



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:36 AM GMT

PDB ID : 2R93  
Title : Elongation complex of RNA polymerase II with a hepatitis delta virus-derived RNA stem loop  
Authors : Lehmann, E.; Brueckner, F.; Cramer, P.  
Deposited on : 2007-09-12  
Resolution : 4.00 Å(reported)

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

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

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



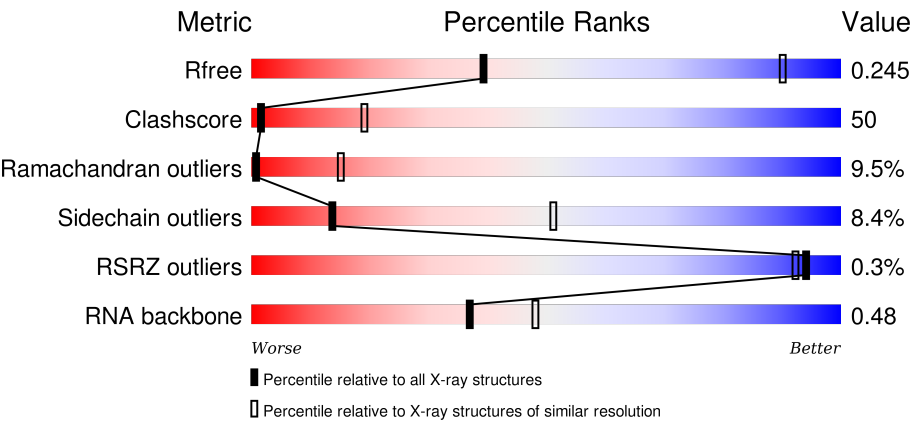
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)
RNA backbone	2183	1079 (5.04-2.80)

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	R	18	<div><div>11%</div><div><div></div><div>28%</div><div>28%</div><div>17%</div><div>6%</div><div>22%</div></div></div>
2	A	1733	<div><div></div><div><div>29%</div><div>44%</div><div>8%</div><div>•</div><div>18%</div></div></div>
3	B	1224	<div><div></div><div><div>28%</div><div>51%</div><div>11%</div><div>•</div><div>9%</div></div></div>
4	C	318	<div><div></div><div><div>26%</div><div>48%</div><div>8%</div><div>•</div><div>16%</div></div></div>

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Mol	Chain	Length	Quality of chain
5	D	221	<div><div></div><div>33%38%9%19%</div></div>
6	E	215	<div><div></div><div>35%57%7%</div></div>
7	F	155	<div><div></div><div>19%32%6%43%</div></div>
8	G	171	<div><div></div><div>30%61%8%</div></div>
9	H	146	<div><div></div><div>2%27%51%14%8%</div></div>
10	I	122	<div><div></div><div>37%46%12%5%</div></div>
11	J	70	<div><div></div><div>20%53%19%7%</div></div>
12	K	120	<div><div></div><div>38%47%9%7%</div></div>
13	L	70	<div><div></div><div>%17%33%14%34%</div></div>



## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 31500 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 RNA chain called RNA (5'-R(\*UP\*GP\*AP\*UP\*UP\*CP\*UP\*CP\*UP\*AP\*UP\*CP\*GP\*GP\*AP\*AP\*UP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	14	Total	C	N	O	P	0	0	0
			289	132	49	96	12			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1422	Total	C	N	O	S	0	0	0
			11194	7054	1959	2119	62			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	1112	Total	C	N	O	S	0	0	0
			8841	5596	1550	1640	55			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	88	Total	C	N	O	S	0	0	0
			712	455	120	134	3			

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	135	Total	C	N	O	S	0	0	0
			1084	683	183	214	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	116	Total	C	N	O	S	0	0	0
			944	581	172	181	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	112	Total	C	N	O	S	0	0	0
			904	580	154	168	2			

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	J	1	Total	Zn	0	0
			1	1		
14	B	1	Total	Zn	0	0
			1	1		
14	I	2	Total	Zn	0	0
			2	2		
14	C	1	Total	Zn	0	0
			1	1		
14	A	2	Total	Zn	0	0
			2	2		
14	L	1	Total	Zn	0	0
			1	1		

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

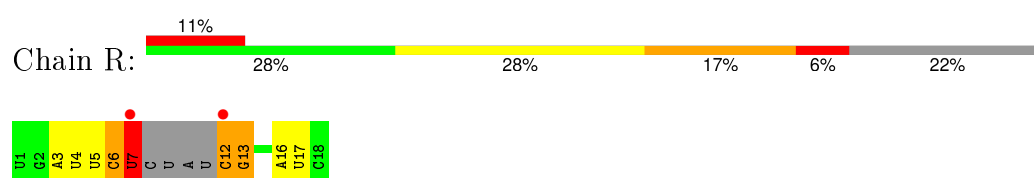
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		



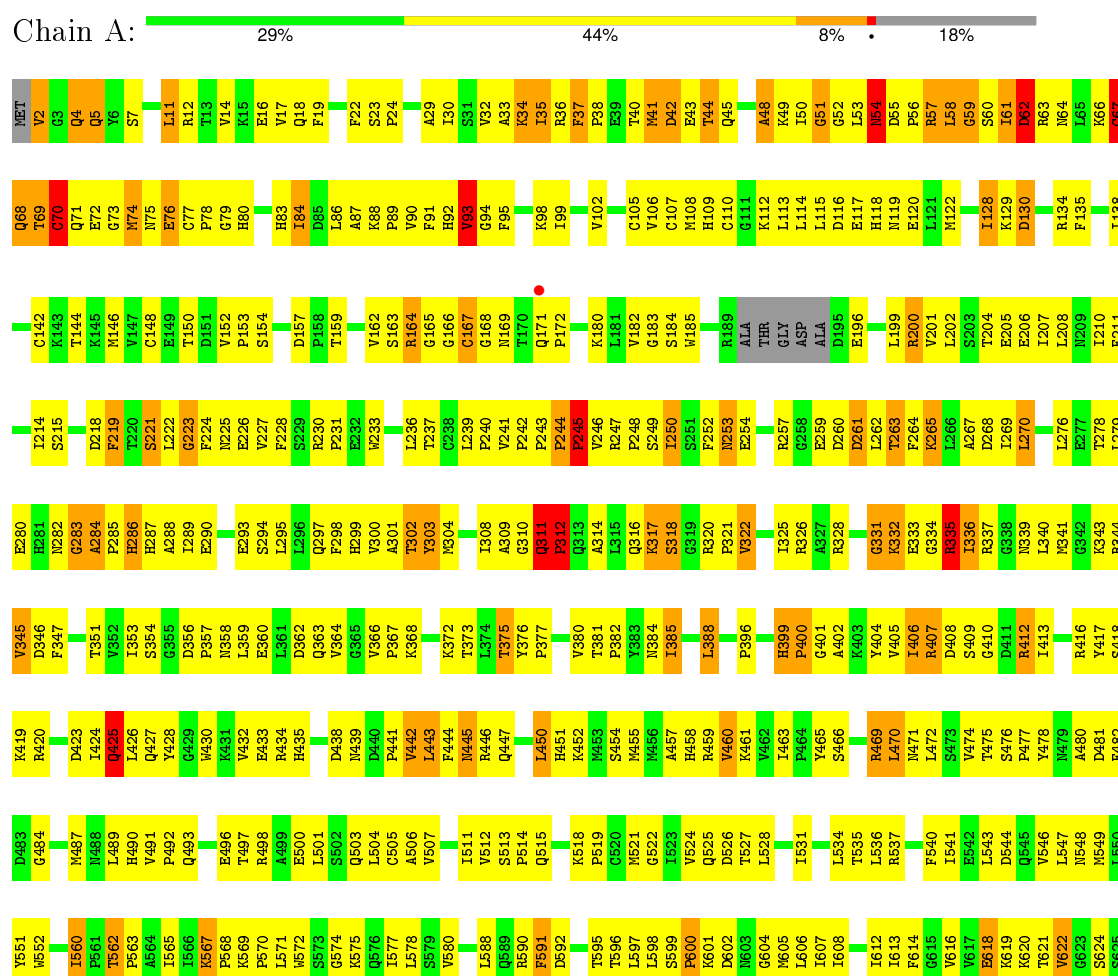
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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: RNA (5'-R(\*UP\*GP\*AP\*UP\*UP\*CP\*UP\*CP\*UP\*AP\*UP\*CP\*GP\*GP\*AP\*AP\*UP\*C)-3')



- Molecule 2: DNA-directed RNA polymerase II subunit RPB1





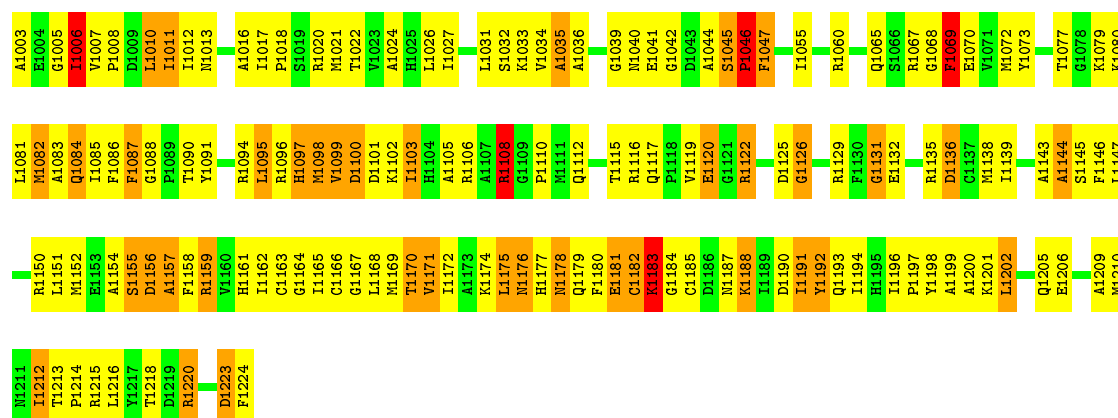




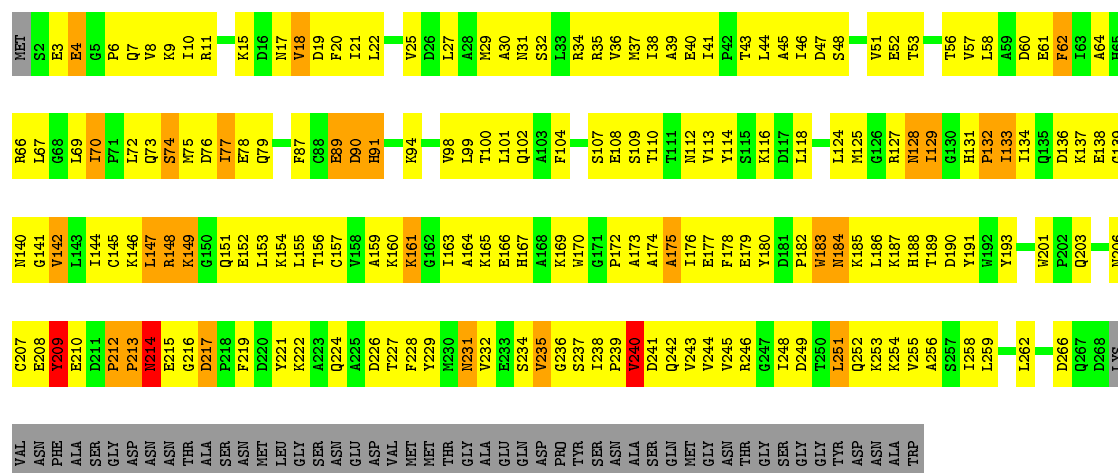
Chain B:  28% 51% 11% 9%



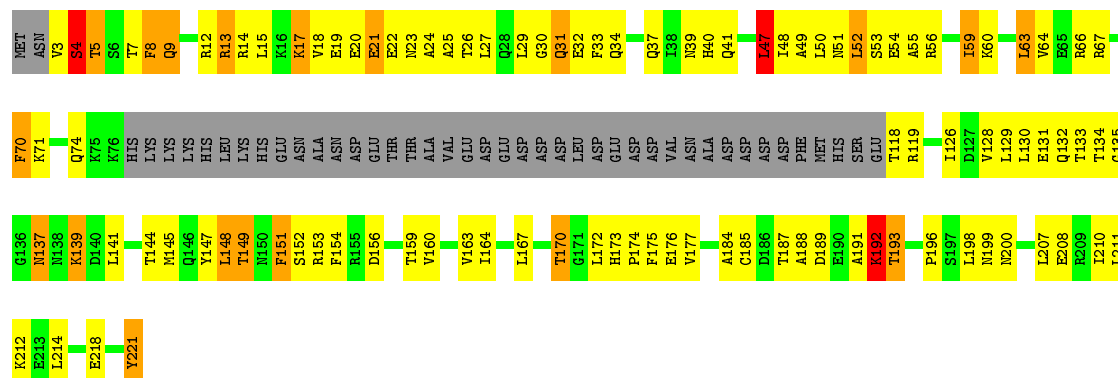




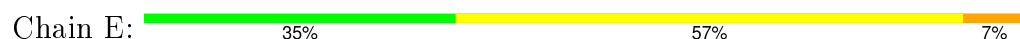
• Molecule 4: DNA-directed RNA polymerase II subunit RPB3



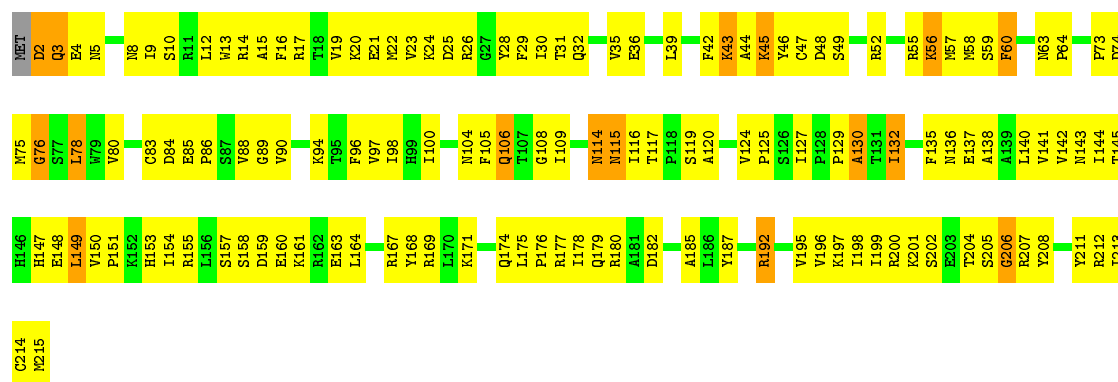
• Molecule 5: DNA-directed RNA polymerase II subunit RPB4



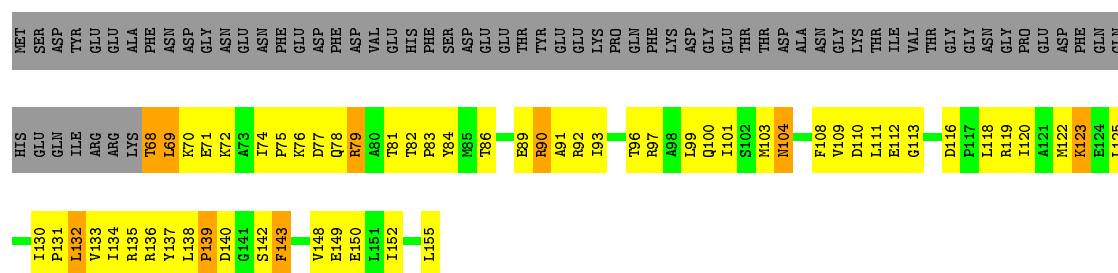
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC1







- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC2



- Molecule 8: DNA-directed RNA polymerase II subunit RPB7

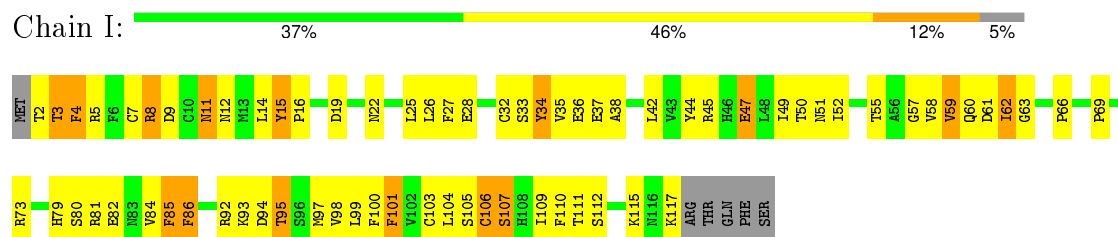


- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3

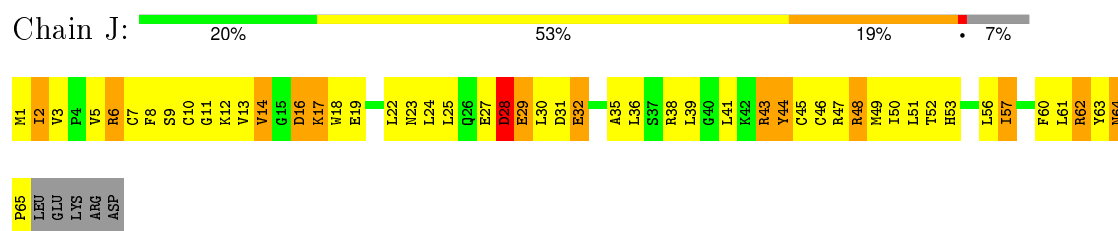




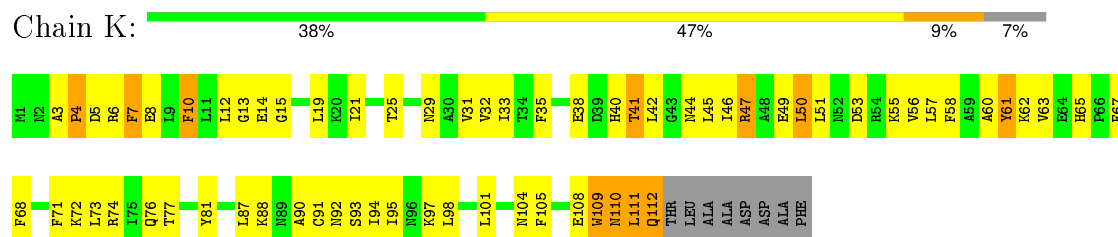
- Molecule 10: DNA-directed RNA polymerase II subunit RPB9



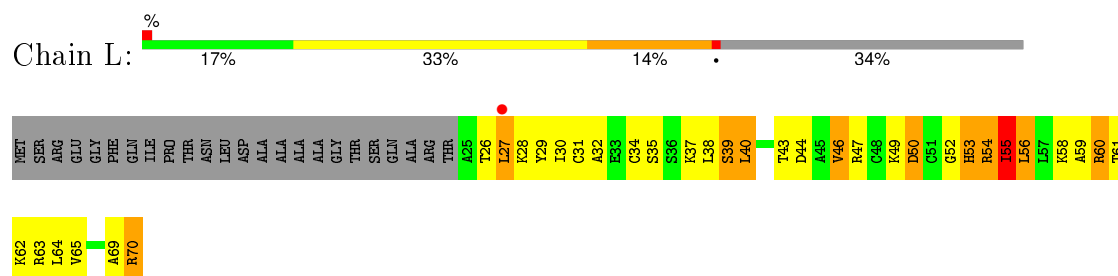
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 12: DNA-directed RNA polymerase II subunit RPB11



- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC4





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	223.34Å 394.88Å 284.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.00 48.28 – 4.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-4.00) 97.2 (48.28-4.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.00 (at 4.00Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.216 , 0.241 0.224 , 0.245	Depositor DCC
$R_{free}$ test set	2068 reflections (2.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	103.2	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 46.8	EDS
Estimated twinning fraction	0.011 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.010 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 105627 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	31500	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	R	0.87	0/321	1.11	3/496 (0.6%)
2	A	0.42	0/11394	0.71	6/15407 (0.0%)
3	B	0.41	0/9013	0.68	0/12152
4	C	0.42	0/2139	0.72	1/2899 (0.0%)
5	D	0.40	0/1444	0.66	0/1935
6	E	0.38	0/1788	0.64	0/2406
7	F	0.53	0/723	0.92	2/974 (0.2%)
8	G	0.44	0/1368	0.72	0/1844
9	H	0.38	0/1102	0.64	0/1492
10	I	0.36	0/962	0.64	0/1295
11	J	0.47	0/541	0.72	0/727
12	K	0.44	0/922	0.65	0/1244
13	L	0.48	0/366	0.72	0/485
All	All	0.42	0/32083	0.70	12/43356 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	70	LYS	N-CA-C	-10.69	82.14	111.00
7	F	69	LEU	CA-CB-CG	9.42	136.97	115.30
1	R	7	U	O4'-C1'-N1	7.69	114.35	108.20
2	A	1176	LEU	N-CA-C	7.45	131.12	111.00
2	A	1176	LEU	CA-CB-CG	7.44	132.41	115.30
1	R	12	C	N1-C1'-C2'	6.79	122.82	114.00
2	A	311	GLN	N-CA-C	5.72	126.46	111.00
2	A	452	LYS	N-CA-C	-5.49	96.17	111.00
2	A	425	GLN	N-CA-C	-5.33	96.61	111.00
1	R	7	U	N1-C1'-C2'	5.17	120.72	114.00
4	C	183	TRP	N-CA-C	-5.17	97.04	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	223	GLY	N-CA-C	5.08	125.80	113.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	289	0	153	11	0
2	A	11194	0	11279	1192	0
3	B	8841	0	8875	1024	0
4	C	2101	0	2056	260	0
5	D	1434	0	1460	119	0
6	E	1752	0	1776	150	0
7	F	712	0	737	108	0
8	G	1340	0	1357	159	0
9	H	1084	0	1057	128	0
10	I	944	0	901	98	0
11	J	532	0	543	90	0
12	K	904	0	911	106	0
13	L	364	0	387	49	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	31500	0	31492	3165	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 50.

All (3165) 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)
7:F:68:THR:HG21	7:F:69:LEU:N	1.59	1.16
7:F:69:LEU:HD23	7:F:71:GLU:CB	1.77	1.14
7:F:69:LEU:HD23	7:F:71:GLU:HB2	1.17	1.12
2:A:58:LEU:HD12	2:A:59:GLY:N	1.65	1.11
2:A:34:LYS:NZ	2:A:57:ARG:HH12	1.50	1.09
6:E:94:LYS:HE2	6:E:98:ILE:HD11	1.32	1.09
3:B:806:THR:HG22	3:B:808:ALA:H	1.10	1.08
2:A:53:LEU:HD23	2:A:54:ASN:H	1.02	1.08
9:H:100:THR:HG23	9:H:138:GLU:HA	1.30	1.08
3:B:510:LYS:HG2	3:B:511:PRO:HD3	1.36	1.08
7:F:68:THR:HB	7:F:69:LEU:CG	1.83	1.07
12:K:47:ARG:HB3	12:K:47:ARG:HH11	1.19	1.07
2:A:1161:THR:HG22	2:A:1163:ILE:H	1.17	1.07
2:A:41:MET:HB3	2:A:49:LYS:HA	1.32	1.07
5:D:40:HIS:HB3	8:G:73:LYS:HZ3	1.16	1.06
2:A:58:LEU:HD12	2:A:59:GLY:H	0.88	1.05
2:A:709:THR:HG22	2:A:711:ARG:H	1.23	1.04
10:I:34:TYR:HD2	10:I:35:VAL:N	1.54	1.04
3:B:343:ILE:HG23	3:B:347:LYS:HB2	1.34	1.04
5:D:40:HIS:HB3	8:G:73:LYS:NZ	1.72	1.02
2:A:225:ASN:HD22	2:A:228:PHE:H	1.04	1.02
2:A:1127:ASP:HB3	2:A:1130:GLN:HB3	1.33	1.02
7:F:68:THR:CB	7:F:69:LEU:HG	1.89	1.02
4:C:101:LEU:HD13	4:C:118:LEU:HD23	1.39	1.02
2:A:535:THR:HG21	2:A:616:VAL:HA	1.40	1.01
3:B:273:LEU:HB2	3:B:276:ILE:HD12	1.40	1.01
4:C:45:ALA:HA	4:C:72:LEU:HD12	1.43	1.01
2:A:114:LEU:HD13	2:A:171:GLN:HE22	1.26	1.00
13:L:32:ALA:HB3	13:L:55:ILE:HD12	1.40	1.00
4:C:47:ASP:HA	13:L:69:ALA:HB3	1.43	1.00
11:J:3:VAL:HG21	11:J:18:TRP:HB2	1.41	1.00
7:F:68:THR:HB	7:F:69:LEU:HG	1.42	1.00
2:A:567:LYS:HB3	9:H:96:VAL:H	1.22	1.00
3:B:364:ILE:HG12	3:B:585:VAL:HG13	1.42	0.99
3:B:515:HIS:H	3:B:518:HIS:HD2	1.06	0.99
8:G:15:PRO:HA	8:G:18:PHE:CD1	1.96	0.99
3:B:214:ALA:HB3	3:B:498:THR:HA	1.42	0.98
2:A:340:LEU:HD13	2:A:1429:ILE:HG23	1.44	0.98
9:H:4:THR:HA	9:H:60:ALA:HB2	1.41	0.97
7:F:68:THR:HB	7:F:69:LEU:CD1	1.94	0.97
8:G:138:THR:HG22	8:G:139:ILE:H	1.27	0.97
7:F:68:THR:CG2	7:F:69:LEU:N	2.27	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:43:THR:HG22	4:C:44:LEU:H	1.28	0.96
2:A:475:THR:HG23	2:A:476:SER:H	1.30	0.96
3:B:589:VAL:HG12	3:B:590:HIS:H	1.31	0.96
2:A:53:LEU:HD22	2:A:54:ASN:HD22	1.29	0.95
3:B:577:ALA:HB1	3:B:589:VAL:HG11	1.45	0.95
2:A:1174:PHE:HA	2:A:1176:LEU:HG	1.44	0.95
2:A:567:LYS:CD	2:A:568:PRO:HD2	1.97	0.95
2:A:567:LYS:CG	2:A:568:PRO:HD2	1.98	0.94
2:A:1373:ASP:HA	2:A:1376:THR:HG22	1.49	0.94
7:F:69:LEU:HD13	7:F:72:LYS:CG	1.98	0.94
7:F:69:LEU:CD2	7:F:71:GLU:HB2	1.97	0.94
3:B:882:THR:HG22	3:B:884:ARG:H	1.32	0.94
10:I:111:THR:HG22	10:I:112:SER:H	1.31	0.94
11:J:64:ASN:HB3	11:J:65:PRO:CD	1.97	0.94
4:C:57:VAL:HG11	11:J:60:PHE:HB3	1.51	0.93
9:H:135:LEU:HD13	9:H:137:GLN:HE21	1.32	0.93
4:C:32:SER:O	4:C:36:VAL:HG23	1.66	0.93
3:B:1097:HIS:H	3:B:1098:MET:HE2	1.31	0.93
2:A:2:VAL:HG21	3:B:1157:ALA:HB1	1.47	0.93
11:J:1:MET:H2	11:J:57:ILE:H	1.13	0.92
2:A:567:LYS:HD2	2:A:568:PRO:HD2	1.49	0.92
2:A:855:THR:HG21	2:A:857:ARG:HE	1.34	0.92
3:B:583:ASN:HD21	3:B:628:THR:HG22	1.34	0.92
9:H:130:ARG:HA	9:H:133:ASN:HD22	1.34	0.92
8:G:23:LYS:HG3	8:G:56:ILE:HD11	1.50	0.92
2:A:14:VAL:H	2:A:1432:GLN:HE22	1.13	0.92
2:A:779:PHE:HE1	2:A:785:PRO:HD3	1.32	0.92
8:G:127:PRO:HG2	8:G:138:THR:HG21	1.49	0.91
2:A:34:LYS:HZ1	2:A:57:ARG:HH12	0.96	0.91
5:D:144:THR:O	5:D:148:LEU:HB2	1.70	0.91
2:A:61:ILE:HG22	2:A:62:ASP:H	1.35	0.91
9:H:130:ARG:H	9:H:130:ARG:HD2	1.34	0.91
3:B:169:ARG:HB2	3:B:454:THR:HG23	1.53	0.91
7:F:68:THR:OG1	7:F:69:LEU:HG	1.71	0.91
3:B:25:ILE:HD11	3:B:653:VAL:O	1.69	0.91
6:E:22:MET:HE3	6:E:26:ARG:HH21	1.35	0.91
2:A:1152:ILE:HG13	10:I:44:TYR:HB3	1.53	0.90
9:H:130:ARG:HB3	9:H:133:ASN:HB2	1.50	0.90
2:A:53:LEU:HD23	2:A:54:ASN:N	1.86	0.90
3:B:510:LYS:HG2	3:B:511:PRO:CD	2.01	0.90
2:A:1152:ILE:HD11	10:I:44:TYR:HD2	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:521:LEU:HD22	3:B:633:VAL:HG12	1.54	0.90
8:G:34:VAL:HG12	8:G:45:ILE:HG21	1.54	0.89
11:J:44:TYR:HA	11:J:47:ARG:HB2	1.54	0.89
4:C:39:ALA:HA	4:C:164:ALA:HB3	1.54	0.89
8:G:13:LEU:HD21	8:G:17:PHE:HB2	1.55	0.89
2:A:269:ILE:HD13	2:A:300:VAL:HG22	1.55	0.89
2:A:34:LYS:HZ1	2:A:57:ARG:NH1	1.70	0.88
3:B:549:THR:HG22	3:B:550:ASP:H	1.38	0.88
5:D:17:LYS:HE3	5:D:17:LYS:HA	1.52	0.88
3:B:622:LYS:HE2	10:I:59:VAL:HG22	1.55	0.88
3:B:1159:ARG:HD3	3:B:1193:GLN:HG3	1.54	0.88
2:A:1444:MET:HG2	8:G:60:ARG:HA	1.55	0.88
3:B:911:ILE:HD11	3:B:941:LEU:HD13	1.56	0.88
3:B:999:MET:HG3	3:B:1000:PRO:HD2	1.53	0.88
2:A:356:ASP:HB2	2:A:469:ARG:NH1	1.88	0.88
6:E:180:ARG:HH21	6:E:192:ARG:HB2	1.37	0.87
7:F:69:LEU:HB3	7:F:72:LYS:H	1.35	0.87
3:B:280:ILE:HB	3:B:285:ILE:HD11	1.55	0.87
3:B:65:GLU:HG3	3:B:66:ASP:H	1.39	0.87
7:F:69:LEU:HB3	7:F:72:LYS:N	1.88	0.87
2:A:1017:LEU:HB2	6:E:206:GLY:H	1.36	0.87
2:A:534:LEU:O	2:A:574:GLY:HA3	1.75	0.87
3:B:801:LYS:O	11:J:52:THR:HG23	1.73	0.86
2:A:563:PRO:HG3	2:A:572:TRP:CZ2	2.10	0.86
2:A:34:LYS:HZ2	2:A:57:ARG:HH22	1.22	0.86
8:G:7:LEU:HB2	8:G:74:TYR:CE2	2.09	0.86
12:K:65:HIS:HD2	12:K:67:PHE:H	1.20	0.86
3:B:944:THR:HG21	3:B:1122:ARG:NH2	1.89	0.86
3:B:1002:THR:HG21	3:B:1006:ILE:HD12	1.58	0.86
10:I:115:LYS:HD3	10:I:117:LYS:HE3	1.55	0.85
2:A:1017:LEU:HB2	6:E:206:GLY:N	1.90	0.85
2:A:1226:VAL:HG22	2:A:1240:CYS:HB3	1.58	0.85
2:A:763:ALA:O	2:A:803:SER:HB3	1.75	0.85
2:A:34:LYS:HG2	2:A:36:ARG:HH21	1.40	0.85
4:C:174:ALA:HB2	4:C:235:VAL:HG22	1.57	0.85
11:J:5:VAL:HG12	11:J:6:ARG:HG3	1.57	0.85
2:A:399:HIS:HB3	2:A:400:PRO:HD3	1.56	0.85
3:B:515:HIS:H	3:B:518:HIS:CD2	1.92	0.85
2:A:58:LEU:CD1	2:A:59:GLY:H	1.84	0.85
8:G:1:MET:SD	8:G:79:PHE:HD1	1.99	0.85
2:A:225:ASN:ND2	2:A:228:PHE:H	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:198:ILE:HD11	6:E:212:ARG:HG3	1.58	0.85
9:H:100:THR:OG1	9:H:138:GLU:HG3	1.77	0.85
6:E:16:PHE:CZ	6:E:20:LYS:HE2	2.11	0.85
3:B:766:ARG:HH22	3:B:1020:ARG:HH11	1.24	0.85
4:C:45:ALA:HA	4:C:72:LEU:CD1	2.06	0.84
8:G:111:THR:HG22	8:G:113:HIS:H	1.42	0.84
5:D:40:HIS:CB	8:G:73:LYS:HZ3	1.89	0.84
2:A:903:ASN:HD22	2:A:904:THR:N	1.74	0.84
2:A:901:LEU:H	2:A:926:GLN:NE2	1.75	0.84
2:A:567:LYS:HB3	9:H:96:VAL:N	1.90	0.84
6:E:14:ARG:HH21	6:E:141:VAL:HG12	1.42	0.84
8:G:49:LEU:HD21	8:G:77:VAL:HG23	1.59	0.83
4:C:36:VAL:HG21	4:C:251:LEU:HD22	1.57	0.83
2:A:1116:LEU:HB2	2:A:1329:THR:OG1	1.78	0.83
3:B:806:THR:HG22	3:B:808:ALA:N	1.93	0.83
2:A:1312:ASN:O	2:A:1316:VAL:HG23	1.78	0.83
2:A:598:LEU:HA	9:H:122:LEU:HD13	1.60	0.83
7:F:86:THR:OG1	7:F:89:GLU:HG3	1.78	0.83
3:B:340:ALA:HB2	3:B:343:ILE:HD12	1.60	0.83
3:B:1072:MET:CE	3:B:1085:ILE:HB	2.09	0.83
3:B:343:ILE:CG2	3:B:347:LYS:HB2	2.07	0.83
2:A:249:SER:O	2:A:250:ILE:HG13	1.79	0.83
2:A:353:ILE:HG21	2:A:487:MET:HE3	1.60	0.83
2:A:567:LYS:NZ	9:H:46:LEU:HB2	1.94	0.83
9:H:93:TYR:HB3	9:H:144:ILE:O	1.79	0.82
2:A:1189:SER:O	2:A:1241:ARG:HD3	1.79	0.82
1:R:12:C:H2'	1:R:13:G:C8	2.13	0.82
3:B:899:ILE:HD11	3:B:911:ILE:HA	1.59	0.82
2:A:1173:HIS:O	2:A:1176:LEU:HD23	1.77	0.82
3:B:594:ALA:HA	3:B:617:ARG:HH12	1.43	0.82
2:A:779:PHE:CE1	2:A:785:PRO:HD3	2.14	0.82
2:A:899:VAL:HB	2:A:929:LEU:HD11	1.62	0.82
2:A:1332:PHE:HD2	2:A:1332:PHE:H	1.27	0.82
3:B:971:THR:OG1	4:C:61:GLU:HG3	1.80	0.82
3:B:798:TYR:HE2	4:C:62:PHE:CE2	1.98	0.82
1:R:7:U:OP1	3:B:942:ARG:NH2	2.13	0.82
8:G:143:ILE:HG22	8:G:144:ARG:N	1.95	0.81
2:A:1227:ILE:HG22	2:A:1228:TRP:H	1.43	0.81
2:A:93:VAL:HG22	2:A:301:ALA:HA	1.62	0.81
2:A:849:MET:HE1	2:A:1061:GLY:HA2	1.60	0.81
2:A:446:ARG:CD	2:A:480:ALA:HB2	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1208:THR:HG22	2:A:1210:GLY:H	1.45	0.81
2:A:1444:MET:HE2	7:F:135:ARG:HB2	1.62	0.81
3:B:770:GLN:OE1	3:B:983:ARG:HA	1.80	0.81
7:F:116:ASP:HB3	7:F:119:ARG:HB2	1.63	0.81
4:C:7:GLN:HG2	12:K:104:ASN:HD22	1.44	0.81
9:H:62:SER:HB2	9:H:64:ASN:HD22	1.45	0.81
2:A:768:GLN:HG2	2:A:816:HIS:HA	1.61	0.81
10:I:34:TYR:CD2	10:I:35:VAL:N	2.45	0.80
2:A:84:ILE:HG22	2:A:239:LEU:HB3	1.63	0.80
7:F:69:LEU:HD13	7:F:72:LYS:HG3	1.61	0.80
2:A:903:ASN:HD22	2:A:904:THR:H	1.27	0.80
2:A:215:SER:HB3	2:A:218:ASP:OD2	1.81	0.80
2:A:537:ARG:HH12	9:H:122:LEU:HG	1.47	0.80
3:B:516:ASN:N	3:B:516:ASN:HD22	1.77	0.80
3:B:35:SER:HA	3:B:811:TYR:HE2	1.46	0.80
4:C:6:PRO:HB3	4:C:25:VAL:HG12	1.63	0.80
11:J:64:ASN:HB3	11:J:65:PRO:HD3	1.61	0.80
2:A:93:VAL:HG13	2:A:301:ALA:HB1	1.63	0.80
2:A:524:VAL:HG12	2:A:525:GLN:H	1.47	0.80
2:A:58:LEU:HD13	2:A:80:HIS:O	1.82	0.80
7:F:68:THR:CB	7:F:69:LEU:CG	2.52	0.80
4:C:239:PRO:HB2	4:C:241:ASP:OD1	1.82	0.80
2:A:34:LYS:CE	2:A:57:ARG:HH12	1.94	0.79
4:C:46:ILE:HG23	4:C:157:CYS:HB3	1.65	0.79
2:A:853:ASP:O	2:A:854:ASN:HB2	1.82	0.79
6:E:19:VAL:O	6:E:23:VAL:HG23	1.81	0.79
2:A:913:LEU:HD12	2:A:914:GLU:H	1.47	0.79
7:F:82:THR:HG22	7:F:84:TYR:H	1.45	0.79
7:F:68:THR:HB	7:F:69:LEU:HD12	1.64	0.79
4:C:47:ASP:HA	13:L:69:ALA:CB	2.12	0.79
3:B:830:TYR:CE2	3:B:1000:PRO:HD3	2.17	0.79
2:A:53:LEU:CD2	2:A:54:ASN:HD22	1.95	0.79
2:A:1445:ILE:H	2:A:1445:ILE:HD12	1.47	0.79
7:F:109:VAL:HG12	7:F:110:ASP:H	1.46	0.79
3:B:60:GLN:O	3:B:63:ILE:HG22	1.82	0.79
3:B:613:VAL:HG13	3:B:627:PHE:O	1.83	0.79
3:B:411:PRO:O	3:B:414:ALA:HB3	1.83	0.79
8:G:143:ILE:HG22	8:G:144:ARG:H	1.47	0.79
7:F:109:VAL:HG12	7:F:110:ASP:N	1.97	0.79
2:A:868:TYR:HD2	2:A:1058:VAL:HG21	1.48	0.79
2:A:1438:THR:HB	3:B:1144:ALA:HB3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:14:VAL:HG12	11:J:50:ILE:HD11	1.65	0.79
7:F:130:ILE:O	7:F:148:VAL:HG21	1.83	0.79
3:B:882:THR:CG2	3:B:884:ARG:HB2	2.13	0.78
2:A:1114:PRO:HB2	2:A:1311:VAL:HG23	1.65	0.78
3:B:245:GLU:O	3:B:246:LYS:HG3	1.81	0.78
8:G:138:THR:HG22	8:G:139:ILE:N	1.98	0.78
4:C:166:GLU:HG3	12:K:10:PHE:HZ	1.48	0.78
2:A:164:ARG:HG3	2:A:165:GLY:H	1.49	0.78
9:H:12:VAL:HG13	9:H:26:ILE:HG23	1.64	0.78
2:A:963:ILE:HD11	2:A:1048:ASN:HB3	1.65	0.78
3:B:953:LEU:HD21	3:B:965:LYS:HB2	1.63	0.78
4:C:66:ARG:NH1	11:J:2:ILE:HG21	1.97	0.78
3:B:710:LEU:HA	3:B:733:HIS:HB3	1.66	0.78
3:B:1095:LEU:HD12	3:B:1095:LEU:H	1.46	0.78
3:B:1197:PRO:HG2	3:B:1200:ALA:HB2	1.66	0.78
2:A:1161:THR:HG22	2:A:1163:ILE:N	1.97	0.78
2:A:1445:ILE:HD11	8:G:68:ALA:HB1	1.63	0.78
10:I:85:PHE:HD2	10:I:85:PHE:H	1.30	0.78
1:R:5:U:H2'	1:R:6:C:O4'	1.84	0.78
2:A:450:LEU:HB3	2:A:838:GLN:HE21	1.47	0.78
5:D:47:LEU:HD11	8:G:3:PHE:CD2	2.19	0.77
3:B:217:ARG:HE	3:B:405:ARG:HB2	1.50	0.77
3:B:579:ARG:HB2	3:B:586:TRP:NE1	1.99	0.77
3:B:828:ALA:HB2	3:B:1085:ILE:HG23	1.65	0.77
3:B:167:ILE:HG22	3:B:453:ILE:HD12	1.66	0.77
2:A:1373:ASP:HA	2:A:1376:THR:CG2	2.15	0.77
3:B:1072:MET:HE3	3:B:1085:ILE:HB	1.64	0.77
10:I:8:ARG:HG3	10:I:34:TYR:HE1	1.49	0.77
9:H:89:LEU:HB3	9:H:91:ASP:OD1	1.84	0.77
2:A:67:CYS:O	2:A:70:CYS:HB3	1.84	0.77
4:C:43:THR:HG22	4:C:44:LEU:N	1.99	0.77
2:A:1329:THR:CG2	2:A:1331:SER:H	1.97	0.77
3:B:825:VAL:CG1	3:B:826:ALA:N	2.47	0.77
2:A:1030:ARG:HG3	2:A:1034:GLU:OE2	1.85	0.77
13:L:32:ALA:HB3	13:L:55:ILE:CD1	2.15	0.77
2:A:783:THR:HG21	2:A:815:PHE:CZ	2.20	0.77
3:B:1085:ILE:HD12	3:B:1085:ILE:N	2.00	0.77
3:B:594:ALA:HA	3:B:617:ARG:NH1	1.98	0.77
2:A:1424:VAL:HG13	2:A:1436:ILE:HD11	1.66	0.77
2:A:70:CYS:O	2:A:72:GLU:HG2	1.85	0.76
3:B:593:PRO:HG2	3:B:617:ARG:NH2	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:758:PHE:HB3	3:B:761:HIS:HD2	1.50	0.76
9:H:42:ILE:HG23	9:H:95:TYR:HE1	1.49	0.76
9:H:4:THR:HA	9:H:60:ALA:CB	2.13	0.76
11:J:12:LYS:O	11:J:14:VAL:HG23	1.84	0.76
4:C:46:ILE:HD12	4:C:67:LEU:HB3	1.66	0.76
2:A:860:LEU:HD11	2:A:1393:ASN:HB2	1.67	0.76
3:B:637:LEU:HD12	3:B:693:ILE:HD12	1.67	0.76
12:K:49:GLU:HG3	12:K:94:ILE:HG12	1.66	0.76
3:B:96:TYR:HB2	3:B:129:PHE:HB2	1.66	0.76
2:A:40:THR:HG22	2:A:41:MET:HG3	1.66	0.76
7:F:90:ARG:HD3	7:F:155:LEU:HD12	1.66	0.76
9:H:100:THR:CG2	9:H:138:GLU:HA	2.14	0.76
4:C:254:LYS:O	4:C:258:ILE:HD13	1.85	0.76
9:H:59:ILE:HG22	9:H:60:ALA:N	2.00	0.76
2:A:351:THR:HB	3:B:1103:ILE:HD12	1.68	0.76
3:B:37:PHE:CE1	3:B:41:LYS:HG3	2.21	0.76
2:A:49:LYS:NZ	2:A:61:ILE:HG13	2.01	0.76
2:A:1420:ASP:HB3	2:A:1422:ARG:HG3	1.68	0.76
2:A:405:VAL:HG22	2:A:432:VAL:HG22	1.67	0.76
2:A:1152:ILE:HD11	10:I:44:TYR:CD2	2.18	0.75
2:A:1121:GLU:HG2	2:A:1122:PRO:HD2	1.67	0.75
3:B:378:LEU:O	3:B:382:ILE:HG13	1.86	0.75
4:C:186:LEU:HD21	4:C:224:GLN:O	1.87	0.75
2:A:629:LEU:O	2:A:633:VAL:HG23	1.86	0.75
2:A:58:LEU:HD11	2:A:244:PRO:HD2	1.66	0.75
2:A:774:ARG:NH2	2:A:797:LYS:HG3	2.00	0.75
3:B:340:ALA:CB	3:B:343:ILE:HD12	2.16	0.75
3:B:273:LEU:CB	3:B:276:ILE:HD12	2.16	0.75
2:A:34:LYS:NZ	2:A:57:ARG:NH1	2.28	0.75
2:A:351:THR:HG22	3:B:1103:ILE:HA	1.66	0.75
3:B:980:PHE:HE1	3:B:990:ILE:HD11	1.51	0.75
3:B:1087:PHE:HD2	3:B:1088:GLY:N	1.84	0.75
10:I:111:THR:HG22	10:I:112:SER:N	2.01	0.74
2:A:608:ILE:HB	2:A:613:ILE:HD11	1.69	0.74
3:B:1159:ARG:HB3	3:B:1159:ARG:HH11	1.52	0.74
3:B:770:GLN:CD	3:B:983:ARG:HA	2.06	0.74
2:A:816:HIS:CD2	3:B:764:SER:HB2	2.21	0.74
3:B:1115:THR:O	3:B:1116:ARG:HB2	1.88	0.74
4:C:38:ILE:HA	4:C:173:ALA:HB2	1.69	0.74
3:B:616:ILE:HG13	3:B:697:GLU:HG3	1.68	0.74
2:A:657:LEU:HD12	2:A:657:LEU:O	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:172:PRO:O	4:C:235:VAL:HG23	1.88	0.74
12:K:45:LEU:HG	12:K:94:ILE:HD13	1.69	0.74
2:A:500:GLU:OE2	2:A:1438:THR:HG21	1.88	0.74
2:A:283:GLY:O	2:A:285:PRO:HD3	1.87	0.74
3:B:847:ASP:HB3	4:C:167:HIS:CD2	2.22	0.74
2:A:901:LEU:HB2	2:A:926:GLN:HG2	1.69	0.74
9:H:102:TYR:OH	9:H:122:LEU:HD22	1.88	0.74
4:C:73:GLN:HB3	4:C:131:HIS:H	1.52	0.74
3:B:193:LYS:NZ	13:L:32:ALA:HB1	2.02	0.74
2:A:382:PRO:HB3	2:A:428:TYR:HE2	1.52	0.74
2:A:475:THR:HG23	2:A:476:SER:N	2.03	0.74
3:B:847:ASP:HB3	4:C:167:HIS:NE2	2.02	0.74
2:A:849:MET:CE	2:A:1061:GLY:HA2	2.18	0.74
11:J:48:ARG:HE	11:J:49:MET:HE2	1.51	0.73
2:A:24:PRO:HD2	2:A:233:TRP:HE1	1.50	0.73
3:B:583:ASN:ND2	3:B:628:THR:HG22	2.03	0.73
2:A:1152:ILE:HG22	2:A:1192:LEU:O	1.88	0.73
2:A:590:ARG:HD3	2:A:604:GLY:HA2	1.70	0.73
2:A:981:LEU:CD2	2:A:1039:LYS:HA	2.18	0.73
2:A:1004:ASN:ND2	6:E:167:ARG:HD2	2.03	0.73
3:B:1065:GLN:HE21	3:B:1067:ARG:H	1.36	0.73
12:K:47:ARG:HB3	12:K:47:ARG:NH1	1.99	0.73
5:D:40:HIS:CB	8:G:73:LYS:NZ	2.47	0.73
3:B:309:GLN:OE1	10:I:52:ILE:HD11	1.88	0.73
3:B:782:LEU:HD12	3:B:788:ARG:HH11	1.53	0.73
2:A:55:ASP:N	2:A:56:PRO:HD3	2.04	0.73
2:A:751:SER:O	2:A:752:LYS:HG2	1.88	0.73
2:A:567:LYS:HZ1	9:H:46:LEU:HB2	1.51	0.73
2:A:1447:GLU:OE2	8:G:23:LYS:HB2	1.89	0.73
4:C:213:PRO:O	4:C:214:ASN:HB2	1.88	0.73
2:A:845:LEU:HD22	2:A:1374:VAL:HG21	1.71	0.73
3:B:217:ARG:NE	3:B:405:ARG:HB2	2.03	0.73
2:A:182:VAL:HG22	2:A:201:VAL:HA	1.69	0.73
2:A:58:LEU:HD11	2:A:243:PRO:CB	2.19	0.73
12:K:65:HIS:CD2	12:K:67:PHE:H	2.07	0.73
3:B:37:PHE:HE1	3:B:41:LYS:HG3	1.52	0.73
2:A:1004:ASN:O	2:A:1008:GLN:HB2	1.89	0.73
13:L:39:SER:O	13:L:40:LEU:HG	1.88	0.73
2:A:738:LYS:HD2	2:A:740:LEU:HD21	1.69	0.73
11:J:3:VAL:HG21	11:J:18:TRP:CB	2.19	0.73
3:B:957:ASN:ND2	3:B:961:LEU:HD12	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:152:GLU:HG2	4:C:153:LEU:H	1.53	0.73
3:B:1166:CYS:HB2	3:B:1215:ARG:NH1	2.04	0.72
7:F:111:LEU:H	7:F:111:LEU:HD12	1.53	0.72
3:B:906:SER:HA	3:B:946:ASN:HB2	1.71	0.72
4:C:262:LEU:HD11	12:K:87:LEU:HD23	1.71	0.72
3:B:1159:ARG:NH1	3:B:1159:ARG:HB3	2.03	0.72
2:A:22:PHE:CD1	3:B:1213:THR:HG22	2.24	0.72
4:C:43:THR:O	4:C:77:ILE:HG13	1.89	0.72
3:B:979:LYS:HG2	3:B:1095:LEU:HD13	1.69	0.72
2:A:230:ARG:H	2:A:233:TRP:HE3	1.35	0.72
2:A:477:PRO:HG2	2:A:521:MET:HG2	1.71	0.72
2:A:528:LEU:HD23	2:A:751:SER:HB3	1.70	0.72
3:B:365:THR:HG23	3:B:367:LEU:H	1.54	0.72
3:B:1220:ARG:NH1	3:B:1220:ARG:HB3	2.05	0.72
2:A:1279:ILE:HD11	2:A:1316:VAL:HG21	1.71	0.72
2:A:1198:ASP:HB3	2:A:1201:ALA:HB3	1.70	0.72
4:C:3:GLU:O	4:C:4:GLU:HB2	1.88	0.72
2:A:709:THR:HB	2:A:712:GLU:HG3	1.72	0.72
4:C:251:LEU:O	4:C:251:LEU:HD12	1.89	0.72
3:B:825:VAL:HG12	3:B:826:ALA:N	2.03	0.72
3:B:708:GLU:O	3:B:710:LEU:N	2.22	0.72
3:B:467:GLY:H	3:B:475:SER:HB3	1.55	0.72
10:I:25:LEU:HB3	10:I:38:ALA:HB2	1.69	0.72
2:A:12:ARG:O	3:B:1194:ILE:HG22	1.88	0.72
12:K:21:ILE:HG23	12:K:31:VAL:HG11	1.71	0.72
6:E:213:ILE:HG12	6:E:214:CYS:H	1.53	0.72
3:B:1006:ILE:HD13	11:J:44:TYR:CE2	2.25	0.72
8:G:96:GLN:HG3	8:G:97:HIS:HD2	1.53	0.72
3:B:859:TYR:OH	3:B:941:LEU:HD12	1.90	0.72
3:B:363:HIS:O	3:B:364:ILE:HB	1.89	0.72
3:B:100:PRO:HD2	3:B:180:TYR:HE1	1.53	0.72
3:B:521:LEU:HB3	3:B:633:VAL:HG11	1.72	0.72
2:A:24:PRO:HD2	2:A:233:TRP:NE1	2.05	0.72
3:B:39:ARG:NH2	3:B:665:GLU:HG2	2.06	0.71
2:A:1254:ALA:O	2:A:1255:GLU:HB2	1.90	0.71
9:H:127:GLY:O	9:H:128:ASN:HB2	1.89	0.71
2:A:798:GLY:HA2	2:A:815:PHE:CD1	2.25	0.71
3:B:862:GLN:HG2	3:B:963:PHE:HD1	1.54	0.71
5:D:134:THR:HG22	5:D:135:GLY:N	2.05	0.71
3:B:1161:HIS:HB3	3:B:1171:VAL:HG11	1.72	0.71
2:A:567:LYS:HD3	9:H:95:TYR:CD2	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:15:ALA:O	6:E:19:VAL:HG23	1.91	0.71
3:B:1065:GLN:HE21	3:B:1067:ARG:N	1.87	0.71
3:B:756:ILE:O	3:B:759:PRO:HD3	1.90	0.71
12:K:111:LEU:HD12	12:K:112:GLN:NE2	2.05	0.71
3:B:1201:LYS:HE2	3:B:1205:GLN:OE1	1.90	0.71
7:F:89:GLU:O	7:F:93:ILE:HG13	1.91	0.71
3:B:746:SER:HB2	3:B:1046:PRO:HG2	1.73	0.71
3:B:312:GLU:O	3:B:315:LYS:HB2	1.91	0.71
3:B:955:THR:CG2	3:B:956:THR:N	2.53	0.71
3:B:53:GLN:HG2	3:B:547:VAL:HG22	1.71	0.71
6:E:207:ARG:HB2	6:E:207:ARG:HH11	1.55	0.71
2:A:53:LEU:CD2	2:A:54:ASN:H	1.93	0.71
3:B:589:VAL:HG12	3:B:590:HIS:N	2.04	0.71
3:B:1097:HIS:N	3:B:1098:MET:HE2	2.04	0.71
3:B:681:TRP:HA	3:B:684:LEU:HD13	1.72	0.71
3:B:825:VAL:CG1	3:B:826:ALA:H	2.03	0.71
2:A:23:SER:HA	2:A:233:TRP:NE1	2.06	0.71
3:B:1069:PHE:HD1	3:B:1069:PHE:H	1.38	0.71
11:J:57:ILE:HA	11:J:60:PHE:HD2	1.54	0.71
2:A:1329:THR:HG22	2:A:1331:SER:H	1.56	0.71
2:A:836:TYR:CE2	2:A:840:ARG:HD2	2.26	0.71
6:E:114:ASN:O	6:E:115:ASN:HB3	1.90	0.71
4:C:209:TYR:HD1	4:C:209:TYR:H	1.37	0.71
2:A:902:LEU:HG	2:A:926:GLN:HG3	1.71	0.71
2:A:1329:THR:HG22	2:A:1331:SER:N	2.06	0.71
3:B:1182:CYS:SG	3:B:1182:CYS:O	2.48	0.71
7:F:79:ARG:NH2	7:F:150:GLU:OE1	2.22	0.71
2:A:1343:ALA:HB2	6:E:150:VAL:HG22	1.73	0.71
8:G:23:LYS:HG3	8:G:56:ILE:CD1	2.21	0.70
2:A:339:ASN:HB3	3:B:1117:GLN:HE22	1.56	0.70
11:J:64:ASN:HD22	11:J:65:PRO:HD3	1.55	0.70
10:I:52:ILE:HG13	10:I:52:ILE:O	1.90	0.70
2:A:1324:PRO:HB2	6:E:142:VAL:HG11	1.72	0.70
3:B:233:PRO:HG2	3:B:234:ILE:HD12	1.73	0.70
4:C:66:ARG:NH2	11:J:3:VAL:O	2.24	0.70
3:B:216:GLU:OE1	3:B:537:LYS:HE2	1.91	0.70
3:B:983:ARG:HH11	3:B:1091:TYR:HB3	1.55	0.70
6:E:135:PHE:HB3	6:E:140:LEU:HD11	1.73	0.70
2:A:252:PHE:O	2:A:253:ASN:HB2	1.90	0.70
3:B:287:ARG:HG2	3:B:292:ILE:HA	1.71	0.70
3:B:35:SER:O	3:B:39:ARG:HG3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1323:ASP:OD1	2:A:1325:THR:HB	1.91	0.70
3:B:905:VAL:HG23	3:B:941:LEU:HD22	1.74	0.70
4:C:40:GLU:HA	4:C:163:ILE:CG2	2.21	0.70
3:B:601:ARG:O	3:B:605:ARG:HG3	1.90	0.70
2:A:855:THR:CG2	2:A:857:ARG:HE	2.05	0.70
2:A:1115:SER:HB3	2:A:1330:ASN:HD21	1.57	0.70
3:B:351:TYR:O	3:B:355:ILE:HG13	1.91	0.70
8:G:15:PRO:HA	8:G:18:PHE:CE1	2.25	0.70
7:F:119:ARG:HG3	7:F:119:ARG:HH11	1.56	0.70
6:E:23:VAL:O	6:E:28:TYR:HB2	1.92	0.70
2:A:842:VAL:HG11	3:B:1136:ASP:OD2	1.92	0.70
6:E:85:GLU:HB2	6:E:88:VAL:HG22	1.74	0.70
5:D:56:ARG:HB2	5:D:148:LEU:HD22	1.72	0.70
9:H:36:CYS:HA	9:H:126:GLU:O	1.92	0.69
4:C:203:GLN:HG2	4:C:207:CYS:SG	2.31	0.69
2:A:34:LYS:HG2	2:A:36:ARG:NH2	2.05	0.69
2:A:63:ARG:HA	2:A:74:MET:CE	2.22	0.69
3:B:976:ILE:O	3:B:990:ILE:HB	1.92	0.69
3:B:684:LEU:H	3:B:684:LEU:HD12	1.58	0.69
3:B:745:PRO:O	3:B:748:ILE:HG12	1.91	0.69
2:A:567:LYS:CB	2:A:568:PRO:HD2	2.21	0.69
3:B:1147:LEU:O	3:B:1151:LEU:HD13	1.92	0.69
2:A:92:HIS:O	2:A:94:GLY:N	2.26	0.69
2:A:1420:ASP:O	2:A:1421:CYS:HB2	1.93	0.69
3:B:467:GLY:H	3:B:475:SER:CB	2.06	0.69
2:A:416:ARG:C	2:A:417:TYR:HD2	1.95	0.69
2:A:1348:LEU:HG	2:A:1372:VAL:HG23	1.74	0.69
2:A:1211:GLN:O	2:A:1214:GLU:HB2	1.93	0.69
2:A:4:GLN:O	2:A:5:GLN:HB2	1.92	0.69
3:B:498:THR:CG2	3:B:537:LYS:HG3	2.22	0.69
2:A:1341:ILE:HD12	2:A:1379:GLY:O	1.92	0.69
6:E:153:HIS:HB3	6:E:196:VAL:CG1	2.22	0.69
2:A:1227:ILE:HG22	2:A:1228:TRP:N	2.07	0.69
2:A:679:ILE:HG12	2:A:732:LEU:HD12	1.75	0.69
2:A:53:LEU:HD22	2:A:54:ASN:ND2	2.04	0.69
2:A:42:ASP:HB3	2:A:45:GLN:H	1.57	0.69
3:B:642:ASP:HA	3:B:649:LYS:HA	1.75	0.69
2:A:526:ASP:HB2	3:B:835:GLN:OE1	1.92	0.69
3:B:294:ASP:O	3:B:296:GLU:N	2.24	0.69
10:I:7:CYS:HB2	10:I:34:TYR:CD1	2.28	0.69
3:B:125:SER:HA	3:B:171:PRO:HA	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:728:LYS:O	2:A:732:LEU:HG	1.91	0.69
2:A:1313:LEU:HD23	2:A:1338:VAL:HG21	1.73	0.69
4:C:98:VAL:O	4:C:99:LEU:HD22	1.93	0.69
3:B:579:ARG:HB2	3:B:586:TRP:HE1	1.56	0.69
10:I:101:PHE:HB2	10:I:110:PHE:CE2	2.28	0.69
2:A:903:ASN:ND2	2:A:904:THR:N	2.41	0.69
9:H:15:VAL:HG22	9:H:26:ILE:HG12	1.75	0.69
2:A:1436:ILE:HD13	3:B:1139:ILE:HG23	1.75	0.69
9:H:38:LEU:HD12	9:H:124:ARG:O	1.93	0.69
2:A:1153:TYR:CE1	10:I:42:LEU:HD13	2.28	0.69
6:E:179:GLN:HB2	6:E:182:ASP:HB2	1.75	0.69
2:A:345:VAL:HG23	2:A:346:ASP:O	1.92	0.69
3:B:654:ARG:HH11	3:B:654:ARG:HG3	1.58	0.69
2:A:1289:ARG:HD2	2:A:1303:GLU:OE2	1.93	0.69
11:J:23:ASN:C	11:J:25:LEU:H	1.95	0.69
4:C:166:GLU:HG3	12:K:10:PHE:CZ	2.26	0.68
2:A:1445:ILE:HG12	8:G:18:PHE:HE2	1.57	0.68
2:A:14:VAL:N	2:A:1432:GLN:HE22	1.89	0.68
2:A:1174:PHE:CA	2:A:1176:LEU:HG	2.19	0.68
1:R:3:A:H4'	2:A:447:GLN:NE2	2.07	0.68
3:B:637:LEU:O	3:B:690:VAL:HG13	1.92	0.68
4:C:212:PRO:HB3	4:C:213:PRO:HD2	1.74	0.68
3:B:424:LEU:O	3:B:428:ILE:HG13	1.93	0.68
8:G:14:HIS:ND1	8:G:15:PRO:HD2	2.09	0.68
2:A:457:ALA:HB3	2:A:506:ALA:HA	1.75	0.68
6:E:202:SER:OG	6:E:204:THR:HG22	1.94	0.68
10:I:105:SER:O	10:I:106:CYS:HB3	1.94	0.68
3:B:944:THR:HG21	3:B:1122:ARG:HH22	1.56	0.68
3:B:393:LYS:HE3	3:B:393:LYS:HA	1.74	0.68
4:C:99:LEU:HD12	4:C:118:LEU:HB3	1.76	0.68
2:A:855:THR:HG21	2:A:857:ARG:NE	2.09	0.68
3:B:1087:PHE:CD2	3:B:1088:GLY:N	2.62	0.68
2:A:135:PHE:CD1	2:A:222:LEU:HD22	2.29	0.68
2:A:1076:ALA:HA	2:A:1079:MET:CE	2.22	0.68
3:B:176:SER:O	3:B:182:SER:HB3	1.93	0.68
3:B:638:PHE:HB3	3:B:651:LEU:HD22	1.75	0.68
2:A:427:GLN:HG3	2:A:430:TRP:CZ2	2.29	0.68
8:G:96:GLN:HG3	8:G:97:HIS:CD2	2.28	0.68
4:C:148:ARG:HD3	4:C:149:LYS:HG3	1.75	0.68
2:A:1094:VAL:HG13	2:A:1113:THR:HG21	1.75	0.68
3:B:175:ARG:HH11	3:B:175:ARG:HG2	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:792:MET:HG3	3:B:855:PHE:HE1	1.59	0.68
3:B:172:ILE:HD13	3:B:178:ASN:HD22	1.58	0.68
3:B:856:PHE:HD2	3:B:967:ARG:HD2	1.58	0.68
3:B:244:LEU:HD21	3:B:366:GLN:NE2	2.09	0.68
5:D:153:ARG:HB3	5:D:154:PHE:CE1	2.29	0.68
2:A:858:ASN:ND2	2:A:860:LEU:H	1.92	0.68
5:D:4:SER:O	5:D:5:THR:HB	1.92	0.68
2:A:61:ILE:HG22	2:A:62:ASP:N	2.08	0.67
2:A:567:LYS:HB2	2:A:568:PRO:CD	2.24	0.67
3:B:975:GLN:O	3:B:990:ILE:HD12	1.93	0.67
3:B:1159:ARG:HE	3:B:1193:GLN:HE21	1.42	0.67
3:B:1162:ILE:HD11	3:B:1194:ILE:HD13	1.74	0.67
3:B:361:LEU:HD21	3:B:377:PHE:CD2	2.28	0.67
2:A:858:ASN:HD22	2:A:858:ASN:C	1.97	0.67
2:A:605:MET:HG2	2:A:621:THR:HG21	1.76	0.67
2:A:958:VAL:HG22	2:A:1052:GLN:HB3	1.77	0.67
9:H:102:TYR:N	9:H:102:TYR:CD2	2.62	0.67
3:B:39:ARG:HG2	3:B:39:ARG:HH11	1.59	0.67
4:C:6:PRO:HB2	12:K:101:LEU:HD12	1.76	0.67
2:A:1193:LEU:HB2	2:A:1260:LEU:HD11	1.76	0.67
3:B:563:MET:CE	3:B:580:VAL:HB	2.23	0.67
2:A:471:ASN:O	2:A:474:VAL:HG12	1.94	0.67
2:A:869:GLY:O	6:E:204:THR:HG21	1.94	0.67
3:B:23:ALA:HB1	3:B:24:PRO:HD2	1.76	0.67
3:B:799:PRO:HB3	3:B:818:PRO:HG2	1.77	0.67
3:B:333:PHE:O	3:B:337:ARG:HG2	1.94	0.67
5:D:56:ARG:HD3	5:D:149:THR:HA	1.75	0.67
2:A:34:LYS:HD3	2:A:57:ARG:NH2	2.10	0.67
12:K:47:ARG:CB	12:K:47:ARG:HH11	2.02	0.67
2:A:335:ARG:HA	2:A:339:ASN:HD22	1.59	0.67
2:A:1239:ARG:HH22	2:A:1241:ARG:NH2	1.92	0.67
4:C:40:GLU:HA	4:C:163:ILE:HG21	1.77	0.67
3:B:810:GLU:HB2	3:B:815:ARG:HH22	1.59	0.67
3:B:1097:HIS:H	3:B:1098:MET:CE	2.04	0.67
2:A:552:TRP:HE1	12:K:62:LYS:HB2	1.59	0.67
4:C:46:ILE:CG2	4:C:157:CYS:HB3	2.24	0.67
3:B:798:TYR:HE2	4:C:62:PHE:CZ	2.13	0.67
2:A:1341:ILE:HG23	2:A:1342:GLU:N	2.10	0.67
11:J:14:VAL:HG12	11:J:14:VAL:O	1.94	0.67
2:A:1015:VAL:HG12	2:A:1019:CYS:SG	2.35	0.67
2:A:528:LEU:O	2:A:531:ILE:HG22	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:172:PRO:HD3	2:A:185:TRP:NE1	2.09	0.67
2:A:547:LEU:HD22	12:K:58:PHE:CE1	2.30	0.67
2:A:828:ALA:CB	3:B:530:GLY:HA2	2.25	0.67
2:A:12:ARG:HD2	3:B:1218:THR:HB	1.77	0.67
2:A:1291:VAL:HG13	2:A:1292:PRO:HD2	1.77	0.67
2:A:1450:LEU:HG	2:A:1450:LEU:O	1.95	0.67
3:B:778:MET:CE	3:B:1094:ARG:HD3	2.25	0.67
2:A:269:ILE:HD11	2:A:300:VAL:HA	1.77	0.67
2:A:899:VAL:HB	2:A:929:LEU:CD1	2.25	0.67
2:A:84:ILE:HD11	2:A:270:LEU:HD22	1.76	0.67
3:B:181:LEU:HD22	3:B:189:LEU:HD22	1.77	0.66
2:A:984:LYS:O	2:A:988:LEU:HB2	1.95	0.66
3:B:1177:HIS:HB2	3:B:1179:GLN:HE21	1.59	0.66
3:B:57:TYR:HD1	3:B:57:TYR:N	1.93	0.66
3:B:100:PRO:HD2	3:B:180:TYR:CE1	2.29	0.66
3:B:1006:ILE:HD13	11:J:44:TYR:HE2	1.61	0.66
6:E:145:THR:HG21	6:E:187:TYR:CE2	2.29	0.66
2:A:443:LEU:HD21	2:A:455:MET:HB3	1.77	0.66
3:B:121:ASN:HA	3:B:207:GLY:HA2	1.75	0.66
2:A:114:LEU:HD13	2:A:171:GLN:NE2	2.05	0.66
2:A:463:ILE:HD11	2:A:469:ARG:HG3	1.77	0.66
2:A:164:ARG:HG3	2:A:165:GLY:N	2.11	0.66
5:D:189:ASP:O	5:D:193:THR:HB	1.95	0.66
2:A:7:SER:HB2	3:B:1175:LEU:HD22	1.77	0.66
6:E:28:TYR:HE1	6:E:78:LEU:HD13	1.60	0.66
2:A:1198:ASP:O	2:A:1202:MET:HG2	1.96	0.66
9:H:40:LEU:HD13	9:H:123:MET:HE3	1.77	0.66
3:B:118:ARG:HG2	3:B:204:ILE:HD13	1.77	0.66
2:A:50:ILE:C	2:A:52:GLY:H	1.98	0.66
3:B:1197:PRO:HG2	3:B:1200:ALA:CB	2.24	0.66
3:B:611:PRO:HB3	3:B:685:LEU:HD11	1.78	0.66
6:E:177:ARG:HD3	6:E:215:MET:HG3	1.77	0.66
2:A:567:LYS:CB	9:H:95:TYR:HA	2.25	0.66
7:F:69:LEU:HD23	7:F:71:GLU:HB3	1.74	0.66
3:B:1161:HIS:NE2	3:B:1175:LEU:HD21	2.11	0.66
2:A:14:VAL:HG21	3:B:1216:LEU:HD12	1.78	0.66
2:A:262:LEU:HD12	2:A:328:ARG:NH2	2.10	0.66
2:A:49:LYS:HZ1	2:A:61:ILE:N	1.94	0.66
6:E:153:HIS:HB3	6:E:196:VAL:HG11	1.76	0.66
3:B:880:THR:O	3:B:881:ASN:HB2	1.94	0.66
3:B:502:ILE:H	3:B:502:ILE:HD12	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:69:THR:C	2:A:71:GLN:H	1.99	0.66
2:A:37:PHE:HB2	2:A:52:GLY:HA3	1.78	0.66
11:J:1:MET:N	11:J:56:LEU:N	2.43	0.66
2:A:472:LEU:O	2:A:475:THR:HG22	1.95	0.66
3:B:957:ASN:O	3:B:959:ASP:N	2.29	0.66
2:A:683:ILE:HG21	2:A:801:GLU:HG3	1.78	0.66
2:A:1319:VAL:HG13	2:A:1320:PRO:HD2	1.78	0.66
2:A:152:VAL:CG1	2:A:153:PRO:HD2	2.26	0.66
2:A:58:LEU:CD1	2:A:59:GLY:N	2.53	0.65
2:A:356:ASP:HB2	2:A:469:ARG:HH11	1.59	0.65
2:A:134:ARG:O	2:A:138:ILE:HG13	1.96	0.65
2:A:202:LEU:HB3	2:A:207:ILE:HD11	1.79	0.65
3:B:98:THR:O	3:B:126:SER:HB2	1.97	0.65
3:B:825:VAL:HG13	3:B:826:ALA:H	1.61	0.65
2:A:1116:LEU:N	2:A:1308:THR:HG22	2.11	0.65
2:A:981:LEU:HD21	2:A:1038:THR:O	1.97	0.65
2:A:34:LYS:O	2:A:35:ILE:HB	1.97	0.65
3:B:882:THR:HG22	3:B:884:ARG:HB2	1.77	0.65
2:A:901:LEU:HD22	2:A:919:ILE:HG22	1.78	0.65
2:A:1116:LEU:HB3	2:A:1308:THR:HG21	1.78	0.65
2:A:90:VAL:CG1	2:A:297:GLN:HA	2.27	0.65
9:H:4:THR:CA	9:H:60:ALA:HB2	2.22	0.65
3:B:1187:ASN:O	3:B:1188:LYS:HB2	1.96	0.65
3:B:642:ASP:HB3	3:B:649:LYS:CD	2.26	0.65
9:H:81:PRO:CB	9:H:82:PRO:HD2	2.26	0.65
3:B:828:ALA:HB2	3:B:1085:ILE:CG2	2.25	0.65
2:A:302:THR:HG22	2:A:303:TYR:N	2.12	0.65
2:A:913:LEU:HD12	2:A:914:GLU:N	2.10	0.65
13:L:49:LYS:O	13:L:50:ASP:HB2	1.97	0.65
3:B:950:ASP:O	3:B:951:GLN:HB2	1.96	0.65
3:B:526:GLU:HG2	3:B:538:ASN:HD22	1.61	0.65
5:D:48:ILE:HG21	8:G:4:ILE:HB	1.79	0.65
11:J:63:TYR:O	11:J:64:ASN:HB2	1.96	0.65
3:B:1159:ARG:NE	3:B:1193:GLN:HE21	1.95	0.65
2:A:709:THR:HG22	2:A:711:ARG:N	2.03	0.65
2:A:1325:THR:O	6:E:148:GLU:HB2	1.96	0.65
3:B:821:GLN:NE2	3:B:851:PHE:HA	2.12	0.65
8:G:61:ILE:HG23	8:G:66:GLY:O	1.97	0.65
9:H:130:ARG:CB	9:H:133:ASN:HB2	2.26	0.65
3:B:579:ARG:HH11	3:B:579:ARG:HG2	1.62	0.65
3:B:955:THR:HG22	3:B:956:THR:N	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:253:ASN:HB3	3:B:935:ARG:CZ	2.26	0.65
2:A:41:MET:HB3	2:A:49:LYS:CA	2.20	0.65
8:G:1:MET:O	8:G:3:PHE:CE1	2.50	0.65
2:A:1370:LEU:O	2:A:1374:VAL:HG23	1.96	0.65
3:B:1096:ARG:O	3:B:1097:HIS:HB2	1.96	0.65
2:A:1209:MET:SD	2:A:1236:LEU:HD22	2.37	0.65
13:L:27:LEU:HD13	13:L:37:LYS:HE2	1.79	0.65
2:A:886:ILE:HG22	2:A:887:GLY:N	2.12	0.65
6:E:17:ARG:O	6:E:21:GLU:HG3	1.97	0.64
2:A:1348:LEU:O	2:A:1352:VAL:HG23	1.96	0.64
3:B:39:ARG:HH21	3:B:665:GLU:CD	2.01	0.64
8:G:81:PRO:HG3	8:G:106:MET:SD	2.37	0.64
2:A:49:LYS:HZ1	2:A:61:ILE:HG13	1.59	0.64
2:A:590:ARG:NH2	2:A:620:LYS:CB	2.60	0.64
9:H:113:ALA:HB2	9:H:126:GLU:HG3	1.78	0.64
2:A:560:ILE:HG13	9:H:78:SER:HB2	1.79	0.64
5:D:33:PHE:HB3	5:D:47:LEU:HD21	1.79	0.64
2:A:1166:ASP:OD2	2:A:1239:ARG:HD2	1.96	0.64
3:B:288:ALA:HA	3:B:331:LEU:HD12	1.79	0.64
3:B:464:GLY:HA2	3:B:479:VAL:O	1.97	0.64
12:K:93:SER:O	12:K:97:LYS:HG3	1.97	0.64
11:J:44:TYR:HD2	11:J:44:TYR:N	1.95	0.64
2:A:138:ILE:CD1	2:A:222:LEU:HD23	2.27	0.64
3:B:516:ASN:ND2	3:B:516:ASN:N	2.46	0.64
6:E:24:LYS:HB3	6:E:30:ILE:HD12	1.79	0.64
2:A:590:ARG:NH2	2:A:620:LYS:HB2	2.12	0.64
5:D:134:THR:HG22	5:D:135:GLY:H	1.60	0.64
3:B:289:LEU:HD13	3:B:375:ALA:HB2	1.78	0.64
2:A:1074:GLU:C	2:A:1076:ALA:H	2.00	0.64
3:B:1084:GLN:NE2	3:B:1084:GLN:H	1.94	0.64
2:A:311:GLN:O	2:A:312:PRO:C	2.35	0.64
5:D:33:PHE:CE2	8:G:80:LYS:NZ	2.65	0.64
2:A:1332:PHE:N	2:A:1332:PHE:CD2	2.65	0.64
3:B:1065:GLN:HB2	4:C:201:TRP:CZ3	2.32	0.64
2:A:808:LEU:HD23	2:A:813:PHE:HA	1.78	0.64
4:C:67:LEU:HD11	4:C:155:LEU:CD1	2.28	0.64
3:B:906:SER:O	3:B:941:LEU:HD23	1.98	0.64
13:L:53:HIS:O	13:L:55:ILE:HG12	1.97	0.64
9:H:89:LEU:C	9:H:91:ASP:H	2.00	0.64
3:B:171:PRO:HD2	3:B:457:LEU:CD1	2.28	0.64
6:E:124:VAL:HB	6:E:125:PRO:HD3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1445:ILE:HG12	8:G:18:PHE:CE2	2.32	0.64
8:G:128:PRO:O	8:G:138:THR:HG23	1.97	0.64
11:J:64:ASN:CB	11:J:65:PRO:CD	2.75	0.64
3:B:840:ILE:HD13	3:B:994:TYR:HE1	1.61	0.64
4:C:107:SER:O	4:C:109:SER:N	2.30	0.64
5:D:119:ARG:HD3	5:D:221:TYR:CD2	2.33	0.64
2:A:34:LYS:CG	2:A:36:ARG:HH21	2.11	0.64
2:A:35:ILE:HA	2:A:52:GLY:O	1.97	0.64
9:H:59:ILE:HG22	9:H:60:ALA:H	1.62	0.64
3:B:583:ASN:HD21	3:B:628:THR:CG2	2.08	0.64
4:C:17:ASN:N	4:C:240:VAL:HG11	2.12	0.64
8:G:145:VAL:HG12	8:G:146:LYS:N	2.11	0.64
3:B:995:ARG:HH12	4:C:165:LYS:HG2	1.62	0.64
4:C:66:ARG:HH21	11:J:5:VAL:H	1.46	0.64
4:C:36:VAL:HG21	4:C:251:LEU:HB2	1.79	0.64
3:B:23:ALA:H	3:B:654:ARG:HB3	1.63	0.64
4:C:100:THR:HG22	4:C:101:LEU:H	1.63	0.64
5:D:145:MET:O	5:D:149:THR:HB	1.98	0.64
2:A:463:ILE:CD1	2:A:469:ARG:HG3	2.28	0.64
6:E:180:ARG:NH2	6:E:192:ARG:HB2	2.12	0.64
2:A:351:THR:HB	3:B:1103:ILE:CD1	2.28	0.64
2:A:353:ILE:HD13	2:A:487:MET:HE2	1.80	0.64
8:G:143:ILE:CG2	8:G:144:ARG:H	2.11	0.64
3:B:171:PRO:HD2	3:B:457:LEU:HD13	1.79	0.64
2:A:12:ARG:NE	3:B:1192:TYR:HE2	1.96	0.64
12:K:53:ASP:OD1	12:K:55:LYS:HB2	1.98	0.64
8:G:117:GLN:C	8:G:119:LEU:H	2.01	0.64
3:B:181:LEU:HD22	3:B:189:LEU:CD2	2.28	0.63
2:A:341:MET:HE1	3:B:1135:ARG:NH1	2.13	0.63
7:F:111:LEU:C	7:F:113:GLY:H	2.00	0.63
2:A:445:ASN:HB2	2:A:454:SER:O	1.97	0.63
10:I:26:LEU:HD23	10:I:37:GLU:HA	1.80	0.63
8:G:153:GLN:HG2	8:G:154:VAL:HG23	1.80	0.63
8:G:122:ASN:ND2	8:G:125:SER:HB3	2.13	0.63
2:A:981:LEU:HD23	2:A:1039:LYS:HA	1.79	0.63
9:H:100:THR:HG22	9:H:101:ALA:N	2.14	0.63
4:C:77:ILE:HA	4:C:129:ILE:HD11	1.79	0.63
6:E:169:ARG:HH12	7:F:74:ILE:HD11	1.63	0.63
4:C:244:VAL:O	4:C:248:ILE:HG13	1.96	0.63
2:A:960:ILE:O	2:A:963:ILE:HG22	1.99	0.63
12:K:31:VAL:HG12	12:K:32:VAL:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:69:LEU:HD13	3:B:429:PHE:HD1	1.63	0.63
2:A:567:LYS:HB3	9:H:95:TYR:HA	1.81	0.63
2:A:868:TYR:CE1	2:A:1064:VAL:HG11	2.33	0.63
3:B:313:MET:O	3:B:316:PRO:HD2	1.99	0.63
2:A:694:THR:O	2:A:698:GLN:HG3	1.99	0.63
2:A:50:ILE:O	2:A:52:GLY:N	2.31	0.63
5:D:39:ASN:HD22	5:D:41:GLN:HB2	1.64	0.63
11:J:1:MET:H1	11:J:56:LEU:N	1.95	0.63
2:A:567:LYS:HB2	2:A:568:PRO:HD2	1.80	0.63
10:I:111:THR:CG2	10:I:112:SER:H	2.10	0.63
11:J:14:VAL:CG1	11:J:50:ILE:HD11	2.28	0.63
3:B:1163:CYS:SG	3:B:1165:ILE:HB	2.38	0.63
2:A:19:PHE:O	2:A:1416:ALA:HA	1.99	0.63
2:A:1323:ASP:C	2:A:1325:THR:H	2.02	0.63
3:B:850:LEU:HD12	3:B:851:PHE:N	2.14	0.63
5:D:53:SER:H	5:D:148:LEU:CD2	2.12	0.63
3:B:707:PRO:HG2	3:B:708:GLU:H	1.64	0.63
4:C:253:LYS:O	4:C:256:ALA:HB3	1.98	0.63
7:F:125:LEU:O	7:F:125:LEU:HG	1.98	0.63
9:H:41:ASP:O	9:H:42:ILE:HG13	1.99	0.63
2:A:1332:PHE:HD2	2:A:1332:PHE:N	1.97	0.63
2:A:767:GLN:NE2	2:A:774:ARG:HB3	2.13	0.63
2:A:477:PRO:CG	2:A:521:MET:HG2	2.29	0.63
2:A:1313:LEU:O	2:A:1315:GLU:N	2.32	0.63
4:C:182:PRO:HG3	4:C:206:ASN:O	1.98	0.63
2:A:1333:ILE:HD13	2:A:1381:LEU:HD12	1.80	0.63
2:A:1006:ILE:CD1	6:E:163:GLU:HG3	2.29	0.63
8:G:51:TYR:O	8:G:54:ILE:HG13	1.99	0.63
8:G:45:ILE:HA	8:G:78:VAL:HG12	1.80	0.63
3:B:899:ILE:CD1	3:B:911:ILE:HA	2.29	0.63
9:H:89:LEU:O	9:H:91:ASP:N	2.28	0.63
8:G:91:VAL:HA	8:G:101:VAL:HA	1.80	0.63
2:A:353:ILE:HG21	2:A:487:MET:CE	2.28	0.63
9:H:62:SER:C	9:H:64:ASN:H	2.01	0.63
2:A:138:ILE:HD13	2:A:222:LEU:HD23	1.80	0.63
2:A:382:PRO:HD3	2:A:428:TYR:CD2	2.34	0.63
6:E:55:ARG:C	6:E:57:MET:H	2.02	0.63
3:B:112:LEU:HD12	3:B:113:TYR:H	1.63	0.63
3:B:192:LEU:O	3:B:193:LYS:HB2	1.99	0.63
2:A:866:PHE:C	2:A:867:ILE:HD12	2.18	0.63
2:A:973:ILE:HG21	2:A:1036:ARG:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:416:ARG:O	2:A:417:TYR:HD2	1.82	0.63
2:A:248:PRO:O	2:A:260:ASP:HB2	1.99	0.63
3:B:758:PHE:HB3	3:B:761:HIS:CD2	2.34	0.62
5:D:71:LYS:HA	5:D:74:GLN:HB2	1.80	0.62
2:A:971:PHE:HE2	2:A:1040:GLN:HG2	1.63	0.62
5:D:47:LEU:HD11	8:G:3:PHE:CE2	2.34	0.62
12:K:90:ALA:O	12:K:94:ILE:HG13	1.99	0.62
11:J:44:TYR:N	11:J:44:TYR:CD2	2.66	0.62
2:A:896:ARG:HD3	2:A:897:TYR:CE1	2.34	0.62
3:B:57:TYR:CD1	3:B:57:TYR:N	2.64	0.62
2:A:781:ASP:O	2:A:789:LYS:HA	1.99	0.62
2:A:852:TYR:CD2	2:A:1060:PRO:HB2	2.34	0.62
3:B:525:ALA:O	3:B:768:THR:HG23	1.99	0.62
7:F:97:ARG:O	7:F:101:ILE:HG13	1.99	0.62
2:A:269:ILE:CD1	2:A:300:VAL:HG22	2.27	0.62
3:B:999:MET:HG2	3:B:1007:VAL:HG22	1.81	0.62
3:B:1178:ASN:O	3:B:1180:PHE:CD1	2.52	0.62
3:B:886:LYS:HE2	3:B:936:ASP:OD1	1.98	0.62
2:A:647:GLY:O	2:A:651:LYS:HG3	2.00	0.62
3:B:1099:VAL:CG1	3:B:1100:ASP:N	2.62	0.62
2:A:68:GLN:C	2:A:70:CYS:H	2.02	0.62
11:J:7:CYS:SG	11:J:49:MET:HE3	2.39	0.62
2:A:458:HIS:CE1	2:A:507:VAL:HG21	2.34	0.62
2:A:2:VAL:HG21	3:B:1157:ALA:CB	2.24	0.62
6:E:176:PRO:O	6:E:212:ARG:HA	1.99	0.62
2:A:446:ARG:HD3	2:A:480:ALA:HB2	1.80	0.62
3:B:294:ASP:HB2	10:I:12:ASN:HA	1.81	0.62
2:A:578:LEU:HD23	2:A:612:ILE:CD1	2.29	0.62
3:B:46:GLN:HG3	3:B:47:GLN:H	1.63	0.62
2:A:1373:ASP:CA	2:A:1376:THR:HG22	2.25	0.62
2:A:798:GLY:HA2	2:A:815:PHE:HD1	1.65	0.62
7:F:69:LEU:HD13	7:F:72:LYS:CB	2.29	0.62
6:E:28:TYR:CE1	6:E:78:LEU:HD13	2.34	0.62
3:B:387:LEU:O	3:B:392:ARG:HB2	2.00	0.62
8:G:28:THR:O	8:G:32:GLU:HG3	1.99	0.62
2:A:33:ALA:HB1	2:A:56:PRO:HB2	1.81	0.62
9:H:25:ARG:HA	9:H:41:ASP:HA	1.81	0.62
2:A:471:ASN:OD1	2:A:472:LEU:N	2.33	0.62
2:A:993:LEU:HD23	2:A:1022:LEU:HD21	1.82	0.62
2:A:321:PRO:O	2:A:322:VAL:HB	1.99	0.62
4:C:147:LEU:HD23	4:C:147:LEU:N	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:100:THR:HG22	4:C:101:LEU:N	2.15	0.62
2:A:857:ARG:HD3	2:A:861:GLY:O	2.00	0.62
2:A:979:SER:OG	2:A:980:ASP:N	2.32	0.62
5:D:63:LEU:HD12	5:D:129:LEU:HG	1.80	0.62
8:G:138:THR:HG22	8:G:139:ILE:HG13	1.80	0.62
2:A:399:HIS:CB	2:A:400:PRO:HD3	2.28	0.62
6:E:46:TYR:CD2	6:E:58:MET:HG2	2.34	0.62
2:A:1115:SER:O	2:A:1311:VAL:HG22	1.99	0.62
2:A:470:LEU:HD22	2:A:487:MET:CE	2.29	0.62
2:A:446:ARG:HD2	2:A:480:ALA:HB2	1.81	0.62
6:E:207:ARG:CB	6:E:207:ARG:HH11	2.13	0.62
3:B:44:VAL:CG1	3:B:199:MET:HG2	2.30	0.62
2:A:535:THR:CG2	2:A:616:VAL:HA	2.23	0.62
2:A:1445:ILE:H	2:A:1445:ILE:CD1	2.09	0.62
3:B:616:ILE:N	3:B:616:ILE:HD12	2.14	0.62
6:E:178:ILE:HG22	6:E:213:ILE:O	1.99	0.62
5:D:159:THR:O	5:D:163:VAL:HG23	1.98	0.62
2:A:34:LYS:HZ2	2:A:57:ARG:NH2	1.97	0.61
3:B:800:GLN:HB3	11:J:52:THR:HG21	1.80	0.61
3:B:821:GLN:HE22	3:B:851:PHE:HA	1.63	0.61
2:A:382:PRO:CB	2:A:428:TYR:HE2	2.13	0.61
8:G:83:LYS:HG2	8:G:149:GLY:HA2	1.81	0.61
7:F:103:MET:O	7:F:104:ASN:HB2	1.98	0.61
2:A:282:ASN:O	2:A:284:ALA:N	2.33	0.61
3:B:278:GLN:HG2	3:B:279:ASP:H	1.65	0.61
3:B:615:MET:HB3	3:B:626:ILE:HG12	1.82	0.61
8:G:47:CYS:O	8:G:76:ALA:HB1	2.00	0.61
3:B:360:PHE:CD2	3:B:361:LEU:HB2	2.35	0.61
2:A:858:ASN:ND2	2:A:861:GLY:H	1.99	0.61
3:B:126:SER:O	3:B:169:ARG:HA	2.00	0.61
6:E:198:ILE:CD1	6:E:212:ARG:HG3	2.30	0.61
3:B:873:THR:O	3:B:914:LYS:HA	2.00	0.61
2:A:743:VAL:O	2:A:747:VAL:HG23	1.99	0.61
11:J:57:ILE:HA	11:J:60:PHE:CD2	2.35	0.61
8:G:26:LEU:HD12	8:G:56:ILE:HG21	1.82	0.61
6:E:169:ARG:HB3	7:F:140:ASP:OD2	2.00	0.61
2:A:372:LYS:HA	2:A:435:HIS:ND1	2.14	0.61
2:A:1349:TYR:HB2	2:A:1372:VAL:HG21	1.80	0.61
2:A:84:ILE:HG23	2:A:84:ILE:O	2.00	0.61
2:A:222:LEU:O	2:A:224:PHE:HD1	1.83	0.61
3:B:1166:CYS:HB2	3:B:1215:ARG:HH12	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:69:THR:C	2:A:71:GLN:N	2.53	0.61
9:H:44:VAL:HG12	9:H:44:VAL:O	2.00	0.61
3:B:172:ILE:CD1	3:B:178:ASN:HD22	2.13	0.61
3:B:1072:MET:HE1	3:B:1085:ILE:HB	1.82	0.61
6:E:213:ILE:HG12	6:E:214:CYS:N	2.15	0.61
4:C:184:ASN:ND2	4:C:187:LYS:HA	2.15	0.61
8:G:119:LEU:HD12	8:G:131:GLN:O	2.00	0.61
2:A:298:PHE:HZ	2:A:314:ALA:HB2	1.66	0.61
2:A:1444:MET:HG2	8:G:60:ARG:CA	2.29	0.61
4:C:7:GLN:HG2	12:K:104:ASN:ND2	2.14	0.61
12:K:42:LEU:HD21	12:K:46:ILE:HD11	1.82	0.61
8:G:14:HIS:CD2	8:G:16:SER:HB2	2.35	0.61
4:C:11:ARG:NH2	4:C:229:TYR:HB3	2.15	0.61
3:B:797:TYR:O	11:J:1:MET:HG2	2.00	0.61
2:A:458:HIS:HE2	2:A:478:TYR:HH	1.47	0.61
10:I:55:THR:HG23	10:I:86:PHE:HZ	1.65	0.61
2:A:24:PRO:HB3	2:A:237:THR:HB	1.82	0.61
2:A:18:GLN:O	3:B:1215:ARG:HG2	2.01	0.61
3:B:1084:GLN:NE2	3:B:1084:GLN:N	2.49	0.61
2:A:720:ARG:O	2:A:724:GLU:HB2	2.01	0.61
2:A:567:LYS:CB	2:A:568:PRO:CD	2.78	0.61
9:H:102:TYR:H	9:H:102:TYR:HD2	1.45	0.61
2:A:863:VAL:HG11	2:A:866:PHE:CE2	2.36	0.61
6:E:78:LEU:HD21	6:E:80:VAL:HG23	1.81	0.61
2:A:450:LEU:HD12	2:A:450:LEU:H	1.66	0.61
3:B:378:LEU:O	3:B:378:LEU:HD12	2.00	0.61
13:L:38:LEU:O	13:L:39:SER:HB3	2.00	0.61
12:K:21:ILE:HG12	12:K:33:ILE:HG12	1.82	0.61
2:A:596:THR:O	2:A:598:LEU:N	2.33	0.61
3:B:498:THR:HG21	3:B:537:LYS:HG3	1.81	0.61
2:A:16:GLU:HB3	2:A:1418:LEU:HD11	1.83	0.61
2:A:22:PHE:CE1	3:B:1213:THR:HG22	2.36	0.61
2:A:451:HIS:CD2	2:A:1074:GLU:HG3	2.36	0.61
3:B:305:VAL:O	3:B:305:VAL:HG12	2.01	0.61
8:G:4:ILE:HG12	8:G:77:VAL:HG22	1.83	0.61
4:C:61:GLU:HA	4:C:64:ALA:HB3	1.83	0.61
11:J:16:ASP:OD1	11:J:17:LYS:HD2	2.01	0.61
2:A:598:LEU:HD22	9:H:25:ARG:NH1	2.15	0.61
3:B:220:GLY:O	3:B:222:ILE:HG13	2.01	0.61
2:A:458:HIS:NE2	2:A:478:TYR:OH	2.31	0.61
4:C:73:GLN:NE2	4:C:75:MET:HB2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:842:ASN:ND2	3:B:845:SER:H	1.99	0.61
2:A:826:ASP:O	2:A:830:LYS:HB2	2.01	0.61
2:A:567:LYS:HD3	9:H:95:TYR:CG	2.35	0.60
4:C:191:TYR:HD2	4:C:201:TRP:CD1	2.19	0.60
2:A:511:ILE:HA	2:A:521:MET:HE3	1.82	0.60
2:A:622:VAL:HG13	2:A:622:VAL:O	2.01	0.60
2:A:58:LEU:HD11	2:A:243:PRO:HB3	1.82	0.60
2:A:105:CYS:O	2:A:114:LEU:HG	2.00	0.60
3:B:102:VAL:CG2	3:B:112:LEU:HD22	2.31	0.60
2:A:567:LYS:CE	9:H:46:LEU:HB2	2.31	0.60
2:A:442:VAL:HB	2:A:489:LEU:HD11	1.83	0.60
3:B:180:TYR:HD1	3:B:180:TYR:H	1.49	0.60
3:B:1011:ILE:O	3:B:1011:ILE:HG22	2.00	0.60
2:A:870:GLU:HG2	6:E:208:TYR:CG	2.36	0.60
2:A:1002:GLY:HA3	2:A:1007:ILE:HG21	1.82	0.60
2:A:1290:LYS:O	2:A:1291:VAL:HG23	2.01	0.60
3:B:215:GLN:OE1	3:B:479:VAL:HG22	2.01	0.60
2:A:821:ARG:HB2	2:A:821:ARG:NH1	2.16	0.60
3:B:653:VAL:CG2	3:B:689:LEU:HB3	2.31	0.60
2:A:1130:GLN:HA	2:A:1133:LEU:HD12	1.83	0.60
4:C:128:ASN:O	4:C:129:ILE:HG13	2.01	0.60
2:A:239:LEU:HD12	2:A:240:PRO:HD2	1.83	0.60
4:C:232:VAL:HG21	4:C:244:VAL:HG22	1.83	0.60
13:L:38:LEU:CD1	13:L:49:LYS:HE2	2.31	0.60
2:A:317:LYS:O	2:A:318:SER:HB3	2.02	0.60
2:A:1336:MET:HE3	2:A:1381:LEU:HG	1.83	0.60
2:A:565:ILE:O	2:A:570:PRO:HA	2.01	0.60
3:B:882:THR:HG21	3:B:884:ARG:HB2	1.84	0.60
4:C:34:ARG:O	4:C:38:ILE:HG13	2.02	0.60
3:B:1016:ALA:O	3:B:1020:ARG:HG3	2.01	0.60
3:B:563:MET:HE1	3:B:580:VAL:HB	1.84	0.60
4:C:43:THR:CG2	4:C:44:LEU:H	1.98	0.60
3:B:859:TYR:CZ	3:B:941:LEU:HD12	2.37	0.60
10:I:58:VAL:HG13	10:I:62:ILE:CD1	2.31	0.60
3:B:282:ILE:HD12	3:B:382:ILE:HD13	1.84	0.60
6:E:147:HIS:HD2	6:E:149:LEU:HB2	1.67	0.60
3:B:190:TYR:CD2	11:J:62:ARG:HB3	2.37	0.60
7:F:68:THR:HG21	7:F:69:LEU:CA	2.31	0.60
4:C:62:PHE:O	4:C:66:ARG:HG3	2.00	0.60
3:B:766:ARG:NH2	3:B:1020:ARG:HD3	2.16	0.60
2:A:135:PHE:HD1	2:A:222:LEU:HD22	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:18:VAL:CG2	4:C:240:VAL:HB	2.31	0.60
2:A:1063:MET:CG	2:A:1436:ILE:HG23	2.32	0.60
3:B:233:PRO:HG2	3:B:234:ILE:CD1	2.31	0.60
4:C:76:ASP:OD2	4:C:128:ASN:N	2.34	0.60
3:B:826:ALA:HB2	3:B:1008:PRO:HB3	1.84	0.60
2:A:1017:LEU:HB3	6:E:205:SER:HA	1.83	0.60
4:C:18:VAL:O	4:C:20:PHE:HD2	1.85	0.60
4:C:214:ASN:HB3	4:C:217:ASP:OD2	2.00	0.60
3:B:955:THR:HG22	3:B:956:THR:O	2.01	0.60
3:B:1180:PHE:O	3:B:1181:GLU:O	2.19	0.60
2:A:265:LYS:HD3	2:A:322:VAL:HG11	1.83	0.60
5:D:188:ALA:O	5:D:192:LYS:HG3	2.02	0.60
2:A:1428:VAL:HG13	3:B:1151:LEU:HD21	1.82	0.60
2:A:863:VAL:HG11	2:A:866:PHE:CD2	2.37	0.60
2:A:857:ARG:NH1	7:F:139:PRO:HB2	2.16	0.60
2:A:466:SER:O	3:B:1103:ILE:HD11	2.01	0.60
8:G:106:MET:HG2	8:G:107:LYS:N	2.17	0.60
3:B:874:PHE:HA	3:B:913:GLY:O	2.02	0.60
5:D:40:HIS:CE1	5:D:41:GLN:HG3	2.37	0.60
2:A:340:LEU:HD13	2:A:1429:ILE:CG2	2.26	0.60
6:E:84:ASP:O	6:E:86:PRO:HD3	2.02	0.60
3:B:642:ASP:HB3	3:B:649:LYS:CG	2.32	0.60
3:B:346:GLU:O	3:B:350:GLN:HB2	2.02	0.60
12:K:7:PHE:HA	12:K:10:PHE:CE2	2.37	0.59
2:A:1173:HIS:O	2:A:1176:LEU:CD2	2.48	0.59
2:A:1208:THR:HG22	2:A:1210:GLY:N	2.16	0.59
9:H:64:ASN:O	9:H:65:LEU:HB2	2.01	0.59
2:A:504:LEU:HD11	7:F:91:ALA:HB1	1.83	0.59
12:K:55:LYS:HB3	12:K:81:TYR:CD1	2.37	0.59
10:I:19:ASP:OD1	10:I:22:ASN:HB2	2.02	0.59
10:I:33:SER:O	10:I:35:VAL:HG23	2.01	0.59
11:J:9:SER:HB2	11:J:45:CYS:HB2	1.85	0.59
2:A:450:LEU:HB3	2:A:838:GLN:NE2	2.16	0.59
2:A:590:ARG:O	2:A:591:PHE:HB2	2.00	0.59
2:A:613:ILE:O	2:A:614:PHE:HB3	2.01	0.59
6:E:207:ARG:HB2	6:E:207:ARG:NH1	2.16	0.59
2:A:685:GLU:HG3	2:A:686:ALA:N	2.17	0.59
2:A:166:GLY:O	2:A:167:CYS:SG	2.60	0.59
2:A:663:SER:OG	2:A:664:THR:N	2.35	0.59
5:D:47:LEU:HD11	8:G:3:PHE:HD2	1.64	0.59
3:B:193:LYS:HZ1	13:L:32:ALA:HB1	1.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:797:TYR:HB2	3:B:852:ARG:O	2.01	0.59
11:J:1:MET:H2	11:J:57:ILE:N	1.94	0.59
2:A:1369:ALA:O	2:A:1372:VAL:HG12	2.02	0.59
6:E:48:ASP:CG	6:E:49:SER:H	2.05	0.59
6:E:117:THR:HG22	6:E:119:SER:H	1.67	0.59
5:D:185:CYS:HB2	5:D:211:LEU:HD21	1.83	0.59
8:G:1:MET:HE3	8:G:80:LYS:O	2.01	0.59
3:B:882:THR:HB	3:B:934:LYS:O	2.02	0.59
11:J:64:ASN:ND2	11:J:65:PRO:HD3	2.17	0.59
4:C:38:ILE:HA	4:C:173:ALA:CB	2.32	0.59
2:A:23:SER:HB3	2:A:233:TRP:CZ2	2.36	0.59
2:A:22:PHE:HE2	2:A:30:ILE:HD12	1.68	0.59
2:A:298:PHE:CZ	2:A:314:ALA:HB2	2.37	0.59
3:B:705:MET:H	3:B:710:LEU:CD1	2.15	0.59
10:I:50:THR:HG22	10:I:52:ILE:H	1.67	0.59
4:C:187:LYS:HG3	4:C:219:PHE:CE1	2.38	0.59
3:B:882:THR:HG22	3:B:884:ARG:N	2.12	0.59
3:B:1001:PHE:CE1	3:B:1073:TYR:HB2	2.38	0.59
4:C:39:ALA:CA	4:C:164:ALA:HB3	2.30	0.59
2:A:399:HIS:O	2:A:401:GLY:N	2.36	0.59
6:E:13:TRP:HB2	6:E:42:PHE:CE2	2.37	0.59
7:F:111:LEU:O	7:F:113:GLY:N	2.31	0.59
2:A:253:ASN:HB3	3:B:935:ARG:NH2	2.17	0.59
2:A:1094:VAL:HG12	2:A:1095:THR:H	1.68	0.59
2:A:650:GLN:O	2:A:654:ASN:ND2	2.36	0.59
3:B:778:MET:HE1	3:B:1094:ARG:HD3	1.83	0.59
3:B:653:VAL:HG22	3:B:689:LEU:HB3	1.84	0.59
3:B:1085:ILE:H	3:B:1085:ILE:HD12	1.65	0.59
2:A:1115:SER:HB3	2:A:1330:ASN:ND2	2.16	0.59
3:B:761:HIS:HB2	3:B:1024:ALA:HB2	1.84	0.59
10:I:106:CYS:O	10:I:107:SER:HB2	2.03	0.59
2:A:1336:MET:CE	2:A:1381:LEU:HG	2.33	0.59
3:B:833:TYR:N	3:B:833:TYR:CD1	2.68	0.59
3:B:798:TYR:CE2	4:C:62:PHE:CE2	2.85	0.59
2:A:442:VAL:HG21	2:A:460:VAL:HG23	1.84	0.59
2:A:475:THR:CG2	2:A:476:SER:H	2.12	0.59
2:A:929:LEU:HD23	2:A:983:ILE:HG21	1.85	0.59
3:B:165:VAL:HG11	3:B:448:ILE:CD1	2.32	0.59
3:B:843:GLN:O	3:B:844:SER:C	2.40	0.59
2:A:1410:PHE:HA	3:B:1212:ILE:HD11	1.85	0.59
2:A:1130:GLN:HE21	2:A:1134:ILE:HD11	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:903:VAL:HG12	3:B:904:ARG:N	2.18	0.59
2:A:1329:THR:H	2:A:1335:ILE:HD11	1.66	0.59
3:B:39:ARG:HG2	3:B:39:ARG:NH1	2.17	0.59
3:B:542:MET:HE2	3:B:743:ILE:HG13	1.84	0.59
3:B:542:MET:HB3	3:B:636:PRO:HD2	1.85	0.59
3:B:365:THR:HG23	3:B:367:LEU:N	2.17	0.59
2:A:698:GLN:HA	10:I:97:MET:O	2.03	0.59
3:B:1077:THR:HG22	12:K:44:ASN:ND2	2.17	0.59
5:D:29:LEU:HD13	8:G:82:PHE:CZ	2.38	0.59
4:C:8:VAL:HG12	4:C:9:LYS:H	1.68	0.59
11:J:64:ASN:HB3	11:J:65:PRO:HD2	1.84	0.59
9:H:135:LEU:HD13	9:H:137:GLN:NE2	2.11	0.59
3:B:994:TYR:HB2	3:B:999:MET:CE	2.32	0.59
2:A:528:LEU:HD23	2:A:751:SER:CB	2.33	0.59
2:A:438:ASP:O	2:A:439:ASN:HB2	2.03	0.59
2:A:1226:VAL:HG22	2:A:1240:CYS:CB	2.31	0.58
2:A:215:SER:HB3	2:A:218:ASP:CG	2.24	0.58
3:B:693:ILE:HD13	3:B:701:ILE:HD13	1.85	0.58
7:F:90:ARG:HG3	7:F:91:ALA:N	2.18	0.58
2:A:675:THR:OG1	2:A:736:ASN:ND2	2.36	0.58
3:B:559:SER:HA	3:B:563:MET:HB3	1.85	0.58
4:C:164:ALA:HA	4:C:167:HIS:O	2.03	0.58
3:B:463:THR:HB	3:B:465:ASN:H	1.68	0.58
3:B:44:VAL:HG11	3:B:199:MET:HG2	1.84	0.58
3:B:1110:PRO:HG3	3:B:1125:ASP:HB3	1.85	0.58
5:D:50:LEU:HD13	5:D:55:ALA:HA	1.84	0.58
2:A:710:LEU:H	2:A:710:LEU:HD12	1.68	0.58
13:L:55:ILE:O	13:L:56:LEU:HB2	2.02	0.58
4:C:66:ARG:NH2	11:J:5:VAL:HG23	2.16	0.58
3:B:65:GLU:HG3	3:B:66:ASP:N	2.16	0.58
7:F:119:ARG:NH1	7:F:119:ARG:HG3	2.18	0.58
7:F:130:ILE:O	7:F:148:VAL:CG2	2.51	0.58
3:B:744:HIS:HD2	3:B:746:SER:OG	1.85	0.58
3:B:121:ASN:HA	3:B:207:GLY:CA	2.33	0.58
2:A:93:VAL:CG2	2:A:301:ALA:HA	2.33	0.58
3:B:1165:ILE:HG22	3:B:1166:CYS:N	2.17	0.58
2:A:254:GLU:HB2	3:B:935:ARG:HH12	1.68	0.58
5:D:198:LEU:O	5:D:200:ASN:N	2.35	0.58
3:B:174:LEU:HD22	3:B:202:TYR:CE1	2.39	0.58
3:B:816:GLU:O	3:B:817:LEU:HD23	2.03	0.58
2:A:244:PRO:HB2	2:A:245:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:2:ILE:HG22	11:J:3:VAL:O	2.03	0.58
10:I:50:THR:HG22	10:I:51:ASN:H	1.68	0.58
12:K:57:LEU:HD12	12:K:77:THR:O	2.03	0.58
2:A:284:ALA:C	2:A:286:HIS:H	2.06	0.58
3:B:54:PHE:CZ	3:B:59:LEU:HD13	2.37	0.58
3:B:258:LEU:O	3:B:258:LEU:HG	2.04	0.58
2:A:1127:ASP:CB	2:A:1130:GLN:HB3	2.22	0.58
2:A:75:ASN:HA	3:B:1116:ARG:HH22	1.67	0.58
2:A:1341:ILE:CG2	2:A:1342:GLU:N	2.66	0.58
7:F:116:ASP:HB3	7:F:119:ARG:CB	2.33	0.58
3:B:706:GLN:HE22	3:B:730:ARG:NH1	2.01	0.58
2:A:889:SER:HB3	2:A:1297:GLU:HG2	1.85	0.58
10:I:16:PRO:HB3	10:I:27:PHE:CD2	2.39	0.58
4:C:56:THR:HG22	4:C:57:VAL:H	1.68	0.58
12:K:10:PHE:CD2	12:K:10:PHE:N	2.70	0.58
3:B:1096:ARG:O	3:B:1097:HIS:CB	2.51	0.58
10:I:62:ILE:HG12	10:I:62:ILE:O	2.04	0.58
2:A:90:VAL:HG13	2:A:297:GLN:HA	1.86	0.58
6:E:124:VAL:HG13	6:E:132:ILE:HD12	1.85	0.58
2:A:496:GLU:HG2	7:F:99:LEU:HD22	1.84	0.58
2:A:974:ASP:HB2	9:H:136:LYS:HZ2	1.68	0.58
2:A:1101:LEU:HD11	2:A:1105:LEU:HD11	1.84	0.58
5:D:160:VAL:O	5:D:164:ILE:HG13	2.03	0.58
11:J:1:MET:H1	11:J:56:LEU:H	1.49	0.58
2:A:853:ASP:OD1	2:A:855:THR:HG22	2.04	0.58
3:B:766:ARG:NH2	3:B:1020:ARG:HH11	1.98	0.58
6:E:157:SER:OG	6:E:160:GLU:HG3	2.04	0.58
5:D:170:THR:HB	5:D:172:LEU:HG	1.85	0.58
2:A:1127:ASP:HB3	2:A:1130:GLN:CB	2.23	0.58
4:C:124:LEU:O	4:C:125:MET:HB2	2.03	0.58
9:H:42:ILE:HG23	9:H:95:TYR:CE1	2.34	0.58
2:A:1438:THR:O	7:F:92:ARG:HD2	2.03	0.58
2:A:381:THR:OG1	2:A:382:PRO:HD2	2.03	0.58
4:C:107:SER:C	4:C:109:SER:H	2.06	0.58
3:B:833:TYR:N	3:B:833:TYR:HD1	2.01	0.58
4:C:89:GLU:O	4:C:90:ASP:HB3	2.02	0.58
2:A:1430:LEU:O	3:B:1196:ILE:HG22	2.04	0.58
2:A:472:LEU:HD11	3:B:835:GLN:NE2	2.18	0.58
3:B:589:VAL:CG1	3:B:590:HIS:H	2.13	0.58
3:B:1156:ASP:HB3	3:B:1198:TYR:H	1.69	0.58
3:B:519:TRP:HE1	3:B:635:ARG:NH2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:520:GLY:HA2	3:B:748:ILE:HG22	1.86	0.58
2:A:665:GLY:O	2:A:667:GLY:N	2.36	0.58
2:A:1350:LYS:O	2:A:1354:ASN:ND2	2.37	0.58
3:B:221:ASN:N	3:B:241:ARG:O	2.34	0.58
12:K:12:LEU:HD12	12:K:12:LEU:H	1.69	0.58
3:B:850:LEU:HD12	3:B:851:PHE:H	1.68	0.57
3:B:971:THR:HG1	4:C:61:GLU:HG3	1.69	0.57
8:G:14:HIS:HD2	8:G:16:SER:HB2	1.67	0.57
2:A:93:VAL:HG23	2:A:304:MET:HE3	1.86	0.57
2:A:407:ARG:HB3	2:A:430:TRP:CE2	2.39	0.57
3:B:997:GLU:H	3:B:997:GLU:CD	2.04	0.57
2:A:821:ARG:HB2	2:A:821:ARG:HH11	1.67	0.57
5:D:47:LEU:HD13	5:D:48:ILE:N	2.19	0.57
4:C:44:LEU:HB2	4:C:77:ILE:HD11	1.85	0.57
9:H:102:TYR:N	9:H:102:TYR:HD2	1.99	0.57
10:I:101:PHE:HE1	10:I:112:SER:HB2	1.70	0.57
3:B:1001:PHE:CZ	3:B:1073:TYR:HB2	2.39	0.57
2:A:1441:PHE:CE2	7:F:89:GLU:HG2	2.40	0.57
3:B:807:ARG:HG2	3:B:1045:SER:OG	2.04	0.57
12:K:21:ILE:HG23	12:K:31:VAL:CG1	2.35	0.57
3:B:1181:GLU:OE1	3:B:1183:LYS:HG3	2.05	0.57
2:A:821:ARG:HD2	2:A:825:ILE:HD11	1.86	0.57
4:C:69:LEU:N	4:C:69:LEU:HD12	2.19	0.57
4:C:70:ILE:HG12	4:C:142:VAL:HG11	1.85	0.57
3:B:324:ILE:HG12	3:B:329:THR:HG22	1.86	0.57
7:F:68:THR:HG21	7:F:69:LEU:CB	2.34	0.57
10:I:14:LEU:HD22	10:I:28:GLU:O	2.05	0.57
2:A:340:LEU:HD21	3:B:1200:ALA:N	2.20	0.57
2:A:401:GLY:C	2:A:435:HIS:HD2	2.06	0.57
3:B:1162:ILE:HD11	3:B:1194:ILE:CD1	2.34	0.57
3:B:916:THR:O	3:B:935:ARG:HG3	2.04	0.57
3:B:642:ASP:HB3	3:B:649:LYS:HG3	1.86	0.57
3:B:603:LEU:HB3	3:B:609:ILE:HG13	1.87	0.57
2:A:308:ILE:HG22	2:A:309:ALA:H	1.68	0.57
9:H:105:GLU:HG2	9:H:106:GLU:N	2.20	0.57
2:A:1120:LEU:CD1	2:A:1120:LEU:N	2.68	0.57
2:A:1152:ILE:CD1	10:I:44:TYR:HD2	2.14	0.57
2:A:899:VAL:CB	2:A:929:LEU:HD11	2.32	0.57
4:C:18:VAL:HG23	4:C:240:VAL:HB	1.86	0.57
2:A:896:ARG:HD3	2:A:897:TYR:HE1	1.69	0.57
3:B:190:TYR:HD2	11:J:62:ARG:O	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:61:THR:HG22	13:L:62:LYS:N	2.19	0.57
5:D:33:PHE:CE1	8:G:80:LYS:HE3	2.40	0.57
8:G:154:VAL:HG12	8:G:155:SER:N	2.19	0.57
4:C:238:ILE:HD11	4:C:246:ARG:NH1	2.18	0.57
2:A:1424:VAL:HG13	2:A:1436:ILE:CD1	2.35	0.57
3:B:1106:ARG:HD3	3:B:1126:GLY:O	2.03	0.57
2:A:1244:ARG:HB3	2:A:1245:PRO:HD2	1.84	0.57
2:A:360:GLU:HG2	2:A:363:GLN:OE1	2.04	0.57
2:A:106:VAL:HG13	2:A:112:LYS:O	2.04	0.57
3:B:193:LYS:HD3	3:B:787:VAL:HG11	1.87	0.57
3:B:515:HIS:N	3:B:518:HIS:HD2	1.89	0.57
2:A:981:LEU:HD21	2:A:1039:LYS:HA	1.85	0.57
2:A:185:TRP:CZ3	2:A:200:ARG:HG2	2.40	0.57
10:I:8:ARG:HG3	10:I:34:TYR:CE1	2.36	0.57
3:B:345:LYS:HA	3:B:348:ARG:HD2	1.85	0.57
2:A:920:LEU:HD23	2:A:921:GLY:N	2.20	0.57
2:A:1305:VAL:HG12	2:A:1306:LEU:N	2.20	0.57
13:L:30:ILE:O	13:L:56:LEU:HA	2.04	0.57
2:A:853:ASP:OD1	2:A:855:THR:N	2.38	0.57
2:A:19:PHE:HB3	2:A:1413:GLY:HA2	1.87	0.57
4:C:147:LEU:HB2	4:C:151:GLN:HB2	1.87	0.57
7:F:103:MET:HE1	8:G:65:ASP:HB2	1.86	0.57
10:I:7:CYS:HB3	10:I:14:LEU:HD21	1.87	0.57
8:G:18:PHE:HA	8:G:22:MET:CE	2.34	0.57
3:B:498:THR:HG22	3:B:537:LYS:HG3	1.87	0.57
3:B:269:ILE:HG21	3:B:282:ILE:HD13	1.87	0.57
2:A:382:PRO:HB3	2:A:428:TYR:CE2	2.35	0.57
2:A:1418:LEU:HD12	2:A:1419:ASP:N	2.19	0.57
2:A:1313:LEU:HD23	2:A:1338:VAL:CG2	2.34	0.57
4:C:148:ARG:CG	4:C:149:LYS:H	2.18	0.57
2:A:548:ASN:HA	12:K:60:ALA:HB1	1.87	0.57
2:A:946:VAL:HG22	6:E:201:LYS:HD2	1.85	0.57
8:G:1:MET:SD	8:G:79:PHE:CD1	2.91	0.56
2:A:332:LYS:HA	2:A:337:ARG:HD2	1.86	0.56
2:A:457:ALA:O	2:A:507:VAL:HG23	2.05	0.56
11:J:64:ASN:CB	11:J:65:PRO:HD3	2.33	0.56
3:B:591:ARG:O	3:B:593:PRO:HD3	2.05	0.56
2:A:18:GLN:HB3	3:B:1215:ARG:HG3	1.87	0.56
5:D:47:LEU:HD13	5:D:48:ILE:H	1.71	0.56
2:A:115:LEU:HB2	2:A:122:MET:HE2	1.87	0.56
3:B:308:TRP:HA	3:B:311:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:955:THR:CG2	3:B:956:THR:H	2.16	0.56
3:B:467:GLY:N	3:B:475:SER:HB3	2.18	0.56
3:B:118:ARG:CG	3:B:204:ILE:HD13	2.35	0.56
2:A:490:HIS:HB3	3:B:1150:ARG:NH1	2.21	0.56
2:A:35:ILE:HG22	2:A:35:ILE:O	2.06	0.56
8:G:43:GLY:HA3	8:G:80:LYS:HB3	1.87	0.56
4:C:79:GLN:HE21	4:C:127:ARG:HD3	1.70	0.56
3:B:363:HIS:HD2	3:B:585:VAL:HG22	1.70	0.56
3:B:1095:LEU:HD12	3:B:1095:LEU:N	2.19	0.56
3:B:658:ILE:HG22	3:B:662:MET:HE2	1.87	0.56
2:A:401:GLY:C	2:A:435:HIS:CD2	2.79	0.56
6:E:17:ARG:O	6:E:20:LYS:HB2	2.05	0.56
4:C:18:VAL:HG12	4:C:18:VAL:O	2.03	0.56
4:C:238:ILE:HG22	4:C:243:VAL:HG23	1.87	0.56
2:A:504:LEU:N	2:A:504:LEU:HD12	2.20	0.56
2:A:794:PRO:HG2	2:A:795:GLU:OE2	2.06	0.56
3:B:1181:GLU:HG3	3:B:1188:LYS:HE3	1.87	0.56
2:A:675:THR:O	2:A:679:ILE:HG13	2.06	0.56
11:J:23:ASN:O	11:J:25:LEU:N	2.38	0.56
3:B:563:MET:HE3	3:B:580:VAL:HB	1.87	0.56
2:A:310:GLY:O	2:A:312:PRO:HD2	2.04	0.56
3:B:794:ASN:O	3:B:795:ILE:HD12	2.06	0.56
2:A:373:THR:HG21	3:B:1105:ALA:HB3	1.87	0.56
7:F:69:LEU:HD13	7:F:72:LYS:CD	2.35	0.56
2:A:1155:ASP:OD2	2:A:1161:THR:HA	2.06	0.56
2:A:537:ARG:HD2	9:H:20:TYR:CE1	2.40	0.56
9:H:130:ARG:N	9:H:130:ARG:HD2	2.12	0.56
5:D:144:THR:HG21	8:G:46:LEU:HD13	1.87	0.56
3:B:983:ARG:HD2	3:B:1091:TYR:HD2	1.69	0.56
4:C:234:SER:CB	4:C:240:VAL:HG13	2.36	0.56
6:E:15:ALA:HA	6:E:140:LEU:O	2.06	0.56
13:L:49:LYS:O	13:L:50:ASP:CB	2.54	0.56
2:A:1076:ALA:HA	2:A:1079:MET:HE2	1.85	0.56
3:B:401:PHE:HA	3:B:404:LYS:HG3	1.86	0.56
2:A:29:ALA:HB1	3:B:1184:GLY:CA	2.36	0.56
2:A:1385:THR:HG22	2:A:1386:ARG:H	1.69	0.56
2:A:106:VAL:HG12	2:A:107:CYS:N	2.20	0.56
8:G:26:LEU:HD12	8:G:56:ILE:CG2	2.36	0.56
4:C:238:ILE:CG2	4:C:242:GLN:HB2	2.35	0.56
2:A:868:TYR:CD2	2:A:1058:VAL:HG21	2.34	0.56
2:A:1030:ARG:NH1	2:A:1035:TYR:OH	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:758:PHE:CE1	3:B:1027:ILE:HG22	2.41	0.56
2:A:606:LEU:HB3	2:A:614:PHE:CE2	2.40	0.56
7:F:76:LYS:O	7:F:79:ARG:HD3	2.04	0.56
9:H:107:VAL:O	9:H:108:SER:O	2.22	0.56
3:B:580:VAL:HG13	3:B:624:LEU:HB3	1.88	0.56
2:A:828:ALA:HB1	3:B:530:GLY:HA2	1.86	0.56
2:A:87:ALA:HB3	2:A:276:LEU:HD23	1.88	0.56
3:B:1007:VAL:CG2	3:B:1008:PRO:HD2	2.36	0.56
3:B:94:LYS:HG2	3:B:95:ILE:N	2.20	0.56
2:A:590:ARG:HD3	2:A:604:GLY:CA	2.35	0.56
5:D:4:SER:O	5:D:5:THR:CB	2.54	0.56
2:A:971:PHE:CE2	2:A:1040:GLN:HG2	2.39	0.56
3:B:1007:VAL:HG22	3:B:1008:PRO:HD2	1.87	0.56
7:F:111:LEU:N	7:F:111:LEU:HD12	2.18	0.56
3:B:1178:ASN:O	3:B:1180:PHE:HD1	1.88	0.56
2:A:552:TRP:HE1	12:K:62:LYS:CB	2.17	0.56
2:A:600:PRO:HG2	2:A:601:LYS:H	1.69	0.56
2:A:1164:PRO:HG2	2:A:1165:GLU:H	1.70	0.56
2:A:1283:VAL:HG12	2:A:1284:MET:N	2.19	0.56
3:B:640:VAL:HG12	3:B:640:VAL:O	2.05	0.56
2:A:58:LEU:CD1	2:A:243:PRO:HB3	2.36	0.56
3:B:195:CYS:SG	3:B:196:PRO:HD2	2.46	0.56
3:B:978:ASP:OD2	3:B:1098:MET:HG2	2.06	0.56
3:B:1072:MET:HE3	3:B:1085:ILE:HD13	1.88	0.56
10:I:80:SER:HB2	10:I:103:CYS:SG	2.45	0.56
8:G:73:LYS:HE2	8:G:74:TYR:O	2.06	0.56
8:G:48:VAL:HA	8:G:76:ALA:HB2	1.88	0.56
4:C:98:VAL:C	4:C:99:LEU:HD22	2.26	0.56
2:A:779:PHE:O	2:A:780:VAL:C	2.44	0.56
3:B:123:THR:OG1	3:B:458:LYS:HE2	2.06	0.56
7:F:103:MET:CE	8:G:65:ASP:HB2	2.36	0.56
11:J:48:ARG:HD2	11:J:49:MET:N	2.21	0.56
6:E:22:MET:HE3	6:E:26:ARG:NH2	2.12	0.56
2:A:1349:TYR:HE1	2:A:1368:MET:HB2	1.71	0.56
3:B:168:GLY:H	3:B:450:ALA:HB1	1.70	0.56
3:B:53:GLN:HG2	3:B:547:VAL:CG2	2.36	0.56
9:H:81:PRO:CB	9:H:82:PRO:CD	2.84	0.56
13:L:28:LYS:O	13:L:29:TYR:HD2	1.89	0.56
2:A:546:VAL:HG13	2:A:577:ILE:HG21	1.88	0.56
3:B:778:MET:HE1	3:B:1094:ARG:CD	2.36	0.55
6:E:13:TRP:CE3	6:E:39:LEU:HD13	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:768:GLN:CG	2:A:816:HIS:HA	2.34	0.55
2:A:722:LEU:HD21	2:A:794:PRO:HB3	1.87	0.55
2:A:18:GLN:H	3:B:1215:ARG:HB2	1.71	0.55
4:C:209:TYR:N	4:C:209:TYR:CD1	2.74	0.55
2:A:102:VAL:HG11	2:A:211:PHE:CE2	2.41	0.55
13:L:61:THR:HG21	13:L:63:ARG:HG2	1.87	0.55
5:D:24:ALA:C	5:D:26:THR:H	2.09	0.55
3:B:704:ALA:HB2	3:B:738:PHE:CD2	2.41	0.55
4:C:52:GLU:HA	13:L:64:LEU:HD22	1.87	0.55
5:D:48:ILE:CG2	8:G:4:ILE:HB	2.36	0.55
10:I:34:TYR:HD2	10:I:35:VAL:H	1.49	0.55
3:B:796:LEU:HD12	3:B:852:ARG:O	2.06	0.55
3:B:361:LEU:HD21	3:B:377:PHE:HD2	1.71	0.55
8:G:114:LEU:HG	8:G:162:SER:HB3	1.89	0.55
3:B:957:ASN:HD22	3:B:961:LEU:HD12	1.70	0.55
2:A:1076:ALA:HA	2:A:1079:MET:HE3	1.87	0.55
4:C:189:THR:HG22	4:C:190:ASP:N	2.21	0.55
2:A:596:THR:C	2:A:598:LEU:H	2.09	0.55
3:B:1159:ARG:CD	3:B:1193:GLN:HE21	2.19	0.55
2:A:1115:SER:O	2:A:1116:LEU:HB3	2.06	0.55
2:A:726:ARG:O	2:A:729:ALA:HB3	2.06	0.55
3:B:295:GLY:O	3:B:299:GLU:HG2	2.06	0.55
8:G:106:MET:CG	8:G:107:LYS:N	2.70	0.55
8:G:7:LEU:CD1	8:G:45:ILE:HD11	2.37	0.55
3:B:953:LEU:CD2	3:B:965:LYS:HB2	2.34	0.55
5:D:52:LEU:HD21	5:D:147:TYR:HE2	1.72	0.55
2:A:367:PRO:HA	2:A:463:ILE:O	2.06	0.55
2:A:260:ASP:OD1	2:A:261:ASP:N	2.39	0.55
6:E:55:ARG:HD2	6:E:83:CYS:O	2.06	0.55
2:A:546:VAL:O	2:A:546:VAL:HG12	2.07	0.55
3:B:1034:VAL:O	3:B:1036:ALA:N	2.39	0.55
2:A:963:ILE:HD11	2:A:1048:ASN:CB	2.35	0.55
2:A:1291:VAL:HG13	2:A:1292:PRO:CD	2.37	0.55
4:C:35:ARG:NH1	12:K:41:THR:N	2.54	0.55
11:J:1:MET:N	11:J:57:ILE:H	1.96	0.55
3:B:1094:ARG:HH21	3:B:1098:MET:HG2	1.70	0.55
2:A:1114:PRO:HB2	2:A:1311:VAL:CG2	2.34	0.55
10:I:58:VAL:HG13	10:I:62:ILE:HD12	1.89	0.55
2:A:783:THR:HG21	2:A:815:PHE:CE2	2.41	0.55
2:A:1074:GLU:H	2:A:1075:PRO:HD2	1.72	0.55
2:A:886:ILE:HD11	2:A:943:LEU:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:954:TRP:HB3	2:A:955:PRO:HD2	1.89	0.55
3:B:1202:LEU:HD23	3:B:1206:GLU:HG3	1.89	0.55
8:G:138:THR:CG2	8:G:139:ILE:H	1.99	0.55
7:F:93:ILE:HD11	7:F:134:ILE:HD11	1.89	0.55
3:B:637:LEU:HD21	3:B:742:GLU:OE2	2.07	0.55
2:A:591:PHE:HA	2:A:595:THR:HG21	1.88	0.55
12:K:110:ASN:O	12:K:111:LEU:CB	2.54	0.55
3:B:642:ASP:HB3	3:B:649:LYS:HD2	1.89	0.55
9:H:40:LEU:HD22	9:H:123:MET:CE	2.37	0.55
4:C:147:LEU:HD12	4:C:151:GLN:O	2.06	0.55
3:B:871:THR:HG22	3:B:872:GLU:N	2.21	0.55
3:B:185:THR:H	3:B:188:ASP:HB2	1.70	0.55
2:A:325:ILE:HG21	3:B:1210:MET:HG3	1.89	0.55
12:K:61:TYR:C	12:K:61:TYR:CD2	2.77	0.55
2:A:32:VAL:HG21	2:A:68:GLN:NE2	2.22	0.55
8:G:37:SER:OG	8:G:45:ILE:HB	2.07	0.55
4:C:235:VAL:HG12	11:J:13:VAL:CG2	2.37	0.55
7:F:99:LEU:HD12	7:F:99:LEU:O	2.06	0.55
6:E:157:SER:C	6:E:159:ASP:H	2.08	0.55
2:A:541:ILE:HG21	2:A:549:MET:HE1	1.88	0.55
3:B:763:GLN:HG2	3:B:765:PRO:HD2	1.88	0.55
2:A:34:LYS:CE	2:A:57:ARG:NH1	2.66	0.55
5:D:39:ASN:ND2	5:D:41:GLN:HB2	2.22	0.55
2:A:1116:LEU:HB3	2:A:1308:THR:CG2	2.37	0.55
9:H:64:ASN:O	9:H:65:LEU:CB	2.55	0.55
2:A:261:ASP:OD1	2:A:322:VAL:HG13	2.07	0.55
3:B:190:TYR:CE2	11:J:62:ARG:HB3	2.42	0.55
2:A:1401:SER:O	2:A:1402:PHE:HB2	2.07	0.55
8:G:153:GLN:CG	8:G:154:VAL:HG23	2.37	0.54
2:A:679:ILE:O	2:A:683:ILE:HG13	2.07	0.54
5:D:172:LEU:HD22	5:D:176:GLU:OE1	2.07	0.54
2:A:1299:VAL:HG12	2:A:1300:LYS:N	2.22	0.54
4:C:226:ASP:O	4:C:227:THR:HB	2.07	0.54
7:F:68:THR:OG1	7:F:68:THR:O	2.23	0.54
8:G:1:MET:O	8:G:3:PHE:CD1	2.60	0.54
4:C:45:ALA:O	4:C:159:ALA:HA	2.07	0.54
10:I:55:THR:HG22	10:I:58:VAL:CG2	2.38	0.54
10:I:85:PHE:CD1	10:I:99:LEU:HD13	2.42	0.54
2:A:718:VAL:O	2:A:722:LEU:HD12	2.06	0.54
2:A:605:MET:HG2	2:A:621:THR:CG2	2.36	0.54
3:B:244:LEU:HD11	3:B:366:GLN:HE22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:639:ILE:HG22	3:B:641:GLU:HG2	1.89	0.54
2:A:406:ILE:HG22	2:A:412:ARG:HA	1.88	0.54
2:A:180:LYS:NZ	2:A:294:SER:HB3	2.22	0.54
3:B:847:ASP:C	3:B:849:GLY:H	2.10	0.54
8:G:143:ILE:CG2	8:G:144:ARG:N	2.63	0.54
2:A:69:THR:O	2:A:71:GLN:N	2.40	0.54
2:A:720:ARG:HB3	2:A:720:ARG:CZ	2.37	0.54
3:B:115:GLN:HG2	3:B:193:LYS:HB2	1.89	0.54
3:B:1117:GLN:HE21	3:B:1199:ALA:HB2	1.72	0.54
6:E:10:SER:O	6:E:14:ARG:HG3	2.08	0.54
10:I:69:PRO:HG2	10:I:85:PHE:CE2	2.42	0.54
2:A:1063:MET:SD	2:A:1436:ILE:HG12	2.47	0.54
2:A:1041:ALA:O	2:A:1045:VAL:HG23	2.07	0.54
2:A:845:LEU:HB3	2:A:848:ILE:HD12	1.90	0.54
2:A:18:GLN:HB2	3:B:1215:ARG:HB2	1.89	0.54
5:D:153:ARG:C	5:D:154:PHE:CD1	2.81	0.54
12:K:6:ARG:O	12:K:8:GLU:N	2.41	0.54
2:A:1293:SER:OG	2:A:1294:PRO:HD2	2.06	0.54
4:C:177:GLU:HB2	4:C:231:ASN:HB3	1.88	0.54
5:D:12:ARG:NE	5:D:14:ARG:HD2	2.22	0.54
3:B:471:LYS:O	3:B:472:ALA:HB2	2.07	0.54
3:B:952:VAL:HG22	3:B:966:VAL:HG13	1.88	0.54
3:B:975:GLN:HG2	3:B:976:ILE:H	1.73	0.54
2:A:382:PRO:HD3	2:A:428:TYR:HD2	1.71	0.54
2:A:17:VAL:HA	3:B:1215:ARG:O	2.08	0.54
3:B:603:LEU:HD12	3:B:609:ILE:HG13	1.89	0.54
2:A:358:ASN:O	2:A:359:LEU:HD23	2.07	0.54
2:A:55:ASP:CG	2:A:55:ASP:O	2.43	0.54
9:H:139:ASN:O	9:H:140:ALA:HB2	2.08	0.54
10:I:14:LEU:HA	10:I:28:GLU:O	2.08	0.54
2:A:144:THR:O	2:A:146:MET:HG3	2.08	0.54
3:B:1001:PHE:CD2	4:C:34:ARG:NH2	2.75	0.54
2:A:1036:ARG:HH11	2:A:1036:ARG:HG2	1.72	0.54
3:B:234:ILE:N	3:B:234:ILE:HD12	2.23	0.54
6:E:145:THR:HG21	6:E:187:TYR:CD2	2.42	0.54
3:B:479:VAL:O	3:B:480:SER:HB3	2.07	0.54
7:F:99:LEU:O	7:F:103:MET:HG2	2.08	0.54
3:B:603:LEU:HD13	3:B:608:ASP:HB2	1.89	0.54
2:A:577:ILE:O	2:A:580:VAL:HG23	2.07	0.54
3:B:803:LEU:HB2	3:B:1032:SER:OG	2.06	0.54
2:A:344:ARG:NH2	3:B:1120:GLU:HB2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:197:LYS:HE2	6:E:199:ILE:HD11	1.90	0.54
5:D:8:PHE:CE2	8:G:73:LYS:HD3	2.42	0.54
2:A:93:VAL:HG21	2:A:301:ALA:O	2.08	0.54
9:H:61:SER:O	9:H:62:SER:CB	2.56	0.54
12:K:111:LEU:O	12:K:111:LEU:HD12	2.08	0.54
3:B:24:PRO:O	3:B:655:LYS:HB2	2.07	0.54
9:H:40:LEU:HD13	9:H:123:MET:CE	2.37	0.54
3:B:360:PHE:CD2	3:B:360:PHE:C	2.80	0.54
2:A:75:ASN:O	2:A:76:GLU:CB	2.56	0.54
3:B:1072:MET:HE2	3:B:1087:PHE:HB2	1.89	0.54
2:A:1329:THR:HG23	2:A:1331:SER:H	1.69	0.54
8:G:88:ASP:HB3	8:G:144:ARG:HA	1.89	0.54
7:F:148:VAL:HG23	7:F:149:GLU:N	2.22	0.54
2:A:504:LEU:HD11	7:F:91:ALA:CB	2.37	0.54
2:A:1260:LEU:O	2:A:1260:LEU:HD12	2.07	0.54
3:B:1084:GLN:HE21	3:B:1084:GLN:H	1.54	0.54
4:C:165:LYS:O	12:K:6:ARG:NH1	2.40	0.54
3:B:661:LEU:HD23	3:B:679:TYR:O	2.08	0.54
3:B:102:VAL:HG23	3:B:112:LEU:HB2	1.89	0.54
4:C:142:VAL:H	11:J:16:ASP:HB3	1.72	0.54
3:B:852:ARG:NH2	13:L:70:ARG:OXT	2.37	0.54
3:B:549:THR:HB	3:B:628:THR:OG1	2.07	0.54
2:A:1038:THR:H	2:A:1041:ALA:HB3	1.72	0.54
3:B:1182:CYS:O	3:B:1183:LYS:O	2.26	0.54
3:B:344:LYS:O	3:B:346:GLU:N	2.41	0.54
2:A:974:ASP:HB2	9:H:136:LYS:NZ	2.23	0.54
13:L:61:THR:HG22	13:L:62:LYS:H	1.73	0.54
2:A:1118:VAL:HG12	2:A:1327:ILE:HG13	1.89	0.54
2:A:79:GLY:HA3	2:A:243:PRO:CG	2.38	0.54
3:B:521:LEU:HB3	3:B:633:VAL:CG1	2.38	0.54
2:A:351:THR:HG21	3:B:1103:ILE:HG13	1.90	0.54
3:B:265:SER:O	3:B:266:ALA:HB3	2.08	0.54
2:A:399:HIS:HB3	2:A:400:PRO:CD	2.32	0.54
3:B:983:ARG:HD2	3:B:1091:TYR:CD2	2.43	0.54
2:A:524:VAL:HG12	2:A:525:GLN:N	2.19	0.54
3:B:955:THR:HG23	3:B:956:THR:H	1.73	0.54
4:C:187:LYS:C	4:C:189:THR:H	2.11	0.54
2:A:492:PRO:HB3	2:A:501:LEU:CD1	2.38	0.54
3:B:1022:THR:HG23	3:B:1022:THR:O	2.08	0.54
10:I:34:TYR:C	10:I:34:TYR:HD2	2.09	0.53
2:A:1323:ASP:O	2:A:1325:THR:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:994:TYR:HB2	3:B:999:MET:HE3	1.90	0.53
11:J:23:ASN:C	11:J:25:LEU:N	2.61	0.53
3:B:842:ASN:O	3:B:846:ILE:HG13	2.09	0.53
3:B:1005:GLY:HA2	4:C:176:ILE:O	2.07	0.53
10:I:2:THR:O	10:I:3:THR:C	2.47	0.53
7:F:69:LEU:CG	7:F:71:GLU:HB2	2.39	0.53
8:G:79:PHE:HE2	8:G:105:PRO:HG2	1.74	0.53
3:B:680:THR:O	3:B:684:LEU:CD1	2.57	0.53
2:A:1151:GLU:HA	10:I:44:TYR:O	2.08	0.53
2:A:84:ILE:O	2:A:84:ILE:CG2	2.56	0.53
2:A:1074:GLU:N	2:A:1075:PRO:HD2	2.23	0.53
2:A:551:TYR:CE2	12:K:62:LYS:HG2	2.44	0.53
2:A:541:ILE:HG21	2:A:549:MET:CE	2.39	0.53
3:B:737:THR:HG21	10:I:66:PRO:HA	1.88	0.53
4:C:221:TYR:CE1	4:C:222:LYS:HG3	2.43	0.53
2:A:1102:LYS:O	2:A:1106:ASN:ND2	2.41	0.53
2:A:34:LYS:HB3	2:A:36:ARG:HE	1.73	0.53
2:A:567:LYS:CG	2:A:568:PRO:CD	2.81	0.53
3:B:653:VAL:HG22	3:B:689:LEU:HD22	1.88	0.53
6:E:14:ARG:HH21	6:E:141:VAL:CG1	2.19	0.53
3:B:983:ARG:HH11	3:B:1091:TYR:CB	2.21	0.53
3:B:36:ALA:HA	3:B:39:ARG:HD2	1.90	0.53
2:A:265:LYS:HD2	2:A:265:LYS:N	2.23	0.53
2:A:152:VAL:HG13	2:A:153:PRO:HD2	1.91	0.53
9:H:81:PRO:HB2	9:H:82:PRO:HD2	1.88	0.53
4:C:179:GLU:HG2	4:C:180:TYR:N	2.23	0.53
2:A:34:LYS:NZ	2:A:57:ARG:HH22	2.02	0.53
2:A:1130:GLN:O	2:A:1134:ILE:HG13	2.08	0.53
8:G:88:ASP:OD2	8:G:88:ASP:N	2.40	0.53
7:F:109:VAL:CG1	7:F:110:ASP:N	2.68	0.53
10:I:98:VAL:HG12	10:I:99:LEU:N	2.24	0.53
2:A:42:ASP:C	2:A:44:THR:H	2.11	0.53
2:A:547:LEU:HD22	12:K:58:PHE:CD1	2.43	0.53
6:E:124:VAL:HB	6:E:125:PRO:CD	2.38	0.53
2:A:852:TYR:CE2	2:A:1060:PRO:HB2	2.43	0.53
3:B:185:THR:O	3:B:186:GLU:C	2.47	0.53
2:A:1409:LEU:O	2:A:1412:ALA:HB3	2.09	0.53
3:B:446:LEU:O	3:B:447:ALA:HB3	2.07	0.53
7:F:69:LEU:HD13	7:F:72:LYS:HB2	1.90	0.53
2:A:567:LYS:HG3	2:A:568:PRO:HD2	1.88	0.53
2:A:567:LYS:HE3	9:H:46:LEU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:683:SER:O	3:B:687:GLU:HB2	2.09	0.53
4:C:133:ILE:CD1	4:C:237:SER:HA	2.39	0.53
2:A:1097:GLY:O	2:A:1100:ARG:HB3	2.08	0.53
12:K:46:ILE:O	12:K:46:ILE:HG22	2.09	0.53
3:B:992:ILE:HG12	3:B:993:THR:N	2.23	0.53
5:D:173:HIS:O	5:D:177:VAL:HG23	2.07	0.53
2:A:709:THR:CG2	2:A:711:ARG:HB2	2.39	0.53
10:I:15:TYR:N	10:I:15:TYR:CD1	2.77	0.53
11:J:8:PHE:H	11:J:49:MET:CE	2.21	0.53
2:A:786:HIS:CD2	3:B:703:ILE:HB	2.44	0.53
2:A:356:ASP:HB2	2:A:469:ARG:HH12	1.72	0.53
2:A:899:VAL:CG1	2:A:908:LEU:HD21	2.39	0.53
2:A:38:PRO:HB3	2:A:270:LEU:HG	1.91	0.53
2:A:316:GLN:HB2	2:A:322:VAL:CG2	2.38	0.53
6:E:164:LEU:HD11	6:E:211:TYR:CE1	2.43	0.53
3:B:1129:ARG:HG2	3:B:1131:GLY:H	1.74	0.53
3:B:912:ILE:O	3:B:938:SER:HB3	2.09	0.53
2:A:385:ILE:CD1	2:A:426:LEU:HB2	2.38	0.53
6:E:161:LYS:HD2	6:E:195:VAL:HG23	1.89	0.53
2:A:1141:THR:OG1	2:A:1205:LYS:HD3	2.08	0.53
2:A:61:ILE:CG2	2:A:62:ASP:H	2.09	0.53
2:A:68:GLN:O	2:A:70:CYS:N	2.41	0.53
8:G:30:LEU:O	8:G:34:VAL:HG23	2.09	0.53
3:B:911:ILE:HD11	3:B:941:LEU:CD1	2.34	0.53
3:B:797:TYR:HE1	3:B:854:LEU:CD2	2.21	0.53
3:B:38:PHE:HD1	3:B:811:TYR:CD2	2.27	0.53
2:A:699:ALA:O	2:A:700:ASN:CB	2.57	0.53
3:B:1039:GLY:HA2	11:J:51:LEU:CD2	2.38	0.53
9:H:116:TYR:HE2	9:H:140:ALA:CB	2.21	0.53
2:A:1445:ILE:N	2:A:1445:ILE:HD12	2.20	0.53
2:A:899:VAL:HG13	2:A:908:LEU:HD21	1.91	0.53
3:B:516:ASN:ND2	3:B:516:ASN:H	2.06	0.53
13:L:61:THR:CG2	13:L:63:ARG:HG2	2.39	0.53
2:A:341:MET:HE2	2:A:1425:SER:HB3	1.91	0.53
8:G:51:TYR:C	8:G:51:TYR:CD2	2.82	0.53
3:B:295:GLY:H	3:B:298:LEU:HD23	1.73	0.53
3:B:570:VAL:CG2	3:B:573:GLN:HB3	2.38	0.53
3:B:1174:LYS:O	3:B:1176:ASN:N	2.42	0.53
2:A:50:ILE:C	2:A:52:GLY:N	2.62	0.53
10:I:34:TYR:C	10:I:34:TYR:CD2	2.80	0.53
3:B:172:ILE:HD13	3:B:178:ASN:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:241:ASP:O	4:C:245:VAL:HG23	2.09	0.53
8:G:96:GLN:HB3	8:G:121:PHE:CE2	2.44	0.53
2:A:622:VAL:O	2:A:622:VAL:CG1	2.57	0.53
5:D:167:LEU:O	5:D:170:THR:OG1	2.26	0.53
3:B:189:LEU:HA	3:B:192:LEU:HD12	1.91	0.52
3:B:840:ILE:HG21	3:B:994:TYR:HD1	1.73	0.52
2:A:219:PHE:CE2	2:A:231:PRO:HD2	2.45	0.52
3:B:129:PHE:HA	3:B:165:VAL:O	2.08	0.52
2:A:381:THR:HG22	2:A:384:ASN:ND2	2.24	0.52
2:A:427:GLN:HG3	2:A:430:TRP:CE2	2.44	0.52
9:H:83:GLN:C	9:H:85:GLY:H	2.12	0.52
2:A:93:VAL:CG2	2:A:304:MET:HE3	2.38	0.52
2:A:1121:GLU:CG	2:A:1122:PRO:HD2	2.35	0.52
2:A:682:THR:HA	2:A:685:GLU:HG2	1.91	0.52
2:A:1074:GLU:C	2:A:1076:ALA:N	2.62	0.52
2:A:34:LYS:CB	2:A:36:ARG:HE	2.22	0.52
8:G:80:LYS:HG2	8:G:80:LYS:O	2.08	0.52
11:J:18:TRP:NE1	11:J:22:LEU:HD22	2.24	0.52
3:B:979:LYS:HG2	3:B:1095:LEU:CD1	2.37	0.52
5:D:59:ILE:HG21	5:D:145:MET:SD	2.50	0.52
2:A:135:PHE:HA	2:A:138:ILE:HD12	1.91	0.52
4:C:242:GLN:C	4:C:244:VAL:H	2.11	0.52
1:R:6:C:H2'	1:R:6:C:O2	2.08	0.52
2:A:629:LEU:HD22	2:A:633:VAL:CG2	2.39	0.52
8:G:110:VAL:HG22	8:G:161:GLY:O	2.08	0.52
2:A:1280:GLU:O	2:A:1282:VAL:HG23	2.09	0.52
3:B:1172:ILE:O	3:B:1172:ILE:HG22	2.09	0.52
8:G:7:LEU:HD11	8:G:45:ILE:HD11	1.92	0.52
13:L:52:GLY:O	13:L:53:HIS:C	2.47	0.52
4:C:56:THR:HG22	4:C:57:VAL:N	2.23	0.52
3:B:613:VAL:HG22	3:B:628:THR:HA	1.92	0.52
2:A:785:PRO:HG2	2:A:786:HIS:CD2	2.45	0.52
6:E:13:TRP:O	6:E:16:PHE:HB3	2.09	0.52
4:C:249:ASP:O	4:C:252:GLN:HB3	2.09	0.52
3:B:309:GLN:CD	10:I:52:ILE:HD11	2.30	0.52
3:B:654:ARG:NH1	3:B:654:ARG:HG3	2.23	0.52
2:A:172:PRO:HB3	2:A:185:TRP:CD2	2.45	0.52
3:B:604:ARG:NH1	3:B:691:GLU:OE2	2.42	0.52
2:A:58:LEU:O	2:A:59:GLY:O	2.28	0.52
2:A:337:ARG:HD3	3:B:1132:GLU:OE1	2.09	0.52
3:B:684:LEU:O	3:B:689:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:996:ARG:HG2	3:B:1007:VAL:HG11	1.91	0.52
2:A:682:THR:HG23	2:A:728:LYS:HE3	1.92	0.52
12:K:58:PHE:HE2	12:K:74:ARG:HE	1.53	0.52
2:A:1118:VAL:O	2:A:1305:VAL:HG13	2.10	0.52
3:B:31:TRP:CE3	3:B:34:ILE:HD12	2.45	0.52
2:A:56:PRO:O	2:A:57:ARG:HG3	2.09	0.52
8:G:15:PRO:HA	8:G:18:PHE:HD1	1.70	0.52
2:A:332:LYS:HB2	2:A:337:ARG:NH1	2.24	0.52
2:A:870:GLU:HB2	6:E:204:THR:HG21	1.92	0.52
4:C:239:PRO:O	4:C:241:ASP:N	2.43	0.52
9:H:12:VAL:HG13	9:H:26:ILE:CG2	2.39	0.52
3:B:129:PHE:HE2	3:B:166:PHE:HD1	1.58	0.52
2:A:848:ILE:HB	2:A:1065:GLY:HA3	1.91	0.52
2:A:22:PHE:CE2	2:A:30:ILE:HD12	2.45	0.52
3:B:1192:TYR:N	3:B:1192:TYR:CD1	2.77	0.52
3:B:1084:GLN:OE1	4:C:189:THR:CG2	2.58	0.52
2:A:1006:ILE:HD11	6:E:163:GLU:HG3	1.91	0.52
2:A:1454:MET:O	2:A:1454:MET:HG3	2.09	0.52
7:F:69:LEU:HD22	7:F:71:GLU:C	2.30	0.52
8:G:44:TYR:O	8:G:78:VAL:HG12	2.09	0.52
3:B:363:HIS:CD2	3:B:585:VAL:HG22	2.44	0.52
8:G:122:ASN:HD22	8:G:125:SER:HB3	1.74	0.52
2:A:442:VAL:CG2	2:A:460:VAL:HG23	2.40	0.52
3:B:944:THR:HG21	3:B:1122:ARG:CZ	2.40	0.52
6:E:135:PHE:HD2	6:E:140:LEU:HD21	1.73	0.52
6:E:30:ILE:HG22	6:E:31:THR:N	2.24	0.52
10:I:55:THR:HG22	10:I:55:THR:O	2.10	0.52
3:B:579:ARG:CB	3:B:586:TRP:HE1	2.23	0.52
2:A:590:ARG:HH22	2:A:620:LYS:HB3	1.74	0.52
2:A:384:ASN:OD1	2:A:388:LEU:HD12	2.09	0.52
3:B:792:MET:HA	3:B:856:PHE:O	2.09	0.52
3:B:860:MET:HG2	3:B:861:ASP:N	2.25	0.52
2:A:344:ARG:CZ	3:B:1120:GLU:HB2	2.40	0.52
2:A:88:LYS:HE3	2:A:280:GLU:OE2	2.10	0.52
3:B:558:LEU:O	3:B:560:GLU:N	2.43	0.52
2:A:1222:ASN:O	2:A:1223:ASP:HB3	2.10	0.52
2:A:1418:LEU:HD12	2:A:1419:ASP:H	1.75	0.52
3:B:22:SER:HA	3:B:654:ARG:CB	2.40	0.52
3:B:211:VAL:O	3:B:480:SER:HA	2.10	0.52
3:B:865:LYS:HE2	3:B:871:THR:OG1	2.09	0.52
3:B:641:GLU:C	3:B:643:ASP:H	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:757:ASN:OD1	3:B:1021:MET:HG3	2.10	0.52
2:A:1042:PHE:CE2	2:A:1046:LEU:HD11	2.45	0.52
3:B:172:ILE:HG22	3:B:173:MET:N	2.25	0.52
7:F:135:ARG:HG2	7:F:137:TYR:CE1	2.43	0.52
6:E:136:ASN:OD1	6:E:137:GLU:N	2.43	0.52
2:A:1059:HIS:ND1	7:F:86:THR:HA	2.24	0.52
2:A:899:VAL:HG22	2:A:1029:ARG:HG2	1.92	0.52
2:A:873:MET:HG3	2:A:1056:SER:O	2.10	0.52
4:C:35:ARG:NH1	12:K:41:THR:H	2.07	0.52
3:B:1047:PHE:N	3:B:1047:PHE:CD1	2.77	0.52
5:D:151:PHE:CD1	5:D:151:PHE:N	2.78	0.52
3:B:240:ILE:HG23	3:B:240:ILE:O	2.09	0.52
2:A:786:HIS:CD2	2:A:786:HIS:N	2.77	0.52
7:F:109:VAL:CG1	7:F:110:ASP:H	2.17	0.52
4:C:213:PRO:O	4:C:214:ASN:CB	2.56	0.52
4:C:3:GLU:O	4:C:4:GLU:CB	2.58	0.52
2:A:1293:SER:OG	2:A:1295:THR:HG23	2.10	0.52
2:A:1144:LYS:HB2	2:A:1268:LEU:O	2.10	0.52
3:B:487:THR:CG2	3:B:488:TYR:N	2.72	0.52
2:A:1005:GLU:O	2:A:1009:ASN:HB2	2.09	0.52
2:A:1446:ASP:HB2	7:F:133:VAL:HG23	1.91	0.52
2:A:75:ASN:O	2:A:76:GLU:HB3	2.10	0.51
8:G:127:PRO:HG2	8:G:138:THR:CG2	2.32	0.51
3:B:1154:ALA:O	3:B:1155:SER:HB2	2.10	0.51
9:H:11:GLN:HA	9:H:53:ASP:O	2.10	0.51
2:A:709:THR:HG21	10:I:93:LYS:O	2.11	0.51
2:A:119:ASN:O	2:A:122:MET:HB3	2.10	0.51
3:B:798:TYR:CE2	4:C:62:PHE:HE2	2.28	0.51
2:A:285:PRO:HG2	2:A:288:ALA:HB3	1.92	0.51
2:A:24:PRO:HD2	2:A:233:TRP:CD1	2.45	0.51
2:A:1006:ILE:HD12	6:E:163:GLU:HG3	1.91	0.51
2:A:548:ASN:OD1	12:K:60:ALA:HB1	2.11	0.51
5:D:67:ARG:HB2	5:D:133:THR:HG21	1.91	0.51
10:I:82:GLU:O	10:I:104:LEU:HG	2.09	0.51
9:H:100:THR:CG2	9:H:101:ALA:N	2.73	0.51
3:B:102:VAL:HG12	3:B:104:GLU:HG2	1.92	0.51
8:G:101:VAL:HG12	8:G:102:GLN:N	2.24	0.51
4:C:36:VAL:CG2	4:C:251:LEU:HD22	2.33	0.51
2:A:1017:LEU:CB	6:E:206:GLY:H	2.18	0.51
4:C:248:ILE:HG23	12:K:98:LEU:HD22	1.92	0.51
3:B:95:ILE:HG13	3:B:130:VAL:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:618:GLU:OE1	2:A:620:LYS:HG3	2.10	0.51
7:F:111:LEU:H	7:F:111:LEU:CD1	2.23	0.51
2:A:262:LEU:O	2:A:264:PHE:N	2.44	0.51
2:A:152:VAL:HG12	2:A:153:PRO:HD2	1.92	0.51
6:E:55:ARG:C	6:E:57:MET:N	2.64	0.51
9:H:145:ARG:O	9:H:146:ARG:HB2	2.10	0.51
2:A:965:GLN:O	2:A:968:GLN:HB2	2.10	0.51
2:A:332:LYS:O	2:A:333:GLU:HB2	2.09	0.51
3:B:685:LEU:C	3:B:687:GLU:H	2.12	0.51
3:B:622:LYS:HE2	10:I:59:VAL:CG2	2.35	0.51
4:C:234:SER:HB3	4:C:240:VAL:HG13	1.93	0.51
2:A:873:MET:HG2	2:A:957:PRO:HB3	1.93	0.51
3:B:542:MET:HG2	3:B:747:MET:HB3	1.92	0.51
2:A:590:ARG:NH2	2:A:620:LYS:HB3	2.23	0.51
2:A:552:TRP:NE1	12:K:62:LYS:HB2	2.23	0.51
8:G:87:VAL:HG23	8:G:103:VAL:HG21	1.91	0.51
7:F:69:LEU:CB	7:F:72:LYS:HB2	2.40	0.51
9:H:47:PHE:CD2	9:H:95:TYR:HD1	2.29	0.51
2:A:92:HIS:CD2	2:A:304:MET:HE1	2.46	0.51
9:H:15:VAL:HG22	9:H:26:ILE:CD1	2.41	0.51
3:B:310:MET:HE3	3:B:387:LEU:HD12	1.92	0.51
3:B:169:ARG:HD2	3:B:454:THR:HG21	1.92	0.51
1:R:7:U:P	3:B:942:ARG:HH22	2.34	0.51
2:A:438:ASP:OD1	2:A:461:LYS:HA	2.10	0.51
3:B:1034:VAL:HG12	3:B:1035:ALA:N	2.23	0.51
2:A:1242:VAL:HG12	2:A:1243:VAL:H	1.75	0.51
2:A:168:GLY:O	2:A:169:ASN:C	2.49	0.51
3:B:893:LEU:HD11	3:B:910:VAL:HG11	1.92	0.51
12:K:47:ARG:C	12:K:47:ARG:HD2	2.30	0.51
3:B:253:THR:HG22	3:B:254:LEU:N	2.26	0.51
2:A:722:LEU:HD22	2:A:799:PHE:CD1	2.45	0.51
2:A:547:LEU:HD22	12:K:58:PHE:HE1	1.73	0.51
2:A:90:VAL:HG11	2:A:297:GLN:HA	1.91	0.51
3:B:641:GLU:HB3	3:B:643:ASP:OD2	2.11	0.51
2:A:696:GLU:OE2	2:A:702:LEU:HD21	2.11	0.51
13:L:32:ALA:CB	13:L:55:ILE:HD12	2.26	0.51
3:B:217:ARG:C	3:B:217:ARG:HD2	2.31	0.51
2:A:334:GLY:O	2:A:336:ILE:N	2.43	0.51
3:B:100:PRO:CD	3:B:180:TYR:HE1	2.22	0.51
3:B:51:PHE:CD2	3:B:173:MET:HB3	2.46	0.51
12:K:41:THR:HG22	12:K:42:LEU:N	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:669:THR:O	2:A:805:LEU:HD22	2.10	0.51
2:A:512:VAL:HG12	2:A:512:VAL:O	2.11	0.51
8:G:91:VAL:HG23	8:G:141:SER:O	2.10	0.51
6:E:169:ARG:NH1	7:F:74:ILE:HD11	2.25	0.51
7:F:143:PHE:C	7:F:143:PHE:CD1	2.84	0.51
3:B:244:LEU:HD21	3:B:366:GLN:HE21	1.76	0.51
2:A:87:ALA:CB	2:A:276:LEU:HD23	2.41	0.51
3:B:640:VAL:O	3:B:641:GLU:C	2.49	0.51
3:B:299:GLU:OE2	3:B:572:HIS:HE1	1.93	0.51
3:B:570:VAL:HG23	3:B:573:GLN:HB3	1.92	0.51
9:H:83:GLN:O	9:H:85:GLY:N	2.41	0.51
2:A:148:CYS:O	2:A:168:GLY:HA2	2.10	0.51
2:A:982:THR:O	2:A:985:ASP:HB2	2.11	0.51
2:A:1273:LEU:HD12	2:A:1273:LEU:N	2.26	0.51
7:F:118:LEU:HD12	7:F:118:LEU:O	2.11	0.51
3:B:1073:TYR:CE2	3:B:1080:LYS:HG2	2.45	0.51
2:A:1444:MET:CE	7:F:135:ARG:HB2	2.35	0.51
4:C:10:ILE:CD1	12:K:108:GLU:HB3	2.41	0.51
10:I:50:THR:HG22	10:I:51:ASN:N	2.26	0.51
3:B:781:PHE:HE2	3:B:793:ALA:HB1	1.75	0.51
7:F:111:LEU:C	7:F:113:GLY:N	2.64	0.51
12:K:21:ILE:CG1	12:K:33:ILE:HG23	2.41	0.51
12:K:31:VAL:CG1	12:K:32:VAL:N	2.73	0.51
5:D:23:ASN:O	8:G:83:LYS:HB2	2.11	0.51
5:D:208:GLU:O	5:D:212:LYS:HG3	2.11	0.51
2:A:782:ARG:NH2	3:B:699:GLU:O	2.42	0.51
3:B:562:GLY:HA3	3:B:590:HIS:CE1	2.46	0.50
4:C:251:LEU:O	4:C:255:VAL:HG23	2.11	0.50
2:A:870:GLU:HG2	6:E:208:TYR:CD2	2.45	0.50
2:A:929:LEU:CD2	2:A:983:ILE:HG21	2.41	0.50
3:B:547:VAL:HG13	3:B:548:GLY:N	2.26	0.50
3:B:288:ALA:O	3:B:331:LEU:HD11	2.10	0.50
3:B:995:ARG:NH1	4:C:165:LYS:HG2	2.25	0.50
4:C:60:ASP:OD1	13:L:60:ARG:NH2	2.40	0.50
9:H:63:LEU:HB3	9:H:90:ALA:HB3	1.93	0.50
4:C:160:LYS:O	4:C:161:LYS:O	2.29	0.50
2:A:709:THR:HB	2:A:712:GLU:H	1.76	0.50
3:B:343:ILE:HG22	3:B:348:ARG:HG3	1.91	0.50
2:A:107:CYS:N	2:A:114:LEU:HD21	2.26	0.50
3:B:899:ILE:CG2	3:B:949:VAL:HG21	2.42	0.50
5:D:59:ILE:HG22	5:D:60:LYS:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1010:LEU:O	3:B:1011:ILE:CG1	2.60	0.50
2:A:899:VAL:CG1	2:A:929:LEU:HD11	2.41	0.50
2:A:806:ARG:NH1	3:B:729:ILE:HG13	2.25	0.50
2:A:341:MET:HE3	2:A:843:LYS:NZ	2.27	0.50
2:A:254:GLU:HB2	3:B:935:ARG:HH22	1.76	0.50
3:B:175:ARG:NH1	3:B:175:ARG:HG2	2.25	0.50
8:G:83:LYS:HE2	8:G:150:CYS:H	1.77	0.50
6:E:197:LYS:HG3	6:E:211:TYR:CE2	2.47	0.50
3:B:446:LEU:HD23	3:B:446:LEU:N	2.26	0.50
9:H:142:LEU:C	9:H:143:LEU:HD12	2.32	0.50
2:A:1389:PHE:CD1	2:A:1389:PHE:C	2.83	0.50
2:A:63:ARG:HA	2:A:74:MET:HE2	1.91	0.50
3:B:29:ASP:HB3	3:B:658:ILE:CD1	2.41	0.50
2:A:588:LEU:O	2:A:606:LEU:HD12	2.11	0.50
2:A:528:LEU:HD23	2:A:751:SER:CA	2.41	0.50
2:A:44:THR:O	2:A:45:GLN:HB2	2.10	0.50
13:L:27:LEU:HD23	13:L:27:LEU:N	2.25	0.50
5:D:12:ARG:HG2	5:D:14:ARG:HG3	1.94	0.50
3:B:303:TYR:N	3:B:303:TYR:CD2	2.78	0.50
5:D:8:PHE:CE2	5:D:40:HIS:HA	2.47	0.50
2:A:535:THR:O	2:A:575:LYS:HG3	2.12	0.50
5:D:56:ARG:HA	5:D:148:LEU:HD13	1.94	0.50
3:B:611:PRO:CB	3:B:685:LEU:HD21	2.41	0.50
6:E:202:SER:HB3	6:E:205:SER:O	2.12	0.50
6:E:39:LEU:O	6:E:42:PHE:HB3	2.10	0.50
3:B:129:PHE:HE2	3:B:166:PHE:CD1	2.29	0.50
3:B:1045:SER:O	3:B:1046:PRO:O	2.29	0.50
2:A:1067:LEU:HD12	2:A:1367:HIS:CE1	2.46	0.50
2:A:836:TYR:CZ	2:A:840:ARG:HD2	2.46	0.50
2:A:683:ILE:HD13	2:A:801:GLU:HG3	1.94	0.50
8:G:149:GLY:O	8:G:159:ALA:HB1	2.11	0.50
2:A:49:LYS:HZ1	2:A:61:ILE:CG1	2.25	0.50
2:A:1445:ILE:HD11	8:G:68:ALA:CB	2.39	0.50
11:J:47:ARG:HH11	11:J:47:ARG:HG2	1.77	0.50
2:A:1225:PHE:HE2	2:A:1227:ILE:HD11	1.76	0.50
2:A:12:ARG:CZ	3:B:1192:TYR:HE2	2.24	0.50
3:B:409:ALA:O	3:B:413:LEU:HG	2.11	0.50
7:F:77:ASP:O	7:F:78:GLN:HB2	2.12	0.50
2:A:70:CYS:O	2:A:70:CYS:SG	2.70	0.50
2:A:1124:HIS:HB3	2:A:1130:GLN:HG2	1.94	0.50
2:A:785:PRO:HG2	2:A:786:HIS:HD2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1102:LYS:O	3:B:1103:ILE:C	2.50	0.50
3:B:654:ARG:H	3:B:657:HIS:HD2	1.59	0.50
2:A:207:ILE:HG22	2:A:211:PHE:CE1	2.47	0.50
6:E:90:VAL:HG22	6:E:90:VAL:O	2.11	0.50
9:H:130:ARG:H	9:H:130:ARG:CD	2.10	0.50
3:B:744:HIS:ND1	3:B:745:PRO:HD2	2.26	0.50
9:H:105:GLU:HG2	9:H:106:GLU:H	1.77	0.50
4:C:113:VAL:O	4:C:144:ILE:HB	2.12	0.50
2:A:339:ASN:HB3	3:B:1117:GLN:NE2	2.25	0.50
3:B:1081:LEU:HD12	3:B:1085:ILE:HD11	1.92	0.50
3:B:705:MET:H	3:B:710:LEU:HD12	1.76	0.50
2:A:172:PRO:HG3	2:A:185:TRP:CZ2	2.46	0.50
2:A:117:GLU:H	2:A:117:GLU:CD	2.15	0.50
2:A:49:LYS:HE2	2:A:61:ILE:HD12	1.93	0.50
2:A:49:LYS:HZ3	2:A:61:ILE:HG13	1.74	0.50
4:C:144:ILE:HG22	4:C:145:CYS:N	2.27	0.50
2:A:444:PHE:HB2	2:A:458:HIS:HD2	1.77	0.50
3:B:757:PRO:HD3	3:B:983:ARG:NH2	2.26	0.50
6:E:86:PRO:O	6:E:114:ASN:HB2	2.12	0.50
8:G:145:VAL:CG1	8:G:146:LYS:N	2.74	0.50
3:B:582:VAL:HG23	3:B:626:ILE:HB	1.94	0.50
3:B:185:THR:O	3:B:188:ASP:N	2.45	0.50
2:A:1385:THR:HG22	2:A:1386:ARG:N	2.27	0.50
2:A:1242:VAL:HG12	2:A:1243:VAL:N	2.27	0.50
2:A:89:PRO:O	2:A:204:THR:HG21	2.12	0.50
3:B:286:PHE:CD1	3:B:297:ILE:HG23	2.47	0.50
8:G:1:MET:C	8:G:1:MET:SD	2.90	0.49
2:A:399:HIS:CB	2:A:400:PRO:CD	2.90	0.49
2:A:899:VAL:CG2	2:A:1029:ARG:HG2	2.41	0.49
1:R:4:U:O2	1:R:16:A:H2	1.94	0.49
3:B:1065:GLN:HG3	3:B:1067:ARG:H	1.76	0.49
3:B:309:GLN:HG3	10:I:52:ILE:HD11	1.93	0.49
13:L:40:LEU:HD22	13:L:44:ASP:CB	2.41	0.49
3:B:284:ILE:HG23	3:B:324:ILE:CD1	2.42	0.49
3:B:1034:VAL:HG21	3:B:1055:ILE:HG23	1.93	0.49
4:C:161:LYS:O	4:C:170:TRP:NE1	2.45	0.49
2:A:1120:LEU:CD1	2:A:1120:LEU:H	2.25	0.49
3:B:549:THR:HG22	3:B:550:ASP:N	2.18	0.49
6:E:192:ARG:HH11	6:E:192:ARG:HG3	1.77	0.49
2:A:92:HIS:O	2:A:95:PHE:N	2.45	0.49
2:A:224:PHE:CD2	2:A:231:PRO:HG3	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:39:ARG:NH2	3:B:665:GLU:CG	2.75	0.49
2:A:385:ILE:HD11	2:A:426:LEU:HB2	1.92	0.49
3:B:893:LEU:HD11	3:B:910:VAL:CG1	2.42	0.49
3:B:785:TYR:C	3:B:785:TYR:CD1	2.85	0.49
3:B:896:ASP:OD2	13:L:58:LYS:HE3	2.12	0.49
2:A:1156:PRO:HA	2:A:1190:PRO:CB	2.42	0.49
3:B:345:LYS:O	3:B:348:ARG:HB2	2.12	0.49
3:B:945:GLU:O	3:B:946:ASN:HB3	2.13	0.49
2:A:335:ARG:CA	2:A:339:ASN:HD22	2.24	0.49
3:B:832:GLY:O	3:B:835:GLN:NE2	2.44	0.49
4:C:251:LEU:HD11	12:K:45:LEU:CD2	2.43	0.49
2:A:901:LEU:O	2:A:921:GLY:N	2.34	0.49
9:H:61:SER:O	9:H:62:SER:HB3	2.12	0.49
3:B:39:ARG:HH21	3:B:665:GLU:CG	2.25	0.49
3:B:453:ILE:O	3:B:457:LEU:HG	2.12	0.49
3:B:616:ILE:CG1	3:B:697:GLU:HA	2.42	0.49
3:B:784:ASN:HD21	3:B:788:ARG:HD2	1.76	0.49
3:B:211:VAL:HG23	3:B:483:LEU:HB2	1.94	0.49
3:B:865:LYS:NZ	3:B:869:SER:HA	2.27	0.49
3:B:873:THR:CG2	3:B:874:PHE:N	2.76	0.49
3:B:281:PRO:HB3	3:B:320:ASP:OD2	2.12	0.49
3:B:800:GLN:HB3	11:J:52:THR:CG2	2.42	0.49
2:A:537:ARG:HD2	9:H:20:TYR:HE1	1.77	0.49
3:B:1156:ASP:O	3:B:1157:ALA:O	2.30	0.49
2:A:1220:PHE:O	2:A:1221:LYS:HB2	2.13	0.49
4:C:238:ILE:HG23	4:C:242:GLN:HB2	1.93	0.49
6:E:29:PHE:O	6:E:30:ILE:HG13	2.12	0.49
10:I:55:THR:HG23	10:I:86:PHE:CZ	2.46	0.49
2:A:629:LEU:HD22	2:A:633:VAL:HG23	1.94	0.49
8:G:117:GLN:O	8:G:119:LEU:N	2.46	0.49
3:B:54:PHE:HA	3:B:58:THR:HB	1.94	0.49
12:K:12:LEU:HD12	12:K:12:LEU:N	2.28	0.49
2:A:29:ALA:HB1	3:B:1184:GLY:HA2	1.93	0.49
3:B:890:TYR:CZ	3:B:910:VAL:HG21	2.48	0.49
4:C:114:TYR:CD2	4:C:140:ASN:HB3	2.47	0.49
9:H:23:VAL:HG22	9:H:43:ASN:HA	1.93	0.49
12:K:88:LYS:O	12:K:91:CYS:HB2	2.13	0.49
2:A:537:ARG:O	2:A:540:PHE:CE1	2.66	0.49
9:H:89:LEU:C	9:H:91:ASP:N	2.65	0.49
3:B:825:VAL:O	3:B:826:ALA:HB2	2.13	0.49
2:A:718:VAL:O	2:A:721:PHE:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1201:LYS:HE2	3:B:1205:GLN:CD	2.33	0.49
3:B:327:ARG:HH22	3:B:371:GLU:HG2	1.77	0.49
9:H:113:ALA:HB1	9:H:125:LEU:O	2.11	0.49
2:A:1410:PHE:HA	3:B:1212:ILE:CD1	2.41	0.49
2:A:1037:LEU:HD12	2:A:1042:PHE:HD1	1.77	0.49
2:A:765:VAL:HG23	2:A:802:ASN:O	2.12	0.49
2:A:54:ASN:HB3	2:A:247:ARG:HH12	1.76	0.49
3:B:343:ILE:CG2	3:B:348:ARG:HG3	2.42	0.49
2:A:868:TYR:CE1	2:A:1064:VAL:CG1	2.95	0.49
1:R:4:U:H2'	1:R:5:U:C6	2.46	0.49
2:A:283:GLY:O	2:A:285:PRO:CD	2.58	0.49
8:G:27:LYS:HD3	8:G:51:TYR:CE2	2.47	0.49
3:B:582:VAL:HG12	3:B:587:HIS:NE2	2.28	0.49
2:A:1410:PHE:HD2	3:B:1212:ILE:HD12	1.77	0.49
3:B:295:GLY:N	3:B:298:LEU:HD23	2.27	0.49
3:B:569:TYR:CE1	3:B:589:VAL:HG21	2.48	0.49
7:F:89:GLU:OE2	7:F:134:ILE:HG21	2.13	0.49
2:A:774:ARG:O	2:A:775:ILE:C	2.51	0.49
2:A:1032:LEU:O	2:A:1036:ARG:HD3	2.12	0.49
2:A:1343:ALA:HB1	6:E:149:LEU:HB3	1.94	0.49
3:B:185:THR:O	3:B:188:ASP:HB2	2.12	0.49
3:B:735:ALA:O	3:B:738:PHE:HE1	1.96	0.49
2:A:862:ASN:HA	6:E:174:GLN:HB3	1.93	0.49
3:B:314:LEU:O	3:B:317:CYS:HB3	2.13	0.49
2:A:1364:ASN:O	2:A:1365:TYR:C	2.51	0.49
2:A:11:LEU:O	2:A:11:LEU:HD23	2.13	0.49
2:A:1120:LEU:O	2:A:1323:ASP:N	2.46	0.49
2:A:535:THR:HG23	2:A:575:LYS:HG2	1.95	0.49
2:A:596:THR:C	2:A:598:LEU:N	2.66	0.49
3:B:1151:LEU:CD1	3:B:1151:LEU:N	2.75	0.49
2:A:457:ALA:HB3	2:A:506:ALA:CA	2.41	0.49
2:A:1349:TYR:CA	2:A:1372:VAL:HG21	2.42	0.49
2:A:1048:ASN:O	2:A:1049:ILE:C	2.51	0.49
2:A:90:VAL:HG12	2:A:297:GLN:NE2	2.28	0.49
7:F:75:PRO:O	7:F:77:ASP:O	2.30	0.49
3:B:948:ILE:O	3:B:968:VAL:HG13	2.13	0.49
2:A:569:LYS:O	2:A:571:LEU:HD13	2.12	0.49
3:B:1196:ILE:HB	3:B:1197:PRO:HD2	1.95	0.49
2:A:442:VAL:O	2:A:457:ALA:HA	2.13	0.49
3:B:882:THR:HG22	3:B:884:ARG:CB	2.42	0.49
10:I:101:PHE:CE1	10:I:112:SER:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:766:ARG:HH22	3:B:1020:ARG:NH1	2.02	0.49
3:B:33:VAL:HG21	3:B:638:PHE:HZ	1.76	0.49
3:B:616:ILE:HG23	3:B:700:SER:OG	2.12	0.49
3:B:956:THR:CG2	3:B:960:GLY:HA2	2.43	0.49
3:B:234:ILE:HG12	3:B:257:LYS:HD3	1.94	0.49
4:C:183:TRP:O	4:C:185:LYS:N	2.45	0.49
2:A:264:PHE:O	2:A:267:ALA:HB3	2.13	0.49
8:G:119:LEU:HD13	8:G:132:SER:HB2	1.94	0.49
2:A:513:SER:OG	2:A:515:GLN:HG2	2.13	0.49
5:D:207:LEU:HD12	5:D:207:LEU:O	2.13	0.49
4:C:76:ASP:O	4:C:79:GLN:HG2	2.13	0.49
3:B:581:PHE:HA	3:B:585:VAL:O	2.12	0.49
3:B:980:PHE:CA	3:B:1095:LEU:HD11	2.43	0.49
7:F:138:LEU:HB2	7:F:142:SER:O	2.13	0.49
2:A:1226:VAL:HG13	2:A:1239:ARG:O	2.13	0.49
2:A:353:ILE:HB	2:A:470:LEU:CD2	2.43	0.49
2:A:302:THR:CG2	2:A:303:TYR:N	2.76	0.49
3:B:311:LEU:O	3:B:312:GLU:C	2.51	0.49
3:B:460:ALA:C	3:B:462:ALA:H	2.17	0.49
12:K:55:LYS:HB3	12:K:81:TYR:HD1	1.77	0.49
4:C:116:LYS:HD3	4:C:140:ASN:HA	1.95	0.49
10:I:73:ARG:O	10:I:81:ARG:HA	2.12	0.49
2:A:108:MET:N	2:A:108:MET:SD	2.85	0.49
2:A:278:THR:O	2:A:278:THR:HG22	2.13	0.49
2:A:49:LYS:NZ	2:A:61:ILE:CG1	2.76	0.48
9:H:101:ALA:HB2	9:H:116:TYR:CE1	2.48	0.48
4:C:235:VAL:HG11	11:J:6:ARG:NH2	2.28	0.48
8:G:18:PHE:HA	8:G:22:MET:HE2	1.94	0.48
5:D:51:ASN:OD1	5:D:54:GLU:HB3	2.12	0.48
6:E:46:TYR:CE2	6:E:58:MET:HA	2.48	0.48
6:E:136:ASN:OD1	6:E:138:ALA:N	2.46	0.48
2:A:1329:THR:CG2	2:A:1331:SER:HB3	2.43	0.48
4:C:20:PHE:HE1	4:C:22:LEU:HB2	1.77	0.48
2:A:503:GLN:C	2:A:504:LEU:HD12	2.33	0.48
3:B:871:THR:HG22	3:B:872:GLU:O	2.13	0.48
2:A:1410:PHE:C	2:A:1412:ALA:H	2.16	0.48
5:D:130:LEU:C	5:D:132:GLN:H	2.15	0.48
2:A:482:PHE:C	2:A:484:GLY:H	2.16	0.48
4:C:47:ASP:CA	13:L:69:ALA:CB	2.88	0.48
4:C:70:ILE:HD11	4:C:144:ILE:CG1	2.44	0.48
2:A:1428:VAL:HG13	3:B:1151:LEU:CD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1017:LEU:CB	6:E:205:SER:HA	2.43	0.48
2:A:1227:ILE:CG2	2:A:1228:TRP:H	2.21	0.48
4:C:25:VAL:HG23	4:C:228:PHE:HE1	1.77	0.48
2:A:1198:ASP:HB3	2:A:1201:ALA:CB	2.41	0.48
12:K:21:ILE:HG12	12:K:33:ILE:HG23	1.94	0.48
3:B:1180:PHE:HB3	3:B:1191:ILE:HD12	1.95	0.48
2:A:527:THR:HG21	2:A:650:GLN:HA	1.95	0.48
3:B:236:HIS:CE1	3:B:389:ALA:HA	2.49	0.48
10:I:16:PRO:HB3	10:I:27:PHE:HD2	1.78	0.48
2:A:1446:ASP:HB2	7:F:133:VAL:CG2	2.43	0.48
8:G:9:LEU:HD12	8:G:10:ASN:H	1.78	0.48
4:C:138:GLU:OE1	4:C:138:GLU:N	2.46	0.48
3:B:459:TYR:CZ	3:B:469:GLN:HG2	2.47	0.48
7:F:131:PRO:C	7:F:132:LEU:HD23	2.33	0.48
2:A:1134:ILE:O	2:A:1138:ILE:HG13	2.12	0.48
11:J:43:ARG:HG3	11:J:45:CYS:SG	2.53	0.48
4:C:242:GLN:C	4:C:244:VAL:N	2.66	0.48
3:B:705:MET:N	3:B:710:LEU:HD12	2.29	0.48
3:B:729:ILE:O	3:B:729:ILE:HG22	2.13	0.48
5:D:191:ALA:C	5:D:193:THR:H	2.16	0.48
3:B:199:MET:N	3:B:199:MET:SD	2.83	0.48
3:B:44:VAL:O	3:B:45:SER:C	2.52	0.48
2:A:1119:TYR:HA	2:A:1305:VAL:HG13	1.95	0.48
3:B:1223:ASP:HB3	3:B:1224:PHE:H	1.43	0.48
10:I:109:ILE:HG22	10:I:109:ILE:O	2.14	0.48
2:A:635:ARG:HH11	2:A:635:ARG:HA	1.78	0.48
2:A:964:ILE:O	2:A:967:ALA:HB3	2.12	0.48
8:G:125:SER:OG	8:G:128:PRO:HA	2.12	0.48
3:B:579:ARG:HG2	3:B:579:ARG:NH1	2.26	0.48
3:B:1065:GLN:NE2	3:B:1067:ARG:H	2.08	0.48
3:B:309:GLN:HG3	10:I:52:ILE:CD1	2.44	0.48
3:B:582:VAL:O	3:B:582:VAL:HG12	2.12	0.48
2:A:1118:VAL:O	2:A:1118:VAL:HG23	2.13	0.48
4:C:91:HIS:O	4:C:91:HIS:ND1	2.47	0.48
2:A:129:LYS:O	2:A:130:ASP:HB2	2.14	0.48
2:A:51:GLY:HA2	2:A:56:PRO:HA	1.96	0.48
2:A:34:LYS:HE3	2:A:57:ARG:HH12	1.76	0.48
3:B:113:TYR:CD2	3:B:192:LEU:HD22	2.48	0.48
10:I:69:PRO:HG2	10:I:85:PHE:CD2	2.48	0.48
3:B:758:PHE:CE1	3:B:1027:ILE:CG2	2.96	0.48
2:A:608:ILE:HG13	2:A:613:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:309:GLN:O	3:B:312:GLU:HB3	2.13	0.48
3:B:873:THR:HG22	3:B:874:PHE:N	2.27	0.48
2:A:206:GLU:O	2:A:210:ILE:HG13	2.13	0.48
3:B:40:GLU:OE1	3:B:682:SER:HB2	2.14	0.48
2:A:709:THR:HG21	2:A:711:ARG:HB2	1.96	0.48
3:B:114:PRO:HG2	3:B:115:GLN:H	1.78	0.48
9:H:128:ASN:O	9:H:128:ASN:OD1	2.31	0.48
3:B:25:ILE:HD11	3:B:653:VAL:C	2.34	0.48
2:A:1116:LEU:CB	2:A:1308:THR:HG21	2.43	0.48
9:H:15:VAL:HG22	9:H:26:ILE:CG1	2.41	0.48
2:A:718:VAL:HG12	2:A:722:LEU:HD11	1.95	0.48
5:D:134:THR:CG2	5:D:135:GLY:N	2.74	0.48
3:B:287:ARG:NH1	3:B:324:ILE:O	2.46	0.48
2:A:1333:ILE:O	2:A:1337:GLU:HG3	2.14	0.48
2:A:578:LEU:HD23	2:A:612:ILE:HD11	1.95	0.48
3:B:997:GLU:HB3	4:C:35:ARG:HB3	1.95	0.48
4:C:21:ILE:HG12	4:C:229:TYR:HD2	1.78	0.48
2:A:518:LYS:HE2	2:A:624:SER:O	2.13	0.48
7:F:69:LEU:CD2	7:F:71:GLU:C	2.82	0.48
3:B:361:LEU:N	3:B:362:PRO:CD	2.77	0.48
2:A:332:LYS:HG3	2:A:333:GLU:HG2	1.96	0.48
6:E:182:ASP:HB3	6:E:185:ALA:CB	2.44	0.48
2:A:445:ASN:HB2	2:A:455:MET:HG2	1.95	0.48
5:D:64:VAL:C	5:D:66:ARG:H	2.17	0.48
13:L:43:THR:O	13:L:43:THR:HG22	2.13	0.48
7:F:68:THR:HG21	7:F:69:LEU:HB2	1.96	0.48
8:G:80:LYS:HD3	8:G:80:LYS:N	2.29	0.48
9:H:95:TYR:CE2	9:H:97:MET:HG3	2.49	0.48
9:H:58:THR:HG22	9:H:59:ILE:N	2.29	0.48
3:B:578:THR:C	3:B:589:VAL:HG13	2.33	0.48
2:A:873:MET:C	2:A:1058:VAL:HG23	2.33	0.48
2:A:896:ARG:NH2	2:A:1030:ARG:HH21	2.12	0.48
6:E:182:ASP:HB3	6:E:185:ALA:HB2	1.95	0.48
3:B:654:ARG:O	3:B:656:GLY:N	2.47	0.48
3:B:902:GLY:O	13:L:65:VAL:HG11	2.13	0.48
4:C:66:ARG:NH1	11:J:2:ILE:CG2	2.72	0.48
4:C:36:VAL:HG21	4:C:251:LEU:CD2	2.38	0.48
2:A:860:LEU:CD1	2:A:1393:ASN:HB2	2.41	0.48
3:B:1158:PHE:CD1	3:B:1159:ARG:N	2.81	0.48
7:F:143:PHE:HD1	7:F:143:PHE:C	2.17	0.48
2:A:1224:LEU:HD12	2:A:1241:ARG:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1349:TYR:CB	2:A:1372:VAL:HG21	2.44	0.48
9:H:62:SER:C	9:H:64:ASN:N	2.67	0.48
4:C:186:LEU:HD12	4:C:186:LEU:N	2.29	0.48
13:L:38:LEU:HD11	13:L:49:LYS:HE2	1.96	0.48
6:E:88:VAL:HG12	6:E:89:GLY:N	2.29	0.48
2:A:547:LEU:HD13	12:K:58:PHE:CD1	2.48	0.48
2:A:541:ILE:HG22	2:A:546:VAL:HG23	1.95	0.48
2:A:1280:GLU:O	2:A:1281:ARG:C	2.52	0.48
4:C:114:TYR:CG	4:C:140:ASN:HB3	2.49	0.48
6:E:116:ILE:HG22	6:E:120:ALA:HB3	1.95	0.48
5:D:18:VAL:O	5:D:18:VAL:HG22	2.13	0.48
2:A:62:ASP:HB3	2:A:64:ASN:ND2	2.28	0.48
5:D:27:LEU:HD22	5:D:173:HIS:CD2	2.49	0.48
2:A:709:THR:HG23	10:I:94:ASP:HA	1.96	0.48
8:G:14:HIS:CE1	8:G:15:PRO:HD2	2.49	0.48
2:A:1376:THR:HG23	2:A:1377:THR:N	2.29	0.48
2:A:2:VAL:CG2	3:B:1157:ALA:HB1	2.33	0.48
3:B:25:ILE:HG23	3:B:658:ILE:HD12	1.96	0.48
4:C:234:SER:HB2	4:C:240:VAL:HG13	1.96	0.48
6:E:28:TYR:HE1	6:E:78:LEU:CD1	2.25	0.48
2:A:666:ILE:HD12	2:A:667:GLY:H	1.79	0.48
2:A:451:HIS:NE2	2:A:1074:GLU:HG3	2.29	0.48
5:D:153:ARG:HB3	5:D:154:PHE:CD1	2.48	0.48
2:A:262:LEU:C	2:A:264:PHE:H	2.16	0.48
12:K:55:LYS:HB2	12:K:81:TYR:HE1	1.79	0.48
5:D:29:LEU:HD22	8:G:82:PHE:CE2	2.48	0.48
3:B:373:ARG:HG2	3:B:566:LEU:HD23	1.95	0.48
2:A:741:ASN:C	2:A:741:ASN:HD22	2.17	0.48
10:I:15:TYR:H	10:I:15:TYR:HD1	1.61	0.47
10:I:34:TYR:HE2	10:I:36:GLU:HB3	1.78	0.47
2:A:1120:LEU:HD13	2:A:1120:LEU:H	1.79	0.47
2:A:1120:LEU:HD12	2:A:1120:LEU:N	2.28	0.47
3:B:240:ILE:HD13	3:B:377:PHE:HE2	1.79	0.47
3:B:824:ILE:HG22	3:B:824:ILE:O	2.13	0.47
6:E:177:ARG:C	6:E:212:ARG:HD3	2.34	0.47
2:A:806:ARG:HH12	3:B:729:ILE:CD1	2.27	0.47
3:B:324:ILE:HD13	3:B:330:ALA:HA	1.95	0.47
2:A:1289:ARG:NH1	2:A:1326:ARG:NH1	2.62	0.47
2:A:98:LYS:O	2:A:102:VAL:HG23	2.14	0.47
3:B:1032:SER:O	3:B:1036:ALA:HB2	2.13	0.47
13:L:34:CYS:SG	13:L:34:CYS:O	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:37:PHE:CD1	2:A:37:PHE:N	2.82	0.47
3:B:806:THR:O	3:B:809:MET:HG3	2.14	0.47
2:A:53:LEU:O	2:A:54:ASN:C	2.53	0.47
3:B:1081:LEU:O	3:B:1082:MET:C	2.52	0.47
2:A:1265:ASN:ND2	3:B:265:SER:HB3	2.29	0.47
3:B:120:ARG:HG2	3:B:955:THR:HG21	1.96	0.47
2:A:30:ILE:HD11	3:B:1168:LEU:HD13	1.96	0.47
2:A:443:LEU:HD12	3:B:1146:PHE:CE2	2.49	0.47
3:B:558:LEU:O	3:B:561:TRP:N	2.47	0.47
2:A:754:SER:O	2:A:757:ASN:HB2	2.13	0.47
2:A:347:PHE:CE2	2:A:375:THR:HG23	2.49	0.47
5:D:175:PHE:HE1	8:G:1:MET:HA	1.78	0.47
3:B:172:ILE:HG21	3:B:178:ASN:HB3	1.95	0.47
5:D:17:LYS:HE3	5:D:17:LYS:CA	2.34	0.47
2:A:1444:MET:HE2	7:F:135:ARG:CB	2.41	0.47
9:H:62:SER:O	9:H:64:ASN:N	2.47	0.47
3:B:129:PHE:CE2	3:B:166:PHE:HD1	2.32	0.47
9:H:107:VAL:O	9:H:111:LEU:HB2	2.15	0.47
3:B:846:ILE:HG23	3:B:974:PRO:HG2	1.96	0.47
3:B:575:PRO:HG2	3:B:576:ASP:H	1.80	0.47
8:G:39:THR:HG22	8:G:41:LYS:H	1.78	0.47
4:C:125:MET:HB2	4:C:127:ARG:HE	1.79	0.47
2:A:1345:ARG:HG3	2:A:1376:THR:HG21	1.96	0.47
10:I:101:PHE:N	10:I:101:PHE:CD1	2.82	0.47
2:A:1116:LEU:CB	2:A:1308:THR:CG2	2.93	0.47
4:C:242:GLN:HB3	4:C:246:ARG:HG3	1.96	0.47
6:E:19:VAL:HG11	6:E:80:VAL:HG11	1.95	0.47
3:B:762:ASN:HD21	3:B:1024:ALA:HB3	1.80	0.47
3:B:957:ASN:O	3:B:958:GLN:C	2.51	0.47
2:A:295:LEU:O	2:A:298:PHE:HB3	2.14	0.47
2:A:527:THR:CG2	2:A:650:GLN:HA	2.45	0.47
2:A:63:ARG:HG2	2:A:74:MET:HE1	1.95	0.47
3:B:903:VAL:CG1	3:B:904:ARG:N	2.78	0.47
2:A:224:PHE:CE2	2:A:231:PRO:HG3	2.49	0.47
7:F:84:TYR:CD2	7:F:152:ILE:HB	2.49	0.47
3:B:37:PHE:C	3:B:37:PHE:CD1	2.85	0.47
3:B:1187:ASN:O	3:B:1188:LYS:CB	2.60	0.47
2:A:262:LEU:C	2:A:264:PHE:N	2.67	0.47
3:B:1077:THR:HG22	12:K:44:ASN:HD21	1.78	0.47
6:E:164:LEU:HD21	6:E:211:TYR:CG	2.49	0.47
5:D:175:PHE:HZ	8:G:85:GLU:HG3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:711:ARG:O	2:A:714:PHE:HB3	2.15	0.47
2:A:567:LYS:HB3	9:H:95:TYR:CA	2.44	0.47
9:H:127:GLY:N	9:H:130:ARG:HH22	2.12	0.47
3:B:25:ILE:HG22	3:B:29:ASP:CB	2.45	0.47
2:A:1263:ILE:O	2:A:1267:MET:HG3	2.15	0.47
3:B:376:PHE:HB3	3:B:586:TRP:CZ3	2.49	0.47
3:B:94:LYS:HG2	3:B:95:ILE:H	1.79	0.47
3:B:1220:ARG:HH11	3:B:1220:ARG:HB3	1.79	0.47
3:B:610:ASN:O	3:B:612:GLU:N	2.48	0.47
3:B:827:ILE:HA	3:B:1012:ILE:O	2.14	0.47
7:F:69:LEU:HD22	7:F:72:LYS:N	2.30	0.47
2:A:61:ILE:O	2:A:63:ARG:N	2.48	0.47
8:G:1:MET:HE3	8:G:80:LYS:C	2.35	0.47
13:L:55:ILE:O	13:L:56:LEU:CB	2.63	0.47
3:B:364:ILE:HG12	3:B:585:VAL:CG1	2.30	0.47
3:B:222:ILE:O	3:B:240:ILE:HA	2.15	0.47
3:B:360:PHE:CE2	3:B:361:LEU:HB2	2.49	0.47
8:G:15:PRO:CG	8:G:66:GLY:HA3	2.45	0.47
3:B:1098:MET:CE	3:B:1098:MET:H	2.27	0.47
3:B:840:ILE:HG21	3:B:994:TYR:CD1	2.50	0.47
3:B:1103:ILE:O	3:B:1122:ARG:NH1	2.48	0.47
6:E:153:HIS:HB3	6:E:196:VAL:HG13	1.96	0.47
3:B:33:VAL:O	3:B:36:ALA:HB3	2.15	0.47
4:C:243:VAL:HG12	4:C:243:VAL:O	2.15	0.47
4:C:22:LEU:HD11	12:K:101:LEU:HD11	1.96	0.47
3:B:706:GLN:NE2	3:B:730:ARG:NH1	2.62	0.47
2:A:1068:ALA:HA	2:A:1367:HIS:ND1	2.30	0.47
5:D:154:PHE:CE2	5:D:163:VAL:HG21	2.49	0.47
3:B:582:VAL:O	3:B:582:VAL:CG1	2.63	0.47
4:C:35:ARG:HH11	12:K:41:THR:N	2.11	0.47
4:C:89:GLU:O	4:C:90:ASP:CB	2.62	0.47
2:A:1272:THR:C	2:A:1273:LEU:HD12	2.35	0.47
5:D:66:ARG:O	5:D:70:PHE:HB2	2.14	0.47
9:H:84:ALA:HA	9:H:87:ARG:HB2	1.95	0.47
2:A:1149:ALA:CB	10:I:47:GLU:HA	2.44	0.47
6:E:47:CYS:HA	6:E:52:ARG:O	2.14	0.47
6:E:13:TRP:HB2	6:E:42:PHE:CD2	2.49	0.47
2:A:1279:ILE:HD11	2:A:1316:VAL:CG2	2.44	0.47
2:A:1225:PHE:CE2	2:A:1227:ILE:HD11	2.50	0.47
3:B:1162:ILE:HG23	3:B:1168:LEU:O	2.14	0.47
3:B:1068:GLY:O	3:B:1069:PHE:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:254:GLU:HB2	3:B:935:ARG:NH1	2.29	0.47
2:A:942:PHE:HD2	2:A:943:LEU:HD23	1.79	0.47
3:B:186:GLU:HG2	11:J:62:ARG:HH22	1.78	0.47
2:A:492:PRO:HB3	2:A:501:LEU:HD12	1.97	0.47
6:E:100:ILE:HG23	6:E:105:PHE:CD1	2.49	0.47
3:B:1079:LYS:N	4:C:27:LEU:HD21	2.30	0.47
8:G:8:SER:HB3	8:G:73:LYS:HD2	1.95	0.47
2:A:1265:ASN:C	2:A:1267:MET:N	2.67	0.47
2:A:84:ILE:CD1	2:A:270:LEU:HD22	2.43	0.47
2:A:218:ASP:O	2:A:219:PHE:C	2.52	0.47
2:A:993:LEU:HD21	2:A:1049:ILE:HG21	1.97	0.47
2:A:844:ALA:C	2:A:845:LEU:HD23	2.35	0.47
4:C:53:THR:O	4:C:153:LEU:HA	2.14	0.47
12:K:111:LEU:O	12:K:112:GLN:CB	2.62	0.47
3:B:642:ASP:CA	3:B:649:LYS:HG3	2.44	0.47
3:B:460:ALA:O	3:B:462:ALA:N	2.48	0.47
4:C:69:LEU:CD1	4:C:69:LEU:N	2.78	0.47
3:B:604:ARG:HH11	3:B:691:GLU:HG2	1.80	0.47
2:A:1283:VAL:HG12	2:A:1284:MET:H	1.79	0.47
2:A:1156:PRO:HA	2:A:1190:PRO:HB3	1.96	0.47
6:E:105:PHE:O	6:E:106:GLN:HB2	2.15	0.47
3:B:889:THR:HG22	3:B:891:ASP:H	1.80	0.47
2:A:673:GLY:O	2:A:676:MET:HB2	2.15	0.47
8:G:48:VAL:HG13	8:G:74:TYR:HD1	1.79	0.47
3:B:905:VAL:CG2	3:B:941:LEU:HD22	2.41	0.47
3:B:361:LEU:O	3:B:363:HIS:O	2.33	0.47
8:G:59:GLY:HA3	8:G:70:PHE:CD2	2.50	0.47
2:A:343:LYS:NZ	3:B:1151:LEU:HB3	2.30	0.47
5:D:13:ARG:HB3	5:D:17:LYS:HZ3	1.80	0.47
3:B:35:SER:HA	3:B:811:TYR:CE2	2.37	0.47
2:A:590:ARG:HB3	2:A:605:MET:N	2.30	0.47
2:A:605:MET:HE3	2:A:614:PHE:O	2.15	0.47
2:A:265:LYS:HD2	2:A:265:LYS:H	1.80	0.47
4:C:8:VAL:O	4:C:9:LYS:HG3	2.15	0.47
3:B:785:TYR:CD1	3:B:786:ASN:N	2.83	0.47
3:B:1224:PHE:CE2	6:E:171:LYS:HG3	2.49	0.47
13:L:30:ILE:HG22	13:L:31:CYS:N	2.30	0.46
3:B:840:ILE:HD13	3:B:994:TYR:CE1	2.47	0.46
6:E:29:PHE:C	6:E:30:ILE:HG13	2.35	0.46
3:B:37:PHE:HD2	3:B:542:MET:SD	2.38	0.46
4:C:152:GLU:OE2	4:C:154:LYS:HE3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:289:LEU:HD13	3:B:375:ALA:CB	2.45	0.46
6:E:55:ARG:O	6:E:57:MET:N	2.47	0.46
2:A:852:TYR:CD1	7:F:136:ARG:HB3	2.50	0.46
6:E:157:SER:C	6:E:159:ASP:N	2.68	0.46
3:B:603:LEU:HB3	3:B:609:ILE:CD1	2.44	0.46
3:B:1039:GLY:HA2	11:J:51:LEU:HD21	1.97	0.46
5:D:128:VAL:O	5:D:132:GLN:HG3	2.14	0.46
2:A:1187:GLN:NE2	2:A:1188:GLN:HE21	2.13	0.46
11:J:35:ALA:O	11:J:39:LEU:HD12	2.16	0.46
4:C:101:LEU:C	4:C:102:GLN:HG3	2.34	0.46
3:B:948:ILE:HG22	3:B:949:VAL:O	2.15	0.46
2:A:343:LYS:HZ3	3:B:1197:PRO:HB3	1.79	0.46
2:A:853:ASP:CG	2:A:855:THR:HG22	2.34	0.46
3:B:942:ARG:O	3:B:944:THR:N	2.49	0.46
2:A:450:LEU:HD12	2:A:450:LEU:N	2.30	0.46
3:B:123:THR:O	3:B:125:SER:N	2.46	0.46
3:B:424:LEU:CD2	3:B:453:ILE:HD11	2.45	0.46
3:B:282:ILE:CD1	3:B:382:ILE:HD13	2.46	0.46
2:A:774:ARG:NH2	2:A:797:LYS:CG	2.76	0.46
4:C:213:PRO:HG2	4:C:214:ASN:H	1.79	0.46
2:A:1191:TRP:HB3	2:A:1260:LEU:HD23	1.97	0.46
3:B:205:ILE:HD12	3:B:205:ILE:N	2.31	0.46
4:C:44:LEU:HD21	4:C:159:ALA:CB	2.45	0.46
11:J:45:CYS:O	11:J:48:ARG:HG3	2.16	0.46
12:K:10:PHE:HD2	12:K:10:PHE:N	2.14	0.46
3:B:777:ALA:HA	3:B:1095:LEU:HA	1.97	0.46
2:A:356:ASP:OD2	12:K:65:HIS:HE1	1.99	0.46
2:A:134:ARG:HD2	2:A:221:SER:O	2.16	0.46
2:A:116:ASP:C	2:A:118:HIS:N	2.67	0.46
3:B:762:ASN:ND2	3:B:1024:ALA:HB3	2.30	0.46
3:B:957:ASN:O	3:B:960:GLY:N	2.48	0.46
12:K:110:ASN:O	12:K:111:LEU:HB3	2.14	0.46
11:J:19:GLU:O	11:J:23:ASN:HB2	2.15	0.46
2:A:1094:VAL:HG12	2:A:1095:THR:N	2.29	0.46
3:B:1099:VAL:HG12	3:B:1100:ASP:N	2.30	0.46
6:E:43:LYS:O	6:E:45:LYS:N	2.47	0.46
2:A:571:LEU:HD22	9:H:46:LEU:HD11	1.98	0.46
3:B:1151:LEU:N	3:B:1151:LEU:HD12	2.31	0.46
2:A:474:VAL:HG22	2:A:478:TYR:HE1	1.80	0.46
6:E:24:LYS:HG3	6:E:25:ASP:N	2.30	0.46
6:E:108:GLY:HA3	6:E:132:ILE:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:71:LYS:HA	5:D:74:GLN:CB	2.45	0.46
7:F:101:ILE:HD13	7:F:120:ILE:CG2	2.46	0.46
2:A:720:ARG:HB3	2:A:720:ARG:NH1	2.30	0.46
11:J:51:LEU:O	11:J:51:LEU:HD12	2.14	0.46
7:F:96:THR:O	7:F:100:GLN:HG3	2.16	0.46
3:B:461:LEU:HD12	3:B:461:LEU:N	2.30	0.46
4:C:101:LEU:HD12	4:C:101:LEU:HA	1.80	0.46
9:H:91:ASP:O	9:H:93:TYR:N	2.45	0.46
9:H:127:GLY:O	9:H:128:ASN:CB	2.60	0.46
2:A:219:PHE:O	2:A:222:LEU:O	2.34	0.46
3:B:166:PHE:C	3:B:167:ILE:HG13	2.36	0.46
2:A:806:ARG:O	3:B:761:HIS:HE1	1.97	0.46
7:F:90:ARG:HD3	7:F:155:LEU:CD1	2.42	0.46
2:A:986:ILE:HD12	2:A:1032:LEU:HD11	1.97	0.46
2:A:1191:TRP:CE3	2:A:1191:TRP:HA	2.51	0.46
2:A:1027:ALA:O	2:A:1031:VAL:HG23	2.15	0.46
11:J:48:ARG:HE	11:J:49:MET:CE	2.23	0.46
9:H:95:TYR:HB3	9:H:144:ILE:HB	1.98	0.46
2:A:340:LEU:HD21	3:B:1200:ALA:CA	2.46	0.46
2:A:335:ARG:NH1	3:B:1202:LEU:HD22	2.30	0.46
11:J:44:TYR:HA	11:J:47:ARG:CB	2.35	0.46
3:B:841:MET:HE2	3:B:1010:LEU:HD11	1.98	0.46
6:E:78:LEU:HD11	6:E:109:ILE:HD12	1.98	0.46
3:B:758:PHE:CZ	3:B:1044:ALA:HA	2.50	0.46
4:C:152:GLU:HG2	4:C:153:LEU:N	2.26	0.46
3:B:1166:CYS:O	3:B:1168:LEU:N	2.42	0.46
4:C:183:TRP:CZ2	4:C:207:CYS:HB3	2.50	0.46
2:A:1193:LEU:HD12	2:A:1194:ARG:N	2.30	0.46
2:A:1244:ARG:HB3	2:A:1245:PRO:CD	2.45	0.46
4:C:259:LEU:HD21	12:K:92:ASN:OD1	2.16	0.46
3:B:373:ARG:CG	3:B:566:LEU:HD23	2.45	0.46
2:A:441:PRO:HD2	2:A:498:ARG:NH2	2.31	0.46
3:B:878:GLN:O	3:B:879:ARG:C	2.52	0.46
6:E:97:VAL:HG13	6:E:127:ILE:HD13	1.97	0.46
9:H:10:PHE:CD1	9:H:10:PHE:N	2.84	0.46
5:D:37:GLN:OE1	8:G:5:LYS:HD2	2.16	0.46
3:B:1001:PHE:CE2	4:C:34:ARG:CZ	2.99	0.46
3:B:830:TYR:CD2	3:B:1000:PRO:HD3	2.51	0.46
2:A:563:PRO:HG3	2:A:572:TRP:CE2	2.48	0.46
2:A:1224:LEU:HD11	2:A:1240:CYS:HB2	1.98	0.46
2:A:1341:ILE:CG2	2:A:1342:GLU:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:116:ASP:OD2	2:A:164:ARG:HD2	2.16	0.46
2:A:588:LEU:O	2:A:606:LEU:HA	2.16	0.46
2:A:666:ILE:N	2:A:666:ILE:HD12	2.31	0.46
2:A:172:PRO:HG3	2:A:185:TRP:CE2	2.51	0.46
3:B:69:LEU:HD13	3:B:429:PHE:CD1	2.48	0.46
12:K:46:ILE:O	12:K:50:LEU:HB2	2.16	0.46
5:D:185:CYS:HB2	5:D:211:LEU:CD2	2.45	0.46
3:B:1125:ASP:O	3:B:1125:ASP:OD1	2.33	0.46
3:B:604:ARG:O	3:B:606:LYS:N	2.49	0.46
3:B:1034:VAL:C	3:B:1036:ALA:H	2.18	0.46
3:B:193:LYS:HZ2	13:L:32:ALA:HB1	1.77	0.46
11:J:6:ARG:HG2	11:J:13:VAL:HA	1.98	0.46
3:B:1098:MET:HE3	3:B:1098:MET:H	1.81	0.46
5:D:52:LEU:CD2	5:D:147:TYR:HE2	2.27	0.46
4:C:18:VAL:O	4:C:19:ASP:C	2.52	0.46
4:C:132:PRO:O	4:C:133:ILE:C	2.54	0.46
3:B:308:TRP:HZ3	10:I:45:ARG:HB3	1.79	0.46
4:C:212:PRO:CB	4:C:213:PRO:HD2	2.42	0.46
2:A:18:GLN:CB	3:B:1215:ARG:HB2	2.46	0.46
12:K:58:PHE:HB3	12:K:76:GLN:HB3	1.96	0.46
2:A:1236:LEU:C	2:A:1237:ILE:HG13	2.36	0.46
3:B:842:ASN:ND2	3:B:845:SER:OG	2.48	0.46
2:A:184:SER:HB3	2:A:199:LEU:CD2	2.46	0.46
2:A:1169:ILE:HG22	2:A:1169:ILE:O	2.15	0.46
2:A:244:PRO:CB	2:A:245:PRO:HD3	2.45	0.46
10:I:7:CYS:O	10:I:11:ASN:HA	2.16	0.46
3:B:899:ILE:HG21	3:B:949:VAL:HG21	1.98	0.46
3:B:216:GLU:HA	3:B:406:LEU:HD23	1.97	0.46
3:B:1198:TYR:CD2	3:B:1198:TYR:O	2.69	0.46
2:A:1342:GLU:OE2	6:E:212:ARG:NH1	2.48	0.46
8:G:111:THR:HB	8:G:114:LEU:HB2	1.98	0.46
6:E:31:THR:O	6:E:35:VAL:HG23	2.16	0.46
3:B:245:GLU:C	3:B:246:LYS:HG3	2.37	0.46
10:I:85:PHE:CE1	10:I:99:LEU:HD13	2.50	0.46
3:B:95:ILE:CG1	3:B:130:VAL:HG22	2.46	0.46
9:H:81:PRO:HB3	9:H:82:PRO:HD2	1.97	0.46
9:H:17:PRO:HB3	9:H:24:CYS:SG	2.55	0.46
3:B:99:LYS:HB3	3:B:100:PRO:HD2	1.98	0.46
3:B:29:ASP:O	3:B:30:SER:C	2.53	0.46
10:I:85:PHE:N	10:I:85:PHE:CD2	2.77	0.46
2:A:783:THR:HG22	2:A:784:LEU:HG	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1436:ILE:O	2:A:1437:GLY:C	2.53	0.46
2:A:1148:ILE:HG23	10:I:49:ILE:HB	1.97	0.46
3:B:327:ARG:NH2	3:B:371:GLU:HG2	2.30	0.46
3:B:648:HIS:CG	3:B:649:LYS:H	2.34	0.46
2:A:90:VAL:HG12	2:A:91:PHE:N	2.31	0.46
8:G:117:GLN:C	8:G:119:LEU:N	2.69	0.46
2:A:687:LYS:O	2:A:690:VAL:HB	2.16	0.46
4:C:46:ILE:CD1	4:C:67:LEU:HB3	2.41	0.45
3:B:994:TYR:HB2	3:B:999:MET:HE1	1.97	0.45
3:B:638:PHE:HB3	3:B:651:LEU:CD2	2.43	0.45
10:I:58:VAL:HG13	10:I:62:ILE:HD13	1.96	0.45
12:K:55:LYS:CB	12:K:81:TYR:CE1	2.99	0.45
3:B:1110:PRO:O	3:B:1119:VAL:HG22	2.16	0.45
2:A:710:LEU:N	2:A:710:LEU:HD12	2.30	0.45
5:D:156:ASP:O	5:D:160:VAL:HG23	2.17	0.45
2:A:697:ALA:HB2	2:A:702:LEU:HD12	1.98	0.45
2:A:514:PRO:CB	2:A:875:ALA:HB3	2.46	0.45
2:A:996:ASN:O	2:A:998:LEU:N	2.45	0.45
2:A:940:ARG:O	2:A:944:ARG:HG3	2.17	0.45
8:G:38:CYS:SG	8:G:44:TYR:CE1	3.09	0.45
4:C:99:LEU:HB2	4:C:157:CYS:HB2	1.97	0.45
9:H:55:LEU:HD22	9:H:144:ILE:CG2	2.46	0.45
3:B:778:MET:CE	3:B:1094:ARG:CD	2.93	0.45
2:A:1443:VAL:C	2:A:1444:MET:HG3	2.36	0.45
2:A:1011:GLN:O	2:A:1015:VAL:HG23	2.16	0.45
3:B:485:ARG:NH2	3:B:782:LEU:HD11	2.31	0.45
3:B:781:PHE:CE2	3:B:793:ALA:HB1	2.51	0.45
2:A:1068:ALA:HB3	2:A:1370:LEU:HD23	1.98	0.45
3:B:293:PRO:HG2	3:B:296:GLU:HB3	1.98	0.45
3:B:615:MET:HA	3:B:625:LYS:O	2.17	0.45
3:B:54:PHE:CE2	3:B:59:LEU:HD13	2.51	0.45
5:D:151:PHE:HD1	5:D:151:PHE:H	1.62	0.45
3:B:449:ASN:C	3:B:451:LYS:H	2.19	0.45
2:A:1010:ALA:O	2:A:1013:ASP:HB2	2.16	0.45
2:A:226:GLU:O	2:A:226:GLU:HG2	2.16	0.45
5:D:137:ASN:ND2	5:D:137:ASN:H	2.15	0.45
2:A:1323:ASP:C	2:A:1325:THR:N	2.69	0.45
3:B:797:TYR:CE1	3:B:854:LEU:HD21	2.52	0.45
2:A:472:LEU:O	2:A:475:THR:CG2	2.63	0.45
3:B:1156:ASP:HB3	3:B:1198:TYR:N	2.31	0.45
2:A:1208:THR:O	2:A:1212:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:19:LEU:HD21	12:K:35:PHE:CE2	2.51	0.45
4:C:179:GLU:HG2	4:C:180:TYR:H	1.81	0.45
2:A:802:ASN:ND2	2:A:812:GLU:OE1	2.48	0.45
5:D:210:ILE:O	5:D:214:LEU:HG	2.15	0.45
3:B:274:PRO:HG3	3:B:359:GLU:O	2.16	0.45
3:B:664:THR:HG23	3:B:678:GLU:N	2.31	0.45
10:I:5:ARG:O	10:I:14:LEU:HG	2.16	0.45
9:H:95:TYR:HE2	9:H:97:MET:CG	2.29	0.45
3:B:515:HIS:O	3:B:518:HIS:HB2	2.16	0.45
3:B:405:ARG:HA	3:B:631:GLY:O	2.17	0.45
2:A:1170:ILE:O	2:A:1174:PHE:HD1	1.99	0.45
11:J:36:LEU:HD22	11:J:41:LEU:HD12	1.98	0.45
2:A:921:GLY:O	2:A:922:ASP:C	2.54	0.45
2:A:405:VAL:O	2:A:413:ILE:HG13	2.16	0.45
3:B:388:CYS:C	3:B:390:LEU:H	2.19	0.45
2:A:767:GLN:OE1	2:A:799:PHE:HB2	2.16	0.45
3:B:616:ILE:HG12	3:B:697:GLU:HA	1.98	0.45
5:D:29:LEU:N	5:D:29:LEU:HD23	2.31	0.45
2:A:1118:VAL:HG23	2:A:1306:LEU:HB2	1.98	0.45
7:F:108:PHE:HE1	7:F:131:PRO:HG3	1.80	0.45
2:A:818:MET:HA	3:B:514:LEU:HB3	1.98	0.45
12:K:13:GLY:O	12:K:14:GLU:C	2.53	0.45
4:C:37:MET:HA	4:C:41:ILE:HD11	1.98	0.45
3:B:1214:PRO:O	3:B:1214:PRO:HG2	2.16	0.45
2:A:1107:VAL:O	2:A:1107:VAL:HG12	2.17	0.45
3:B:492:LEU:HB2	3:B:751:VAL:HG11	1.98	0.45
3:B:822:ASN:HD22	11:J:52:THR:HG21	1.80	0.45
4:C:235:VAL:HG12	11:J:13:VAL:HG23	1.99	0.45
2:A:336:ILE:HG22	2:A:337:ARG:N	2.32	0.45
2:A:855:THR:HG23	2:A:857:ARG:HG3	1.97	0.45
5:D:51:ASN:O	5:D:52:LEU:C	2.55	0.45
7:F:89:GLU:HB3	7:F:134:ILE:CD1	2.47	0.45
2:A:219:PHE:CD2	2:A:231:PRO:HD2	2.52	0.45
4:C:15:LYS:O	4:C:240:VAL:HG22	2.16	0.45
4:C:236:GLY:C	4:C:238:ILE:N	2.70	0.45
6:E:135:PHE:CD2	6:E:140:LEU:HD21	2.50	0.45
2:A:182:VAL:CG1	2:A:183:GLY:N	2.80	0.45
2:A:254:GLU:CB	3:B:935:ARG:HH22	2.30	0.45
2:A:416:ARG:C	2:A:417:TYR:CD2	2.83	0.45
3:B:211:VAL:CG2	3:B:483:LEU:HB2	2.47	0.45
2:A:852:TYR:CD2	2:A:1060:PRO:CB	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:710:LEU:H	2:A:710:LEU:CD1	2.30	0.45
2:A:889:SER:HB3	2:A:1297:GLU:CG	2.47	0.45
2:A:754:SER:H	2:A:757:ASN:HD22	1.64	0.45
2:A:89:PRO:C	2:A:204:THR:HG21	2.37	0.45
2:A:48:ALA:O	2:A:49:LYS:HG2	2.17	0.45
8:G:38:CYS:HB3	8:G:155:SER:HA	1.98	0.45
2:A:14:VAL:HB	2:A:1430:LEU:HD13	1.99	0.45
2:A:335:ARG:N	2:A:339:ASN:HD22	2.15	0.45
3:B:100:PRO:HD3	3:B:172:ILE:HD12	1.98	0.45
6:E:175:LEU:HD23	6:E:176:PRO:HD2	1.98	0.45
2:A:1311:VAL:HG11	2:A:1329:THR:HG21	1.98	0.45
3:B:1090:THR:HG22	3:B:1091:TYR:N	2.30	0.45
6:E:24:LYS:HB2	6:E:24:LYS:HE3	1.76	0.45
3:B:620:ARG:NH2	10:I:86:PHE:CD2	2.84	0.45
2:A:341:MET:CE	2:A:843:LYS:NZ	2.80	0.45
2:A:1313:LEU:C	2:A:1315:GLU:H	2.17	0.45
3:B:56:ASP:CB	3:B:57:TYR:HD1	2.30	0.45
2:A:261:ASP:O	2:A:264:PHE:HB2	2.16	0.45
3:B:864:LYS:N	3:B:872:GLU:OE1	2.50	0.45
3:B:258:LEU:O	3:B:258:LEU:CG	2.62	0.45
6:E:96:PHE:CE1	6:E:100:ILE:HD11	2.51	0.45
6:E:106:GLN:HA	6:E:130:ALA:CB	2.46	0.45
2:A:567:LYS:CB	9:H:96:VAL:H	2.12	0.45
4:C:255:VAL:HG12	4:C:255:VAL:O	2.17	0.45
4:C:31:ASN:O	4:C:34:ARG:HB3	2.16	0.45
12:K:56:VAL:HA	12:K:77:THR:HG22	1.99	0.45
2:A:259:GLU:OE1	2:A:263:THR:HG21	2.16	0.45
2:A:1259:MET:C	2:A:1261:LYS:H	2.20	0.45
3:B:1060:ARG:HD2	3:B:1060:ARG:HA	1.61	0.45
2:A:1405:THR:HB	2:A:1406:VAL:H	1.59	0.45
10:I:92:ARG:HG2	10:I:94:ASP:OD1	2.17	0.45
2:A:75:ASN:HA	3:B:1116:ARG:NH2	2.32	0.45
4:C:246:ARG:HA	4:C:249:ASP:HB3	1.98	0.45
1:R:3:A:H2'	1:R:4:U:C6	2.51	0.45
3:B:1220:ARG:CZ	3:B:1220:ARG:HB3	2.46	0.45
3:B:1183:LYS:HE3	3:B:1183:LYS:N	2.32	0.45
3:B:792:MET:HG3	3:B:855:PHE:CE1	2.45	0.45
3:B:872:GLU:CD	3:B:914:LYS:HE2	2.37	0.45
3:B:843:GLN:O	3:B:846:ILE:N	2.49	0.45
7:F:118:LEU:O	7:F:122:MET:HG3	2.16	0.45
2:A:1187:GLN:NE2	2:A:1188:GLN:NE2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1261:LYS:O	2:A:1264:GLU:HB3	2.17	0.45
3:B:402:GLY:HA2	3:B:695:ALA:HB3	1.99	0.45
3:B:731:VAL:HG12	3:B:732:SER:N	2.32	0.45
8:G:45:ILE:HD13	8:G:78:VAL:HG13	1.98	0.45
8:G:18:PHE:HA	8:G:22:MET:HE3	1.99	0.45
3:B:980:PHE:CE1	3:B:990:ILE:HD11	2.41	0.45
2:A:562:THR:HA	2:A:563:PRO:HD3	1.85	0.45
2:A:788:SER:HB3	10:I:69:PRO:HB3	1.99	0.45
4:C:131:HIS:O	4:C:133:ILE:N	2.37	0.45
6:E:124:VAL:HA	6:E:132:ILE:HD12	1.99	0.45
4:C:8:VAL:HG21	12:K:105:PHE:HA	1.99	0.45
9:H:104:PHE:CZ	9:H:136:LYS:HA	2.52	0.45
3:B:487:THR:HG22	3:B:488:TYR:N	2.31	0.45
4:C:77:ILE:HD13	4:C:77:ILE:HA	1.69	0.45
3:B:189:LEU:HD12	3:B:196:PRO:HA	1.97	0.45
3:B:549:THR:CG2	3:B:550:ASP:H	2.15	0.45
6:E:177:ARG:O	6:E:212:ARG:CD	2.65	0.45
2:A:1332:PHE:CE1	2:A:1348:LEU:HD13	2.51	0.45
3:B:811:TYR:N	3:B:811:TYR:CD1	2.85	0.45
3:B:424:LEU:HD22	3:B:453:ILE:HD11	1.98	0.45
2:A:590:ARG:HH22	2:A:620:LYS:CB	2.28	0.45
13:L:40:LEU:HD22	13:L:44:ASP:HB3	1.99	0.45
9:H:107:VAL:HG21	9:H:126:GLU:OE2	2.16	0.45
2:A:1214:GLU:O	2:A:1218:GLN:HG2	2.17	0.45
3:B:642:ASP:CA	3:B:649:LYS:HA	2.47	0.45
3:B:1034:VAL:C	3:B:1036:ALA:N	2.70	0.45
8:G:10:ASN:OD1	8:G:71:ASN:HA	2.15	0.45
2:A:1149:ALA:HB2	10:I:47:GLU:HA	1.99	0.45
3:B:889:THR:HG23	3:B:891:ASP:OD2	2.17	0.45
3:B:70:ILE:O	3:B:70:ILE:HG22	2.16	0.45
2:A:227:VAL:HG12	5:D:15:LEU:HD23	1.99	0.45
5:D:34:GLN:O	5:D:47:LEU:HD23	2.16	0.44
11:J:10:CYS:SG	11:J:11:GLY:N	2.90	0.44
3:B:562:GLY:C	3:B:590:HIS:HD1	2.16	0.44
2:A:1011:GLN:NE2	2:A:1015:VAL:HG21	2.32	0.44
2:A:396:PRO:HG3	2:A:416:ARG:HB3	1.98	0.44
3:B:654:ARG:C	3:B:656:GLY:H	2.19	0.44
3:B:525:ALA:O	3:B:768:THR:HA	2.17	0.44
5:D:29:LEU:HB3	8:G:82:PHE:HE2	1.81	0.44
3:B:890:TYR:CE1	3:B:910:VAL:HG21	2.52	0.44
7:F:108:PHE:CE1	7:F:131:PRO:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1138:MET:HE2	3:B:1143:ALA:HB3	2.00	0.44
8:G:115:MET:HB3	8:G:163:ILE:HD11	1.99	0.44
2:A:927:VAL:O	2:A:931:GLU:HB2	2.17	0.44
3:B:290:GLY:C	3:B:291:ILE:HG13	2.37	0.44
2:A:40:THR:HB	2:A:41:MET:HE3	1.99	0.44
2:A:1120:LEU:CD1	2:A:1304:TRP:O	2.66	0.44
3:B:905:VAL:HG23	3:B:941:LEU:CD2	2.46	0.44
4:C:166:GLU:OE1	13:L:70:ARG:NH2	2.43	0.44
2:A:1445:ILE:HD12	8:G:59:GLY:O	2.17	0.44
3:B:980:PHE:HE2	3:B:1094:ARG:HB2	1.81	0.44
3:B:1159:ARG:HD2	3:B:1159:ARG:O	2.17	0.44
2:A:562:THR:HB	9:H:98:TYR:CD2	2.52	0.44
2:A:898:ARG:O	2:A:1029:ARG:NH1	2.51	0.44
2:A:605:MET:CE	2:A:607:ILE:HG12	2.47	0.44
3:B:1177:HIS:CB	3:B:1179:GLN:HE21	2.29	0.44
3:B:56:ASP:HB3	3:B:57:TYR:CD1	2.52	0.44
3:B:205:ILE:HG21	3:B:462:ALA:HB2	1.99	0.44
2:A:717:ASN:HA	2:A:720:ARG:HH12	1.82	0.44
3:B:487:THR:O	3:B:490:SER:HB3	2.18	0.44
2:A:684:ALA:O	2:A:687:LYS:HB2	2.16	0.44
2:A:1394:THR:HG21	2:A:1398:MET:SD	2.58	0.44
11:J:28:ASP:O	11:J:29:GLU:C	2.56	0.44
5:D:31:GLN:O	5:D:34:GLN:HG3	2.17	0.44
8:G:85:GLU:HG2	8:G:86:VAL:N	2.31	0.44
3:B:1151:LEU:CD1	3:B:1151:LEU:H	2.31	0.44
3:B:1202:LEU:O	3:B:1206:GLU:HG3	2.17	0.44
3:B:776:GLN:O	3:B:1095:LEU:HA	2.17	0.44
2:A:867:ILE:N	2:A:867:ILE:HD12	2.32	0.44
2:A:164:ARG:CG	2:A:165:GLY:N	2.75	0.44
2:A:605:MET:HE1	2:A:607:ILE:HG12	1.98	0.44
3:B:1065:GLN:NE2	3:B:1067:ARG:HG2	2.32	0.44
5:D:5:THR:O	5:D:5:THR:HG23	2.16	0.44
13:L:58:LYS:O	13:L:58:LYS:HG2	2.16	0.44
8:G:39:THR:HG22	8:G:40:GLY:N	2.32	0.44
9:H:99:GLY:HA3	9:H:118:PHE:HA	1.99	0.44
2:A:961:ARG:HH11	2:A:961:ARG:HG3	1.83	0.44
2:A:114:LEU:O	2:A:115:LEU:HG	2.17	0.44
2:A:1152:ILE:CG1	10:I:44:TYR:HB3	2.36	0.44
2:A:356:ASP:OD2	12:K:65:HIS:CE1	2.71	0.44
2:A:1441:PHE:CZ	7:F:89:GLU:HA	2.52	0.44
2:A:774:ARG:CZ	2:A:797:LYS:HG3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:133:ILE:HD12	4:C:237:SER:HA	1.97	0.44
2:A:102:VAL:HG11	2:A:211:PHE:HE2	1.82	0.44
3:B:215:GLN:NE2	3:B:215:GLN:HA	2.32	0.44
2:A:1397:LEU:HB2	2:A:1426:GLU:OE1	2.17	0.44
12:K:68:PHE:CD2	12:K:68:PHE:N	2.83	0.44
7:F:68:THR:CB	7:F:69:LEU:CB	2.96	0.44
2:A:1450:LEU:HD21	8:G:18:PHE:O	2.18	0.44
2:A:332:LYS:H	2:A:337:ARG:HB3	1.82	0.44
3:B:1070:GLU:OE1	11:J:44:TYR:OH	2.34	0.44
3:B:1072:MET:CE	3:B:1087:PHE:HB2	2.48	0.44
2:A:1265:ASN:O	2:A:1267:MET:N	2.50	0.44
10:I:86:PHE:CE1	10:I:100:PHE:HB2	2.52	0.44
3:B:168:GLY:N	3:B:450:ALA:HB1	2.31	0.44
2:A:843:LYS:HD3	2:A:846:GLU:OE2	2.17	0.44
2:A:825:ILE:HG22	2:A:826:ASP:N	2.32	0.44
3:B:604:ARG:C	3:B:606:LYS:H	2.21	0.44
2:A:1305:VAL:CG1	2:A:1306:LEU:N	2.80	0.44
2:A:744:LYS:HG2	2:A:748:MET:HE2	1.98	0.44
12:K:51:LEU:HA	12:K:51:LEU:HD12	1.82	0.44
4:C:94:LYS:HB2	4:C:94:LYS:HE3	1.80	0.44
8:G:154:VAL:HG12	8:G:155:SER:H	1.83	0.44
9:H:58:THR:HG22	9:H:59:ILE:H	1.82	0.44
3:B:27:ALA:O	3:B:29:ASP:N	2.51	0.44
4:C:258:ILE:N	4:C:258:ILE:HD12	2.32	0.44
2:A:1213:GLY:O	2:A:1214:GLU:C	2.56	0.44
2:A:1095:THR:O	2:A:1100:ARG:HB2	2.18	0.44
2:A:357:PRO:HD2	3:B:833:TYR:CE1	2.52	0.44
2:A:1066:VAL:O	2:A:1069:ALA:HB3	2.18	0.44
10:I:4:PHE:C	10:I:4:PHE:CD1	2.91	0.44
2:A:244:PRO:O	2:A:246:VAL:N	2.50	0.44
3:B:510:LYS:CG	3:B:511:PRO:HD3	2.26	0.44
5:D:173:HIS:CD2	5:D:175:PHE:H	2.36	0.44
4:C:124:LEU:O	4:C:127:ARG:HG2	2.18	0.44
2:A:1160:SER:HA	2:A:1170:ILE:CD1	2.48	0.44
3:B:824:ILE:HG22	3:B:1008:PRO:HA	2.00	0.44
3:B:757:PRO:HD3	3:B:983:ARG:HH21	1.82	0.44
2:A:666:ILE:HD11	3:B:1067:ARG:O	2.17	0.44
2:A:78:PRO:HA	3:B:1201:LYS:NZ	2.32	0.44
3:B:642:ASP:CB	3:B:649:LYS:HG3	2.47	0.44
5:D:3:VAL:O	5:D:4:SER:CB	2.66	0.44
2:A:90:VAL:CG1	2:A:297:GLN:NE2	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:6:ARG:C	12:K:8:GLU:H	2.20	0.44
3:B:496:ARG:NH1	3:B:539:LEU:HB2	2.33	0.44
2:A:600:PRO:C	2:A:602:ASP:H	2.20	0.44
2:A:418:SER:C	2:A:420:ARG:H	2.20	0.44
6:E:5:ASN:O	6:E:9:ILE:HG13	2.18	0.44
2:A:1025:ARG:O	2:A:1026:LEU:HD23	2.17	0.44
3:B:259:TYR:H	3:B:259:TYR:HD1	1.66	0.44
3:B:800:GLN:HB2	3:B:821:GLN:HA	1.99	0.44
2:A:681:GLU:O	2:A:685:GLU:HG2	2.18	0.44
2:A:42:ASP:C	2:A:44:THR:N	2.70	0.44
2:A:90:VAL:HG13	2:A:297:GLN:CD	2.38	0.44
2:A:720:ARG:CB	2:A:720:ARG:NH1	2.81	0.44
3:B:1125:ASP:O	3:B:1126:GLY:O	2.36	0.44
3:B:606:LYS:HD2	3:B:608:ASP:OD2	2.18	0.44
2:A:1273:LEU:CD1	2:A:1273:LEU:N	2.81	0.44
7:F:75:PRO:HG3	7:F:78:GLN:OE1	2.18	0.44
10:I:61:ASP:C	10:I:63:GLY:H	2.21	0.44
13:L:47:ARG:HH21	13:L:54:ARG:NH2	2.14	0.44
2:A:56:PRO:O	2:A:57:ARG:NE	2.47	0.44
2:A:366:VAL:HG21	2:A:460:VAL:HG22	1.99	0.44
2:A:853:ASP:OD2	2:A:855:THR:HG22	2.18	0.44
2:A:785:PRO:HG2	3:B:703:ILE:HD12	1.99	0.44
3:B:840:ILE:CG2	3:B:994:TYR:HD1	2.30	0.44
5:D:3:VAL:O	5:D:4:SER:HB3	2.18	0.44
3:B:526:GLU:O	3:B:526:GLU:HG2	2.18	0.44
7:F:125:LEU:O	7:F:125:LEU:CG	2.65	0.44
2:A:1299:VAL:CG1	2:A:1300:LYS:N	2.80	0.44
5:D:37:GLN:OE1	8:G:5:LYS:NZ	2.35	0.44
3:B:224:GLN:O	3:B:238:ALA:HA	2.18	0.44
3:B:1164:GLY:HA3	3:B:1190:ASP:OD2	2.18	0.44
2:A:40:THR:CG2	2:A:41:MET:HG3	2.44	0.43
5:D:51:ASN:O	5:D:52:LEU:O	2.36	0.43
3:B:1081:LEU:O	3:B:1083:ALA:N	2.50	0.43
3:B:635:ARG:NH1	3:B:742:GLU:OE2	2.51	0.43
3:B:309:GLN:CG	10:I:52:ILE:HD11	2.47	0.43
3:B:1183:LYS:N	3:B:1183:LYS:CE	2.81	0.43
2:A:1313:LEU:CD2	2:A:1338:VAL:HG21	2.45	0.43
3:B:22:SER:HA	3:B:654:ARG:HG3	2.00	0.43
5:D:63:LEU:O	5:D:129:LEU:HD11	2.18	0.43
2:A:599:SER:HA	2:A:600:PRO:HD2	1.89	0.43
3:B:763:GLN:HG2	3:B:765:PRO:CG	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:LEU:HA	2:A:505:CYS:HB2	2.00	0.43
2:A:964:ILE:O	2:A:967:ALA:N	2.51	0.43
2:A:923:LEU:O	2:A:927:VAL:HG23	2.18	0.43
3:B:644:GLU:OE2	3:B:646:LEU:HB2	2.18	0.43
10:I:8:ARG:H	10:I:8:ARG:HG3	1.61	0.43
4:C:44:LEU:HD21	4:C:159:ALA:HB1	1.98	0.43
4:C:174:ALA:O	4:C:175:ALA:HB2	2.18	0.43
2:A:914:GLU:HB2	2:A:979:SER:O	2.17	0.43
2:A:874:ASP:HA	2:A:1058:VAL:HG22	1.99	0.43
3:B:244:LEU:HD11	3:B:366:GLN:NE2	2.33	0.43
2:A:1260:LEU:O	2:A:1260:LEU:CG	2.66	0.43
3:B:563:MET:HE2	3:B:588:GLY:C	2.39	0.43
8:G:106:MET:HB3	8:G:106:MET:HE2	1.87	0.43
2:A:971:PHE:O	2:A:972:HIS:C	2.56	0.43
3:B:977:GLY:HA3	3:B:1099:VAL:CG2	2.48	0.43
2:A:809:THR:H	2:A:812:GLU:HB2	1.82	0.43
3:B:866:TYR:O	3:B:867:GLY:C	2.56	0.43
2:A:630:ILE:HD13	2:A:646:PHE:CZ	2.53	0.43
3:B:48:LEU:O	3:B:49:ASP:C	2.56	0.43
3:B:797:TYR:HE1	3:B:854:LEU:HD21	1.83	0.43
2:A:858:ASN:HD22	2:A:861:GLY:H	1.64	0.43
6:E:153:HIS:CD2	6:E:198:ILE:HG12	2.54	0.43
3:B:388:CYS:C	3:B:390:LEU:N	2.72	0.43
2:A:230:ARG:HB2	2:A:233:TRP:CE3	2.53	0.43
3:B:247:GLY:C	3:B:249:ARG:H	2.22	0.43
3:B:603:LEU:HB3	3:B:609:ILE:CG1	2.48	0.43
2:A:412:ARG:HH21	3:B:1108:ARG:NH1	2.16	0.43
3:B:469:GLN:HB2	3:B:470:LYS:H	1.54	0.43
8:G:45:ILE:HD13	8:G:78:VAL:CG1	2.48	0.43
2:A:146:MET:HB3	2:A:171:GLN:O	2.18	0.43
13:L:70:ARG:HG2	13:L:70:ARG:HH11	1.84	0.43
8:G:14:HIS:HD2	8:G:16:SER:CB	2.30	0.43
2:A:817:ALA:HA	3:B:764:SER:OG	2.18	0.43
4:C:10:ILE:HA	4:C:20:PHE:HB2	1.99	0.43
4:C:239:PRO:C	4:C:241:ASP:H	2.21	0.43
3:B:635:ARG:NH2	3:B:742:GLU:OE2	2.50	0.43
3:B:269:ILE:HD11	3:B:386:LEU:HD21	1.99	0.43
2:A:43:GLU:O	2:A:44:THR:HB	2.19	0.43
2:A:321:PRO:O	2:A:322:VAL:CB	2.66	0.43
4:C:184:ASN:HD21	4:C:187:LYS:HA	1.79	0.43
4:C:187:LYS:HG3	4:C:219:PHE:HE1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:35:ARG:NH1	12:K:40:HIS:HB2	2.34	0.43
4:C:35:ARG:HH11	12:K:41:THR:CA	2.30	0.43
2:A:347:PHE:N	2:A:347:PHE:CD1	2.86	0.43
8:G:115:MET:HA	8:G:163:ILE:HG13	2.00	0.43
9:H:118:PHE:O	9:H:120:GLY:N	2.52	0.43
3:B:1040:ASN:O	3:B:1042:GLY:N	2.51	0.43
6:E:75:MET:O	6:E:76:GLY:O	2.37	0.43
2:A:279:LEU:HD12	2:A:289:ILE:HG12	2.00	0.43
3:B:552:MET:O	3:B:554:ILE:N	2.51	0.43
2:A:34:LYS:O	2:A:35:ILE:CB	2.66	0.43
8:G:80:LYS:HD3	8:G:80:LYS:H	1.82	0.43
8:G:26:LEU:HD11	8:G:70:PHE:CD1	2.53	0.43
2:A:339:ASN:O	2:A:343:LYS:HG2	2.19	0.43
2:A:1116:LEU:CA	2:A:1308:THR:HG22	2.48	0.43
4:C:73:GLN:CB	4:C:131:HIS:H	2.26	0.43
2:A:254:GLU:HG3	3:B:935:ARG:HH22	1.84	0.43
2:A:1215:ARG:HA	2:A:1218:GLN:HG2	1.99	0.43
2:A:316:GLN:HG2	2:A:317:LYS:N	2.33	0.43
3:B:1099:VAL:HG12	3:B:1100:ASP:H	1.82	0.43
2:A:1205:LYS:O	2:A:1206:ASP:C	2.57	0.43
3:B:210:LYS:HG3	3:B:461:LEU:O	2.17	0.43
2:A:745:GLN:HA	2:A:748:MET:HE3	2.00	0.43
2:A:289:ILE:O	2:A:293:GLU:N	2.51	0.43
3:B:552:MET:C	3:B:554:ILE:H	2.22	0.43
2:A:1162:VAL:HG12	2:A:1162:VAL:O	2.18	0.43
2:A:853:ASP:C	2:A:853:ASP:OD1	2.56	0.43
3:B:684:LEU:N	3:B:684:LEU:HD12	2.30	0.43
3:B:1033:LYS:NZ	3:B:1070:GLU:OE1	2.49	0.43
2:A:463:ILE:HD12	2:A:469:ARG:HD2	2.01	0.43
2:A:894:GLU:O	2:A:898:ARG:HB3	2.19	0.43
2:A:1438:THR:HB	3:B:1144:ALA:CB	2.42	0.43
12:K:53:ASP:HB3	12:K:56:VAL:HG23	2.00	0.43
5:D:185:CYS:O	5:D:211:LEU:HD22	2.19	0.43
2:A:976:THR:OG1	2:A:977:LYS:N	2.51	0.43
2:A:1118:VAL:CG2	2:A:1306:LEU:HB2	2.48	0.43
3:B:210:LYS:HD3	3:B:481:GLN:O	2.18	0.43
2:A:362:ASP:OD2	2:A:459:ARG:HD3	2.18	0.43
2:A:67:CYS:SG	2:A:77:CYS:SG	3.16	0.43
11:J:3:VAL:HA	11:J:53:HIS:CE1	2.54	0.43
2:A:1345:ARG:HD2	2:A:1373:ASP:OD1	2.19	0.43
3:B:658:ILE:HG22	3:B:659:ALA:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:834:ASN:O	3:B:1013:ASN:HB2	2.19	0.43
2:A:1239:ARG:HB3	2:A:1239:ARG:NH1	2.33	0.43
2:A:849:MET:HE1	2:A:1061:GLY:CA	2.41	0.43
4:C:10:ILE:HA	4:C:20:PHE:CB	2.49	0.43
4:C:25:VAL:HG23	4:C:228:PHE:CE1	2.52	0.43
2:A:1004:ASN:HD21	6:E:167:ARG:HD2	1.81	0.43
2:A:17:VAL:HG23	2:A:1419:ASP:HB3	2.01	0.43
6:E:144:ILE:HG13	6:E:145:THR:N	2.32	0.43
3:B:861:ASP:OD1	3:B:914:LYS:HD2	2.19	0.43
2:A:713:SER:O	2:A:717:ASN:ND2	2.51	0.43
8:G:87:VAL:CG2	8:G:103:VAL:HG21	2.49	0.43
2:A:1364:ASN:O	2:A:1366:ARG:N	2.52	0.43
2:A:376:TYR:OH	2:A:498:ARG:HD2	2.19	0.43
4:C:208:GLU:O	4:C:210:GLU:N	2.51	0.43
3:B:954:VAL:HG22	3:B:964:VAL:HG22	1.99	0.43
3:B:230:ALA:HB3	3:B:231:PRO:HD3	2.01	0.43
2:A:35:ILE:HD13	2:A:241:VAL:HG11	1.98	0.43
3:B:787:VAL:O	3:B:787:VAL:HG12	2.19	0.43
8:G:22:MET:O	8:G:23:LYS:C	2.56	0.43
3:B:1147:LEU:HD23	3:B:1147:LEU:C	2.38	0.43
2:A:92:HIS:O	2:A:93:VAL:C	2.57	0.43
3:B:130:VAL:HB	3:B:167:ILE:CD1	2.49	0.43
3:B:37:PHE:HE1	3:B:41:LYS:CG	2.28	0.43
3:B:308:TRP:CZ3	10:I:45:ARG:HB3	2.53	0.43
2:A:1100:ARG:NH2	2:A:1351:GLU:HG2	2.34	0.43
2:A:172:PRO:HD3	2:A:185:TRP:HE1	1.83	0.43
3:B:803:LEU:HD12	3:B:1032:SER:HB3	2.00	0.43
3:B:558:LEU:C	3:B:560:GLU:N	2.72	0.43
2:A:1219:THR:HG21	2:A:1271:ILE:CD1	2.49	0.43
6:E:151:PRO:HB3	6:E:200:ARG:HB3	2.01	0.43
5:D:118:THR:HG22	5:D:118:THR:O	2.18	0.43
3:B:254:LEU:HD23	3:B:381:MET:HE1	1.99	0.43
3:B:840:ILE:HB	3:B:1011:ILE:HB	2.01	0.43
2:A:1220:PHE:CD1	2:A:1224:LEU:HD23	2.53	0.43
2:A:353:ILE:CD1	2:A:487:MET:HE2	2.46	0.43
2:A:302:THR:O	2:A:304:MET:N	2.52	0.43
3:B:758:PHE:CE2	3:B:1044:ALA:HA	2.53	0.43
3:B:327:ARG:O	3:B:331:LEU:HD13	2.18	0.43
4:C:107:SER:C	4:C:109:SER:N	2.70	0.43
3:B:1099:VAL:HG13	3:B:1100:ASP:N	2.34	0.43
9:H:118:PHE:CD1	9:H:118:PHE:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1169:MET:O	3:B:1170:THR:C	2.58	0.43
4:C:44:LEU:CD2	4:C:159:ALA:HB1	2.49	0.43
2:A:901:LEU:HD22	2:A:919:ILE:CG2	2.48	0.43
2:A:138:ILE:HD12	2:A:222:LEU:HD23	1.99	0.43
2:A:1001:ARG:O	2:A:1002:GLY:O	2.37	0.43
2:A:500:GLU:OE2	3:B:1145:SER:HB2	2.19	0.43
10:I:99:LEU:C	10:I:100:PHE:HD1	2.21	0.43
3:B:542:MET:CE	3:B:743:ILE:HG13	2.46	0.43
2:A:767:GLN:HB2	2:A:799:PHE:HD1	1.83	0.43
3:B:483:LEU:HD12	3:B:484:ASN:N	2.34	0.43
10:I:16:PRO:HB3	10:I:27:PHE:CE2	2.54	0.43
2:A:108:MET:O	2:A:109:HIS:HB3	2.19	0.43
2:A:157:ASP:C	2:A:159:THR:H	2.21	0.43
3:B:527:THR:OG1	3:B:528:PRO:HD2	2.19	0.43
12:K:63:VAL:HG23	12:K:63:VAL:O	2.19	0.43
7:F:69:LEU:HB2	7:F:72:LYS:HB2	2.01	0.42
2:A:72:GLU:OE2	3:B:1175:LEU:HD12	2.19	0.42
3:B:114:PRO:O	3:B:116:GLU:N	2.52	0.42
3:B:953:LEU:HB2	13:L:56:LEU:O	2.19	0.42
4:C:175:ALA:HB2	11:J:10:CYS:HB2	2.00	0.42
3:B:822:ASN:O	11:J:48:ARG:NH1	2.52	0.42
2:A:332:LYS:O	2:A:333:GLU:CB	2.67	0.42
2:A:14:VAL:CG2	3:B:1216:LEU:HD12	2.47	0.42
6:E:13:TRP:CZ3	6:E:39:LEU:HB2	2.54	0.42
3:B:710:LEU:CA	3:B:733:HIS:HB3	2.45	0.42
2:A:1063:MET:HG3	2:A:1436:ILE:HG23	2.00	0.42
6:E:167:ARG:HD3	6:E:167:ARG:HA	1.75	0.42
2:A:4:GLN:O	2:A:5:GLN:CB	2.65	0.42
3:B:205:ILE:O	3:B:207:GLY:N	2.51	0.42
5:D:29:LEU:HB3	8:G:82:PHE:CE2	2.54	0.42
2:A:29:ALA:HB1	3:B:1184:GLY:HA3	2.00	0.42
2:A:541:ILE:HD13	2:A:549:MET:CE	2.49	0.42
2:A:1206:ASP:HB3	2:A:1274:ARG:HH12	1.83	0.42
2:A:765:VAL:HG12	2:A:766:GLY:N	2.33	0.42
3:B:459:TYR:CE1	3:B:469:GLN:HG2	2.54	0.42
6:E:32:GLN:HG3	6:E:36:GLU:OE2	2.19	0.42
6:E:12:LEU:HD12	6:E:12:LEU:O	2.19	0.42
2:A:242:PRO:HD3	3:B:1209:ALA:CB	2.49	0.42
2:A:58:LEU:CD1	2:A:244:PRO:HD2	2.42	0.42
3:B:953:LEU:O	3:B:953:LEU:HD23	2.19	0.42
3:B:216:GLU:OE1	3:B:537:LYS:CE	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:331:GLY:O	2:A:332:LYS:O	2.37	0.42
2:A:1174:PHE:C	2:A:1176:LEU:N	2.73	0.42
3:B:980:PHE:CE2	3:B:1094:ARG:HG3	2.53	0.42
7:F:138:LEU:HB3	7:F:139:PRO:HD2	2.01	0.42
2:A:779:PHE:CE2	3:B:517:THR:HG22	2.54	0.42
3:B:653:VAL:CG2	3:B:689:LEU:HD22	2.49	0.42
3:B:770:GLN:OE1	3:B:983:ARG:CA	2.60	0.42
2:A:590:ARG:HD3	2:A:604:GLY:C	2.40	0.42
3:B:244:LEU:HD13	3:B:247:GLY:O	2.19	0.42
9:H:56:THR:HB	9:H:145:ARG:HG2	2.00	0.42
9:H:7:ASP:O	9:H:8:ASP:HB2	2.19	0.42
5:D:139:LYS:HE2	5:D:139:LYS:HB2	1.88	0.42
2:A:34:LYS:HD3	2:A:57:ARG:HH22	1.80	0.42
10:I:92:ARG:HB3	10:I:95:THR:OG1	2.19	0.42
3:B:911:ILE:O	3:B:911:ILE:HG22	2.20	0.42
11:J:8:PHE:H	11:J:49:MET:HE3	1.84	0.42
3:B:659:ALA:HA	3:B:662:MET:HE2	2.00	0.42
2:A:466:SER:HB3	3:B:1103:ILE:HG12	2.00	0.42
2:A:353:ILE:HB	2:A:470:LEU:HD23	2.01	0.42
3:B:746:SER:CB	3:B:1046:PRO:HG2	2.45	0.42
2:A:722:LEU:O	2:A:725:ALA:HB3	2.19	0.42
2:A:590:ARG:HG3	2:A:590:ARG:NH1	2.35	0.42
2:A:606:LEU:HD11	2:A:608:ILE:CG1	2.50	0.42
2:A:1036:ARG:HH11	2:A:1036:ARG:CG	2.32	0.42
13:L:28:LYS:C	13:L:29:TYR:HD2	2.22	0.42
2:A:1346:ALA:O	2:A:1350:LYS:HB2	2.20	0.42
2:A:491:VAL:HG12	2:A:492:PRO:O	2.19	0.42
3:B:827:ILE:HD12	3:B:1086:PHE:HD2	1.84	0.42
5:D:214:LEU:HD23	5:D:214:LEU:N	2.34	0.42
2:A:658:LEU:HG	2:A:659:HIS:ND1	2.34	0.42
5:D:30:GLY:O	5:D:32:GLU:N	2.52	0.42
5:D:141:LEU:HA	5:D:141:LEU:HD12	1.86	0.42
8:G:34:VAL:HG12	8:G:45:ILE:CG2	2.37	0.42
4:C:48:SER:O	4:C:157:CYS:HA	2.19	0.42
10:I:59:VAL:HG12	10:I:60:GLN:N	2.34	0.42
2:A:849:MET:CE	2:A:1061:GLY:CA	2.95	0.42
2:A:270:LEU:HD12	2:A:270:LEU:O	2.19	0.42
3:B:38:PHE:CD1	3:B:811:TYR:CD2	3.07	0.42
2:A:850:VAL:HG23	2:A:1064:VAL:HG21	2.02	0.42
3:B:744:HIS:CG	3:B:745:PRO:HD2	2.54	0.42
3:B:745:PRO:C	3:B:747:MET:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:390:LEU:O	3:B:392:ARG:HG3	2.19	0.42
2:A:285:PRO:O	2:A:287:HIS:N	2.52	0.42
2:A:384:ASN:CG	2:A:388:LEU:HD12	2.40	0.42
3:B:810:GLU:HA	3:B:815:ARG:HH12	1.84	0.42
3:B:582:VAL:HA	3:B:626:ILE:O	2.19	0.42
2:A:166:GLY:O	2:A:167:CYS:CB	2.67	0.42
4:C:176:ILE:HG22	4:C:177:GLU:O	2.19	0.42
3:B:31:TRP:CZ3	3:B:34:ILE:HD12	2.54	0.42
9:H:63:LEU:HD11	9:H:141:TYR:CD2	2.54	0.42
2:A:1366:ARG:HG2	2:A:1366:ARG:HH11	1.82	0.42
8:G:112:LYS:NZ	8:G:120:THR:HA	2.33	0.42
2:A:86:LEU:HD12	2:A:236:LEU:O	2.19	0.42
4:C:99:LEU:HA	4:C:99:LEU:HD13	1.90	0.42
5:D:148:LEU:O	5:D:152:SER:OG	2.33	0.42
2:A:1019:CYS:O	2:A:1022:LEU:HB3	2.18	0.42
3:B:128:LEU:HD11	3:B:170:LEU:CB	2.50	0.42
3:B:165:VAL:HG11	3:B:448:ILE:HD13	2.00	0.42
6:E:85:GLU:HB2	6:E:88:VAL:CG2	2.48	0.42
12:K:55:LYS:HB3	12:K:81:TYR:CE1	2.54	0.42
3:B:69:LEU:HD22	3:B:429:PHE:CE1	2.54	0.42
7:F:99:LEU:O	7:F:103:MET:CG	2.67	0.42
4:C:134:ILE:HG22	4:C:136:ASP:H	1.84	0.42
2:A:637:LYS:HB3	2:A:641:VAL:HG11	2.02	0.42
3:B:466:TRP:HA	3:B:466:TRP:CE3	2.53	0.42
9:H:91:ASP:C	9:H:93:TYR:H	2.22	0.42
2:A:851:HIS:CD2	2:A:857:ARG:HB2	2.54	0.42
7:F:138:LEU:O	7:F:140:ASP:N	2.52	0.42
3:B:1010:LEU:O	3:B:1011:ILE:HG13	2.19	0.42
3:B:830:TYR:C	3:B:831:SER:HG	2.21	0.42
2:A:1114:PRO:O	2:A:1115:SER:O	2.36	0.42
4:C:248:ILE:HD13	12:K:101:LEU:HD23	2.01	0.42
7:F:109:VAL:HG11	7:F:123:LYS:HD3	2.00	0.42
2:A:1434:ALA:O	2:A:1436:ILE:N	2.52	0.42
3:B:310:MET:O	3:B:313:MET:HB2	2.19	0.42
13:L:40:LEU:HD22	13:L:44:ASP:CG	2.40	0.42
3:B:1181:GLU:O	3:B:1182:CYS:CB	2.68	0.42
5:D:119:ARG:HD3	5:D:221:TYR:CE2	2.54	0.42
2:A:19:PHE:HE1	2:A:1396:ALA:HB3	1.84	0.42
3:B:603:LEU:CD1	3:B:608:ASP:HB2	2.50	0.42
2:A:180:LYS:HZ1	2:A:294:SER:HB3	1.85	0.42
2:A:210:ILE:O	2:A:214:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:423:LYS:O	3:B:427:ASP:HB2	2.20	0.42
10:I:84:VAL:HG13	10:I:84:VAL:O	2.19	0.42
5:D:175:PHE:CE1	8:G:1:MET:HA	2.55	0.42
2:A:1265:ASN:C	2:A:1267:MET:H	2.23	0.42
2:A:470:LEU:HD22	2:A:487:MET:HE1	2.02	0.42
4:C:6:PRO:HG2	12:K:101:LEU:HB2	2.01	0.42
3:B:170:LEU:HA	3:B:171:PRO:HD2	1.92	0.42
3:B:856:PHE:HD2	3:B:967:ARG:CD	2.30	0.42
12:K:58:PHE:HB3	12:K:76:GLN:HE21	1.83	0.42
4:C:112:ASN:HB2	4:C:114:TYR:CE1	2.55	0.42
6:E:116:ILE:CG2	6:E:120:ALA:HB3	2.50	0.42
2:A:418:SER:O	2:A:420:ARG:N	2.53	0.42
3:B:237:VAL:HG12	3:B:238:ALA:N	2.35	0.42
11:J:36:LEU:HD12	11:J:47:ARG:NH1	2.34	0.42
3:B:448:ILE:O	3:B:450:ALA:N	2.52	0.42
3:B:37:PHE:CE2	3:B:542:MET:HA	2.54	0.42
2:A:973:ILE:HD11	2:A:1041:ALA:HB2	2.01	0.42
12:K:111:LEU:O	12:K:112:GLN:HB3	2.19	0.42
3:B:234:ILE:H	3:B:234:ILE:HD12	1.85	0.42
3:B:294:ASP:C	3:B:296:GLU:H	2.17	0.42
3:B:1099:VAL:C	3:B:1101:ASP:H	2.23	0.42
3:B:212:LEU:HD12	3:B:409:ALA:HB1	2.01	0.42
3:B:900:ALA:O	3:B:902:GLY:N	2.53	0.42
2:A:347:PHE:CE2	2:A:493:GLN:OE1	2.73	0.42
11:J:27:GLU:C	11:J:29:GLU:H	2.20	0.42
2:A:128:ILE:O	2:A:128:ILE:HG22	2.20	0.42
2:A:208:LEU:HD23	2:A:208:LEU:C	2.39	0.42
2:A:444:PHE:CB	2:A:458:HIS:HD2	2.33	0.42
3:B:847:ASP:C	3:B:849:GLY:N	2.72	0.42
3:B:265:SER:O	3:B:266:ALA:CB	2.68	0.42
3:B:593:PRO:HG2	3:B:617:ARG:CZ	2.49	0.42
2:A:784:LEU:HD11	2:A:815:PHE:CE2	2.55	0.42
2:A:207:ILE:CG2	2:A:211:PHE:CE1	3.03	0.42
3:B:871:THR:CG2	3:B:872:GLU:N	2.82	0.42
3:B:1039:GLY:HA2	11:J:51:LEU:HD22	2.01	0.42
2:A:814:PHE:O	2:A:818:MET:HG3	2.20	0.42
3:B:476:ARG:NH2	3:B:501:PRO:HG3	2.35	0.42
2:A:162:VAL:HG12	2:A:163:SER:N	2.35	0.42
9:H:32:THR:HG22	9:H:33:GLN:OE1	2.19	0.42
9:H:110:ASP:OD1	9:H:110:ASP:N	2.53	0.42
5:D:25:ALA:HB2	8:G:84:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:216:GLU:HG2	3:B:217:ARG:N	2.35	0.42
3:B:1001:PHE:CE2	4:C:34:ARG:NE	2.88	0.42
2:A:1420:ASP:O	2:A:1421:CYS:CB	2.64	0.42
3:B:56:ASP:HB3	3:B:57:TYR:HD1	1.85	0.42
12:K:42:LEU:O	12:K:46:ILE:HG13	2.19	0.42
9:H:103:LYS:HG2	9:H:104:PHE:N	2.35	0.42
2:A:412:ARG:NH2	3:B:1108:ARG:NH1	2.68	0.42
2:A:1009:ASN:HA	2:A:1012:ARG:NH1	2.35	0.42
4:C:91:HIS:HD1	4:C:91:HIS:C	2.23	0.42
3:B:210:LYS:HA	3:B:481:GLN:O	2.20	0.42
2:A:761:MET:HA	2:A:804:TYR:HB2	2.02	0.42
8:G:140:LYS:HG2	8:G:140:LYS:H	1.68	0.42
3:B:262:GLU:HG2	3:B:262:GLU:O	2.19	0.42
2:A:68:GLN:C	2:A:70:CYS:N	2.70	0.41
8:G:45:ILE:HA	8:G:78:VAL:CG1	2.48	0.41
2:A:106:VAL:HG13	2:A:112:LYS:C	2.40	0.41
13:L:53:HIS:HB3	13:L:55:ILE:CD1	2.50	0.41
3:B:180:TYR:CD1	3:B:180:TYR:N	2.85	0.41
4:C:25:VAL:CG2	4:C:228:PHE:HE1	2.33	0.41
4:C:29:MET:HE1	12:K:98:LEU:HG	2.02	0.41
3:B:705:MET:HB3	3:B:706:GLN:H	1.71	0.41
3:B:745:PRO:C	3:B:747:MET:N	2.73	0.41
3:B:386:LEU:C	3:B:388:CYS:N	2.73	0.41
2:A:1410:PHE:HD2	3:B:1212:ILE:CD1	2.33	0.41
3:B:298:LEU:CD2	3:B:298:LEU:N	2.83	0.41
6:E:4:GLU:O	6:E:8:ASN:HB2	2.19	0.41
2:A:150:THR:HG22	2:A:150:THR:O	2.20	0.41
2:A:7:SER:HB2	3:B:1175:LEU:CD2	2.49	0.41
2:A:7:SER:CB	3:B:1175:LEU:HD22	2.46	0.41
3:B:273:LEU:O	3:B:276:ILE:HB	2.20	0.41
8:G:15:PRO:HG2	8:G:66:GLY:HA3	2.01	0.41
2:A:858:ASN:ND2	2:A:858:ASN:C	2.68	0.41
3:B:1002:THR:HG23	3:B:1006:ILE:O	2.20	0.41
6:E:42:PHE:HZ	6:E:58:MET:HE1	1.85	0.41
2:A:1329:THR:HG21	2:A:1331:SER:HB3	2.01	0.41
2:A:896:ARG:NH2	2:A:1030:ARG:NH2	2.68	0.41
2:A:284:ALA:C	2:A:286:HIS:N	2.73	0.41
2:A:167:CYS:O	2:A:167:CYS:SG	2.78	0.41
6:E:100:ILE:CG2	6:E:105:PHE:HB2	2.50	0.41
2:A:923:LEU:HD23	2:A:923:LEU:HA	1.90	0.41
11:J:27:GLU:O	11:J:29:GLU:N	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:146:LYS:HB2	11:J:61:LEU:HD11	2.02	0.41
6:E:2:ASP:HB3	6:E:3:GLN:H	1.41	0.41
2:A:364:VAL:O	2:A:364:VAL:HG13	2.18	0.41
2:A:1376:THR:HG23	2:A:1377:THR:H	1.84	0.41
12:K:65:HIS:C	12:K:65:HIS:CD2	2.93	0.41
6:E:23:VAL:HB	6:E:30:ILE:HD11	2.01	0.41
3:B:171:PRO:HD2	3:B:457:LEU:HD12	2.00	0.41
2:A:1030:ARG:HG3	2:A:1034:GLU:CD	2.41	0.41
3:B:37:PHE:C	3:B:37:PHE:HD1	2.22	0.41
4:C:191:TYR:CD2	4:C:201:TRP:CD1	3.04	0.41
4:C:152:GLU:CG	4:C:153:LEU:H	2.27	0.41
9:H:40:LEU:CD1	9:H:123:MET:HE3	2.49	0.41
2:A:852:TYR:HA	2:A:1060:PRO:HB3	2.02	0.41
4:C:35:ARG:HH12	12:K:40:HIS:HB2	1.84	0.41
12:K:3:ALA:O	12:K:4:PRO:O	2.39	0.41
11:J:31:ASP:O	11:J:32:GLU:C	2.58	0.41
3:B:621:GLU:O	3:B:621:GLU:HG3	2.20	0.41
5:D:25:ALA:C	5:D:27:LEU:H	2.21	0.41
5:D:8:PHE:O	5:D:9:GLN:HB2	2.21	0.41
3:B:898:LEU:HD13	3:B:952:VAL:HG11	2.02	0.41
8:G:91:VAL:HB	8:G:139:ILE:O	2.20	0.41
4:C:251:LEU:C	4:C:251:LEU:HD12	2.39	0.41
3:B:976:ILE:HD13	3:B:991:GLY:O	2.21	0.41
3:B:828:ALA:O	3:B:834:ASN:ND2	2.53	0.41
1:R:12:C:H5'	2:A:320:ARG:NH2	2.34	0.41
3:B:758:PHE:HZ	3:B:1031:LEU:HD22	1.86	0.41
3:B:781:PHE:O	3:B:782:LEU:HD23	2.19	0.41
2:A:182:VAL:HG12	2:A:183:GLY:N	2.35	0.41
12:K:35:PHE:HE1	12:K:73:LEU:HB3	1.83	0.41
2:A:1206:ASP:O	2:A:1274:ARG:NH1	2.53	0.41
5:D:130:LEU:O	5:D:132:GLN:N	2.48	0.41
2:A:375:THR:OG1	2:A:376:TYR:N	2.52	0.41
2:A:290:GLU:HA	2:A:293:GLU:HB3	2.03	0.41
3:B:1003:ALA:HA	4:C:178:PHE:O	2.20	0.41
2:A:1177:LEU:HD23	2:A:1177:LEU:HA	1.74	0.41
8:G:44:TYR:CD2	8:G:105:PRO:HB2	2.56	0.41
3:B:952:VAL:HG12	3:B:953:LEU:N	2.35	0.41
11:J:48:ARG:HD2	11:J:48:ARG:C	2.41	0.41
8:G:22:MET:C	8:G:24:GLN:N	2.73	0.41
2:A:343:LYS:HZ1	3:B:1151:LEU:HB3	1.85	0.41
6:E:16:PHE:CE2	6:E:20:LYS:HE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1115:SER:OG	2:A:1116:LEU:N	2.53	0.41
2:A:816:HIS:CD2	3:B:764:SER:H	2.39	0.41
4:C:18:VAL:O	4:C:20:PHE:CD2	2.70	0.41
12:K:101:LEU:HD23	12:K:101:LEU:O	2.20	0.41
7:F:82:THR:HA	7:F:83:PRO:HD3	1.83	0.41
13:L:38:LEU:O	13:L:39:SER:CB	2.64	0.41
2:A:738:LYS:C	2:A:740:LEU:H	2.24	0.41
9:H:24:CYS:HB2	9:H:44:VAL:HG21	2.02	0.41
2:A:373:THR:HG21	3:B:1105:ALA:CB	2.50	0.41
3:B:298:LEU:N	3:B:298:LEU:HD22	2.36	0.41
3:B:304:ASP:OD1	3:B:306:ASN:HB2	2.21	0.41
3:B:326:ASP:OD2	3:B:328:GLU:HB2	2.21	0.41
3:B:20:ASP:O	3:B:21:GLU:C	2.58	0.41
2:A:756:ILE:O	2:A:759:ALA:HB3	2.21	0.41
2:A:1111:MET:H	2:A:1111:MET:HG2	1.59	0.41
2:A:41:MET:HA	2:A:50:ILE:H	1.86	0.41
2:A:120:GLU:C	2:A:122:MET:N	2.72	0.41
3:B:899:ILE:CG2	3:B:903:VAL:HG21	2.51	0.41
2:A:1427:ASN:HB3	2:A:1432:GLN:O	2.20	0.41
3:B:681:TRP:O	3:B:683:SER:N	2.53	0.41
3:B:1085:ILE:CD1	3:B:1085:ILE:N	2.69	0.41
1:R:12:C:H2'	1:R:13:G:H8	1.79	0.41
4:C:236:GLY:O	4:C:238:ILE:N	2.53	0.41
4:C:6:PRO:HB3	4:C:25:VAL:CG1	2.42	0.41
2:A:427:GLN:O	2:A:428:TYR:C	2.59	0.41
2:A:845:LEU:O	2:A:846:GLU:C	2.59	0.41
3:B:862:GLN:CG	3:B:963:PHE:HD1	2.28	0.41
3:B:284:ILE:HG12	3:B:324:ILE:HD12	2.02	0.41
3:B:288:ALA:N	3:B:330:ALA:HB1	2.35	0.41
3:B:46:GLN:HE22	3:B:496:ARG:HA	1.86	0.41
3:B:303:TYR:N	3:B:303:TYR:HD2	2.18	0.41
6:E:154:ILE:HG22	6:E:155:ARG:O	2.19	0.41
2:A:693:VAL:O	2:A:693:VAL:HG12	2.20	0.41
3:B:769:TYR:CD1	3:B:987:LYS:NZ	2.89	0.41
3:B:1115:THR:HG21	3:B:1117:GLN:HB2	2.03	0.41
3:B:1152:MET:O	3:B:1157:ALA:HB2	2.21	0.41
6:E:168:TYR:C	6:E:169:ARG:HG3	2.41	0.41
11:J:41:LEU:N	11:J:41:LEU:HD23	2.33	0.41
2:A:138:ILE:HD11	2:A:221:SER:O	2.21	0.41
3:B:37:PHE:CD2	3:B:542:MET:SD	3.14	0.41
3:B:284:ILE:HG23	3:B:324:ILE:HD12	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1074:GLU:O	2:A:1076:ALA:N	2.54	0.41
12:K:76:GLN:HE21	12:K:76:GLN:HB3	1.66	0.41
3:B:1099:VAL:O	3:B:1101:ASP:N	2.54	0.41
2:A:974:ASP:OD2	2:A:976:THR:OG1	2.37	0.41
4:C:176:ILE:HG22	4:C:177:GLU:N	2.36	0.41
2:A:754:SER:O	2:A:755:PHE:C	2.58	0.41
4:C:137:LYS:HB3	4:C:138:GLU:OE1	2.20	0.41
3:B:552:MET:C	3:B:554:ILE:N	2.74	0.41
2:A:404:TYR:HB2	2:A:433:GLU:HB2	2.02	0.41
2:A:648:ASN:O	2:A:649:ILE:C	2.56	0.41
6:E:60:PHE:C	6:E:60:PHE:CD2	2.93	0.41
10:I:32:CYS:SG	10:I:33:SER:N	2.93	0.41
4:C:169:LYS:NZ	13:L:69:ALA:HB3	2.36	0.41
4:C:175:ALA:CB	11:J:43:ARG:HH12	2.34	0.41
5:D:53:SER:CB	5:D:152:SER:HB3	2.51	0.41
6:E:138:ALA:HA	6:E:141:VAL:HG23	2.03	0.41
2:A:768:GLN:HG2	2:A:816:HIS:CA	2.42	0.41
10:I:85:PHE:HD1	10:I:99:LEU:HD13	1.86	0.41
6:E:178:ILE:HG23	6:E:178:ILE:O	2.20	0.41
2:A:1343:ALA:CB	6:E:150:VAL:HG22	2.45	0.41
3:B:324:ILE:CG2	3:B:325:GLN:N	2.84	0.41
3:B:339:THR:HB	3:B:351:TYR:CE2	2.55	0.41
2:A:207:ILE:CG2	2:A:211:PHE:HE1	2.33	0.41
13:L:27:LEU:O	13:L:28:LYS:HG2	2.21	0.41
2:A:1334:ASP:O	2:A:1336:MET:N	2.53	0.41
10:I:19:ASP:CG	10:I:22:ASN:HB2	2.41	0.41
6:E:157:SER:OG	6:E:159:ASP:HB2	2.21	0.41
2:A:809:THR:HG23	2:A:812:GLU:OE1	2.21	0.41
2:A:497:THR:O	2:A:498:ARG:C	2.59	0.41
3:B:711:GLU:HB2	3:B:712:PRO:CD	2.50	0.41
2:A:268:ASP:HB3	2:A:299:HIS:CE1	2.54	0.41
2:A:425:GLN:N	2:A:425:GLN:OE1	2.54	0.41
3:B:557:PHE:CD2	3:B:557:PHE:C	2.94	0.41
7:F:68:THR:OG1	7:F:69:LEU:CG	2.55	0.41
2:A:32:VAL:HG21	2:A:68:GLN:HE21	1.84	0.41
10:I:15:TYR:O	10:I:28:GLU:HG2	2.21	0.41
4:C:98:VAL:HG12	4:C:99:LEU:N	2.35	0.41
4:C:43:THR:CG2	4:C:44:LEU:N	2.66	0.41
4:C:74:SER:CB	4:C:77:ILE:HG12	2.51	0.41
3:B:797:TYR:CE1	3:B:854:LEU:CD2	3.03	0.41
3:B:797:TYR:HE1	3:B:854:LEU:HD23	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:101:VAL:CG1	8:G:102:GLN:N	2.84	0.41
2:A:457:ALA:HB3	2:A:506:ALA:N	2.36	0.41
2:A:444:PHE:CB	2:A:458:HIS:CD2	3.04	0.41
2:A:857:ARG:HG2	2:A:863:VAL:HA	2.03	0.41
3:B:126:SER:OG	3:B:172:ILE:HD11	2.20	0.41
3:B:611:PRO:HG2	3:B:685:LEU:HD21	2.03	0.41
11:J:44:TYR:CA	11:J:47:ARG:HB2	2.37	0.41
3:B:1159:ARG:HD2	3:B:1159:ARG:C	2.41	0.41
2:A:1443:VAL:O	2:A:1443:VAL:HG23	2.20	0.41
2:A:562:THR:HB	9:H:98:TYR:HD2	1.86	0.41
2:A:351:THR:CG2	3:B:1103:ILE:HG13	2.50	0.41
8:G:144:ARG:HG2	8:G:168:LEU:HD23	2.03	0.41
2:A:222:LEU:O	2:A:224:PHE:N	2.53	0.41
4:C:22:LEU:HD21	4:C:25:VAL:HG11	2.02	0.41
3:B:37:PHE:HE2	3:B:542:MET:HA	1.85	0.41
3:B:520:GLY:CA	3:B:748:ILE:HG22	2.50	0.41
12:K:19:LEU:HD22	12:K:33:ILE:CG2	2.51	0.41
3:B:53:GLN:HB2	3:B:547:VAL:HG21	2.02	0.41
3:B:1182:CYS:O	3:B:1183:LYS:C	2.58	0.41
2:A:254:GLU:HB2	3:B:935:ARG:NH2	2.35	0.41
2:A:683:ILE:HD13	2:A:801:GLU:CG	2.50	0.41
10:I:106:CYS:O	10:I:107:SER:CB	2.68	0.41
5:D:153:ARG:NH2	5:D:184:ALA:HA	2.36	0.41
2:A:152:VAL:HG12	2:A:153:PRO:CD	2.50	0.41
3:B:211:VAL:HG21	3:B:483:LEU:HD13	2.03	0.41
5:D:188:ALA:O	5:D:192:LYS:CG	2.69	0.41
9:H:143:LEU:N	9:H:143:LEU:HD12	2.35	0.41
4:C:259:LEU:CD1	12:K:88:LYS:HA	2.50	0.41
3:B:1079:LYS:CA	4:C:27:LEU:HD21	2.51	0.41
2:A:1398:MET:HB2	2:A:1426:GLU:OE2	2.21	0.41
9:H:99:GLY:HA3	9:H:117:SER:O	2.21	0.41
2:A:1219:THR:OG1	2:A:1271:ILE:HD11	2.21	0.41
3:B:21:GLU:HG3	3:B:21:GLU:H	1.64	0.41
3:B:557:PHE:O	3:B:557:PHE:CD2	2.74	0.41
9:H:31:THR:O	9:H:31:THR:HG22	2.21	0.41
6:E:63:ASN:HA	6:E:64:PRO:HD3	1.88	0.41
3:B:203:PHE:N	3:B:203:PHE:CD1	2.89	0.41
4:C:100:THR:CG2	4:C:101:LEU:N	2.84	0.41
3:B:1198:TYR:CD2	3:B:1198:TYR:C	2.93	0.41
2:A:1220:PHE:CE2	2:A:1263:ILE:HG23	2.56	0.41
4:C:22:LEU:CD2	4:C:25:VAL:HG11	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:109:VAL:HG11	7:F:123:LYS:CD	2.51	0.41
3:B:1220:ARG:HH11	3:B:1220:ARG:CB	2.34	0.41
2:A:1214:GLU:HA	2:A:1214:GLU:OE1	2.21	0.41
2:A:1315:GLU:C	2:A:1317:MET:N	2.74	0.41
2:A:1100:ARG:O	2:A:1103:GLU:HB3	2.21	0.41
12:K:38:GLU:HB3	12:K:71:PHE:HE2	1.86	0.41
2:A:172:PRO:HB3	2:A:185:TRP:CG	2.56	0.41
3:B:278:GLN:HG2	3:B:279:ASP:N	2.33	0.41
3:B:184:ALA:HB1	3:B:188:ASP:HB3	2.03	0.41
3:B:221:ASN:OD1	3:B:242:SER:HA	2.21	0.41
3:B:779:GLY:O	3:B:795:ILE:HA	2.21	0.41
3:B:732:SER:HB2	3:B:734:HIS:CD2	2.57	0.41
2:A:997:LEU:HD13	2:A:1018:PHE:CE2	2.55	0.41
8:G:48:VAL:HA	8:G:76:ALA:CB	2.50	0.40
3:B:797:TYR:CE1	3:B:971:THR:HG23	2.56	0.40
4:C:56:THR:HG22	4:C:58:LEU:HD23	2.02	0.40
4:C:66:ARG:NH1	4:C:144:ILE:O	2.54	0.40
4:C:70:ILE:HG22	4:C:70:ILE:O	2.21	0.40
2:A:300:VAL:O	2:A:300:VAL:HG12	2.21	0.40
2:A:1116:LEU:HB2	2:A:1329:THR:HG1	1.80	0.40
2:A:1349:TYR:N	2:A:1372:VAL:HG21	2.36	0.40
8:G:144:ARG:O	8:G:168:LEU:HD22	2.21	0.40
4:C:232:VAL:HG11	4:C:244:VAL:HG22	2.03	0.40
2:A:1057:VAL:HG12	2:A:1058:VAL:N	2.37	0.40
2:A:719:VAL:O	2:A:721:PHE:N	2.54	0.40
2:A:24:PRO:CD	2:A:233:TRP:CD1	3.05	0.40
12:K:109:TRP:O	12:K:111:LEU:N	2.54	0.40
6:E:143:ASN:ND2	6:E:145:THR:OG1	2.54	0.40
2:A:443:LEU:HD12	3:B:1146:PHE:HE2	1.85	0.40
5:D:191:ALA:O	5:D:193:THR:N	2.54	0.40
2:A:98:LYS:O	2:A:99:ILE:C	2.59	0.40
12:K:61:TYR:HA	12:K:72:LYS:O	2.21	0.40
2:A:962:ARG:O	2:A:964:ILE:N	2.54	0.40
5:D:64:VAL:C	5:D:66:ARG:N	2.74	0.40
11:J:30:LEU:HD11	11:J:38:ARG:HH12	1.86	0.40
3:B:307:ASP:OD1	3:B:307:ASP:O	2.39	0.40
2:A:737:LEU:HD23	2:A:737:LEU:HA	1.88	0.40
3:B:899:ILE:O	3:B:952:VAL:HG21	2.21	0.40
3:B:821:GLN:HE22	3:B:851:PHE:CA	2.32	0.40
3:B:377:PHE:O	3:B:380:TYR:N	2.54	0.40
3:B:1095:LEU:H	3:B:1095:LEU:CD1	2.13	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:920:LEU:HD23	2:A:920:LEU:C	2.41	0.40
3:B:167:ILE:HG22	3:B:167:ILE:O	2.21	0.40
6:E:56:LYS:HE3	6:E:84:ASP:HB2	2.03	0.40
3:B:289:LEU:HD22	3:B:371:GLU:O	2.20	0.40
3:B:657:HIS:O	3:B:660:LYS:HB3	2.21	0.40
3:B:792:MET:H	3:B:857:ARG:HA	1.85	0.40
12:K:62:LYS:O	12:K:71:PHE:HB2	2.21	0.40
12:K:42:LEU:CD2	12:K:46:ILE:HD11	2.50	0.40
9:H:22:LYS:O	9:H:23:VAL:HG23	2.21	0.40
3:B:1138:MET:CE	3:B:1143:ALA:HB3	2.51	0.40
3:B:237:VAL:CG1	3:B:238:ALA:N	2.84	0.40
2:A:522:GLY:O	2:A:646:PHE:HE2	2.04	0.40
3:B:868:MET:O	3:B:870:ILE:HG13	2.21	0.40
13:L:46:VAL:HG12	13:L:46:VAL:O	2.20	0.40
2:A:368:LYS:HB2	2:A:368:LYS:HE3	1.78	0.40
2:A:34:LYS:N	2:A:34:LYS:CD	2.85	0.40
2:A:334:GLY:O	2:A:335:ARG:C	2.60	0.40
4:C:31:ASN:O	4:C:32:SER:C	2.59	0.40
5:D:52:LEU:O	5:D:53:SER:OG	2.31	0.40
7:F:135:ARG:HD3	7:F:143:PHE:CD2	2.56	0.40
2:A:1308:THR:HG21	2:A:1310:GLY:O	2.22	0.40
4:C:252:GLN:NE2	12:K:95:ILE:HG23	2.36	0.40
2:A:524:VAL:CG1	2:A:525:GLN:H	2.26	0.40
2:A:666:ILE:HG23	3:B:1026:LEU:HB3	2.03	0.40
2:A:511:ILE:O	2:A:519:PRO:HA	2.21	0.40
3:B:1181:GLU:O	3:B:1182:CYS:HB2	2.21	0.40
9:H:38:LEU:HD13	9:H:125:LEU:HD13	2.03	0.40
2:A:883:LEU:HD13	2:A:943:LEU:HD13	2.03	0.40
3:B:463:THR:HB	3:B:464:GLY:H	1.71	0.40
3:B:872:GLU:OE2	3:B:914:LYS:HE2	2.21	0.40
2:A:977:LYS:HB3	2:A:978:PRO:HD2	2.02	0.40
3:B:992:ILE:CG1	3:B:993:THR:N	2.84	0.40
3:B:728:ARG:HH12	3:B:1047:PHE:HB3	1.86	0.40
3:B:213:ILE:HD12	3:B:497:ARG:HB3	2.03	0.40
2:A:49:LYS:HZ2	2:A:60:SER:HA	1.86	0.40
2:A:57:ARG:O	2:A:68:GLN:HG3	2.22	0.40
3:B:822:ASN:ND2	11:J:52:THR:HG21	2.35	0.40
3:B:240:ILE:CG2	3:B:254:LEU:HB3	2.51	0.40
2:A:1447:GLU:O	2:A:1447:GLU:OE1	2.40	0.40
3:B:1010:LEU:HA	3:B:1010:LEU:HD12	1.79	0.40
3:B:824:ILE:CG2	3:B:1087:PHE:CE2	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1239:ARG:HH22	2:A:1241:ARG:HH22	1.68	0.40
2:A:1227:ILE:CG2	2:A:1228:TRP:N	2.78	0.40
2:A:1001:ARG:NE	7:F:83:PRO:HD3	2.36	0.40
10:I:100:PHE:N	10:I:100:PHE:CD1	2.89	0.40
3:B:388:CYS:O	3:B:391:ASP:N	2.51	0.40
4:C:186:LEU:CD1	4:C:186:LEU:N	2.84	0.40
2:A:23:SER:HA	2:A:233:TRP:CD1	2.56	0.40
4:C:262:LEU:HA	4:C:262:LEU:HD23	1.88	0.40
2:A:1148:ILE:HD11	2:A:1198:ASP:HA	2.03	0.40
5:D:154:PHE:CD1	5:D:154:PHE:N	2.90	0.40
3:B:502:ILE:N	3:B:502:ILE:HD12	2.34	0.40
2:A:777:PHE:CD1	2:A:781:ASP:HA	2.56	0.40
2:A:1297:GLU:H	2:A:1297:GLU:HG3	1.60	0.40
2:A:1402:PHE:CE1	2:A:1403:GLU:HG3	2.57	0.40
2:A:180:LYS:HZ2	2:A:294:SER:HB3	1.86	0.40
2:A:184:SER:HB3	2:A:199:LEU:HD23	2.04	0.40
2:A:402:ALA:HB1	2:A:433:GLU:O	2.22	0.40
8:G:99:PHE:O	8:G:109:PHE:HD1	2.05	0.40
5:D:49:ALA:CB	5:D:174:PRO:O	2.69	0.40
2:A:628:GLY:O	2:A:632:VAL:HG23	2.22	0.40
2:A:79:GLY:HA3	2:A:243:PRO:HG3	2.02	0.40
12:K:47:ARG:O	12:K:47:ARG:HD2	2.21	0.40
2:A:1120:LEU:HD23	2:A:1124:HIS:O	2.22	0.40
3:B:276:ILE:HA	3:B:338:GLY:HA2	2.02	0.40
11:J:1:MET:O	11:J:2:ILE:HB	2.21	0.40
12:K:7:PHE:CD1	12:K:7:PHE:C	2.95	0.40
3:B:100:PRO:HD3	3:B:172:ILE:CD1	2.51	0.40
3:B:834:ASN:ND2	3:B:1013:ASN:HA	2.36	0.40
4:C:10:ILE:H	4:C:10:ILE:HG13	1.58	0.40
4:C:6:PRO:CG	12:K:101:LEU:HB2	2.51	0.40
4:C:239:PRO:C	4:C:241:ASP:N	2.75	0.40
3:B:63:ILE:HD12	3:B:63:ILE:HA	1.95	0.40
2:A:417:TYR:CD2	2:A:417:TYR:N	2.90	0.40
2:A:683:ILE:HG21	2:A:801:GLU:CG	2.49	0.40
2:A:1100:ARG:HH21	2:A:1351:GLU:CD	2.25	0.40
5:D:4:SER:OG	5:D:5:THR:N	2.49	0.40
3:B:1177:HIS:C	3:B:1179:GLN:H	2.25	0.40
2:A:1319:VAL:CG1	2:A:1320:PRO:HD2	2.49	0.40
8:G:145:VAL:HG12	8:G:146:LYS:H	1.86	0.40
4:C:11:ARG:HH21	4:C:229:TYR:HB3	1.85	0.40
3:B:236:HIS:HB2	3:B:258:LEU:HD23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:763:GLN:HG2	3:B:765:PRO:CD	2.51	0.40
3:B:570:VAL:HA	3:B:571:PRO:HD2	1.75	0.40
2:A:377:PRO:HD3	2:A:493:GLN:OE1	2.22	0.40
4:C:27:LEU:O	4:C:30:ALA:HB3	2.21	0.40
9:H:118:PHE:HD1	9:H:121:LEU:O	2.05	0.40
3:B:227:LYS:HB2	3:B:395:GLN:OE1	2.22	0.40
8:G:21:ARG:HD3	8:G:21:ARG:HA	1.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	1412/1733 (82%)	1032 (73%)	252 (18%)	128 (9%)	1	16
3	B	1096/1224 (90%)	781 (71%)	206 (19%)	109 (10%)	1	13
4	C	265/318 (83%)	169 (64%)	66 (25%)	30 (11%)	0	10
5	D	174/221 (79%)	133 (76%)	27 (16%)	14 (8%)	1	19
6	E	212/215 (99%)	166 (78%)	32 (15%)	14 (7%)	1	25
7	F	85/155 (55%)	70 (82%)	11 (13%)	4 (5%)	3	33
8	G	169/171 (99%)	128 (76%)	32 (19%)	9 (5%)	2	31
9	H	131/146 (90%)	78 (60%)	33 (25%)	20 (15%)	0	5
10	I	114/122 (93%)	76 (67%)	26 (23%)	12 (10%)	1	11
11	J	63/70 (90%)	37 (59%)	16 (25%)	10 (16%)	0	5
12	K	110/120 (92%)	88 (80%)	15 (14%)	7 (6%)	2	26
13	L	44/70 (63%)	20 (46%)	12 (27%)	12 (27%)	0	0
All	All	3875/4565 (85%)	2778 (72%)	728 (19%)	369 (10%)	1	15

All (369) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
2	A	42	ASP
2	A	48	ALA
2	A	54	ASN
2	A	57	ARG
2	A	62	ASP
2	A	69	THR
2	A	93	VAL
2	A	130	ASP
2	A	154	SER
2	A	167	CYS
2	A	223	GLY
2	A	250	ILE
2	A	253	ASN
2	A	286	HIS
2	A	311	GLN
2	A	312	PRO
2	A	318	SER
2	A	332	LYS
2	A	335	ARG
2	A	536	LEU
2	A	567	LYS
2	A	597	LEU
2	A	666	ILE
2	A	765	VAL
2	A	780	VAL
2	A	968	GLN
2	A	969	GLN
2	A	1002	GLY
2	A	1115	SER
2	A	1116	LEU
2	A	1120	LEU
2	A	1124	HIS
2	A	1212	VAL
2	A	1223	ASP
2	A	1255	GLU
2	A	1314	SER
2	A	1365	TYR
3	B	20	ASP
3	B	45	SER
3	B	108	VAL
3	B	186	GLU
3	B	206	ASN
3	B	266	ALA

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Mol	Chain	Res	Type
3	B	340	ALA
3	B	345	LYS
3	B	367	LEU
3	B	401	PHE
3	B	470	LYS
3	B	708	GLU
3	B	709	ASP
3	B	731	VAL
3	B	751	VAL
3	B	825	VAL
3	B	826	ALA
3	B	881	ASN
3	B	909	ASP
3	B	943	SER
3	B	958	GLN
3	B	1011	ILE
3	B	1041	GLU
3	B	1046	PRO
3	B	1069	PHE
3	B	1097	HIS
3	B	1155	SER
3	B	1156	ASP
3	B	1157	ALA
3	B	1171	VAL
3	B	1175	LEU
3	B	1181	GLU
3	B	1182	CYS
3	B	1183	LYS
3	B	1188	LYS
4	C	4	GLU
4	C	133	ILE
4	C	149	LYS
4	C	161	LYS
4	C	184	ASN
4	C	212	PRO
4	C	214	ASN
4	C	215	GLU
5	D	4	SER
5	D	5	THR
5	D	20	GLU
5	D	199	ASN
6	E	59	SER

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Mol	Chain	Res	Type
6	E	106	GLN
8	G	63	PRO
8	G	139	ILE
9	H	62	SER
9	H	64	ASN
9	H	108	SER
9	H	128	ASN
9	H	140	ALA
10	I	79	HIS
10	I	106	CYS
11	J	6	ARG
11	J	32	GLU
11	J	64	ASN
12	K	7	PHE
12	K	110	ASN
12	K	111	LEU
13	L	35	SER
13	L	50	ASP
13	L	53	HIS
13	L	59	ALA
13	L	60	ARG
2	A	4	GLN
2	A	44	THR
2	A	59	GLY
2	A	67	CYS
2	A	73	GLY
2	A	74	MET
2	A	76	GLU
2	A	283	GLY
2	A	303	TYR
2	A	331	GLY
2	A	336	ILE
2	A	380	VAL
2	A	410	GLY
2	A	543	LEU
2	A	661	GLY
2	A	753	GLY
2	A	755	PHE
2	A	789	LYS
2	A	846	GLU
2	A	854	ASN
2	A	871	ASP

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Mol	Chain	Res	Type
2	A	986	ILE
2	A	1016	THR
2	A	1036	ARG
2	A	1127	ASP
2	A	1221	LYS
2	A	1378	GLN
2	A	1402	PHE
2	A	1405	THR
3	B	22	SER
3	B	28	GLU
3	B	65	GLU
3	B	184	ALA
3	B	259	TYR
3	B	260	GLY
3	B	295	GLY
3	B	365	THR
3	B	394	ASP
3	B	460	ALA
3	B	461	LEU
3	B	467	GLY
3	B	559	SER
3	B	591	ARG
3	B	605	ARG
3	B	643	ASP
3	B	655	LYS
3	B	827	ILE
3	B	867	GLY
3	B	879	ARG
3	B	907	GLY
3	B	951	GLN
3	B	978	ASP
3	B	1035	ALA
3	B	1100	ASP
3	B	1108	ARG
3	B	1126	GLY
3	B	1131	GLY
4	C	51	VAL
4	C	87	PHE
4	C	90	ASP
4	C	108	GLU
4	C	110	THR
4	C	132	PRO

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Mol	Chain	Res	Type
4	C	213	PRO
4	C	217	ASP
4	C	231	ASN
4	C	240	VAL
5	D	9	GLN
5	D	21	GLU
5	D	52	LEU
5	D	192	LYS
5	D	218	GLU
6	E	44	ALA
6	E	45	LYS
6	E	73	PRO
6	E	76	GLY
6	E	130	ALA
6	E	192	ARG
7	F	81	THR
7	F	112	GLU
8	G	19	GLY
8	G	118	ASP
8	G	167	TYR
9	H	21	ASN
9	H	59	ILE
9	H	63	LEU
9	H	81	PRO
9	H	82	PRO
9	H	84	ALA
9	H	90	ALA
10	I	3	THR
10	I	11	ASN
10	I	47	GLU
10	I	57	GLY
10	I	95	THR
11	J	2	ILE
11	J	24	LEU
11	J	28	ASP
11	J	29	GLU
12	K	15	GLY
12	K	109	TRP
13	L	54	ARG
2	A	35	ILE
2	A	58	LEU
2	A	113	LEU

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Mol	Chain	Res	Type
2	A	263	THR
2	A	322	VAL
2	A	399	HIS
2	A	423	ASP
2	A	465	TYR
2	A	591	PHE
2	A	592	ASP
2	A	738	LYS
2	A	847	ASP
2	A	1122	PRO
2	A	1233	ASP
2	A	1281	ARG
2	A	1377	THR
3	B	115	GLN
3	B	258	LEU
3	B	308	TRP
3	B	369	GLY
3	B	450	ALA
3	B	531	GLN
3	B	641	GLU
3	B	642	ASP
3	B	711	GLU
3	B	712	PRO
3	B	727	LYS
3	B	792	MET
3	B	891	ASP
3	B	901	PRO
3	B	1006	ILE
3	B	1082	MET
3	B	1167	GLY
3	B	1178	ASN
4	C	141	GLY
4	C	142	VAL
4	C	148	ARG
4	C	156	THR
4	C	209	TYR
5	D	31	GLN
5	D	131	GLU
6	E	115	ASN
9	H	17	PRO
9	H	77	ARG
10	I	8	ARG

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Mol	Chain	Res	Type
10	I	107	SER
12	K	29	ASN
13	L	26	THR
2	A	5	GLN
2	A	66	LYS
2	A	400	PRO
2	A	409	SER
2	A	419	LYS
2	A	424	ILE
2	A	544	ASP
2	A	619	LYS
2	A	706	HIS
2	A	739	ASP
2	A	958	VAL
2	A	1266	THR
2	A	1366	ARG
2	A	1392	SER
3	B	46	GLN
3	B	58	THR
3	B	368	GLU
3	B	571	PRO
3	B	575	PRO
3	B	613	VAL
3	B	680	THR
3	B	705	MET
3	B	869	SER
3	B	945	GLU
4	C	78	GLU
4	C	139	GLY
4	C	188	HIS
5	D	196	PRO
6	E	3	GLN
6	E	43	LYS
6	E	56	LYS
6	E	206	GLY
8	G	20	PRO
8	G	35	GLU
8	G	154	VAL
9	H	119	GLY
11	J	17	LYS
11	J	57	ILE
2	A	70	CYS

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Mol	Chain	Res	Type
2	A	84	ILE
2	A	164	ARG
2	A	245	PRO
2	A	257	ARG
2	A	1176	LEU
2	A	1231	ASP
3	B	124	TYR
3	B	267	ARG
3	B	474	SER
3	B	832	GLY
3	B	946	ASN
4	C	18	VAL
4	C	175	ALA
7	F	104	ASN
9	H	60	ALA
9	H	92	ASP
9	H	105	GLU
10	I	9	ASP
12	K	4	PRO
13	L	40	LEU
2	A	61	ILE
2	A	219	PHE
2	A	317	LYS
2	A	700	ASN
2	A	720	ARG
2	A	868	TYR
2	A	910	PRO
2	A	1071	SER
2	A	1114	PRO
2	A	1324	PRO
2	A	1437	GLY
3	B	291	ILE
3	B	611	PRO
3	B	713	ALA
3	B	1017	ILE
3	B	1018	PRO
3	B	1112	GLN
3	B	1144	ALA
5	D	47	LEU
11	J	14	VAL
13	L	39	SER
13	L	55	ILE

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Mol	Chain	Res	Type
13	L	56	LEU
2	A	51	GLY
2	A	284	ALA
2	A	639	PRO
2	A	673	GLY
2	A	963	ILE
2	A	1094	VAL
3	B	305	VAL
3	B	1045	SER
2	A	600	PRO
2	A	1395	GLY
3	B	1103	ILE
5	D	59	ILE
9	H	44	VAL
10	I	59	VAL
2	A	128	ILE
2	A	244	PRO
2	A	1335	ILE
3	B	282	ILE
3	B	362	PRO
6	E	129	PRO
7	F	139	PRO
8	G	115	MET
10	I	62	ILE
2	A	196	GLU
2	A	1435	PRO
3	B	478	GLY
4	C	70	ILE
4	C	216	GLY
9	H	107	VAL
2	A	756	ILE
13	L	46	VAL

### 5.3.2 Protein sidechains ⓘ

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	1245/1520 (82%)	1136 (91%)	109 (9%)	12	48
3	B	964/1061 (91%)	882 (92%)	82 (8%)	13	51
4	C	235/274 (86%)	219 (93%)	16 (7%)	20	59
5	D	160/200 (80%)	138 (86%)	22 (14%)	4	29
6	E	196/197 (100%)	187 (95%)	9 (5%)	33	70
7	F	78/137 (57%)	72 (92%)	6 (8%)	16	55
8	G	152/152 (100%)	133 (88%)	19 (12%)	6	32
9	H	119/128 (93%)	115 (97%)	4 (3%)	44	77
10	I	110/116 (95%)	104 (94%)	6 (6%)	27	66
11	J	60/65 (92%)	53 (88%)	7 (12%)	7	35
12	K	97/102 (95%)	89 (92%)	8 (8%)	14	51
13	L	40/57 (70%)	37 (92%)	3 (8%)	17	56
All	All	3456/4009 (86%)	3165 (92%)	291 (8%)	14	51

All (291) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2	VAL
2	A	11	LEU
2	A	34	LYS
2	A	37	PHE
2	A	41	MET
2	A	54	ASN
2	A	62	ASP
2	A	67	CYS
2	A	68	GLN
2	A	70	CYS
2	A	83	HIS
2	A	93	VAL
2	A	110	CYS
2	A	142	CYS
2	A	200	ARG
2	A	205	GLU
2	A	221	SER
2	A	245	PRO
2	A	261	ASP
2	A	265	LYS
2	A	270	LEU
2	A	302	THR

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Mol	Chain	Res	Type
2	A	312	PRO
2	A	326	ARG
2	A	335	ARG
2	A	345	VAL
2	A	354	SER
2	A	375	THR
2	A	385	ILE
2	A	388	LEU
2	A	406	ILE
2	A	407	ARG
2	A	408	ASP
2	A	412	ARG
2	A	425	GLN
2	A	434	ARG
2	A	442	VAL
2	A	443	LEU
2	A	445	ASN
2	A	450	LEU
2	A	460	VAL
2	A	469	ARG
2	A	470	LEU
2	A	481	ASP
2	A	560	ILE
2	A	562	THR
2	A	618	GLU
2	A	622	VAL
2	A	626	ASN
2	A	629	LEU
2	A	635	ARG
2	A	659	HIS
2	A	666	ILE
2	A	692	ASP
2	A	720	ARG
2	A	727	ASP
2	A	739	ASP
2	A	741	ASN
2	A	768	GLN
2	A	779	PHE
2	A	821	ARG
2	A	827	THR
2	A	834	THR
2	A	858	ASN

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Mol	Chain	Res	Type
2	A	871	ASP
2	A	886	ILE
2	A	890	ASP
2	A	903	ASN
2	A	929	LEU
2	A	939	ASP
2	A	941	LYS
2	A	969	GLN
2	A	1001	ARG
2	A	1009	ASN
2	A	1029	ARG
2	A	1035	TYR
2	A	1052	GLN
2	A	1067	LEU
2	A	1111	MET
2	A	1116	LEU
2	A	1120	LEU
2	A	1122	PRO
2	A	1127	ASP
2	A	1138	ILE
2	A	1146	VAL
2	A	1152	ILE
2	A	1166	ASP
2	A	1175	SER
2	A	1187	GLN
2	A	1206	ASP
2	A	1240	CYS
2	A	1264	GLU
2	A	1271	ILE
2	A	1291	VAL
2	A	1295	THR
2	A	1297	GLU
2	A	1309	ASP
2	A	1329	THR
2	A	1332	PHE
2	A	1333	ILE
2	A	1359	ASP
2	A	1364	ASN
2	A	1372	VAL
2	A	1389	PHE
2	A	1394	THR
2	A	1405	THR

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Mol	Chain	Res	Type
2	A	1442	ASP
2	A	1445	ILE
2	A	1447	GLU
3	B	37	PHE
3	B	57	TYR
3	B	61	ASP
3	B	106	ASP
3	B	175	ARG
3	B	180	TYR
3	B	199	MET
3	B	217	ARG
3	B	250	PHE
3	B	258	LEU
3	B	268	THR
3	B	286	PHE
3	B	303	TYR
3	B	365	THR
3	B	371	GLU
3	B	393	LYS
3	B	401	PHE
3	B	416	LEU
3	B	427	ASP
3	B	429	PHE
3	B	463	THR
3	B	466	TRP
3	B	473	MET
3	B	476	ARG
3	B	485	ARG
3	B	498	THR
3	B	502	ILE
3	B	516	ASN
3	B	537	LYS
3	B	539	LEU
3	B	557	PHE
3	B	582	VAL
3	B	591	ARG
3	B	593	PRO
3	B	603	LEU
3	B	615	MET
3	B	635	ARG
3	B	644	GLU
3	B	724	ASP

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Mol	Chain	Res	Type
3	B	737	THR
3	B	780	VAL
3	B	785	TYR
3	B	791	THR
3	B	795	ILE
3	B	830	TYR
3	B	833	TYR
3	B	835	GLN
3	B	839	MET
3	B	844	SER
3	B	878	GLN
3	B	894	ASP
3	B	909	ASP
3	B	944	THR
3	B	957	ASN
3	B	978	ASP
3	B	999	MET
3	B	1002	THR
3	B	1006	ILE
3	B	1010	LEU
3	B	1046	PRO
3	B	1047	PHE
3	B	1069	PHE
3	B	1084	GLN
3	B	1087	PHE
3	B	1095	LEU
3	B	1098	MET
3	B	1099	VAL
3	B	1108	ARG
3	B	1120	GLU
3	B	1122	ARG
3	B	1136	ASP
3	B	1159	ARG
3	B	1170	THR
3	B	1176	ASN
3	B	1183	LYS
3	B	1185	CYS
3	B	1191	ILE
3	B	1192	TYR
3	B	1202	LEU
3	B	1212	ILE
3	B	1220	ARG

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Mol	Chain	Res	Type
3	B	1223	ASP
4	C	62	PHE
4	C	74	SER
4	C	77	ILE
4	C	89	GLU
4	C	91	HIS
4	C	104	PHE
4	C	128	ASN
4	C	129	ILE
4	C	147	LEU
4	C	193	TYR
4	C	209	TYR
4	C	214	ASN
4	C	235	VAL
4	C	240	VAL
4	C	251	LEU
4	C	266	ASP
5	D	4	SER
5	D	7	THR
5	D	8	PHE
5	D	13	ARG
5	D	17	LYS
5	D	19	GLU
5	D	21	GLU
5	D	22	GLU
5	D	47	LEU
5	D	63	LEU
5	D	70	PHE
5	D	126	ILE
5	D	137	ASN
5	D	139	LYS
5	D	148	LEU
5	D	149	THR
5	D	151	PHE
5	D	170	THR
5	D	187	THR
5	D	192	LYS
5	D	193	THR
5	D	221	TYR
6	E	2	ASP
6	E	60	PHE
6	E	74	ASP

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Mol	Chain	Res	Type
6	E	78	LEU
6	E	104	ASN
6	E	114	ASN
6	E	132	ILE
6	E	149	LEU
6	E	158	SER
7	F	68	THR
7	F	79	ARG
7	F	90	ARG
7	F	123	LYS
7	F	132	LEU
7	F	143	PHE
8	G	1	MET
8	G	11	ILE
8	G	13	LEU
8	G	21	ARG
8	G	26	LEU
8	G	33	GLU
8	G	45	ILE
8	G	49	LEU
8	G	51	TYR
8	G	52	ASP
8	G	64	THR
8	G	74	TYR
8	G	78	VAL
8	G	79	PHE
8	G	80	LYS
8	G	88	ASP
8	G	115	MET
8	G	126	ASN
8	G	171	ILE
9	H	10	PHE
9	H	95	TYR
9	H	102	TYR
9	H	130	ARG
10	I	4	PHE
10	I	15	TYR
10	I	34	TYR
10	I	85	PHE
10	I	86	PHE
10	I	101	PHE
11	J	16	ASP

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Mol	Chain	Res	Type
11	J	28	ASP
11	J	43	ARG
11	J	44	TYR
11	J	46	CYS
11	J	48	ARG
11	J	62	ARG
12	K	5	ASP
12	K	10	PHE
12	K	25	THR
12	K	41	THR
12	K	47	ARG
12	K	50	LEU
12	K	61	TYR
12	K	112	GLN
13	L	27	LEU
13	L	55	ILE
13	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	54	ASN
2	A	64	ASN
2	A	92	HIS
2	A	109	HIS
2	A	171	GLN
2	A	225	ASN
2	A	306	ASN
2	A	339	ASN
2	A	435	HIS
2	A	447	GLN
2	A	479	ASN
2	A	517	ASN
2	A	654	ASN
2	A	717	ASN
2	A	736	ASN
2	A	741	ASN
2	A	768	GLN
2	A	786	HIS
2	A	858	ASN
2	A	903	ASN
2	A	926	GLN

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Mol	Chain	Res	Type
2	A	1106	ASN
2	A	1124	HIS
2	A	1130	GLN
2	A	1187	GLN
2	A	1188	GLN
2	A	1203	ASN
2	A	1265	ASN
2	A	1354	ASN
2	A	1432	GLN
3	B	46	GLN
3	B	53	GLN
3	B	60	GLN
3	B	121	ASN
3	B	178	ASN
3	B	236	HIS
3	B	363	HIS
3	B	366	GLN
3	B	465	ASN
3	B	499	ASN
3	B	513	GLN
3	B	515	HIS
3	B	516	ASN
3	B	518	HIS
3	B	538	ASN
3	B	706	GLN
3	B	744	HIS
3	B	763	GLN
3	B	821	GLN
3	B	842	ASN
3	B	957	ASN
3	B	975	GLN
3	B	1015	HIS
3	B	1062	HIS
3	B	1065	GLN
3	B	1084	GLN
3	B	1117	GLN
3	B	1176	ASN
3	B	1179	GLN
3	B	1193	GLN
4	C	24	ASN
4	C	73	GLN
4	C	79	GLN

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Mol	Chain	Res	Type
4	C	102	GLN
4	C	112	ASN
4	C	131	HIS
4	C	167	HIS
4	C	184	ASN
4	C	252	GLN
5	D	39	ASN
5	D	137	ASN
5	D	173	HIS
5	D	179	GLN
6	E	8	ASN
6	E	101	GLN
6	E	104	ASN
6	E	114	ASN
6	E	143	ASN
6	E	147	HIS
8	G	14	HIS
8	G	53	ASN
8	G	97	HIS
8	G	122	ASN
8	G	126	ASN
9	H	64	ASN
9	H	133	ASN
9	H	134	ASN
9	H	137	GLN
10	I	12	ASN
10	I	90	GLN
11	J	53	HIS
11	J	64	ASN
12	K	44	ASN
12	K	65	HIS
12	K	76	GLN
12	K	104	ASN
12	K	112	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	12/18 (66%)	4 (33%)	0

All (4) RNA backbone outliers are listed below:



Mol	Chain	Res	Type
1	R	6	C
1	R	7	U
1	R	13	G
1	R	17	U

There are no RNA pucker outliers to report.

## 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 [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	R	14/18 (77%)	0.81	2 (14%) 4 4	128, 147, 176, 188	0
2	A	1422/1733 (82%)	-0.37	2 (0%) 95 95	57, 116, 171, 200	0
3	B	1112/1224 (90%)	-0.33	4 (0%) 93 90	61, 126, 184, 200	0
4	C	267/318 (83%)	-0.39	0 100 100	73, 111, 159, 176	0
5	D	178/221 (80%)	-0.32	0 100 100	88, 133, 179, 192	0
6	E	214/215 (99%)	-0.34	0 100 100	93, 154, 191, 199	0
7	F	88/155 (56%)	-0.52	0 100 100	61, 93, 130, 153	0
8	G	171/171 (100%)	-0.38	0 100 100	88, 116, 155, 163	0
9	H	135/146 (92%)	0.18	3 (2%) 65 54	131, 161, 187, 196	0
10	I	116/122 (95%)	-0.16	0 100 100	110, 161, 191, 196	0
11	J	65/70 (92%)	-0.50	0 100 100	79, 109, 145, 149	0
12	K	112/120 (93%)	-0.42	0 100 100	76, 115, 140, 158	0
13	L	46/70 (65%)	0.07	1 (2%) 65 54	107, 170, 191, 193	0
All	All	3940/4583 (85%)	-0.33	12 (0%) 94 92	57, 122, 182, 200	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	471	LYS	3.5
2	A	1455	PRO	3.0
2	A	171	GLN	2.4
9	H	140	ALA	2.3
9	H	136	LYS	2.2
9	H	134	ASN	2.2
3	B	132	VAL	2.2
3	B	882	THR	2.1
1	R	7	U	2.1

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Mol	Chain	Res	Type	RSRZ
3	B	340	ALA	2.0
13	L	27	LEU	2.0
1	R	12	C	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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
14	ZN	I	203	1/1	0.99	0.18	0.49	113,113,113,113	0
14	ZN	B	1307	1/1	0.99	0.20	-0.31	78,78,78,78	0
14	ZN	J	101	1/1	0.99	0.24	-0.50	86,86,86,86	0
14	ZN	C	302	1/1	0.99	0.13	-0.80	71,71,71,71	0
14	ZN	A	1508	1/1	0.99	0.14	-1.22	79,79,79,79	0
14	ZN	I	204	1/1	0.89	0.04	-1.84	190,190,190,190	0
14	ZN	A	1506	1/1	0.97	0.07	-4.52	119,119,119,119	0
15	MG	A	1	1/1	0.97	0.14	-	68,68,68,68	0
14	ZN	L	105	1/1	0.96	0.06	-	156,156,156,156	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.