:O	2:X:212:MET:HG3	2.14	0.46
1:A:1247:MET:HB2	1:A:1247:MET:HE3	1.77	0.46
1:A:1488:LEU:HD12	1:A:1488:LEU:C	2.34	0.46
1:B:1016:VAL:O	1:B:1018:VAL:N	2.48	0.46
1:B:1087:GLY:HA3	1:B:1155:ALA:HA	1.96	0.46
1:B:975:ARG:HB3	1:B:1363:THR:HA	1.96	0.46
1:B:386:VAL:O	1:B:410:VAL:HG13	2.16	0.46
1:B:488:PRO:HG2	1:B:499:TYR:OH	2.15	0.46
1:B:600:VAL:HG12	1:B:601:ALA:H	1.80	0.46
1:B:968:VAL:HG23	1:B:971:THR:HG21	1.98	0.46
1:B:976:ILE:HG22	1:B:977:LEU:H	1.79	0.46
1:A:1202:HIS:CD2	1:A:1204:GLN:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1310:SER:O	1:A:1311:MET:O	2.32	0.46
1:A:964:PRO:HG2	1:A:1365:VAL:HG11	1.98	0.46
1:A:461:SER:C	1:A:463:SER:H	2.18	0.46
1:A:520:ASP:CG	1:A:521:ALA:N	2.68	0.46
1:A:477:LEU:HA	1:A:564:GLU:CG	2.45	0.46
1:B:1024:TYR:CE2	1:B:1030:HIS:HD2	2.27	0.46
1:B:1440:LYS:NZ	1:B:1453:TYR:OH	2.45	0.46
1:B:1003:LEU:CD1	1:B:1498:TYR:CE1	2.98	0.46
1:B:24:VAL:HG11	1:B:543:TYR:OH	2.15	0.46
1:B:25:ILE:HD13	1:B:41:ILE:HB	1.98	0.46
1:B:697:LYS:HE3	1:B:701:ASP:OD2	2.15	0.46
2:Y:183:THR:HB	2:Y:230:GLN:HB3	1.97	0.46
1:A:1003:LEU:CD1	1:A:1498:TYR:CE1	2.97	0.46
1:A:1129:LEU:HD23	1:A:1246:ARG:HH12	1.79	0.46
1:A:1256:LEU:HD21	1:A:1295:GLU:HG2	1.97	0.46
1:A:1251:THR:OG1	1:A:1273:TRP:HZ3	1.94	0.46
1:A:1244:THR:O	1:A:1285:TYR:HD2	1.98	0.46
1:A:976:ILE:O	1:A:1361:VAL:HG22	2.16	0.46
1:A:220:LYS:HG2	1:A:763:PRO:HB3	1.97	0.46
1:A:234:GLU:HG3	1:A:247:GLU:HB3	1.98	0.46
1:A:313:TYR:CE2	1:A:321:LYS:HD2	2.50	0.46
1:A:373:VAL:HG23	1:A:374:GLN:H	1.80	0.46
1:A:385:GLY:H	1:A:411:THR:HG23	1.79	0.46
1:A:478:VAL:CG1	1:A:478:VAL:O	2.62	0.46
1:A:544:TYR:HE1	1:A:555:VAL:CG1	2.27	0.46
1:B:1129:LEU:CD1	1:B:1139:GLU:HB3	2.45	0.46
1:B:1162:VAL:CG2	1:B:1163:LYS:H	2.15	0.46
1:B:240:TYR:C	1:B:240:TYR:CD1	2.86	0.46
1:B:544:TYR:CE1	1:B:555:VAL:CG1	2.99	0.46
1:A:1008:ALA:O	1:A:1009:GLU:C	2.53	0.46
1:A:1008:ALA:HB3	1:A:1078:LEU:CD1	2.46	0.46
1:A:123:ASN:C	1:A:123:ASN:ND2	2.66	0.46
1:A:191:PRO:C	1:A:193:ASN:N	2.69	0.46
1:A:365:PRO:HD2	1:A:464:TYR:CE2	2.49	0.46
1:A:73:LEU:HD12	1:A:79:PHE:CD2	2.49	0.46
1:B:1263:ASP:OD1	1:B:1266:TYR:HB2	2.16	0.46
1:B:966:ASP:O	1:B:1368:THR:HG23	2.16	0.46
1:B:189:LYS:HG3	1:B:190:ILE:O	2.15	0.46
1:B:157:ARG:NH1	1:B:209:PHE:CD1	2.84	0.46
1:B:685:GLU:HG3	1:B:686:ILE:HD13	1.96	0.46
1:B:987:ILE:CD1	1:B:1294:ILE:CD1	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1085:VAL:O	1:A:1089:VAL:HG23	2.15	0.46
1:A:1320:LYS:HG2	1:A:1342:LEU:CD1	2.45	0.46
1:A:830:PRO:HG3	1:A:1483:PHE:CZ	2.51	0.46
1:A:23:TYR:HE1	1:A:656:ASN:H	1.63	0.46
1:A:588:VAL:HG11	1:A:790:LEU:HD11	1.97	0.46
1:A:916:THR:HG22	1:A:917:TRP:N	2.31	0.46
1:A:933:GLY:HA3	1:A:1367:LYS:O	2.15	0.46
1:B:193:ASN:OD1	1:B:1070:LYS:HE2	2.15	0.46
1:B:1104:LEU:HD12	1:B:1159:CYS:HB3	1.98	0.46
1:B:1307:LEU:H	1:B:1307:LEU:HD12	1.81	0.46
1:B:144:ARG:HG2	1:B:775:TRP:CZ2	2.50	0.46
1:B:1492:THR:HG22	1:B:1508:PHE:CD1	2.50	0.46
1:B:388:VAL:HG21	1:B:418:ALA:CB	2.46	0.46
1:B:503:ILE:HB	1:B:511:HIS:HB2	1.96	0.46
1:B:608:ALA:O	1:B:609:VAL:O	2.34	0.46
1:B:656:ASN:O	1:B:657:ALA:HB2	2.16	0.46
1:B:711:CYS:HB3	1:B:729:THR:HG22	1.97	0.46
1:B:799:ILE:CG1	1:B:799:ILE:O	2.64	0.46
1:A:1008:ALA:HB3	1:A:1078:LEU:HD11	1.98	0.46
1:A:1097:GLN:O	1:A:1099:SER:N	2.49	0.46
1:A:1249:GLU:HG2	1:A:1253:TYR:CE2	2.50	0.46
1:A:987:ILE:CD1	1:A:1294:ILE:CD1	2.94	0.46
1:A:504:LEU:CD1	1:A:509:ILE:HG12	2.46	0.46
1:A:576:SER:HB3	1:A:577:PRO:HD3	1.96	0.46
1:A:855:PHE:CE1	1:A:886:GLN:CB	2.98	0.46
1:A:978:SER:OG	1:A:980:LYS:HD3	2.15	0.46
1:B:1317:TYR:HB2	1:B:1320:LYS:HB3	1.97	0.46
1:B:313:TYR:CZ	1:B:321:LYS:HD2	2.51	0.46
1:B:586:GLN:O	1:B:790:LEU:HD12	2.14	0.46
1:B:862:VAL:HG21	1:B:909:ASN:O	2.16	0.46
2:X:134:THR:CG2	2:X:153:PHE:HB3	2.43	0.46
1:A:1028:GLY:O	1:A:1030:HIS:CD2	2.69	0.46
1:A:1205:PHE:CZ	1:A:1209:VAL:HG21	2.51	0.46
1:A:1263:ASP:OD1	1:A:1266:TYR:HB2	2.15	0.46
1:A:161:LEU:HD13	1:A:163:PHE:CE1	2.51	0.46
1:A:234:GLU:HB3	1:A:235:TYR:HD2	1.79	0.46
1:A:265:VAL:HG23	1:A:292:LEU:N	2.29	0.46
1:A:397:VAL:C	1:A:399:GLN:H	2.19	0.46
1:A:478:VAL:HG12	1:A:564:GLU:OE1	2.16	0.46
1:B:1117:SER:HB3	1:B:1174:PHE:CE1	2.51	0.46
1:B:102:VAL:O	1:B:116:ARG:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:TYR:CZ	1:B:141:VAL:HG22	2.51	0.46
1:B:144:ARG:O	1:B:145:VAL:HG23	2.16	0.46
1:B:272:ARG:O	1:B:273:GLU:OE2	2.34	0.46
1:B:363:LEU:HD21	1:B:431:LEU:HB2	1.97	0.46
1:B:594:THR:HB	1:B:596:MET:O	2.16	0.46
1:A:1280:TYR:HD1	1:A:1362:THR:HG22	1.81	0.46
1:A:137:PRO:HG3	1:A:196:TYR:OH	2.16	0.46
1:A:849:ARG:CG	1:A:853:MET:HE1	2.41	0.46
1:B:1180:LEU:HD23	1:B:1180:LEU:HA	1.63	0.46
1:B:31:PHE:HB2	1:B:119:ILE:HB	1.98	0.46
1:B:1244:THR:CG2	1:B:1245:ALA:N	2.78	0.46
1:B:1348:VAL:HG21	1:B:1359:VAL:CG1	2.42	0.46
1:B:30:ILE:CG2	1:B:119:ILE:HA	2.46	0.46
1:B:324:TYR:CD2	1:B:324:TYR:C	2.88	0.46
1:B:330:ILE:HA	1:B:337:SER:HA	1.98	0.46
1:B:504:LEU:HD12	1:B:509:ILE:HA	1.97	0.46
1:B:857:VAL:HA	1:B:913:SER:O	2.15	0.46
1:B:967:LEU:HD12	1:B:968:VAL:H	1.81	0.46
2:Y:143:GLY:C	2:Y:145:ASN:N	2.68	0.46
2:Y:179:LEU:O	2:Y:180:TYR:HB2	2.16	0.46
2:Y:222:ASN:O	2:Y:223:LYS:HG3	2.16	0.46
1:A:1043:GLN:OE1	1:A:1043:GLN:HA	2.15	0.46
1:A:1273:TRP:CZ3	1:A:1274:LEU:CD2	2.99	0.46
1:A:1318:LYS:HA	1:A:1347:ILE:HD11	1.98	0.46
1:A:486:VAL:HG21	1:A:526:ILE:CD1	2.45	0.46
1:A:694:VAL:O	1:A:698:CYS:SG	2.74	0.46
1:A:834:VAL:O	1:A:835:ARG:C	2.52	0.46
1:B:1049:LEU:HD21	1:B:1089:VAL:HG13	1.97	0.46
1:B:115:LYS:HE2	1:B:117:MET:CE	2.46	0.46
1:B:327:VAL:HG12	1:B:328:THR:N	2.31	0.46
1:B:492:TYR:OH	1:B:548:GLY:HA2	2.16	0.46
1:B:834:VAL:HG12	1:B:835:ARG:O	2.15	0.46
1:A:1225:TYR:CE1	1:A:1272:LYS:HG3	2.51	0.45
1:A:1283:GLY:CA	1:A:1290:THR:CG2	2.92	0.45
1:A:1439:LEU:HD13	1:A:1453:TYR:HD2	1.81	0.45
1:A:177:ILE:HG13	1:A:177:ILE:O	2.16	0.45
1:A:227:PHE:CE1	1:A:338:GLU:HB2	2.51	0.45
1:A:466:TYR:CD1	1:A:467:ILE:N	2.83	0.45
1:A:540:LEU:CD1	1:A:540:LEU:C	2.84	0.45
1:A:539:ARG:NH2	1:A:634:CYS:C	2.69	0.45
1:A:653:PHE:CE1	1:A:660:ASP:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:950:TYR:CE1	1:A:1271:ILE:HD11	2.50	0.45
1:B:157:ARG:O	1:B:178:ASP:CB	2.63	0.45
1:B:271:ILE:HG22	1:B:272:ARG:H	1.81	0.45
1:B:543:TYR:HA	1:B:555:VAL:O	2.16	0.45
1:A:1012:LEU:O	1:A:1015:VAL:HG13	2.16	0.45
1:A:984:VAL:CG1	1:A:1024:TYR:CE1	2.84	0.45
1:A:1169:ILE:C	1:A:1171:ALA:N	2.67	0.45
1:A:1412:ARG:O	1:A:1413:GLU:HB2	2.17	0.45
1:A:1432:ILE:HG21	1:A:1479:ILE:HD12	1.97	0.45
1:A:183:ILE:HG22	1:A:185:PHE:CE2	2.52	0.45
1:A:235:TYR:HD2	1:A:235:TYR:N	2.13	0.45
1:A:387:PRO:HG2	1:A:438:ASP:C	2.37	0.45
1:A:609:VAL:CG2	1:A:610:TYR:N	2.51	0.45
1:A:625:GLN:C	1:A:629:LYS:HE2	2.36	0.45
1:B:1041:GLU:O	1:B:1045:LEU:HG	2.16	0.45
1:B:977:LEU:HD21	1:B:1315:VAL:HG21	1.99	0.45
1:B:938:SER:CB	1:B:1362:THR:HA	2.47	0.45
1:B:1503:LYS:CD	1:B:1503:LYS:N	2.78	0.45
1:B:177:ILE:O	1:B:177:ILE:HG13	2.15	0.45
1:B:42:GLN:HB2	1:B:80:GLN:NE2	2.32	0.45
2:X:217:ASN:ND2	2:X:220:ASP:OD2	2.47	0.45
1:A:1244:THR:N	1:A:1285:TYR:CE2	2.85	0.45
1:A:1313:ILE:HG22	1:A:1314:ASP:H	1.78	0.45
1:A:1317:TYR:CB	1:A:1320:LYS:HB3	2.47	0.45
1:A:1488:LEU:HD11	1:A:1510:SER:OG	2.16	0.45
1:A:316:GLU:HB3	1:A:317:ASP:H	1.54	0.45
1:A:829:ILE:HD11	1:A:925:LYS:HG2	1.98	0.45
1:B:37:GLU:HA	1:B:37:GLU:OE1	2.17	0.45
1:B:592:MET:HG2	1:B:600:VAL:HG21	1.97	0.45
1:B:57:LYS:HG2	1:B:64:PHE:O	2.16	0.45
1:B:654:LEU:HA	1:B:654:LEU:HD12	1.55	0.45
2:X:159:GLU:HG2	2:X:159:GLU:O	2.17	0.45
1:A:1049:LEU:O	1:A:1050:LYS:C	2.54	0.45
1:A:109:LYS:HD2	1:A:110:HIS:HB2	1.98	0.45
1:A:1466:SER:C	1:A:1468:PRO:HD3	2.37	0.45
1:A:160:VAL:O	1:A:160:VAL:HG12	2.13	0.45
1:A:23:TYR:CD1	1:A:23:TYR:N	2.81	0.45
1:A:544:TYR:CE1	1:A:555:VAL:CG1	2.98	0.45
1:A:754:MET:O	1:A:755:LYS:CG	2.65	0.45
1:A:835:ARG:NH1	1:A:835:ARG:CG	2.77	0.45
1:B:1008:ALA:N	1:B:1068:VAL:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LYS:HD2	1:B:105:GLU:OE1	2.17	0.45
1:B:1023:HIS:CD2	1:B:1092:TYR:OH	2.69	0.45
1:B:1202:HIS:O	1:B:1205:PHE:N	2.49	0.45
1:B:432:GLU:OE2	1:B:453:ARG:NH2	2.50	0.45
1:B:586:GLN:O	1:B:789:ALA:HA	2.16	0.45
1:B:927:LEU:HD22	1:B:929:VAL:HG22	1.97	0.45
1:A:1143:TYR:CE2	1:A:1147:PHE:HD1	2.35	0.45
1:A:1200:LYS:HE3	1:A:1261:LEU:CD2	2.46	0.45
1:A:977:LEU:HD13	1:A:1346:LEU:HD21	1.99	0.45
1:A:161:LEU:H	1:A:161:LEU:HG	1.61	0.45
1:A:319:ASN:OD1	1:A:321:LYS:HG2	2.17	0.45
1:A:412:ARG:HD3	1:A:414:ASP:OD2	2.16	0.45
1:A:685:GLU:HG3	1:A:686:ILE:HD13	1.98	0.45
1:A:729:THR:O	1:A:733:VAL:HG23	2.16	0.45
1:B:1040:ILE:HA	1:B:1040:ILE:HD13	1.78	0.45
1:B:1311:MET:HG2	1:B:1350:THR:OG1	2.17	0.45
1:B:498:HIS:HB3	1:B:514:THR:HG21	1.98	0.45
1:B:599:TRP:CE3	1:B:778:HIS:O	2.70	0.45
1:A:1188:LEU:HA	1:A:1188:LEU:HD12	1.70	0.45
1:A:148:LEU:HD23	1:A:152:LEU:HD12	1.98	0.45
1:A:23:TYR:H	1:A:23:TYR:HD1	1.65	0.45
1:A:27:ALA:O	1:A:28:PRO:O	2.35	0.45
1:A:656:ASN:O	1:A:657:ALA:HB2	2.17	0.45
1:B:1080:ALA:O	1:B:1083:LEU:HB2	2.17	0.45
1:B:1509:TYR:CD2	1:B:1509:TYR:C	2.87	0.45
1:B:240:TYR:O	1:B:240:TYR:CD1	2.70	0.45
1:B:290:THR:O	1:B:290:THR:HG22	2.17	0.45
1:B:397:VAL:C	1:B:399:GLN:H	2.20	0.45
1:B:498:HIS:HB3	1:B:514:THR:HG23	1.99	0.45
1:B:590:LEU:HD12	1:B:591:ASN:N	2.31	0.45
1:B:42:GLN:HB2	1:B:80:GLN:CD	2.37	0.45
1:B:913:SER:HA	1:B:921:GLU:O	2.17	0.45
2:X:184:THR:O	2:X:185:LYS:HB3	2.16	0.45
1:A:1007:SER:OG	1:A:1008:ALA:N	2.50	0.45
1:A:100:SER:O	1:A:101:TYR:HD2	2.00	0.45
1:A:1205:PHE:CE2	1:A:1209:VAL:HG21	2.52	0.45
1:A:1274:LEU:CB	1:A:1297:LEU:HD11	2.44	0.45
1:A:169:SER:O	1:A:171:VAL:HG23	2.17	0.45
1:A:659:ALA:C	1:A:661:ASP:H	2.20	0.45
1:A:589:SER:HA	1:A:787:GLN:HA	1.98	0.45
1:B:194:PRO:HA	1:B:1058:SER:OG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:976:ILE:HG21	1:B:1280:TYR:CE1	2.50	0.45
1:B:232:GLU:HA	1:B:233:PRO:HD3	1.57	0.45
1:B:492:TYR:C	1:B:492:TYR:CD2	2.87	0.45
1:B:820:PHE:CZ	1:B:848:TYR:HD2	2.34	0.45
1:B:820:PHE:HE2	1:B:848:TYR:HD2	1.62	0.45
2:Y:138:VAL:HG11	2:Y:177:TYR:CD2	2.51	0.45
2:Y:140:LYS:O	2:Y:146:LEU:CD2	2.65	0.45
1:A:1228:TRP:CZ3	1:A:1270:VAL:HG22	2.51	0.45
1:B:1217:LEU:CD2	1:B:1235:LYS:HE3	2.46	0.45
1:B:1245:ALA:HA	1:B:1285:TYR:HB3	1.99	0.45
1:B:1307:LEU:HB2	1:B:1355:GLY:HA2	1.97	0.45
1:B:981:GLY:HA3	1:B:1309:LEU:CD1	2.47	0.45
1:B:1460:VAL:O	1:B:1460:VAL:HG12	2.16	0.45
1:B:122:ASP:OD2	1:B:211:THR:HG22	2.17	0.45
1:B:243:PHE:CZ	1:B:316:GLU:HA	2.51	0.45
1:B:315:LEU:HB2	1:B:318:LEU:HD12	1.99	0.45
1:B:386:VAL:N	1:B:411:THR:HG22	2.25	0.45
1:B:605:VAL:CG1	1:B:606:ASP:N	2.80	0.45
1:B:979:VAL:C	1:B:980:LYS:HD2	2.37	0.45
2:X:194:LYS:HA	2:X:194:LYS:HD2	1.80	0.45
1:A:1050:LYS:O	1:A:1053:MET:CB	2.63	0.45
1:A:1104:LEU:HD13	1:A:1164:ILE:CD1	2.44	0.45
1:A:441:ASP:OD2	1:A:441:ASP:N	2.37	0.45
1:A:498:HIS:HB3	1:A:514:THR:HG23	1.99	0.45
1:A:519:SER:O	1:A:520:ASP:C	2.55	0.45
1:A:623:VAL:HG11	1:A:809:ILE:HD13	1.97	0.45
1:A:646:PHE:O	1:A:649:ALA:HB3	2.16	0.45
1:A:50:PHE:CE2	1:A:79:PHE:CE2	3.05	0.45
1:A:983:LEU:HD23	1:A:1271:ILE:HD13	1.98	0.45
1:B:31:PHE:CZ	1:B:104:LEU:HD22	2.40	0.45
1:B:104:LEU:O	1:B:114:SER:CB	2.65	0.45
1:B:1056:ILE:HD11	1:B:1066:TYR:CE2	2.52	0.45
1:B:1180:LEU:CD1	1:B:1207:SER:HB3	2.47	0.45
1:B:1204:GLN:O	1:B:1207:SER:N	2.50	0.45
1:B:1249:GLU:OE2	1:B:1288:GLN:HB3	2.17	0.45
1:B:1280:TYR:HD1	1:B:1362:THR:CG2	2.30	0.45
1:B:162:THR:O	1:B:164:ILE:HG13	2.17	0.45
1:B:435:VAL:CG1	1:B:436:LYS:N	2.80	0.45
1:B:469:TRP:HB2	1:B:483:ASN:O	2.17	0.45
1:B:531:THR:HG23	1:B:533:ASN:N	2.32	0.45
1:A:100:SER:O	1:A:101:TYR:CB	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1104:LEU:O	1:A:1107:LEU:HD12	2.17	0.45
1:A:1185:THR:HG21	1:A:1228:TRP:HB3	1.99	0.45
1:A:1150:ILE:HD11	1:A:1190:ILE:CG2	2.42	0.45
1:A:1467:ILE:N	1:A:1468:PRO:CD	2.80	0.45
1:A:1423:VAL:CG2	1:A:1496:TYR:HE1	2.29	0.45
1:A:227:PHE:CD1	1:A:227:PHE:O	2.70	0.45
1:A:259:VAL:HG23	1:A:260:VAL:O	2.16	0.45
1:A:240:TYR:CZ	1:A:443:PRO:HD2	2.51	0.45
1:A:590:LEU:HD12	1:A:591:ASN:H	1.81	0.45
1:A:644:ASN:HD21	1:A:648:LEU:CD1	2.20	0.45
1:A:599:TRP:CZ3	1:A:779:LEU:HB2	2.52	0.45
1:A:837:GLU:OE2	1:A:1488:LEU:CB	2.63	0.45
1:A:956:ARG:HG3	1:A:1349:SER:CB	2.37	0.45
1:A:977:LEU:HD12	1:A:1361:VAL:HG23	1.96	0.45
1:B:1200:LYS:HG2	1:B:1200:LYS:H	1.39	0.45
1:B:1332:ASN:O	1:B:1332:ASN:CG	2.53	0.45
1:B:138:ASP:N	1:B:190:ILE:HB	2.32	0.45
1:B:25:ILE:O	1:B:654:LEU:N	2.43	0.45
1:B:54:ILE:HG22	1:B:55:SER:N	2.31	0.45
1:B:41:ILE:CG2	1:B:81:ASN:O	2.64	0.45
1:B:888:VAL:HG12	1:B:894:HIS:HB2	1.97	0.45
1:B:901:LEU:HA	1:B:902:PRO:HD3	1.81	0.45
1:A:101:TYR:CE1	1:A:116:ARG:NE	2.85	0.44
1:A:159:THR:O	1:A:175:GLU:HA	2.17	0.44
1:A:243:PHE:CZ	1:A:316:GLU:CG	2.92	0.44
1:A:315:LEU:HB2	1:A:318:LEU:HD12	1.98	0.44
1:A:31:PHE:CZ	1:A:104:LEU:HD13	2.51	0.44
1:A:469:TRP:HB2	1:A:483:ASN:O	2.17	0.44
1:A:575:LEU:HD23	1:A:575:LEU:HA	1.74	0.44
1:A:758:LEU:O	1:A:760:VAL:N	2.50	0.44
1:A:587:THR:HG22	1:A:789:ALA:HB2	1.99	0.44
1:A:936:ARG:CZ	1:A:1002:HIS:HE1	2.30	0.44
1:B:323:LEU:HG	1:B:347:TYR:HE2	1.82	0.44
1:B:424:LEU:HA	1:B:425:PRO:HD3	1.79	0.44
1:B:396:ASP:O	1:B:429:THR:HG21	2.17	0.44
1:B:431:LEU:C	1:B:431:LEU:HD22	2.37	0.44
1:B:350:SER:OG	1:B:446:ASN:O	2.27	0.44
1:B:363:LEU:CD2	1:B:454:ALA:HB3	2.46	0.44
1:B:608:ALA:HB1	1:B:769:PHE:HE1	1.82	0.44
1:B:849:ARG:HB3	1:B:853:MET:CE	2.46	0.44
2:X:190:THR:HA	2:X:199:GLN:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:153:PHE:CG	2:Y:154:SER:N	2.85	0.44
1:A:1056:ILE:HD11	1:A:1066:TYR:HE2	1.82	0.44
1:A:1225:TYR:CD1	1:A:1273:TRP:HB2	2.53	0.44
1:A:1300:TYR:CD2	1:A:1300:TYR:C	2.90	0.44
1:A:1439:LEU:CD1	1:A:1453:TYR:HD2	2.29	0.44
1:A:25:ILE:HD13	1:A:41:ILE:HA	1.99	0.44
1:A:412:ARG:HG2	1:A:413:VAL:H	1.82	0.44
1:A:492:TYR:C	1:A:492:TYR:CD2	2.90	0.44
1:A:57:LYS:HG2	1:A:64:PHE:O	2.17	0.44
1:A:88:GLN:HB3	1:A:89:PRO:CD	2.47	0.44
1:B:1053:MET:HE3	1:B:1086:LEU:HD13	1.99	0.44
1:B:1210:SER:O	1:B:1214:ARG:N	2.45	0.44
1:B:1265:ASN:HA	1:B:1268:ASN:ND2	2.32	0.44
1:B:540:LEU:C	1:B:540:LEU:CD1	2.85	0.44
1:B:583:SER:HA	1:B:584:PRO:HD3	1.87	0.44
1:B:699:CYS:O	1:B:702:GLY:HA3	2.18	0.44
1:B:980:LYS:HB3	1:B:980:LYS:HE3	1.70	0.44
1:A:1244:THR:HG22	1:A:1245:ALA:N	2.32	0.44
1:A:1438:ASP:O	1:A:1441:ALA:HB3	2.17	0.44
1:A:227:PHE:CE1	1:A:338:GLU:HB3	2.53	0.44
1:B:1378:TYR:CE2	1:B:1409:LYS:HG2	2.53	0.44
1:B:183:ILE:HG22	1:B:185:PHE:CE2	2.52	0.44
1:B:515:ARG:HH22	1:B:527:ASN:CA	2.30	0.44
1:B:590:LEU:HD12	1:B:591:ASN:H	1.82	0.44
1:B:944:LEU:HD23	1:B:944:LEU:HA	1.61	0.44
1:B:991:VAL:HG21	1:B:1017:PRO:O	2.17	0.44
2:Y:226:VAL:HG12	2:Y:227:THR:N	2.32	0.44
1:A:1226:ARG:CZ	1:A:1266:TYR:HE1	2.30	0.44
1:A:1339:GLU:O	1:A:1341:LEU:HD22	2.18	0.44
1:A:961:TYR:CE2	1:A:1343:ASN:HA	2.53	0.44
1:A:165:ASP:HA	1:A:166:PRO:HD3	1.78	0.44
1:A:494:ASP:C	1:A:496:ILE:HD12	2.38	0.44
1:A:847:ASN:O	1:A:848:TYR:CD1	2.71	0.44
1:A:820:PHE:CZ	1:A:848:TYR:HB2	2.42	0.44
1:B:1012:LEU:O	1:B:1015:VAL:CG1	2.65	0.44
1:B:1255:LEU:HD11	1:B:1259:LEU:HD11	1.99	0.44
1:B:1323:LEU:CG	1:B:1324:HIS:N	2.80	0.44
1:B:1432:ILE:HD13	1:B:1481:GLU:HG2	2.00	0.44
1:B:173:MET:C	1:B:174:VAL:HG12	2.38	0.44
1:B:183:ILE:CG2	1:B:185:PHE:CE2	3.01	0.44
1:B:361:LEU:HD12	1:B:361:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:PHE:CE2	1:B:79:PHE:CD2	3.06	0.44
1:B:544:TYR:CE1	1:B:555:VAL:HG12	2.52	0.44
1:B:754:MET:O	1:B:755:LYS:CG	2.65	0.44
2:X:211:ARG:O	2:X:214:ASP:HB2	2.17	0.44
1:A:1041:GLU:O	1:A:1045:LEU:HG	2.18	0.44
1:A:1047:LYS:C	1:A:1049:LEU:N	2.68	0.44
1:A:1105:LEU:HA	1:A:1108:VAL:HG11	2.00	0.44
1:A:1175:LEU:HA	1:A:1175:LEU:HD23	1.79	0.44
1:A:325:ILE:O	1:A:342:ILE:N	2.30	0.44
1:A:773:TRP:HZ3	1:A:788:PHE:CE1	2.34	0.44
1:B:1127:ILE:HD12	1:B:1127:ILE:O	2.16	0.44
1:B:1228:TRP:N	1:B:1228:TRP:CE3	2.86	0.44
1:B:1229:LYS:HD2	1:B:1239:VAL:CG1	2.42	0.44
1:B:1279:ARG:CD	1:B:1284:PHE:CG	2.98	0.44
1:B:1259:LEU:HD11	1:B:1300:TYR:HB2	1.99	0.44
1:B:33:VAL:HB	1:B:209:PHE:CE2	2.51	0.44
1:B:500:ASN:O	1:B:542:VAL:HA	2.18	0.44
1:B:61:ASP:CG	1:B:61:ASP:O	2.56	0.44
1:B:735:ALA:HB1	1:B:754:MET:CE	2.45	0.44
1:B:777:VAL:HG12	1:B:778:HIS:N	2.32	0.44
2:Y:140:LYS:O	2:Y:146:LEU:HA	2.17	0.44
1:A:1047:LYS:O	1:A:1048:LYS:C	2.56	0.44
1:A:1225:TYR:OH	1:A:1272:LYS:HE3	2.18	0.44
1:A:600:VAL:HG12	1:A:601:ALA:H	1.82	0.44
1:B:1018:VAL:O	1:B:1019:PHE:C	2.56	0.44
1:B:1037:ASP:OD1	1:B:1038:PRO:N	2.51	0.44
1:B:1136:GLU:OE1	1:B:1415:SER:HB3	2.17	0.44
1:B:1497:GLU:O	1:B:1498:TYR:C	2.55	0.44
1:B:415:ASP:OD1	1:B:417:VAL:HG23	2.18	0.44
1:B:834:VAL:HG11	1:B:1489:SER:HB3	2.00	0.44
2:X:166:ASP:OD2	2:X:201:ILE:HD13	2.17	0.44
2:X:192:ASN:HB2	2:X:223:LYS:O	2.18	0.44
2:Y:150:ILE:HD12	2:Y:151:ASP:N	2.32	0.44
1:A:1104:LEU:HD12	1:A:1159:CYS:HB3	1.98	0.44
1:A:1243:GLY:HA3	1:A:1285:TYR:CE2	2.53	0.44
1:A:271:ILE:HG22	1:A:272:ARG:H	1.82	0.44
1:A:290:THR:O	1:A:291:MET:O	2.35	0.44
1:A:450:GLU:HB3	1:A:452:TYR:HE2	1.81	0.44
1:A:912:PHE:O	1:A:922:ILE:HA	2.18	0.44
1:B:227:PHE:CZ	1:B:338:GLU:HB2	2.53	0.44
1:B:867:THR:HG23	1:B:900:VAL:CG1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:981:GLY:C	1:B:982:LEU:HD23	2.38	0.44
1:A:1037:ASP:HA	1:A:1038:PRO:HD3	1.76	0.44
1:A:1061:ASN:HB2	1:A:1065:SER:O	2.18	0.44
1:A:1135:VAL:HG12	1:A:1136:GLU:N	2.33	0.44
1:A:1323:LEU:CG	1:A:1324:HIS:H	2.31	0.44
1:A:153:LYS:O	1:A:155:ALA:N	2.51	0.44
1:A:159:THR:CG2	1:A:160:VAL:N	2.81	0.44
1:A:367:ILE:HG23	1:A:368:PRO:CD	2.47	0.44
1:A:412:ARG:HG2	1:A:413:VAL:N	2.32	0.44
1:A:489:LYS:O	1:A:491:PRO:HD2	2.17	0.44
1:A:478:VAL:CG1	1:A:566:LYS:HD3	2.47	0.44
1:A:609:VAL:HG23	1:A:610:TYR:CD2	2.53	0.44
1:B:1016:VAL:O	1:B:1017:PRO:C	2.56	0.44
1:B:1161:LEU:HG	1:B:1164:ILE:HG23	1.99	0.44
1:B:1379:LEU:HD22	1:B:1493:PHE:HE2	1.77	0.44
1:B:1496:TYR:HD2	1:B:1504:GLN:OE1	2.01	0.44
1:B:284:GLN:O	1:B:310:LEU:HD13	2.18	0.44
1:B:367:ILE:CD1	1:B:466:TYR:HB3	2.48	0.44
1:B:544:TYR:CD1	1:B:544:TYR:N	2.84	0.44
2:Y:183:THR:CB	2:Y:230:GLN:HB3	2.48	0.44
1:A:938:SER:OG	1:A:1279:ARG:NE	2.50	0.44
1:A:494:ASP:O	1:A:496:ILE:N	2.46	0.44
1:A:56:ILE:O	1:A:66:TYR:CD2	2.70	0.44
1:A:576:SER:CB	1:A:577:PRO:CD	2.95	0.44
1:A:609:VAL:CG2	1:A:610:TYR:CD2	3.01	0.44
1:A:859:MET:HE2	1:A:912:PHE:CZ	2.52	0.44
1:A:930:VAL:HG12	1:A:931:PRO:N	2.33	0.44
1:A:968:VAL:HG22	1:A:1366:HIS:O	2.18	0.44
1:B:1084:ARG:O	1:B:1088:GLN:HG3	2.17	0.44
1:B:107:VAL:HG12	1:B:108:SER:N	2.33	0.44
1:B:1083:LEU:HD11	1:B:1107:LEU:HD11	1.99	0.44
1:B:1125:GLN:O	1:B:1421:HIS:N	2.49	0.44
1:B:1133:LEU:N	1:B:1134:PRO:CD	2.81	0.44
1:B:1190:ILE:HG12	1:B:1253:TYR:CD1	2.53	0.44
1:B:1401:ARG:HB2	1:B:1478:ARG:CA	2.48	0.44
1:B:1069:TRP:NE1	1:B:1463:GLN:NE2	2.60	0.44
1:B:1423:VAL:HG22	1:B:1496:TYR:CE1	2.51	0.44
1:B:220:LYS:HG2	1:B:763:PRO:HB3	2.00	0.44
1:B:272:ARG:CG	1:B:273:GLU:N	2.81	0.44
1:B:388:VAL:O	1:B:420:PHE:HZ	2.00	0.44
1:B:423:ASN:ND2	1:B:423:ASN:H	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ASP:OD1	1:B:63:LYS:HB2	2.18	0.44
1:B:621:GLU:O	1:B:622:ARG:C	2.56	0.44
1:B:667:GLU:N	1:B:667:GLU:OE1	2.51	0.44
1:A:1057:MET:O	1:A:1060:ARG:HB3	2.18	0.43
1:A:1019:PHE:HE2	1:A:1088:GLN:HE21	1.64	0.43
1:A:1226:ARG:HB3	1:A:1270:VAL:HG23	2.01	0.43
1:A:1243:GLY:HA3	1:A:1285:TYR:HE2	1.82	0.43
1:A:1300:TYR:CE1	1:A:1304:VAL:HG21	2.53	0.43
1:A:1429:PRO:O	1:A:1432:ILE:CG1	2.66	0.43
1:A:144:ARG:O	1:A:145:VAL:HG23	2.18	0.43
1:A:1435:ASN:ND2	1:A:1478:ARG:HB2	2.27	0.43
1:A:303:SER:HB3	1:A:347:TYR:OH	2.18	0.43
1:A:439:ALA:O	1:A:447:GLN:NE2	2.50	0.43
1:A:442:LEU:O	1:A:443:PRO:C	2.52	0.43
1:A:606:ASP:C	1:A:608:ALA:N	2.71	0.43
1:A:724:CYS:O	1:A:727:ALA:N	2.51	0.43
1:A:768:TYR:HE2	1:A:770:PRO:HA	1.83	0.43
1:A:88:GLN:HE21	1:A:88:GLN:HB3	1.63	0.43
1:B:1081:PHE:O	1:B:1081:PHE:CD2	2.71	0.43
1:B:1188:LEU:HA	1:B:1188:LEU:HD12	1.73	0.43
1:B:1228:TRP:N	1:B:1228:TRP:HE3	2.16	0.43
1:B:1305:LYS:HE3	1:B:1305:LYS:HB2	1.68	0.43
1:B:158:GLU:CB	1:B:206:LYS:HE2	2.48	0.43
1:B:465:LEU:HD22	1:B:542:VAL:O	2.18	0.43
1:B:701:ASP:OD1	1:B:702:GLY:N	2.51	0.43
2:X:172:HIS:O	2:X:176:ASN:N	2.49	0.43
1:A:1031:TRP:CE3	1:A:1031:TRP:HA	2.53	0.43
1:A:1052:GLY:O	1:A:1055:SER:HB3	2.17	0.43
1:A:1370:THR:HG21	1:A:1506:THR:O	2.18	0.43
1:A:190:ILE:HG22	1:A:194:PRO:CG	2.47	0.43
1:A:319:ASN:OD1	1:A:321:LYS:CG	2.66	0.43
1:A:777:VAL:CG1	1:A:778:HIS:N	2.81	0.43
1:A:994:GLN:NE2	1:A:998:ASN:HD22	2.16	0.43
1:B:113:LYS:HZ3	1:B:656:ASN:HD21	1.65	0.43
1:B:1247:MET:O	1:B:1251:THR:HG23	2.18	0.43
1:B:259:VAL:HG23	1:B:260:VAL:O	2.17	0.43
1:B:271:ILE:HD11	1:B:307:VAL:CG2	2.48	0.43
1:B:356:LEU:CD1	1:B:452:TYR:CD1	3.00	0.43
1:B:454:ALA:C	1:B:455:ILE:HG13	2.38	0.43
1:B:531:THR:O	1:B:534:MET:HG3	2.18	0.43
1:B:582:TYR:HB2	1:B:819:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:665:ASN:O	1:B:666:ASP:HB3	2.18	0.43
1:B:53:THR:HA	1:B:69:GLY:O	2.18	0.43
1:B:840:GLN:O	1:B:1483:PHE:CD2	2.70	0.43
1:B:257:ASN:ND2	1:B:893:SER:O	2.51	0.43
1:B:896:VAL:C	1:B:897:THR:CG2	2.86	0.43
2:X:193:LEU:HD23	2:X:221:ILE:HG12	1.99	0.43
1:A:1169:ILE:O	1:A:1170:LYS:C	2.57	0.43
1:A:1176:LEU:H	1:A:1176:LEU:HG	1.51	0.43
1:A:1206:ARG:CG	1:A:1206:ARG:NH1	2.73	0.43
1:A:968:VAL:CG1	1:A:1368:THR:CG2	2.86	0.43
1:A:838:GLN:HB3	1:A:1486:GLY:CA	2.48	0.43
1:A:1126:PRO:C	1:A:1499:HIS:HD1	2.21	0.43
1:A:23:TYR:HA	1:A:43:VAL:HG23	2.00	0.43
1:A:469:TRP:CD1	1:A:482:LEU:HD21	2.53	0.43
1:A:541:LEU:HD23	1:A:541:LEU:C	2.38	0.43
1:A:758:LEU:HD22	1:A:760:VAL:H	1.84	0.43
1:B:1024:TYR:CD2	1:B:1025:LEU:N	2.83	0.43
1:B:511:HIS:NE2	1:B:531:THR:HG21	2.31	0.43
2:Y:224:ILE:C	2:Y:225:GLU:HG3	2.39	0.43
1:A:1087:GLY:HA3	1:A:1155:ALA:HA	2.01	0.43
1:A:1352:PHE:CG	1:A:1353:GLY:N	2.83	0.43
1:A:59:TYR:CD2	1:A:60:PRO:CD	2.97	0.43
1:A:59:TYR:CG	1:A:60:PRO:CD	2.97	0.43
1:A:647:HIS:C	1:A:649:ALA:H	2.22	0.43
1:A:975:ARG:O	1:A:1339:GLU:HA	2.19	0.43
1:B:1480:PHE:O	1:B:1481:GLU:C	2.56	0.43
1:B:1422:ALA:HA	1:B:1498:TYR:H	1.83	0.43
1:B:166:PRO:HD3	1:B:199:TRP:CE2	2.53	0.43
1:B:216:TYR:CD2	1:B:216:TYR:N	2.86	0.43
1:B:50:PHE:HE2	1:B:79:PHE:CE2	2.35	0.43
1:B:515:ARG:CZ	1:B:526:ILE:HG23	2.49	0.43
1:B:554:LEU:O	1:B:555:VAL:HG23	2.18	0.43
1:B:571:LEU:HD12	1:B:571:LEU:C	2.29	0.43
1:B:758:LEU:O	1:B:760:VAL:N	2.50	0.43
2:X:140:LYS:O	2:X:146:LEU:HA	2.17	0.43
2:Y:136:LEU:HD23	2:Y:136:LEU:H	1.83	0.43
2:Y:153:PHE:HZ	2:Y:168:LYS:HD2	1.84	0.43
1:A:115:LYS:HG3	1:A:116:ARG:H	1.77	0.43
1:A:1203:PRO:O	1:A:1206:ARG:N	2.52	0.43
1:A:1435:ASN:HB3	1:A:1438:ASP:CG	2.38	0.43
1:A:496:ILE:CD1	1:A:517:LYS:NZ	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:TYR:N	1:A:544:TYR:CD1	2.81	0.43
1:A:605:VAL:O	1:A:797:TRP:HE3	2.01	0.43
1:A:61:ASP:C	1:A:63:LYS:H	2.20	0.43
1:A:641:ASN:O	1:A:642:ASN:C	2.57	0.43
1:A:820:PHE:HZ	1:A:848:TYR:CB	2.27	0.43
1:B:625:GLN:O	1:B:626:PHE:C	2.56	0.43
1:B:699:CYS:SG	1:B:727:ALA:O	2.76	0.43
2:Y:217:ASN:ND2	2:Y:220:ASP:OD2	2.47	0.43
1:A:106:VAL:CG1	1:A:107:VAL:N	2.81	0.43
1:A:494:ASP:HA	1:A:496:ILE:HD11	2.00	0.43
1:A:560:TRP:CH2	1:A:562:ASN:CB	2.99	0.43
1:A:609:VAL:HG23	1:A:610:TYR:CG	2.53	0.43
1:A:832:SER:O	1:A:1430:THR:HG23	2.19	0.43
1:B:1128:LYS:NZ	1:B:1415:SER:HB3	2.34	0.43
1:B:1352:PHE:CG	1:B:1353:GLY:N	2.84	0.43
1:B:128:ILE:HA	1:B:145:VAL:HG22	2.00	0.43
1:B:488:PRO:CG	1:B:499:TYR:OH	2.66	0.43
2:X:158:GLU:HA	2:X:219:LYS:HZ1	1.83	0.43
1:A:1120:GLU:OE2	1:A:1121:ASN:N	2.51	0.43
1:A:1158:ILE:HG13	1:A:1158:ILE:H	1.63	0.43
1:A:1206:ARG:O	1:A:1210:SER:HB3	2.19	0.43
1:A:223:VAL:HG12	1:A:224:LEU:N	2.33	0.43
1:A:231:ILE:HD12	1:A:327:VAL:HG23	2.01	0.43
1:A:560:TRP:HZ3	1:A:562:ASN:HB2	1.74	0.43
1:A:743:SER:OG	1:A:752:LEU:HD22	2.19	0.43
1:A:974:LYS:HE3	1:A:1339:GLU:OE1	2.17	0.43
1:A:995:GLU:O	1:A:996:GLY:O	2.36	0.43
1:B:1068:VAL:HA	1:B:1078:LEU:HD13	2.01	0.43
1:B:1082:ALA:O	1:B:1086:LEU:N	2.49	0.43
1:B:1286:SER:OG	1:B:1287:THR:N	2.50	0.43
1:B:1342:LEU:C	1:B:1343:ASN:HD22	2.22	0.43
1:B:1429:PRO:O	1:B:1432:ILE:HG12	2.19	0.43
1:B:342:ILE:HG22	1:B:343:PRO:HD2	2.01	0.43
1:B:323:LEU:O	1:B:345:ILE:HB	2.17	0.43
1:B:472:ASN:OD1	1:B:473:HIS:CE1	2.72	0.43
1:B:820:PHE:CZ	1:B:821:LYS:O	2.72	0.43
1:B:982:LEU:N	1:B:982:LEU:CD2	2.81	0.43
1:A:1016:VAL:O	1:A:1017:PRO:C	2.55	0.43
1:A:1054:LEU:C	1:A:1056:ILE:H	2.23	0.43
1:A:1096:ASN:ND2	1:A:1096:ASN:C	2.71	0.43
1:A:1318:LYS:HE2	1:A:1345:ASP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:VAL:HG12	1:A:328:THR:N	2.33	0.43
1:A:387:PRO:HA	1:A:410:VAL:HG22	1.99	0.43
1:A:557:ASP:CG	1:A:558:SER:H	2.22	0.43
1:A:599:TRP:HE3	1:A:778:HIS:O	2.01	0.43
1:A:78:LYS:HE3	2:X:143:GLY:O	2.18	0.43
1:A:834:VAL:HG11	1:A:1489:SER:HB3	2.00	0.43
1:A:859:MET:CE	1:A:912:PHE:CZ	3.02	0.43
1:A:90:LYS:HB2	1:A:91:GLN:H	1.58	0.43
1:A:968:VAL:O	1:A:969:PRO:O	2.37	0.43
1:B:988:LEU:CD2	1:B:1021:VAL:HG13	2.49	0.43
1:B:1091:LYS:HE2	1:B:1091:LYS:HB3	1.73	0.43
1:B:1133:LEU:H	1:B:1133:LEU:CD1	2.32	0.43
1:B:1132:THR:CG2	1:B:1134:PRO:HD2	2.49	0.43
1:B:101:TYR:HD1	1:B:116:ARG:CG	2.31	0.43
1:B:1372:GLU:HG3	1:B:1373:GLU:HG3	2.01	0.43
1:B:292:LEU:C	1:B:292:LEU:HD13	2.38	0.43
1:B:504:LEU:HD21	1:B:651:LEU:CG	2.46	0.43
1:B:609:VAL:HG23	1:B:610:TYR:CG	2.52	0.43
1:B:647:HIS:C	1:B:649:ALA:N	2.71	0.43
1:B:951:GLY:O	1:B:952:THR:HG22	2.19	0.43
1:A:1307:LEU:HD12	1:A:1307:LEU:H	1.84	0.43
1:A:1438:ASP:OD2	1:A:1478:ARG:N	2.49	0.43
1:A:127:PHE:HE1	1:A:626:PHE:CE2	2.36	0.43
1:B:979:VAL:HB	1:B:1326:TYR:OH	2.19	0.43
1:B:208:ASP:O	1:B:209:PHE:CG	2.72	0.43
1:B:51:ASP:OD1	1:B:72:HIS:ND1	2.49	0.43
1:B:644:ASN:HD22	1:B:644:ASN:C	2.22	0.43
1:B:707:ASN:HB3	1:B:739:ARG:CZ	2.49	0.43
1:B:773:TRP:HZ3	1:B:788:PHE:CE1	2.37	0.43
1:B:50:PHE:HE2	1:B:79:PHE:CD2	2.37	0.43
2:X:192:ASN:HB2	2:X:223:LYS:H	1.83	0.43
2:X:227:THR:C	2:X:228:LEU:HD23	2.39	0.43
1:A:1042:LYS:HG2	1:A:1046:LYS:HE3	2.01	0.43
1:A:1259:LEU:HD21	1:A:1300:TYR:HD1	1.84	0.43
1:A:133:PRO:O	1:A:134:VAL:CG2	2.53	0.43
1:A:1383:THR:HG22	1:A:1402:ILE:HG12	2.00	0.43
1:A:198:MET:CE	1:A:218:GLU:HB2	2.49	0.43
1:A:269:PHE:CB	1:A:283:MET:HE3	2.48	0.43
1:A:356:LEU:HG	1:A:452:TYR:CZ	2.53	0.43
1:A:465:LEU:CD2	1:A:542:VAL:O	2.66	0.43
1:A:685:GLU:HG3	1:A:686:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:PHE:CZ	1:A:821:LYS:O	2.72	0.43
1:A:971:THR:OG1	1:A:971:THR:O	2.36	0.43
1:B:1068:VAL:HG22	1:B:1069:TRP:N	2.34	0.43
1:B:1283:GLY:O	1:B:1290:THR:OG1	2.36	0.43
1:B:1328:MET:O	1:B:1329:THR:CG2	2.66	0.43
1:B:634:CYS:SG	1:B:672:ILE:HG22	2.59	0.43
1:B:641:ASN:C	1:B:643:ALA:N	2.67	0.43
2:X:146:LEU:C	2:X:146:LEU:HD13	2.39	0.43
1:A:1082:ALA:O	1:A:1086:LEU:HD23	2.19	0.42
1:A:1149:VAL:HA	1:A:1152:ILE:HD12	2.01	0.42
1:A:947:ARG:NH1	1:A:1354:SER:HB3	2.33	0.42
1:A:162:THR:HG21	1:A:204:LYS:HE2	2.00	0.42
1:A:386:VAL:HA	1:A:387:PRO:HD3	1.71	0.42
1:A:760:VAL:O	1:A:761:SER:HB3	2.18	0.42
1:B:1053:MET:HE1	1:B:1086:LEU:CD2	2.46	0.42
1:B:1068:VAL:HG22	1:B:1069:TRP:CD2	2.54	0.42
1:B:121:TYR:O	1:B:210:SER:N	2.43	0.42
1:B:1440:LYS:O	1:B:1444:GLU:CB	2.67	0.42
1:B:170:GLU:O	1:B:171:VAL:HG23	2.19	0.42
4:B:2001:NAG:HO3	4:B:2002:NAG:C1	2.32	0.42
1:B:270:GLY:N	1:B:324:TYR:O	2.52	0.42
1:B:330:ILE:HB	1:B:336:PHE:O	2.19	0.42
1:B:386:VAL:CG1	1:B:387:PRO:HD2	2.39	0.42
1:B:392:ALA:HB3	1:B:404:LEU:CD1	2.45	0.42
1:B:561:LEU:O	1:B:563:ILE:HG23	2.19	0.42
1:B:562:ASN:OD1	1:B:563:ILE:N	2.52	0.42
2:X:138:VAL:HG11	2:X:177:TYR:CD2	2.54	0.42
1:A:1050:LYS:O	1:A:1053:MET:N	2.52	0.42
1:A:1129:LEU:CD1	1:A:1139:GLU:HB3	2.49	0.42
1:A:1225:TYR:HE1	1:A:1272:LYS:HG3	1.84	0.42
1:A:367:ILE:HD12	1:A:466:TYR:HB2	2.00	0.42
1:A:350:SER:HB2	1:A:446:ASN:C	2.39	0.42
1:A:472:ASN:OD1	1:A:473:HIS:CE1	2.72	0.42
1:A:700:TYR:CE1	1:A:758:LEU:CB	2.99	0.42
1:A:735:ALA:O	1:A:754:MET:SD	2.77	0.42
1:A:834:VAL:HG12	1:A:835:ARG:O	2.18	0.42
1:A:988:LEU:HA	1:A:988:LEU:HD23	1.89	0.42
1:B:1023:HIS:HD2	1:B:1092:TYR:OH	2.03	0.42
1:B:1438:ASP:OD2	1:B:1478:ARG:N	2.50	0.42
1:B:1467:ILE:N	1:B:1468:PRO:CD	2.82	0.42
1:B:1381:ILE:HG21	1:B:1509:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:VAL:HG12	1:B:224:LEU:N	2.34	0.42
1:B:232:GLU:OE2	1:B:251:LYS:CE	2.60	0.42
1:B:297:ALA:O	1:B:298:GLN:CG	2.65	0.42
1:B:505:SER:HB3	1:B:510:ILE:CD1	2.49	0.42
1:B:691:LYS:O	1:B:692:HIS:HB2	2.20	0.42
1:B:722:PRO:HA	1:B:725:ILE:HG13	2.01	0.42
1:B:88:GLN:HE21	1:B:88:GLN:HB3	1.64	0.42
1:B:909:ASN:N	1:B:926:THR:HG22	2.33	0.42
2:Y:134:THR:CG2	2:Y:153:PHE:HB3	2.47	0.42
1:A:142:LYS:HD3	1:A:775:TRP:CD1	2.54	0.42
1:A:502:LEU:HD12	1:A:502:LEU:HA	1.81	0.42
1:A:592:MET:HB3	1:A:780:VAL:HG11	2.01	0.42
1:A:61:ASP:O	1:A:61:ASP:CG	2.57	0.42
1:A:762:LYS:HA	1:A:763:PRO:HD3	1.91	0.42
1:A:829:ILE:HG22	1:A:830:PRO:CD	2.49	0.42
1:A:968:VAL:HG23	1:A:971:THR:CG2	2.49	0.42
1:B:1008:ALA:HB2	1:B:1068:VAL:O	2.20	0.42
1:B:1093:VAL:O	1:B:1094:GLU:C	2.58	0.42
1:B:1206:ARG:O	1:B:1210:SER:HB3	2.19	0.42
1:B:1376:SER:OG	1:B:1503:LYS:HA	2.20	0.42
1:B:161:LEU:HD13	1:B:163:PHE:CE1	2.54	0.42
1:B:128:ILE:HB	1:B:215:ALA:HB2	2.00	0.42
1:B:354:LEU:HD12	1:B:435:VAL:HG12	2.00	0.42
1:B:561:LEU:O	1:B:563:ILE:HG22	2.18	0.42
1:B:56:ILE:HD13	1:B:86:THR:H	1.84	0.42
1:B:576:SER:HB3	1:B:577:PRO:HD3	2.01	0.42
1:B:61:ASP:OD1	1:B:61:ASP:O	2.38	0.42
1:B:847:ASN:HD22	1:B:888:VAL:CG2	2.32	0.42
1:B:859:MET:HE2	1:B:912:PHE:CZ	2.54	0.42
1:B:922:ILE:O	1:B:922:ILE:HG22	2.18	0.42
2:X:146:LEU:HD11	2:X:148:ALA:CB	2.45	0.42
1:B:501:TYR:OH	2:Y:147:ASP:HB3	2.19	0.42
1:A:1028:GLY:O	1:A:1029:ASN:O	2.38	0.42
1:A:111:PHE:CD2	1:A:112:SER:N	2.86	0.42
1:A:1203:PRO:O	1:A:1206:ARG:CB	2.68	0.42
1:A:132:LYS:NZ	1:A:139:GLN:NE2	2.67	0.42
1:A:214:THR:HG22	1:A:215:ALA:H	1.84	0.42
1:A:961:TYR:OH	1:A:1343:ASN:CG	2.58	0.42
1:B:1244:THR:HB	1:B:1247:MET:HB3	2.01	0.42
1:B:1428:LEU:HA	1:B:1429:PRO:HD3	1.87	0.42
1:B:191:PRO:HD2	1:B:194:PRO:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:SER:HB2	1:B:446:ASN:C	2.40	0.42
1:B:352:TYR:CD1	1:B:375:VAL:CG1	3.01	0.42
1:B:540:LEU:O	1:B:540:LEU:HD12	2.20	0.42
1:B:735:ALA:O	1:B:754:MET:SD	2.77	0.42
1:B:844:THR:HG22	1:B:895:LEU:HG	2.00	0.42
1:B:88:GLN:HB3	1:B:89:PRO:HD2	2.02	0.42
2:X:194:LYS:HG3	2:X:195:ASP:N	2.35	0.42
2:X:189:ILE:CD1	2:X:203:LEU:HD21	2.48	0.42
2:Y:190:THR:HA	2:Y:199:GLN:O	2.19	0.42
2:Y:211:ARG:O	2:Y:214:ASP:HB2	2.19	0.42
1:A:1011:GLU:HG3	1:A:1055:SER:OG	2.20	0.42
1:A:1283:GLY:H	1:A:1290:THR:HG21	1.84	0.42
1:A:1427:SER:CB	1:A:1491:ALA:HB1	2.50	0.42
1:A:205:TYR:HD1	1:A:211:THR:OG1	2.03	0.42
1:A:461:SER:C	1:A:463:SER:N	2.72	0.42
1:A:55:SER:HB3	1:A:68:SER:CB	2.50	0.42
1:A:55:SER:CB	1:A:67:SER:O	2.68	0.42
1:A:685:GLU:C	1:A:687:ALA:H	2.22	0.42
1:A:796:THR:HG23	1:A:818:LYS:HB3	2.02	0.42
1:A:981:GLY:O	1:A:982:LEU:CB	2.68	0.42
1:B:1185:THR:HG21	1:B:1228:TRP:HB3	2.01	0.42
1:B:1129:LEU:HD23	1:B:1246:ARG:HH12	1.84	0.42
1:B:272:ARG:HG2	1:B:273:GLU:H	1.84	0.42
1:B:350:SER:OG	1:B:448:ALA:N	2.52	0.42
1:B:504:LEU:CD1	1:B:509:ILE:HG12	2.49	0.42
1:B:829:ILE:CG2	1:B:830:PRO:HD2	2.48	0.42
1:B:830:PRO:HG3	1:B:1483:PHE:HZ	1.85	0.42
1:A:1019:PHE:CE2	1:A:1020:TYR:CD1	3.08	0.42
1:A:284:GLN:O	1:A:310:LEU:CD1	2.68	0.42
1:A:349:LEU:HD22	1:A:446:ASN:HD22	1.84	0.42
1:A:489:LYS:C	1:A:491:PRO:HD2	2.40	0.42
1:A:502:LEU:HD12	1:A:512:PHE:HB3	2.01	0.42
1:B:1175:LEU:O	1:B:1179:THR:OG1	2.36	0.42
1:B:1199:ASP:C	1:B:1199:ASP:OD1	2.58	0.42
1:B:950:TYR:HE1	1:B:1271:ILE:HD11	1.83	0.42
1:B:159:THR:O	1:B:175:GLU:HA	2.19	0.42
1:B:31:PHE:HZ	1:B:104:LEU:CD2	2.25	0.42
1:B:518:PHE:O	1:B:519:SER:C	2.58	0.42
1:B:738:LEU:O	1:B:742:ILE:HG13	2.19	0.42
1:B:589:SER:HA	1:B:787:GLN:HA	2.00	0.42
1:B:834:VAL:HG11	1:B:1489:SER:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ILE:HD13	2:Y:135:HIS:CD2	2.55	0.42
1:B:84:ILE:HG13	1:B:84:ILE:O	2.19	0.42
1:B:855:PHE:HD1	1:B:856:CYS:N	2.18	0.42
1:B:862:VAL:O	1:B:863:GLU:C	2.58	0.42
2:Y:227:THR:C	2:Y:228:LEU:HD23	2.40	0.42
1:A:1003:LEU:HA	1:A:1004:PRO:HD2	1.49	0.42
1:A:1108:VAL:HG22	1:A:1109:GLU:N	2.35	0.42
1:A:935:LYS:O	1:A:1365:VAL:O	2.36	0.42
1:A:1434:ALA:CB	1:A:1477:PHE:HE1	2.32	0.42
1:A:38:ASN:C	1:A:39:ILE:HD13	2.38	0.42
1:A:503:ILE:HG12	1:A:540:LEU:CB	2.48	0.42
1:A:577:PRO:HD2	1:A:588:VAL:CG2	2.37	0.42
1:A:610:TYR:HB2	1:A:611:GLY:H	1.68	0.42
1:A:626:PHE:O	1:A:628:GLU:N	2.53	0.42
1:B:1083:LEU:O	1:B:1086:LEU:HB2	2.19	0.42
1:B:1159:CYS:N	1:B:1160:PRO:CD	2.82	0.42
1:B:1278:GLN:NE2	1:B:1278:GLN:CA	2.83	0.42
1:B:1429:PRO:O	1:B:1430:THR:C	2.58	0.42
1:B:840:GLN:HB2	1:B:1484:GLU:HB2	2.02	0.42
1:B:166:PRO:HG3	1:B:199:TRP:CD1	2.54	0.42
1:B:137:PRO:HD3	1:B:220:LYS:O	2.19	0.42
1:B:254:TYR:CE2	1:B:260:VAL:HG22	2.53	0.42
1:B:438:ASP:O	1:B:439:ALA:O	2.38	0.42
1:B:617:LYS:O	1:B:618:LYS:CG	2.49	0.42
1:B:982:LEU:C	1:B:984:VAL:H	2.22	0.42
2:X:192:ASN:HD22	2:X:223:LYS:HB2	1.85	0.42
1:A:100:SER:O	1:A:101:TYR:CD2	2.72	0.42
1:A:1022:PHE:O	1:A:1026:GLU:HB3	2.20	0.42
1:A:1024:TYR:HD2	1:A:1025:LEU:N	2.17	0.42
1:A:1161:LEU:CD1	1:A:1162:VAL:HG22	2.46	0.42
1:A:1317:TYR:HB2	1:A:1320:LYS:HB3	2.02	0.42
1:A:136:THR:HA	1:A:220:LYS:O	2.20	0.42
1:A:1496:TYR:CD1	1:A:1496:TYR:C	2.93	0.42
1:A:253:ARG:HG3	1:A:253:ARG:O	2.19	0.42
1:A:292:LEU:HD13	1:A:292:LEU:C	2.39	0.42
1:A:359:THR:HG21	1:A:372:LYS:N	2.23	0.42
1:A:41:ILE:O	1:A:81:ASN:N	2.49	0.42
1:A:497:THR:HG23	1:A:498:HIS:N	2.29	0.42
1:A:515:ARG:HH22	1:A:527:ASN:H	1.68	0.42
1:A:500:ASN:O	1:A:542:VAL:HA	2.20	0.42
1:A:982:LEU:HD11	1:A:1306:GLN:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1012:LEU:C	1:B:1014:SER:H	2.23	0.42
1:B:1379:LEU:HD12	1:B:1507:MET:HE2	2.01	0.42
1:B:1379:LEU:HD21	1:B:1495:VAL:CG1	2.48	0.42
1:B:396:ASP:N	1:B:400:GLU:O	2.50	0.42
1:B:240:TYR:CZ	1:B:443:PRO:HD3	2.53	0.42
1:B:831:TYR:O	1:B:928:ARG:HB2	2.19	0.42
2:Y:192:ASN:HB2	2:Y:223:LYS:O	2.20	0.42
2:Y:217:ASN:HB2	2:Y:220:ASP:OD2	2.19	0.42
1:A:1069:TRP:NE1	1:A:1463:GLN:NE2	2.68	0.42
1:A:159:THR:HG22	1:A:160:VAL:H	1.84	0.42
1:A:284:GLN:HG2	1:A:310:LEU:HD13	2.02	0.42
1:A:350:SER:HA	1:A:351:PRO:HD3	1.74	0.42
1:A:497:THR:OG1	1:A:498:HIS:ND1	2.52	0.42
1:A:592:MET:HG2	1:A:600:VAL:HG21	2.01	0.42
1:A:855:PHE:CD1	1:A:856:CYS:N	2.87	0.42
1:A:902:PRO:O	1:A:903:LEU:HD13	2.20	0.42
1:A:907:LEU:HD12	1:A:908:HIS:N	2.34	0.42
1:B:1148:THR:OG1	1:B:1152:ILE:HD11	2.19	0.42
1:B:125:PHE:N	1:B:125:PHE:CD1	2.87	0.42
1:B:1307:LEU:HD13	1:B:1356:LEU:HD12	2.02	0.42
1:B:1408:TYR:O	1:B:1410:PRO:HD3	2.20	0.42
1:B:23:TYR:OH	1:B:656:ASN:HB2	2.20	0.42
1:B:415:ASP:OD1	1:B:417:VAL:CG2	2.67	0.42
1:B:369:TYR:HE2	1:B:433:PHE:HE1	1.66	0.42
1:B:531:THR:CG2	1:B:533:ASN:HB2	2.49	0.42
1:B:61:ASP:C	1:B:63:LYS:H	2.21	0.42
1:A:1054:LEU:C	1:A:1056:ILE:N	2.71	0.42
1:A:1227:PHE:HB2	1:A:1251:THR:HG21	2.02	0.42
1:A:191:PRO:O	1:A:194:PRO:HD3	2.20	0.42
1:A:216:TYR:O	1:A:217:PHE:HB3	2.19	0.42
1:A:337:SER:HB3	1:A:1437:GLU:CD	2.40	0.42
1:A:616:ALA:O	1:A:617:LYS:C	2.57	0.42
1:B:1307:LEU:CD1	1:B:1356:LEU:HD12	2.49	0.42
1:B:157:ARG:CZ	1:B:209:PHE:CE1	3.03	0.42
1:B:331:GLU:OE1	1:B:336:PHE:HD1	2.02	0.42
1:B:42:GLN:CG	1:B:80:GLN:NE2	2.81	0.42
1:B:504:LEU:HD12	1:B:509:ILE:HG23	2.02	0.42
1:B:576:SER:CB	1:B:577:PRO:CD	2.97	0.42
1:A:1113:LEU:C	1:A:1115:ASN:H	2.23	0.41
1:A:140:SER:OG	1:A:187:ASP:HB3	2.20	0.41
1:A:1435:ASN:O	1:A:1436:GLU:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLY:N	1:A:283:MET:CE	2.83	0.41
1:A:356:LEU:CD1	1:A:452:TYR:CD1	3.03	0.41
1:A:665:ASN:CG	1:A:666:ASP:H	2.23	0.41
1:A:667:GLU:N	1:A:667:GLU:OE1	2.53	0.41
1:A:839:ILE:HG13	1:A:840:GLN:N	2.35	0.41
1:A:967:LEU:HD12	1:A:968:VAL:N	2.34	0.41
1:A:976:ILE:O	1:A:1361:VAL:HA	2.20	0.41
1:B:110:HIS:O	1:B:110:HIS:CD2	2.73	0.41
1:B:1117:SER:HA	1:B:1145:THR:CG2	2.48	0.41
1:B:1176:LEU:H	1:B:1176:LEU:HG	1.39	0.41
1:B:1180:LEU:HD11	1:B:1207:SER:HB3	2.02	0.41
1:B:123:ASN:ND2	1:B:123:ASN:C	2.70	0.41
1:B:123:ASN:C	1:B:211:THR:HG21	2.40	0.41
1:B:396:ASP:HB3	1:B:398:ASN:N	2.35	0.41
1:B:440:PRO:CD	1:B:441:ASP:H	2.33	0.41
1:B:972:GLU:HG2	1:B:972:GLU:H	1.51	0.41
2:X:164:GLU:O	2:X:168:LYS:HG3	2.20	0.41
2:X:179:LEU:HD11	2:X:185:LYS:HA	2.03	0.41
1:A:1019:PHE:CD2	1:A:1020:TYR:CE1	3.08	0.41
1:A:1096:ASN:ND2	1:A:1099:SER:H	2.19	0.41
1:A:1112:GLN:HG3	1:A:1118:PHE:CE1	2.55	0.41
1:A:719:SER:CB	1:A:1123:GLN:HE21	2.33	0.41
1:A:1227:PHE:CA	1:A:1228:TRP:CE3	3.03	0.41
1:A:173:MET:C	1:A:174:VAL:HG12	2.41	0.41
1:A:415:ASP:OD1	1:A:417:VAL:CG2	2.68	0.41
1:A:617:LYS:O	1:A:618:LYS:CG	2.46	0.41
1:A:824:PHE:CE1	1:A:846:TYR:CD1	2.93	0.41
1:A:862:VAL:O	1:A:863:GLU:C	2.57	0.41
1:A:980:LYS:HB3	1:A:980:LYS:HE3	1.78	0.41
1:B:1037:ASP:HA	1:B:1038:PRO:HD3	1.74	0.41
1:B:1162:VAL:O	1:B:1165:ASP:N	2.52	0.41
1:B:1324:HIS:CE1	1:B:1326:TYR:CE2	3.07	0.41
1:B:1435:ASN:HB2	1:B:1478:ARG:O	2.20	0.41
1:B:357:VAL:O	1:B:359:THR:HG23	2.19	0.41
1:B:405:ASP:HA	1:B:406:PRO:HD3	1.60	0.41
1:B:468:ASP:O	1:B:484:ILE:HG13	2.19	0.41
1:B:604:ALA:O	1:B:772:SER:HB3	2.21	0.41
1:B:610:TYR:HB2	1:B:611:GLY:H	1.67	0.41
1:B:695:VAL:HA	1:B:698:CYS:HB2	2.02	0.41
1:B:889:GLU:H	1:B:889:GLU:CD	2.24	0.41
1:B:930:VAL:HG12	1:B:931:PRO:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:947:ARG:C	1:B:949:ILE:N	2.70	0.41
2:Y:179:LEU:HD11	2:Y:185:LYS:HA	2.02	0.41
1:A:1180:LEU:HD11	1:A:1208:ILE:N	2.35	0.41
1:A:33:VAL:HG23	1:A:120:THR:O	2.20	0.41
1:A:1440:LYS:HD3	1:A:1453:TYR:CZ	2.56	0.41
1:A:185:PHE:HB3	1:A:186:PRO:HD3	2.00	0.41
1:A:295:GLY:C	1:A:296:ILE:CG1	2.88	0.41
1:A:504:LEU:HD12	1:A:509:ILE:HA	2.01	0.41
1:A:66:TYR:CE1	1:A:90:LYS:CG	2.97	0.41
1:B:984:VAL:CG1	1:B:1024:TYR:CE1	2.92	0.41
1:B:1081:PHE:CD2	1:B:1081:PHE:C	2.93	0.41
1:B:1175:LEU:HA	1:B:1175:LEU:HD23	1.69	0.41
1:B:369:TYR:HA	1:B:370:PRO:HD3	1.66	0.41
1:B:387:PRO:C	1:B:388:VAL:HG23	2.41	0.41
1:B:743:SER:OG	1:B:752:LEU:HD22	2.20	0.41
2:X:224:ILE:C	2:X:225:GLU:HG3	2.41	0.41
1:A:120:THR:CG2	1:A:121:TYR:N	2.59	0.41
1:A:292:LEU:HD22	1:A:296:ILE:O	2.21	0.41
1:A:420:PHE:O	1:A:421:VAL:HG23	2.20	0.41
1:A:653:PHE:CZ	1:A:660:ASP:CA	2.92	0.41
1:B:1030:HIS:O	1:B:1033:ILE:CG1	2.64	0.41
1:B:1132:THR:N	1:B:1135:VAL:HB	2.35	0.41
1:B:1152:ILE:O	1:B:1153:ARG:C	2.58	0.41
1:B:1401:ARG:HB2	1:B:1478:ARG:CB	2.50	0.41
1:B:1378:TYR:CE1	1:B:1409:LYS:HE3	2.55	0.41
1:B:1429:PRO:HG2	1:B:1511:THR:CB	2.44	0.41
1:B:171:VAL:O	1:B:171:VAL:HG12	2.19	0.41
1:B:262:GLU:HG2	1:B:332:SER:HB2	2.03	0.41
1:B:244:LYS:HA	1:B:302:ASP:OD2	2.20	0.41
1:B:700:TYR:CE1	1:B:758:LEU:CB	3.02	0.41
1:B:841:LEU:HD12	1:B:859:MET:CE	2.42	0.41
1:B:93:PRO:HG2	1:B:96:GLN:OE1	2.21	0.41
2:Y:194:LYS:HA	2:Y:194:LYS:HD2	1.84	0.41
1:A:1401:ARG:HB2	1:A:1478:ARG:CG	2.48	0.41
1:A:262:GLU:HG2	1:A:332:SER:HB2	2.02	0.41
1:A:44:TYR:OH	1:A:497:THR:HB	2.21	0.41
1:A:935:LYS:HD2	1:A:935:LYS:HA	1.83	0.41
1:B:936:ARG:CZ	1:B:1002:HIS:HE1	2.34	0.41
1:B:1191:SER:O	1:B:1195:LEU:HG	2.20	0.41
1:B:244:LYS:HE3	1:B:304:GLU:OE2	2.21	0.41
1:B:461:SER:C	1:B:463:SER:H	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:PHE:HE1	1:B:638:GLY:O	2.04	0.41
1:B:903:LEU:N	1:B:903:LEU:HD13	2.35	0.41
2:X:199:GLN:C	2:X:200:GLU:HG3	2.40	0.41
1:A:1076:THR:HG22	1:A:1120:GLU:CD	2.41	0.41
1:A:1148:THR:O	1:A:1152:ILE:CD1	2.69	0.41
1:A:1279:ARG:HE	1:A:1279:ARG:HB3	1.65	0.41
1:A:1244:THR:O	1:A:1285:TYR:CD2	2.73	0.41
1:A:30:ILE:HG22	1:A:31:PHE:O	2.20	0.41
1:A:337:SER:HB3	1:A:1437:GLU:OE2	2.21	0.41
1:A:700:TYR:O	1:A:702:GLY:N	2.53	0.41
1:A:256:TYR:HB2	1:A:895:LEU:HD12	2.02	0.41
1:B:1000:LEU:HD23	1:B:1000:LEU:HA	1.87	0.41
1:B:1227:PHE:HA	1:B:1228:TRP:CE3	2.55	0.41
1:B:1278:GLN:CA	1:B:1278:GLN:HE21	2.33	0.41
1:B:938:SER:HB3	1:B:1362:THR:HA	2.03	0.41
1:B:185:PHE:HB3	1:B:186:PRO:HD3	2.02	0.41
1:B:388:VAL:HG12	1:B:420:PHE:HZ	1.85	0.41
1:B:436:LYS:HD2	1:B:437:THR:O	2.20	0.41
1:B:752:LEU:C	1:B:753:HIS:CG	2.93	0.41
2:Y:184:THR:O	2:Y:185:LYS:HB3	2.20	0.41
2:Y:186:TYR:HD2	2:Y:229:LYS:HD3	1.80	0.41
1:A:1144:LEU:O	1:A:1148:THR:CG2	2.67	0.41
1:A:1153:ARG:O	1:A:1155:ALA:N	2.53	0.41
1:A:1427:SER:HB3	1:A:1492:THR:N	2.29	0.41
1:A:1440:LYS:O	1:A:1444:GLU:CB	2.68	0.41
1:A:1456:LYS:O	1:A:1459:HIS:N	2.46	0.41
1:A:150:ASP:O	1:A:152:LEU:HD22	2.20	0.41
1:A:166:PRO:HG3	1:A:199:TRP:CD1	2.56	0.41
1:A:545:ILE:HG12	1:A:554:LEU:HD21	2.03	0.41
1:A:644:ASN:C	1:A:644:ASN:ND2	2.74	0.41
1:A:798:GLU:O	1:A:798:GLU:HG2	2.19	0.41
1:B:1005:LYS:HE3	1:B:1005:LYS:HB3	1.86	0.41
1:B:1148:THR:O	1:B:1152:ILE:CG1	2.67	0.41
1:B:1100:ILE:HG13	1:B:1158:ILE:HD12	2.03	0.41
1:B:1162:VAL:O	1:B:1164:ILE:N	2.53	0.41
1:B:1342:LEU:HD23	1:B:1342:LEU:H	1.85	0.41
1:B:1364:VAL:HG12	1:B:1365:VAL:N	2.35	0.41
1:B:1488:LEU:HD12	1:B:1488:LEU:C	2.40	0.41
1:B:165:ASP:HA	1:B:166:PRO:HD3	1.82	0.41
1:B:169:SER:C	1:B:170:GLU:O	2.57	0.41
1:B:35:ALA:O	1:B:37:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:VAL:HG12	1:B:420:PHE:CZ	2.56	0.41
1:B:431:LEU:HD13	1:B:433:PHE:CD1	2.56	0.41
1:B:477:LEU:HA	1:B:564:GLU:CG	2.51	0.41
1:B:502:LEU:HA	1:B:502:LEU:HD12	1.77	0.41
1:B:560:TRP:CH2	1:B:562:ASN:CB	2.97	0.41
1:B:719:SER:HB2	1:B:1123:GLN:HE21	1.85	0.41
1:B:729:THR:O	1:B:733:VAL:HG23	2.20	0.41
1:A:107:VAL:HG12	1:A:108:SER:N	2.36	0.41
1:A:1096:ASN:HD22	1:A:1099:SER:H	1.69	0.41
1:A:102:VAL:HG13	1:A:119:ILE:HG21	2.03	0.41
1:A:149:ASN:HB2	1:A:150:ASP:OD2	2.21	0.41
1:A:237:PHE:O	1:A:238:ILE:CG1	2.69	0.41
1:A:35:ALA:HA	1:A:150:ASP:OD1	2.21	0.41
1:A:43:VAL:HG22	1:A:44:TYR:N	2.36	0.41
1:A:553:GLU:OE1	1:A:555:VAL:HG23	2.21	0.41
1:A:56:ILE:CD1	1:A:66:TYR:HB2	2.51	0.41
1:A:703:ALA:CB	1:A:732:CYS:HA	2.51	0.41
1:A:840:GLN:HB3	1:A:840:GLN:HE21	1.75	0.41
1:A:897:THR:C	1:A:898:PHE:CD2	2.94	0.41
1:B:1076:THR:HG22	1:B:1120:GLU:CD	2.41	0.41
1:B:1176:LEU:O	1:B:1178:ASN:N	2.54	0.41
1:B:1324:HIS:HE1	1:B:1326:TYR:CE2	2.39	0.41
1:B:1405:CYS:N	1:B:1474:CYS:SG	2.87	0.41
1:B:162:THR:OG1	1:B:162:THR:O	2.32	0.41
1:B:56:ILE:O	1:B:66:TYR:CD2	2.74	0.41
1:A:1117:SER:HA	1:A:1145:THR:HG21	2.02	0.41
1:A:1173:ASN:O	1:A:1174:PHE:C	2.59	0.41
1:A:1212:LEU:O	1:A:1215:GLU:N	2.53	0.41
1:A:987:ILE:CG1	1:A:1294:ILE:HD12	2.51	0.41
1:A:1497:GLU:O	1:A:1498:TYR:C	2.58	0.41
1:A:324:TYR:OH	1:A:326:ALA:HB2	2.20	0.41
1:A:438:ASP:C	1:A:439:ALA:O	2.58	0.41
1:A:54:ILE:O	1:A:55:SER:HB3	2.21	0.41
1:A:654:LEU:HD12	1:A:654:LEU:HA	1.57	0.41
1:A:944:LEU:HD23	1:A:944:LEU:HA	1.77	0.41
1:A:946:PRO:CD	1:A:947:ARG:H	2.30	0.41
1:B:193:ASN:OD1	1:B:1070:LYS:CE	2.69	0.41
1:B:1284:PHE:CD2	1:B:1285:TYR:CD1	3.08	0.41
1:B:1443:VAL:CG2	1:B:1444:GLU:N	2.84	0.41
1:B:1489:SER:HA	1:B:1490:PRO:HD3	1.95	0.41
1:B:257:ASN:O	1:B:257:ASN:CG	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:GLN:CD	1:B:310:LEU:HD22	2.41	0.41
1:B:760:VAL:O	1:B:761:SER:HB3	2.21	0.41
1:B:589:SER:CB	1:B:785:GLN:HE21	2.33	0.41
1:B:80:GLN:HB3	1:B:512:PHE:HE1	1.84	0.41
1:B:909:ASN:H	1:B:926:THR:HA	1.86	0.41
2:X:217:ASN:HB2	2:X:220:ASP:CG	2.41	0.41
1:A:1040:ILE:HD13	1:A:1040:ILE:HA	1.86	0.41
1:A:50:PHE:CB	1:A:109:LYS:HE2	2.51	0.41
1:A:1127:ILE:HD12	1:A:1127:ILE:O	2.21	0.41
1:A:1166:THR:HG22	1:A:1167:ALA:N	2.35	0.41
1:A:1290:THR:O	1:A:1294:ILE:CG1	2.67	0.41
1:A:144:ARG:HG2	1:A:775:TRP:HZ2	1.84	0.41
1:A:149:ASN:O	1:A:150:ASP:C	2.58	0.41
1:A:33:VAL:HB	1:A:209:PHE:HE2	1.86	0.41
1:A:431:LEU:O	1:A:453:ARG:HA	2.21	0.41
1:A:614:ARG:O	1:A:615:GLY:C	2.59	0.41
1:B:1023:HIS:HA	1:B:1092:TYR:OH	2.21	0.41
1:B:1193:TYR:CZ	1:B:1256:LEU:HD13	2.55	0.41
1:B:313:TYR:CE2	1:B:321:LYS:HD2	2.56	0.41
1:B:350:SER:HA	1:B:351:PRO:HD3	1.74	0.41
1:B:504:LEU:HA	1:B:509:ILE:HA	2.03	0.41
1:B:515:ARG:NH1	1:B:526:ILE:HA	2.36	0.41
1:B:599:TRP:CZ3	1:B:779:LEU:HB2	2.56	0.41
1:B:587:THR:HA	1:B:789:ALA:HA	2.03	0.41
1:B:838:GLN:HB3	1:B:1486:GLY:CA	2.50	0.41
1:B:855:PHE:CD2	1:B:888:VAL:HG13	2.56	0.41
1:B:897:THR:O	1:B:898:PHE:CD2	2.74	0.41
2:Y:158:GLU:HA	2:Y:219:LYS:HZ1	1.85	0.41
2:Y:162:LEU:HA	2:Y:165:LEU:CB	2.50	0.41
1:A:1069:TRP:HE1	1:A:1463:GLN:HE21	1.67	0.41
1:A:1500:ARG:HA	1:A:1501:PRO:HD2	1.95	0.41
1:A:27:ALA:HB1	1:A:28:PRO:HD2	2.03	0.41
1:A:308:LYS:HB2	1:A:308:LYS:HE3	1.83	0.41
1:A:355:ASN:O	1:A:356:LEU:C	2.58	0.41
1:A:387:PRO:C	1:A:388:VAL:HG23	2.41	0.41
1:A:440:PRO:CD	1:A:441:ASP:H	2.33	0.41
1:A:709:GLU:CA	1:A:713:GLN:OE1	2.69	0.41
1:A:620:LEU:CD1	1:A:811:VAL:H	2.31	0.41
1:A:886:GLN:HG3	1:A:887:LYS:H	1.86	0.41
1:B:1020:TYR:CZ	1:B:1295:GLU:HB2	2.56	0.41
1:B:935:LYS:O	1:B:1365:VAL:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1475:VAL:CG2	1:B:1476:ARG:N	2.84	0.41
1:B:837:GLU:CG	1:B:1488:LEU:HA	2.46	0.41
1:B:23:TYR:HA	1:B:43:VAL:HG23	2.01	0.41
1:B:325:ILE:HD13	1:B:325:ILE:HG21	1.81	0.41
1:B:356:LEU:HD12	1:B:452:TYR:CD1	2.55	0.41
1:B:409:SER:OG	1:B:410:VAL:N	2.53	0.41
1:B:412:ARG:HD3	1:B:414:ASP:OD2	2.20	0.41
1:B:240:TYR:CE1	1:B:443:PRO:CG	3.04	0.41
1:B:614:ARG:O	1:B:615:GLY:C	2.59	0.41
1:B:639:GLY:N	1:B:645:VAL:HA	2.36	0.41
1:B:765:ILE:HD11	1:B:769:PHE:HE2	1.84	0.41
1:B:978:SER:HB2	1:B:1280:TYR:CD2	2.56	0.41
2:X:143:GLY:C	2:X:145:ASN:N	2.66	0.41
2:X:186:TYR:HD2	2:X:229:LYS:HB3	1.86	0.41
1:A:1008:ALA:O	1:A:1011:GLU:N	2.54	0.40
1:A:1202:HIS:HD2	1:A:1204:GLN:N	2.12	0.40
1:A:1443:VAL:CG2	1:A:1444:GLU:N	2.82	0.40
1:A:157:ARG:O	1:A:178:ASP:CB	2.66	0.40
1:A:141:VAL:CG2	1:A:190:ILE:HD11	2.51	0.40
1:A:394:THR:HG21	1:A:428:VAL:HG23	2.02	0.40
1:A:465:LEU:HD13	1:A:544:TYR:CD1	2.57	0.40
1:A:518:PHE:O	1:A:519:SER:C	2.60	0.40
1:A:689:LYS:HB3	1:A:689:LYS:HE2	1.81	0.40
1:A:722:PRO:HA	1:A:725:ILE:HG13	2.03	0.40
1:A:903:LEU:HD13	1:A:903:LEU:N	2.34	0.40
1:B:1061:ASN:HB3	1:B:1062:ALA:H	1.62	0.40
1:B:1077:TRP:HB2	1:B:1120:GLU:OE1	2.21	0.40
1:B:1084:ARG:HB2	1:B:1151:GLY:HA2	2.02	0.40
1:B:1232:LEU:HG	1:B:1232:LEU:O	2.21	0.40
1:B:1278:GLN:N	1:B:1278:GLN:HE21	2.19	0.40
1:B:1259:LEU:HD13	1:B:1300:TYR:HB2	2.02	0.40
1:B:1280:TYR:OH	1:B:1337:PRO:CG	2.69	0.40
1:B:136:THR:HA	1:B:220:LYS:O	2.22	0.40
1:B:305:THR:HB	1:B:306:ALA:H	1.73	0.40
1:B:308:LYS:HA	1:B:313:TYR:O	2.20	0.40
1:B:254:TYR:OH	1:B:331:GLU:HG3	2.22	0.40
1:B:348:VAL:HG12	1:B:350:SER:N	2.36	0.40
1:B:512:PHE:CE2	2:Y:148:ALA:HB3	2.56	0.40
1:B:478:VAL:HG12	1:B:564:GLU:OE1	2.20	0.40
1:B:768:TYR:HE2	1:B:770:PRO:HA	1.83	0.40
1:B:912:PHE:O	1:B:922:ILE:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:179:LEU:HA	2:X:184:THR:HB	2.03	0.40
2:X:186:TYR:O	2:X:229:LYS:HB3	2.21	0.40
1:A:1022:PHE:HE2	1:A:1092:TYR:CD1	2.39	0.40
1:A:1193:TYR:CE2	1:A:1197:LEU:HD11	2.56	0.40
1:A:1464:LEU:HD12	1:A:1464:LEU:N	2.36	0.40
1:A:227:PHE:CZ	1:A:338:GLU:HB2	2.57	0.40
1:A:424:LEU:HA	1:A:424:LEU:HD23	1.73	0.40
1:A:495:LYS:HA	1:A:495:LYS:CE	2.51	0.40
1:A:541:LEU:HG	1:A:556:SER:OG	2.21	0.40
1:A:914:LEU:HD12	1:A:914:LEU:O	2.22	0.40
1:B:1255:LEU:HB2	1:B:1270:VAL:CG1	2.44	0.40
1:B:170:GLU:O	1:B:171:VAL:CG2	2.68	0.40
1:B:189:LYS:HG3	1:B:190:ILE:N	2.33	0.40
1:B:576:SER:OG	1:B:589:SER:CB	2.58	0.40
1:B:144:ARG:NH2	1:B:602:LEU:O	2.50	0.40
1:B:942:VAL:HG22	1:B:957:LYS:CD	2.50	0.40
1:A:1153:ARG:O	1:A:1156:PHE:N	2.46	0.40
1:A:1143:TYR:CE1	1:A:1186:PHE:CZ	3.07	0.40
1:A:1186:PHE:HD1	1:A:1250:THR:CG2	2.28	0.40
1:A:1200:LYS:H	1:A:1200:LYS:HG2	1.39	0.40
1:A:1303:LEU:C	1:A:1303:LEU:HD13	2.41	0.40
1:A:960:PRO:HB3	1:A:1345:ASP:OD1	2.22	0.40
1:A:1446:VAL:O	1:A:1446:VAL:HG12	2.20	0.40
1:A:816:LYS:O	1:A:817:ALA:HB2	2.22	0.40
1:A:832:SER:HB2	1:A:930:VAL:CG2	2.50	0.40
1:A:963:ILE:HA	1:A:964:PRO:HD3	1.94	0.40
1:A:991:VAL:CG1	1:A:991:VAL:O	2.69	0.40
1:B:1042:LYS:HG2	1:B:1046:LYS:HE3	2.03	0.40
1:B:115:LYS:HG3	1:B:116:ARG:H	1.79	0.40
1:B:1180:LEU:HD11	1:B:1208:ILE:N	2.36	0.40
1:B:1295:GLU:O	1:B:1296:GLY:O	2.40	0.40
1:B:936:ARG:HB3	1:B:1364:VAL:HG22	2.01	0.40
1:B:23:TYR:N	1:B:23:TYR:CD1	2.88	0.40
1:B:457:TYR:HD2	1:B:458:SER:O	2.05	0.40
1:B:486:VAL:HG21	1:B:526:ILE:CD1	2.52	0.40
1:B:360:PRO:CA	1:B:636:ALA:HB3	2.45	0.40
1:B:896:VAL:HG12	1:B:897:THR:H	1.86	0.40
1:B:907:LEU:HD12	1:B:908:HIS:N	2.37	0.40
1:B:940:SER:HB2	1:B:959:PHE:CE1	2.49	0.40
2:Y:193:LEU:CD2	2:Y:221:ILE:HG12	2.51	0.40
1:A:1204:GLN:O	1:A:1208:ILE:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1280:TYR:CD2	1:A:1281:GLY:N	2.89	0.40
1:A:1295:GLU:O	1:A:1299:GLU:HB2	2.20	0.40
1:A:1323:LEU:CG	1:A:1324:HIS:N	2.84	0.40
1:A:1368:THR:O	1:A:1508:PHE:CE2	2.71	0.40
1:A:1401:ARG:HG3	1:A:1478:ARG:HG2	2.03	0.40
1:A:224:LEU:HD13	1:A:225:PRO:CD	2.52	0.40
1:A:254:TYR:CE2	1:A:260:VAL:HG22	2.57	0.40
1:A:310:LEU:HD23	1:A:310:LEU:N	2.37	0.40
1:A:357:VAL:O	1:A:358:ALA:C	2.59	0.40
1:A:404:LEU:HB3	1:A:405:ASP:H	1.76	0.40
1:A:610:TYR:HB3	1:A:614:ARG:HD2	2.00	0.40
1:A:77:ASN:HD21	1:A:81:ASN:ND2	2.19	0.40
1:A:987:ILE:HG22	1:A:1021:VAL:CG2	2.52	0.40
1:B:1019:PHE:CE2	1:B:1020:TYR:CD1	3.08	0.40
1:B:1062:ALA:C	1:B:1064:TYR:H	2.23	0.40
1:B:1104:LEU:O	1:B:1108:VAL:HG12	2.21	0.40
1:B:1280:TYR:HD1	1:B:1362:THR:HG22	1.86	0.40
1:B:1446:VAL:HG12	1:B:1446:VAL:O	2.22	0.40
1:B:545:ILE:HG12	1:B:554:LEU:HD21	2.02	0.40
1:B:132:LYS:HB2	1:B:609:VAL:HG11	2.02	0.40
1:B:721:GLY:HA2	1:B:722:PRO:HD3	1.97	0.40
1:B:946:PRO:CD	1:B:947:ARG:H	2.35	0.40
1:A:1037:ASP:OD1	1:A:1038:PRO:N	2.54	0.40
1:A:981:GLY:CA	1:A:1309:LEU:HD11	2.47	0.40
1:A:1454:GLN:HG3	1:A:1454:GLN:O	2.22	0.40
1:A:1461:ILE:HG22	1:A:1461:ILE:O	2.22	0.40
1:A:342:ILE:O	1:A:343:PRO:C	2.60	0.40
1:A:357:VAL:CG2	1:A:374:GLN:HB3	2.52	0.40
1:A:758:LEU:C	1:A:760:VAL:N	2.73	0.40
1:B:1161:LEU:HD12	1:B:1162:VAL:CG2	2.52	0.40
1:B:1271:ILE:CD1	1:B:1271:ILE:C	2.86	0.40
1:B:1364:VAL:CG1	1:B:1365:VAL:N	2.84	0.40
1:B:148:LEU:HD12	1:B:148:LEU:HA	1.77	0.40
1:B:309:GLU:HG3	1:B:309:GLU:O	2.22	0.40
1:B:424:LEU:HA	1:B:424:LEU:HD23	1.88	0.40
1:B:576:SER:HB2	1:B:577:PRO:HD3	2.03	0.40
1:B:682:LYS:HD2	1:B:682:LYS:O	2.22	0.40
1:B:987:ILE:O	1:B:1021:VAL:HG21	2.21	0.40
2:Y:219:LYS:CD	2:Y:219:LYS:N	2.73	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	1449/1676 (86%)	1039 (72%)	255 (18%)	155 (11%)	0	10
1	B	1449/1676 (86%)	1026 (71%)	274 (19%)	149 (10%)	0	11
2	X	100/103 (97%)	86 (86%)	9 (9%)	5 (5%)	2	28
2	Y	100/103 (97%)	84 (84%)	11 (11%)	5 (5%)	2	28
All	All	3098/3558 (87%)	2235 (72%)	549 (18%)	314 (10%)	1	12

All (314) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	TYR
1	A	86	THR
1	A	97	ASN
1	A	99	VAL
1	A	170	GLU
1	A	174	VAL
1	A	207	GLU
1	A	209	PHE
1	A	282	MET
1	A	289	ASN
1	A	291	MET
1	A	305	THR
1	A	316	GLU
1	A	317	ASP
1	A	318	LEU
1	A	426	SER
1	A	457	TYR
1	A	477	LEU
1	A	480	GLU
1	A	489	LYS
1	A	490	SER
1	A	519	SER

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Mol	Chain	Res	Type
1	A	520	ASP
1	A	522	SER
1	A	609	VAL
1	A	610	TYR
1	A	638	GLY
1	A	657	ALA
1	A	662	SER
1	A	700	TYR
1	A	704	CYS
1	A	720	LEU
1	A	863	GLU
1	A	1231	ASN
1	A	1264	ILE
1	A	1275	SER
1	A	1284	PHE
1	A	1286	SER
1	A	1297	LEU
1	A	1304	VAL
1	A	1311	MET
1	A	1335	GLY
1	A	1342	LEU
1	A	1373	GLU
1	A	1433	SER
2	X	185	LYS
1	B	59	TYR
1	B	97	ASN
1	B	99	VAL
1	B	133	PRO
1	B	174	VAL
1	B	207	GLU
1	B	209	PHE
1	B	282	MET
1	B	289	ASN
1	B	305	THR
1	B	426	SER
1	B	457	TYR
1	B	490	SER
1	B	520	ASP
1	B	522	SER
1	B	609	VAL
1	B	610	TYR
1	B	638	GLY

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Mol	Chain	Res	Type
1	B	657	ALA
1	B	661	ASP
1	B	700	TYR
1	B	704	CYS
1	B	720	LEU
1	B	863	GLU
1	B	949	ILE
1	B	1068	VAL
1	B	1097	GLN
1	B	1231	ASN
1	B	1264	ILE
1	B	1284	PHE
1	B	1311	MET
1	B	1335	GLY
1	B	1342	LEU
1	B	1373	GLU
1	B	1433	SER
2	Y	185	LYS
1	A	90	LYS
1	A	101	TYR
1	A	150	ASP
1	A	302	ASP
1	A	304	GLU
1	A	306	ALA
1	A	307	VAL
1	A	308	LYS
1	A	523	TYR
1	A	615	GLY
1	A	619	PRO
1	A	661	ASP
1	A	669	CYS
1	A	705	VAL
1	A	814	THR
1	A	817	ALA
1	A	909	ASN
1	A	931	PRO
1	A	996	GLY
1	A	1007	SER
1	A	1029	ASN
1	A	1055	SER
1	A	1097	GLN
1	A	1166	THR

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Mol	Chain	Res	Type
1	A	1216	ALA
1	A	1296	GLY
1	A	1312	ASP
1	A	1321	GLY
1	A	1352	PHE
1	A	1457	ASP
1	A	1486	GLY
2	X	144	GLY
1	B	28	PRO
1	B	86	THR
1	B	90	LYS
1	B	101	TYR
1	B	170	GLU
1	B	291	MET
1	B	302	ASP
1	B	304	GLU
1	B	307	VAL
1	B	308	LYS
1	B	378	SER
1	B	388	VAL
1	B	480	GLU
1	B	489	LYS
1	B	495	LYS
1	B	607	SER
1	B	612	VAL
1	B	619	PRO
1	B	662	SER
1	B	669	CYS
1	B	710	THR
1	B	814	THR
1	B	817	ALA
1	B	909	ASN
1	B	931	PRO
1	B	948	GLY
1	B	996	GLY
1	B	1029	ASN
1	B	1098	ASN
1	B	1162	VAL
1	B	1177	GLU
1	B	1216	ALA
1	B	1286	SER
1	B	1296	GLY

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Mol	Chain	Res	Type
1	B	1297	LEU
1	B	1304	VAL
1	B	1310	SER
2	Y	144	GLY
2	Y	195	ASP
1	A	85	LEU
1	A	133	PRO
1	A	173	MET
1	A	231	ILE
1	A	272	ARG
1	A	356	LEU
1	A	388	VAL
1	A	491	PRO
1	A	612	VAL
1	A	625	GLN
1	A	648	LEU
1	A	660	ASP
1	A	663	GLN
1	A	691	LYS
1	A	793	SER
1	A	1240	PRO
1	A	1247	MET
1	A	1263	ASP
1	A	1308	ARG
1	A	1310	SER
2	X	195	ASP
1	B	36	SER
1	B	150	ASP
1	B	186	PRO
1	B	240	TYR
1	B	306	ALA
1	B	356	LEU
1	B	445	GLU
1	B	491	PRO
1	B	519	SER
1	B	617	LYS
1	B	627	LEU
1	B	660	ASP
1	B	663	GLN
1	B	666	ASP
1	B	691	LYS
1	B	793	SER

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Mol	Chain	Res	Type
1	B	856	CYS
1	B	1105	LEU
1	B	1240	PRO
1	B	1269	PRO
1	B	1280	TYR
1	B	1308	ARG
1	B	1312	ASP
1	B	1341	LEU
1	B	1352	PHE
1	B	1457	ASP
1	A	62	LYS
1	A	129	HIS
1	A	141	VAL
1	A	166	PRO
1	A	186	PRO
1	A	425	PRO
1	A	492	TYR
1	A	495	LYS
1	A	607	SER
1	A	627	LEU
1	A	717	ARG
1	A	815	VAL
1	A	856	CYS
1	A	993	SER
1	A	1016	VAL
1	A	1101	CYS
1	A	1113	LEU
1	A	1114	ASP
1	A	1153	ARG
1	A	1177	GLU
1	A	1280	TYR
1	A	1341	LEU
1	A	1349	SER
1	A	1444	GLU
1	A	1468	PRO
1	B	62	LYS
1	B	166	PRO
1	B	173	MET
1	B	398	ASN
1	B	425	PRO
1	B	492	TYR
1	B	625	GLN

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Mol	Chain	Res	Type
1	B	759	PRO
1	B	952	THR
1	B	982	LEU
1	B	1007	SER
1	B	1055	SER
1	B	1057	MET
1	B	1084	ARG
1	B	1153	ARG
1	B	1444	GLU
1	A	497	THR
1	A	536	PRO
1	A	666	ASP
1	A	710	THR
1	A	759	PRO
1	A	892	SER
1	A	969	PRO
1	A	1122	SER
1	A	1481	GLU
1	A	1501	PRO
1	B	78	LYS
1	B	85	LEU
1	B	312	TYR
1	B	320	ASN
1	B	536	PRO
1	B	664	GLU
1	B	667	GLU
1	B	892	SER
1	B	993	SER
1	B	1126	PRO
1	B	1218	VAL
1	B	1239	VAL
1	B	1468	PRO
1	B	1501	PRO
1	A	299	VAL
1	A	617	LYS
1	A	667	GLU
1	A	760	VAL
1	A	1036	SER
1	A	1126	PRO
1	A	1181	PRO
1	A	1432	ILE
1	B	111	PHE

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Mol	Chain	Res	Type
1	B	343	PRO
1	B	565	GLU
1	B	760	VAL
1	B	815	VAL
1	B	1009	GLU
1	B	1263	ASP
1	B	1486	GLY
1	A	686	ILE
1	A	1269	PRO
2	X	178	GLY
1	A	1108	VAL
2	X	196	GLY
1	B	705	VAL
1	B	1016	VAL
1	B	1268	ASN
1	B	1347	ILE
2	Y	196	GLY
1	A	92	LEU
1	A	765	ILE
1	A	1135	VAL
1	A	1218	VAL
1	A	1239	VAL
1	B	92	LEU
1	B	231	ILE
1	B	615	GLY
1	B	1038	PRO
1	B	1432	ILE
1	A	28	PRO
1	A	296	ILE
1	A	510	ILE
1	A	1162	VAL
1	B	171	VAL
1	B	345	ILE
1	B	686	ILE
2	Y	178	GLY
1	A	238	ILE
1	A	668	PRO
1	A	1038	PRO
1	A	1068	VAL
1	B	668	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1296/1484 (87%)	1061 (82%)	235 (18%)	2	14
1	B	1296/1484 (87%)	1051 (81%)	245 (19%)	2	13
2	X	93/94 (99%)	87 (94%)	6 (6%)	20	55
2	Y	93/94 (99%)	86 (92%)	7 (8%)	16	50
All	All	2778/3156 (88%)	2285 (82%)	493 (18%)	2	16

All (493) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	23	TYR
1	A	41	ILE
1	A	42	GLN
1	A	51	ASP
1	A	56	ILE
1	A	64	PHE
1	A	73	LEU
1	A	81	ASN
1	A	88	GLN
1	A	100	SER
1	A	109	LYS
1	A	112	SER
1	A	114	SER
1	A	116	ARG
1	A	119	ILE
1	A	123	ASN
1	A	125	PHE
1	A	126	LEU
1	A	128	ILE
1	A	130	THR
1	A	131	ASP
1	A	140	SER
1	A	143	VAL

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Mol	Chain	Res	Type
1	A	144	ARG
1	A	151	ASP
1	A	161	LEU
1	A	162	THR
1	A	163	PHE
1	A	169	SER
1	A	175	GLU
1	A	176	GLU
1	A	177	ILE
1	A	180	ILE
1	A	184	SER
1	A	192	SER
1	A	195	ARG
1	A	224	LEU
1	A	231	ILE
1	A	232	GLU
1	A	235	TYR
1	A	242	ASN
1	A	249	THR
1	A	264	ASP
1	A	273	GLU
1	A	280	LYS
1	A	296	ILE
1	A	299	VAL
1	A	312	TYR
1	A	313	TYR
1	A	324	TYR
1	A	333	THR
1	A	349	LEU
1	A	354	LEU
1	A	363	LEU
1	A	364	LYS
1	A	373	VAL
1	A	378	SER
1	A	381	GLN
1	A	383	VAL
1	A	386	VAL
1	A	389	THR
1	A	393	GLN
1	A	394	THR
1	A	403	ASP
1	A	411	THR

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Mol	Chain	Res	Type
1	A	419	SER
1	A	421	VAL
1	A	422	LEU
1	A	423	ASN
1	A	431	LEU
1	A	433	PHE
1	A	436	LYS
1	A	441	ASP
1	A	457	TYR
1	A	461	SER
1	A	466	TYR
1	A	469	TRP
1	A	473	HIS
1	A	476	LEU
1	A	482	LEU
1	A	484	ILE
1	A	492	TYR
1	A	493	ILE
1	A	495	LYS
1	A	497	THR
1	A	504	LEU
1	A	518	PHE
1	A	528	ILE
1	A	535	VAL
1	A	539	ARG
1	A	540	LEU
1	A	541	LEU
1	A	544	TYR
1	A	556	SER
1	A	563	ILE
1	A	570	GLN
1	A	573	VAL
1	A	588	VAL
1	A	589	SER
1	A	594	THR
1	A	624	PHE
1	A	631	ASP
1	A	640	LEU
1	A	641	ASN
1	A	644	ASN
1	A	648	LEU
1	A	652	THR

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Mol	Chain	Res	Type
1	A	653	PHE
1	A	667	GLU
1	A	673	LEU
1	A	680	GLN
1	A	705	VAL
1	A	710	THR
1	A	711	CYS
1	A	712	GLU
1	A	724	CYS
1	A	729	THR
1	A	753	HIS
1	A	758	LEU
1	A	767	SER
1	A	786	LEU
1	A	790	LEU
1	A	799	ILE
1	A	800	GLN
1	A	802	ILE
1	A	804	ILE
1	A	809	ILE
1	A	814	THR
1	A	840	GLN
1	A	866	CYS
1	A	867	THR
1	A	886	GLN
1	A	887	LYS
1	A	891	SER
1	A	894	HIS
1	A	895	LEU
1	A	897	THR
1	A	900	VAL
1	A	901	LEU
1	A	903	LEU
1	A	908	HIS
1	A	921	GLU
1	A	924	VAL
1	A	926	THR
1	A	927	LEU
1	A	935	LYS
1	A	936	ARG
1	A	942	VAL
1	A	949	ILE

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Mol	Chain	Res	Type
1	A	952	THR
1	A	957	LYS
1	A	961	TYR
1	A	962	ARG
1	A	973	ILE
1	A	979	VAL
1	A	980	LYS
1	A	982	LEU
1	A	983	LEU
1	A	986	GLU
1	A	995	GLU
1	A	998	ASN
1	A	1001	THR
1	A	1003	LEU
1	A	1015	VAL
1	A	1024	TYR
1	A	1027	THR
1	A	1029	ASN
1	A	1033	ILE
1	A	1039	LEU
1	A	1040	ILE
1	A	1053	MET
1	A	1056	ILE
1	A	1076	THR
1	A	1084	ARG
1	A	1096	ASN
1	A	1101	CYS
1	A	1115	ASN
1	A	1127	ILE
1	A	1128	LYS
1	A	1132	THR
1	A	1140	ASN
1	A	1147	PHE
1	A	1148	THR
1	A	1158	ILE
1	A	1161	LEU
1	A	1164	ILE
1	A	1168	LEU
1	A	1200	LYS
1	A	1208	ILE
1	A	1210	SER
1	A	1217	LEU

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Mol	Chain	Res	Type
1	A	1218	VAL
1	A	1228	TRP
1	A	1229	LYS
1	A	1232	LEU
1	A	1251	THR
1	A	1257	THR
1	A	1274	LEU
1	A	1278	GLN
1	A	1291	ILE
1	A	1297	LEU
1	A	1301	SER
1	A	1307	LEU
1	A	1311	MET
1	A	1313	ILE
1	A	1316	SER
1	A	1318	LYS
1	A	1325	ASN
1	A	1332	ASN
1	A	1334	LEU
1	A	1336	ARG
1	A	1342	LEU
1	A	1343	ASN
1	A	1345	ASP
1	A	1347	ILE
1	A	1365	VAL
1	A	1376	SER
1	A	1383	THR
1	A	1401	ARG
1	A	1437	GLU
1	A	1443	VAL
1	A	1464	LEU
1	A	1465	ASN
1	A	1476	ARG
1	A	1480	PHE
1	A	1483	PHE
1	A	1487	PHE
1	A	1488	LEU
1	A	1496	TYR
1	A	1500	ARG
1	A	1503	LYS
1	A	1507	MET
1	A	1509	TYR

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Mol	Chain	Res	Type
1	A	1511	THR
2	X	134	THR
2	X	136	LEU
2	X	146	LEU
2	X	150	ILE
2	X	166	ASP
2	X	184	THR
1	B	23	TYR
1	B	24	VAL
1	B	26	SER
1	B	41	ILE
1	B	42	GLN
1	B	51	ASP
1	B	56	ILE
1	B	59	TYR
1	B	64	PHE
1	B	73	LEU
1	B	81	ASN
1	B	88	GLN
1	B	100	SER
1	B	109	LYS
1	B	112	SER
1	B	114	SER
1	B	116	ARG
1	B	119	ILE
1	B	123	ASN
1	B	125	PHE
1	B	126	LEU
1	B	128	ILE
1	B	130	THR
1	B	131	ASP
1	B	148	LEU
1	B	151	ASP
1	B	160	VAL
1	B	161	LEU
1	B	162	THR
1	B	163	PHE
1	B	175	GLU
1	B	176	GLU
1	B	177	ILE
1	B	180	ILE
1	B	184	SER

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Mol	Chain	Res	Type
1	B	188	PHE
1	B	189	LYS
1	B	194	PRO
1	B	195	ARG
1	B	212	THR
1	B	224	LEU
1	B	231	ILE
1	B	232	GLU
1	B	235	TYR
1	B	242	ASN
1	B	249	THR
1	B	253	ARG
1	B	257	ASN
1	B	264	ASP
1	B	273	GLU
1	B	280	LYS
1	B	290	THR
1	B	296	ILE
1	B	299	VAL
1	B	312	TYR
1	B	317	ASP
1	B	318	LEU
1	B	324	TYR
1	B	333	THR
1	B	349	LEU
1	B	354	LEU
1	B	363	LEU
1	B	364	LYS
1	B	373	VAL
1	B	378	SER
1	B	379	LEU
1	B	383	VAL
1	B	386	VAL
1	B	389	THR
1	B	393	GLN
1	B	394	THR
1	B	403	ASP
1	B	411	THR
1	B	421	VAL
1	B	422	LEU
1	B	423	ASN
1	B	431	LEU

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Mol	Chain	Res	Type
1	B	433	PHE
1	B	436	LYS
1	B	441	ASP
1	B	457	TYR
1	B	461	SER
1	B	463	SER
1	B	466	TYR
1	B	469	TRP
1	B	473	HIS
1	B	476	LEU
1	B	484	ILE
1	B	492	TYR
1	B	493	ILE
1	B	495	LYS
1	B	497	THR
1	B	500	ASN
1	B	502	LEU
1	B	509	ILE
1	B	517	LYS
1	B	528	ILE
1	B	535	VAL
1	B	539	ARG
1	B	540	LEU
1	B	541	LEU
1	B	544	TYR
1	B	553	GLU
1	B	556	SER
1	B	563	ILE
1	B	570	GLN
1	B	573	VAL
1	B	588	VAL
1	B	589	SER
1	B	594	THR
1	B	624	PHE
1	B	640	LEU
1	B	641	ASN
1	B	644	ASN
1	B	648	LEU
1	B	652	THR
1	B	653	PHE
1	B	667	GLU
1	B	669	CYS

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Mol	Chain	Res	Type
1	B	673	LEU
1	B	680	GLN
1	B	699	CYS
1	B	704	CYS
1	B	705	VAL
1	B	707	ASN
1	B	711	CYS
1	B	729	THR
1	B	753	HIS
1	B	758	LEU
1	B	767	SER
1	B	786	LEU
1	B	790	LEU
1	B	795	THR
1	B	799	ILE
1	B	802	ILE
1	B	804	ILE
1	B	809	ILE
1	B	814	THR
1	B	840	GLN
1	B	866	CYS
1	B	867	THR
1	B	886	GLN
1	B	887	LYS
1	B	891	SER
1	B	894	HIS
1	B	895	LEU
1	B	897	THR
1	B	900	VAL
1	B	901	LEU
1	B	903	LEU
1	B	908	HIS
1	B	924	VAL
1	B	926	THR
1	B	927	LEU
1	B	932	GLU
1	B	935	LYS
1	B	936	ARG
1	B	952	THR
1	B	961	TYR
1	B	962	ARG
1	B	972	GLU

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Mol	Chain	Res	Type
1	B	973	ILE
1	B	975	ARG
1	B	976	ILE
1	B	980	LYS
1	B	982	LEU
1	B	983	LEU
1	B	986	GLU
1	B	995	GLU
1	B	998	ASN
1	B	1001	THR
1	B	1003	LEU
1	B	1015	VAL
1	B	1024	TYR
1	B	1027	THR
1	B	1029	ASN
1	B	1040	ILE
1	B	1053	MET
1	B	1056	ILE
1	B	1069	TRP
1	B	1096	ASN
1	B	1108	VAL
1	B	1115	ASN
1	B	1127	ILE
1	B	1128	LYS
1	B	1132	THR
1	B	1140	ASN
1	B	1147	PHE
1	B	1148	THR
1	B	1158	ILE
1	B	1161	LEU
1	B	1164	ILE
1	B	1168	LEU
1	B	1200	LYS
1	B	1206	ARG
1	B	1208	ILE
1	B	1210	SER
1	B	1213	LYS
1	B	1217	LEU
1	B	1218	VAL
1	B	1226	ARG
1	B	1228	TRP
1	B	1232	LEU

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Mol	Chain	Res	Type
1	B	1251	THR
1	B	1257	THR
1	B	1269	PRO
1	B	1271	ILE
1	B	1278	GLN
1	B	1279	ARG
1	B	1280	TYR
1	B	1297	LEU
1	B	1301	SER
1	B	1307	LEU
1	B	1311	MET
1	B	1313	ILE
1	B	1316	SER
1	B	1318	LYS
1	B	1325	ASN
1	B	1332	ASN
1	B	1334	LEU
1	B	1336	ARG
1	B	1342	LEU
1	B	1343	ASN
1	B	1344	ASP
1	B	1345	ASP
1	B	1347	ILE
1	B	1358	THR
1	B	1376	SER
1	B	1383	THR
1	B	1401	ARG
1	B	1443	VAL
1	B	1464	LEU
1	B	1465	ASN
1	B	1474	CYS
1	B	1476	ARG
1	B	1480	PHE
1	B	1483	PHE
1	B	1487	PHE
1	B	1488	LEU
1	B	1496	TYR
1	B	1500	ARG
1	B	1502	ASP
1	B	1503	LYS
1	B	1507	MET
1	B	1509	TYR

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Mol	Chain	Res	Type
2	Y	134	THR
2	Y	136	LEU
2	Y	138	VAL
2	Y	146	LEU
2	Y	150	ILE
2	Y	184	THR
2	Y	210	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	81	ASN
1	A	88	GLN
1	A	110	HIS
1	A	123	ASN
1	A	139	GLN
1	A	226	HIS
1	A	242	ASN
1	A	279	GLN
1	A	298	GLN
1	A	320	ASN
1	A	393	GLN
1	A	423	ASN
1	A	481	HIS
1	A	625	GLN
1	A	656	ASN
1	A	737	GLN
1	A	785	GLN
1	A	787	GLN
1	A	840	GLN
1	A	886	GLN
1	A	894	HIS
1	A	994	GLN
1	A	1002	HIS
1	A	1023	HIS
1	A	1029	ASN
1	A	1030	HIS
1	A	1090	ASN
1	A	1095	GLN
1	A	1096	ASN
1	A	1115	ASN

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Mol	Chain	Res	Type
1	A	1123	GLN
1	A	1140	ASN
1	A	1173	ASN
1	A	1202	HIS
1	A	1221	ASN
1	A	1260	ASN
1	A	1278	GLN
1	A	1306	GLN
1	A	1325	ASN
1	A	1343	ASN
1	A	1366	HIS
1	A	1435	ASN
1	A	1459	HIS
1	A	1463	GLN
1	A	1465	ASN
1	A	1504	GLN
2	X	135	HIS
2	X	192	ASN
1	B	77	ASN
1	B	80	GLN
1	B	88	GLN
1	B	110	HIS
1	B	123	ASN
1	B	139	GLN
1	B	226	HIS
1	B	242	ASN
1	B	257	ASN
1	B	298	GLN
1	B	320	ASN
1	B	381	GLN
1	B	393	GLN
1	B	423	ASN
1	B	481	HIS
1	B	625	GLN
1	B	656	ASN
1	B	737	GLN
1	B	785	GLN
1	B	787	GLN
1	B	840	GLN
1	B	886	GLN
1	B	894	HIS
1	B	994	GLN

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Mol	Chain	Res	Type
1	B	1002	HIS
1	B	1023	HIS
1	B	1029	ASN
1	B	1030	HIS
1	B	1090	ASN
1	B	1096	ASN
1	B	1115	ASN
1	B	1123	GLN
1	B	1140	ASN
1	B	1173	ASN
1	B	1202	HIS
1	B	1221	ASN
1	B	1268	ASN
1	B	1278	GLN
1	B	1306	GLN
1	B	1325	ASN
1	B	1343	ASN
1	B	1366	HIS
1	B	1435	ASN
1	B	1463	GLN
1	B	1465	ASN
1	B	1504	GLN
2	Y	135	HIS
2	Y	176	ASN
2	Y	230	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

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
4	NAG	A	1680	1	14,14,15	0.66	0	15,19,21	0.72	0
4	NAG	A	2001	1,4	14,14,15	0.52	0	15,19,21	1.13	1 (6%)
4	NAG	A	2002	4	14,14,15	0.47	0	15,19,21	1.00	1 (6%)
4	NAG	B	1679	1	14,14,15	0.71	1 (7%)	15,19,21	0.94	1 (6%)
4	NAG	B	2001	1,4	14,14,15	0.55	0	15,19,21	0.99	0
4	NAG	B	2002	4	14,14,15	0.47	0	15,19,21	0.92	1 (6%)

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
4	NAG	A	1680	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2002	4	-	0/6/23/26	0/1/1/1
4	NAG	B	1679	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2002	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1679	NAG	C1-C2	2.04	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1679	NAG	O5-C1-C2	2.03	114.30	111.47
4	B	2002	NAG	C1-O5-C5	2.60	115.75	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2001	NAG	C1-O5-C5	2.95	116.23	112.17
4	A	2002	NAG	C1-O5-C5	2.95	116.23	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	NAG	2	0
4	B	2001	NAG	3	0
4	B	2002	NAG	1	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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1459/1676 (87%)	-0.62	11 (0%) 86 79	81, 190, 311, 455	0
1	B	1459/1676 (87%)	-0.63	10 (0%) 87 82	85, 190, 308, 475	0
2	X	102/103 (99%)	0.04	9 (8%) 11 9	157, 292, 386, 530	0
2	Y	102/103 (99%)	0.02	5 (4%) 30 24	156, 292, 377, 494	0
All	All	3122/3558 (87%)	-0.58	35 (1%) 80 72	81, 194, 328, 530	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	671	GLU	4.8
2	Y	193	LEU	4.4
2	X	193	LEU	4.4
1	B	671	GLU	4.0
1	A	670	LYS	3.6
1	B	668	PRO	3.4
2	Y	159	GLU	3.4
1	B	615	GLY	3.4
1	A	672	ILE	3.3
2	X	159	GLU	2.9
1	A	668	PRO	2.8
1	B	670	LYS	2.8
1	A	759	PRO	2.8
2	X	158	GLU	2.7
2	Y	192	ASN	2.7
1	A	883	CYS	2.6
1	A	309	GLU	2.6
2	X	197	GLU	2.5
2	Y	157	LYS	2.5
1	B	309	GLU	2.5
1	A	258	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	X	129	SER	2.3
1	A	613	GLN	2.3
2	X	192	ASN	2.2
1	B	47	THR	2.2
1	B	613	GLN	2.2
1	B	672	ILE	2.2
2	X	228	LEU	2.2
2	X	227	THR	2.1
2	Y	158	GLU	2.1
1	A	47	THR	2.1
1	A	615	GLY	2.1
2	X	157	LYS	2.1
1	B	759	PRO	2.1
1	B	258	LYS	2.1

## 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CD	A	1678	1/1	0.87	0.44	2.30	481,481,481,481	0
3	CD	B	1677	1/1	0.90	0.38	1.04	466,466,466,466	0
3	CD	A	1679	1/1	0.22	0.12	-	402,402,402,402	0
3	CD	A	1677	1/1	0.89	0.09	-	229,229,229,229	1
4	NAG	B	2001	14/15	0.79	0.30	-	280,280,280,280	0
4	NAG	A	2001	14/15	0.85	0.28	-	293,293,293,293	0
4	NAG	A	1680	14/15	0.51	0.36	-	301,301,301,301	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	2002	14/15	0.73	0.50	-	363,363,363,363	0
4	NAG	A	2002	14/15	0.66	0.46	-	343,343,343,343	0
4	NAG	B	1679	14/15	0.59	0.35	-	290,290,290,290	0
3	CD	B	1678	1/1	0.39	0.11	-	397,397,397,397	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.