



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 07:03 PM EST

PDB ID : 4QIW  
Title : Crystal structure of euryarchaeal RNA polymerase from *Thermococcus kodakarensis*  
Authors : Jun, S.-H.; Murakami, K.S.  
Deposited on : 2014-06-02  
Resolution : 3.50 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

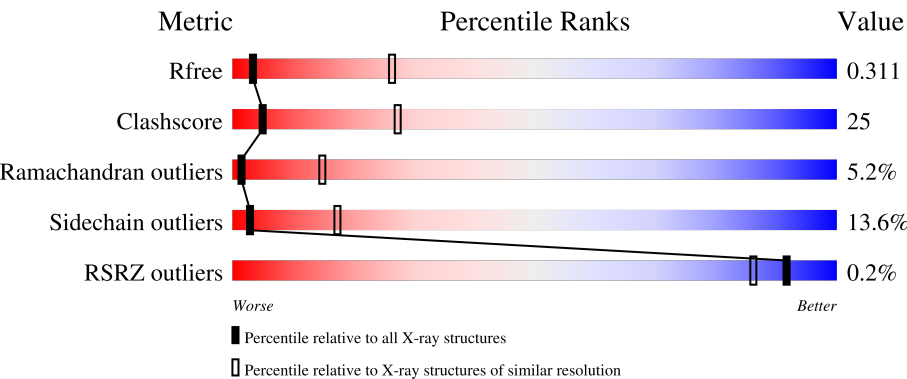
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
$R_{free}$	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	906	<div><div>52%</div><div>35%</div><div>7%</div><div>• 5%</div></div>
1	I	906	<div><div>50%</div><div>36%</div><div>8%</div><div>• 5%</div></div>
2	B	1123	<div><div>48%</div><div>37%</div><div>9%</div><div>• 5%</div></div>
2	J	1123	<div><div>47%</div><div>39%</div><div>9%</div><div>• 5%</div></div>
3	C	391	<div><div>39%</div><div>41%</div><div>13%</div><div>• 6%</div></div>
3	M	391	<div><div>38%</div><div>43%</div><div>12%</div><div>• 6%</div></div>

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Mol	Chain	Length	Quality of chain
4	D	259	
4	O	259	
5	E	190	
5	Q	190	
6	F	122	
6	R	122	
7	H	82	
7	S	82	
8	K	57	
8	T	57	
9	L	100	
9	U	100	
10	N	65	
10	V	65	
11	P	49	
11	W	49	

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 51069 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	863	Total	C	N	O	S	0	0	0
			6891	4357	1221	1275	38			
1	I	862	Total	C	N	O	S	0	0	0
			6875	4347	1220	1270	38			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1069	Total	C	N	O	S	0	0	0
			8536	5396	1520	1584	36			
2	J	1069	Total	C	N	O	S	0	0	0
			8536	5396	1520	1584	36			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit A''.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	369	Total	C	N	O	S	0	0	0
			2882	1819	498	555	10			
3	M	369	Total	C	N	O	S	0	0	0
			2879	1816	498	555	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	258	Total	C	N	O	S	0	0	0
			2066	1330	341	390	5			
4	O	258	Total	C	N	O	S	0	0	0
			2066	1330	341	390	5			

- Molecule 5 is a protein called DNA-directed RNA polymerase, subunit E'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	181	Total	C	N	O	S	0	0	0
			1465	939	250	267	9			
5	Q	181	Total	C	N	O	S	0	0	0
			1465	939	250	267	9			

- Molecule 6 is a protein called DNA-directed RNA polymerase, subunit F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	122	Total	C	N	O	S	0	0	0
			1020	654	169	193	4			
6	R	122	Total	C	N	O	S	0	0	0
			1020	654	169	193	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	115	ILE	-	expression tag	UNP Q5JI52
F	116	ASP	-	expression tag	UNP Q5JI52
F	117	GLU	-	expression tag	UNP Q5JI52
F	118	TYR	-	expression tag	UNP Q5JI52
F	119	ARG	-	expression tag	UNP Q5JI52
F	120	PRO	-	expression tag	UNP Q5JI52
F	121	LEU	-	expression tag	UNP Q5JI52
F	122	GLU	-	expression tag	UNP Q5JI52
R	115	ILE	-	expression tag	UNP Q5JI52
R	116	ASP	-	expression tag	UNP Q5JI52
R	117	GLU	-	expression tag	UNP Q5JI52
R	118	TYR	-	expression tag	UNP Q5JI52
R	119	ARG	-	expression tag	UNP Q5JI52
R	120	PRO	-	expression tag	UNP Q5JI52
R	121	LEU	-	expression tag	UNP Q5JI52
R	122	GLU	-	expression tag	UNP Q5JI52

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit H.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	H	76	Total	C	N	O	0	0	0
			627	408	105	114			
7	S	76	Total	C	N	O	0	0	0
			627	408	105	114			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	K	56	Total 433	C 284	N 75	O 73	S 1	0	0	0
8	T	56	Total 433	C 284	N 75	O 73	S 1	0	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	L	94	Total 775	C 493	N 134	O 146	S 2	0	0	0
9	U	94	Total 775	C 493	N 134	O 146	S 2	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	95	HIS	-	expression tag	UNP Q5JE88
L	96	HIS	-	expression tag	UNP Q5JE88
L	97	HIS	-	expression tag	UNP Q5JE88
L	98	HIS	-	expression tag	UNP Q5JE88
L	99	HIS	-	expression tag	UNP Q5JE88
L	100	HIS	-	expression tag	UNP Q5JE88
U	95	HIS	-	expression tag	UNP Q5JE88
U	96	HIS	-	expression tag	UNP Q5JE88
U	97	HIS	-	expression tag	UNP Q5JE88
U	98	HIS	-	expression tag	UNP Q5JE88
U	99	HIS	-	expression tag	UNP Q5JE88
U	100	HIS	-	expression tag	UNP Q5JE88

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	N	63	Total 510	C 326	N 87	O 91	S 6	0	0	0
10	V	63	Total 510	C 326	N 87	O 91	S 6	0	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	P	42	Total 329	C 206	N 65	O 54	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	W	42	Total	C	N	O	S	0	0	0
			329	206	65	54	4			

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	2	Total	Mg	0	0
			2	2		
12	I	2	Total	Mg	0	0
			2	2		

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	2	Total	Zn	0	0
			2	2		
13	B	1	Total	Zn	0	0
			1	1		
13	N	1	Total	Zn	0	0
			1	1		
13	P	1	Total	Zn	0	0
			1	1		
13	I	2	Total	Zn	0	0
			2	2		
13	J	1	Total	Zn	0	0
			1	1		
13	V	1	Total	Zn	0	0
			1	1		
13	W	1	Total	Zn	0	0
			1	1		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	O	0	0
			1	1		
14	B	1	Total	O	0	0
			1	1		
14	C	1	Total	O	0	0
			1	1		
14	I	1	Total	O	0	0
			1	1		

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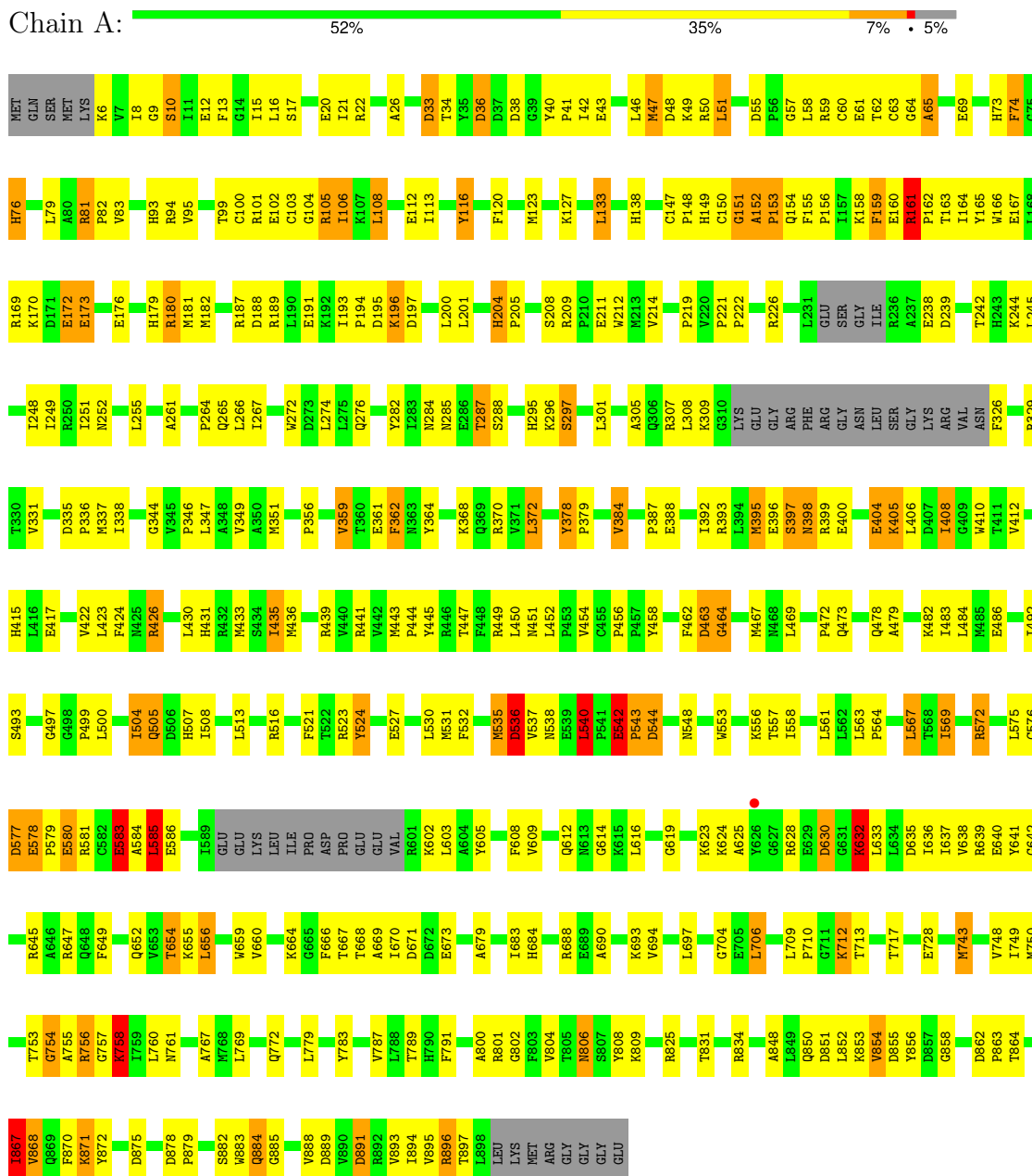
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	J	1	Total	O	0	0
			1	1		
14	M	1	Total	O	0	0
			1	1		



### 3 Residue-property plots

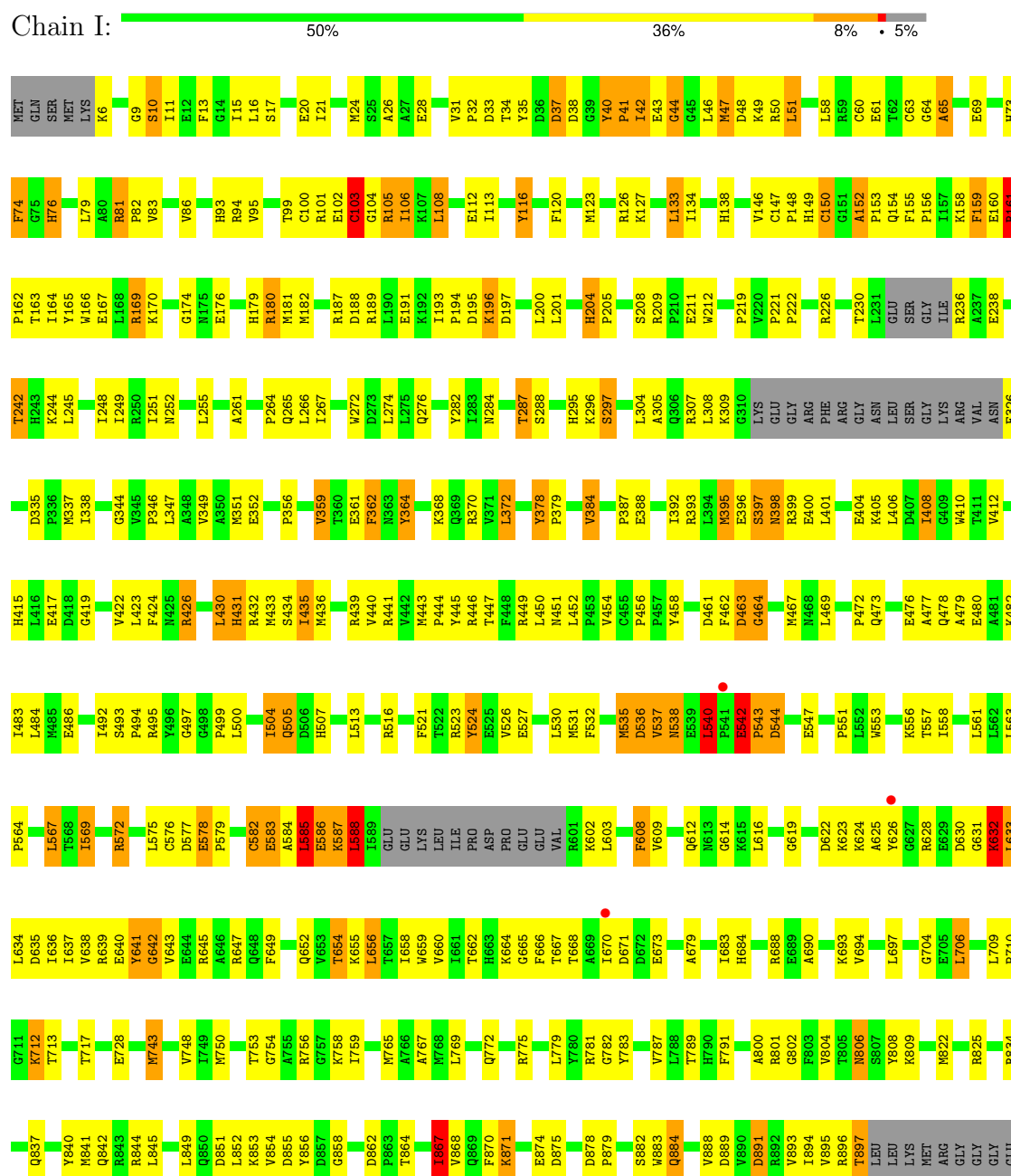
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: DNA-directed RNA polymerase



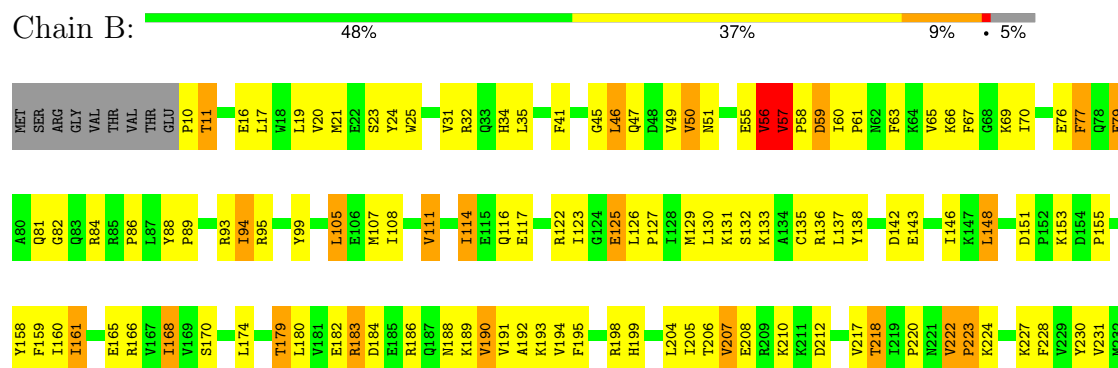
- Molecule 1: DNA-directed RNA polymerase

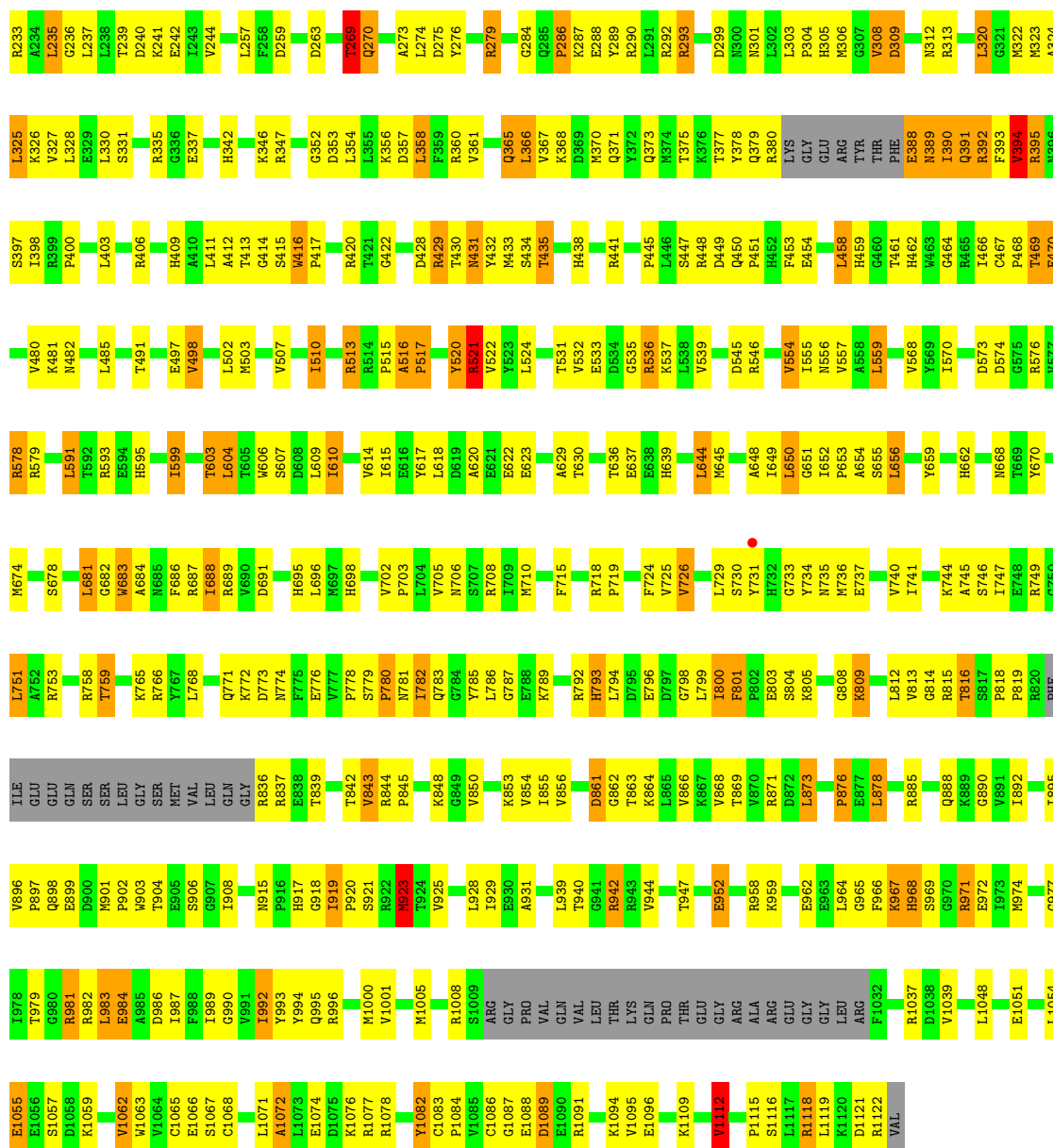
## Chain I:



- Molecule 2: DNA-directed RNA polymerase

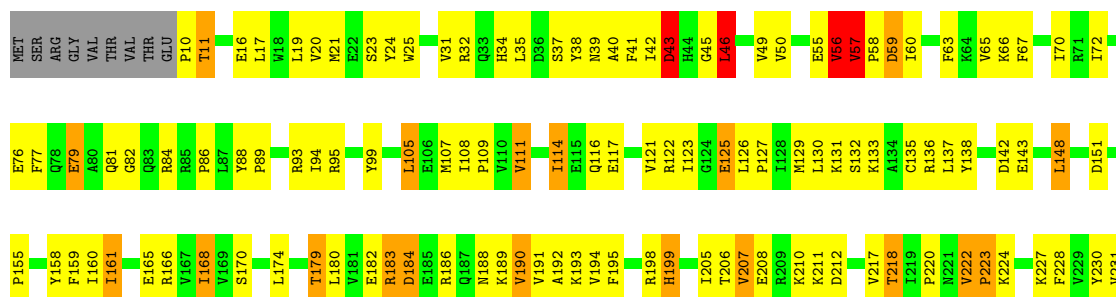
## Chain B:



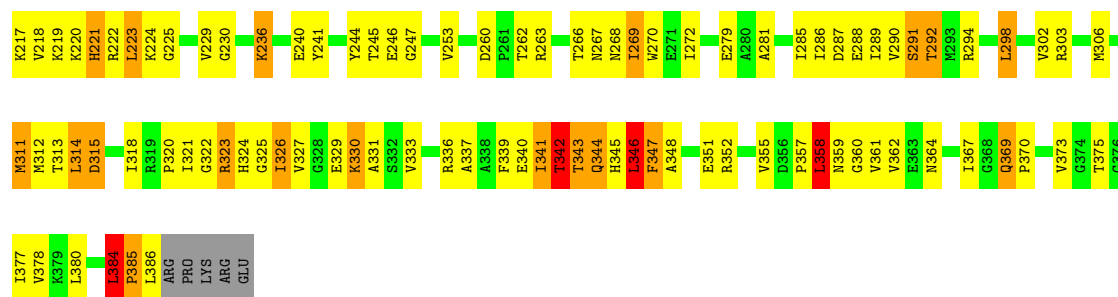


## • Molecule 2: DNA-directed RNA polymerase

Chain J:  47% 39% 9% • 5%

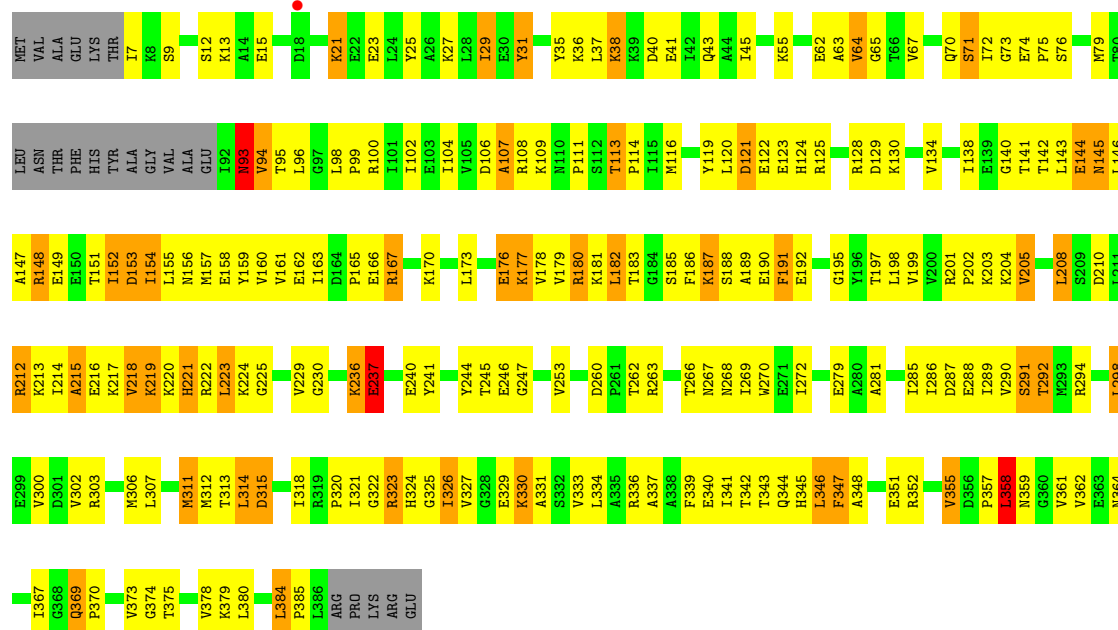






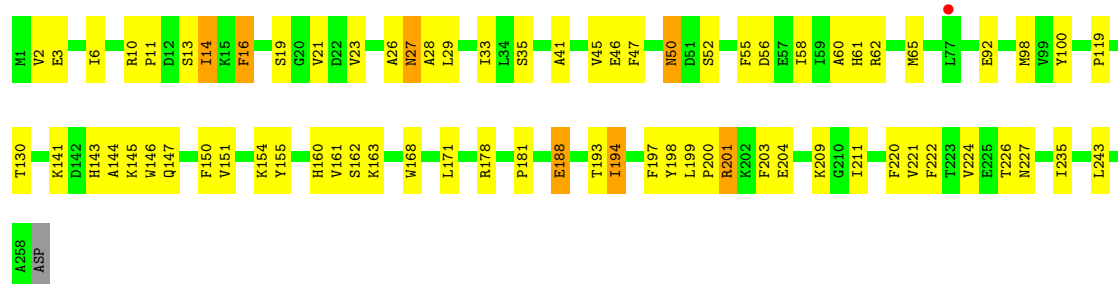
• Molecule 3: DNA-directed RNA polymerase subunit A"

Chain M: 38% 43% 12% 6%



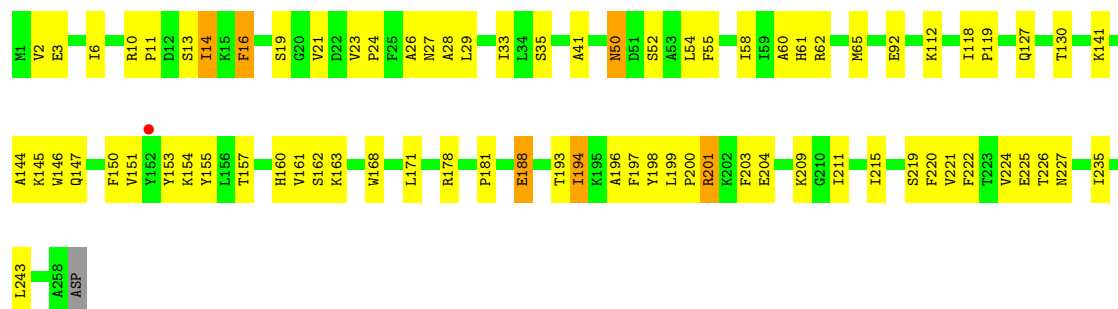
• Molecule 4: DNA-directed RNA polymerase subunit D

Chain D: 71% 25% 4%



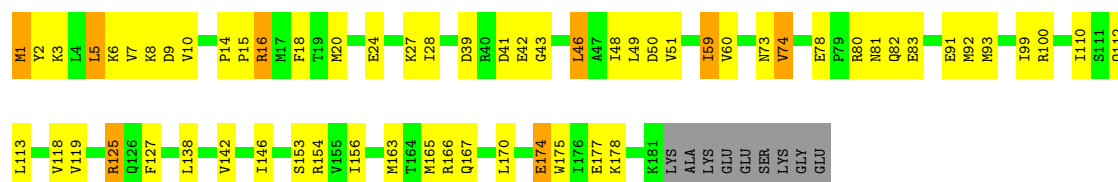
• Molecule 4: DNA-directed RNA polymerase subunit D

Chain O: 70% 27% 3%



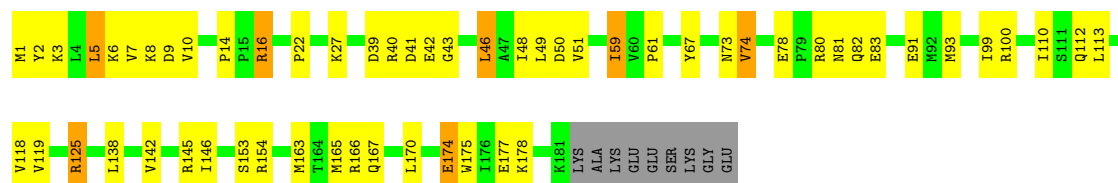
- Molecule 5: DNA-directed RNA polymerase, subunit E'

Chain E': 63% 28% 5%



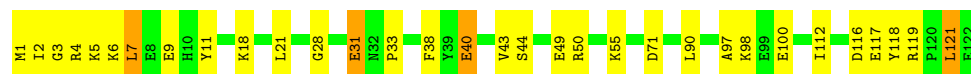
- Molecule 5: DNA-directed RNA polymerase, subunit E'

Chain Q: 65% 27% 5%



- Molecule 6: DNA-directed RNA polymerase, subunit F

Chain F: 74% 23% 5%



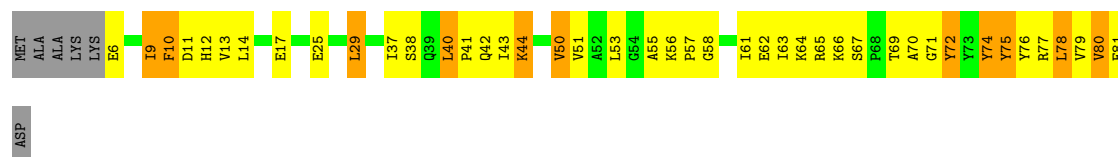
- Molecule 6: DNA-directed RNA polymerase, subunit F

Chain R: 72% 26% 5%

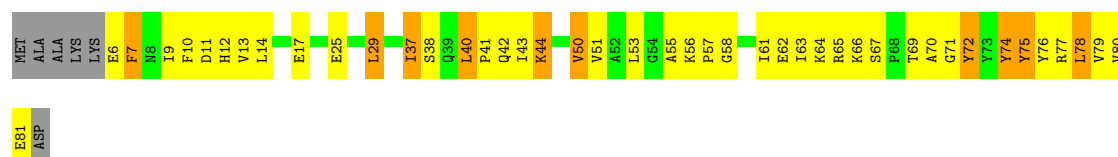


- Molecule 7: DNA-directed RNA polymerase subunit H

Chain H: 40% 39% 13% 7%



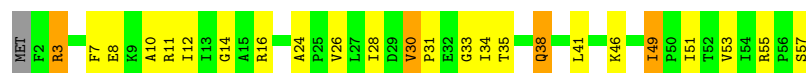
- Molecule 7: DNA-directed RNA polymerase subunit H



- Molecule 8: DNA-directed RNA polymerase subunit K



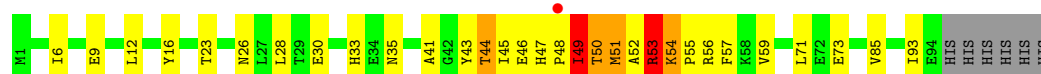
- Molecule 8: DNA-directed RNA polymerase subunit K



- Molecule 9: DNA-directed RNA polymerase subunit L



- Molecule 9: DNA-directed RNA polymerase subunit L



- Molecule 10: DNA-directed RNA polymerase subunit N



- Molecule 10: DNA-directed RNA polymerase subunit N

Chain V:  54% 34% 9% .



- Molecule 11: DNA-directed RNA polymerase subunit P

Chain P:  31% 51% . . 14%



- Molecule 11: DNA-directed RNA polymerase subunit P

Chain W:  41% 37% 6% . 14%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.97Å 206.61Å 365.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 3.50 49.73 – 3.50	Depositor EDS
% Data completeness (in resolution range)	96.3 (49.73-3.50) 95.1 (49.73-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, $R_{free}$	0.277 , 0.316 0.278 , 0.311	Depositor DCC
$R_{free}$ test set	5249 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	88.2	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 178.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	51069	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A	0.26	0/7028	0.50	1/9489 (0.0%)
1	I	0.29	2/7011 (0.0%)	0.52	1/9465 (0.0%)
2	B	0.29	1/8706 (0.0%)	0.53	3/11765 (0.0%)
2	J	0.28	1/8706 (0.0%)	0.52	3/11765 (0.0%)
3	C	0.27	0/2917	0.55	2/3936 (0.1%)
3	M	0.26	0/2914	0.53	1/3932 (0.0%)
4	D	0.27	0/2111	0.43	0/2858
4	O	0.28	0/2111	0.43	0/2858
5	E	0.23	0/1491	0.44	0/2008
5	Q	0.22	0/1491	0.43	0/2008
6	F	0.22	0/1040	0.40	0/1399
6	R	0.22	0/1040	0.40	0/1399
7	H	0.61	4/641 (0.6%)	0.57	0/866
7	S	0.60	4/641 (0.6%)	0.56	0/866
8	K	0.26	0/441	0.52	0/598
8	T	0.26	0/441	0.53	0/598
9	L	0.39	0/790	0.51	1/1066 (0.1%)
9	U	0.41	0/790	0.56	2/1066 (0.2%)
10	N	0.26	0/518	0.57	0/695
10	V	0.27	0/518	0.58	0/695
11	P	0.27	0/333	0.60	0/445
11	W	0.27	0/333	0.56	0/445
All	All	0.29	12/52012 (0.0%)	0.51	14/70222 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	4
2	J	0	1
All	All	0	6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	72	TYR	CE2-CZ	7.29	1.48	1.38
7	H	72	TYR	CE1-CZ	7.14	1.47	1.38
7	S	72	TYR	CE2-CZ	7.13	1.47	1.38
7	S	72	TYR	CG-CD1	7.11	1.48	1.39
1	I	150	CYS	CB-SG	-7.05	1.70	1.82
7	H	72	TYR	CG-CD1	6.68	1.47	1.39
7	H	72	TYR	CG-CD2	6.64	1.47	1.39
7	S	72	TYR	CG-CD2	6.42	1.47	1.39
7	S	72	TYR	CE1-CZ	6.42	1.46	1.38
2	B	1086	CYS	CB-SG	-5.84	1.72	1.81
1	I	103	CYS	CB-SG	-5.64	1.72	1.81
2	J	1086	CYS	CB-SG	5.41	1.91	1.82

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	125	GLU	CA-CB-CG	7.21	129.26	113.40
3	C	164	ASP	C-N-CD	-6.97	105.27	120.60
1	I	150	CYS	CB-CA-C	-6.86	96.68	110.40
2	J	57	VAL	C-N-CD	-6.80	105.63	120.60
2	B	57	VAL	C-N-CD	-6.70	105.86	120.60
9	U	47	HIS	C-N-CD	6.07	141.14	128.40
9	L	47	HIS	C-N-CD	6.06	141.13	128.40
9	U	54	LYS	C-N-CD	6.03	141.06	128.40
2	J	952	GLU	CA-CB-CG	5.80	126.16	113.40
3	C	314	LEU	CA-CB-CG	5.79	128.62	115.30
3	M	314	LEU	CA-CB-CG	5.78	128.59	115.30
1	A	642	GLY	N-CA-C	5.65	127.23	113.10
2	J	125	GLU	CA-CB-CG	5.63	125.80	113.40
2	B	923	MET	CG-SD-CE	5.12	108.40	100.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	536	ASP	Peptide
1	I	582	CYS	Peptide
1	I	632	LYS	Peptide
1	I	641	TYR	Peptide
1	I	642	GLY	Peptide
2	J	513	ARG	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6891	0	6945	310	0
1	I	6875	0	6927	382	1
2	B	8536	0	8585	463	10
2	J	8536	0	8583	578	0
3	C	2882	0	2982	305	0
3	M	2879	0	2973	247	0
4	D	2066	0	2080	59	0
4	O	2066	0	2080	66	0
5	E	1465	0	1503	74	2
5	Q	1465	0	1503	68	3
6	F	1020	0	1024	41	12
6	R	1020	0	1024	48	7
7	H	627	0	642	29	0
7	S	627	0	642	34	0
8	K	433	0	466	16	0
8	T	433	0	466	19	0
9	L	775	0	770	51	0
9	U	775	0	770	67	0
10	N	510	0	523	43	0
10	V	510	0	523	26	0
11	P	329	0	356	27	5
11	W	329	0	355	15	0
12	A	2	0	0	0	0
12	I	2	0	0	0	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	N	1	0	0	0	0
13	P	1	0	0	1	0
13	V	1	0	0	0	0
13	W	1	0	0	0	0
14	A	1	0	0	0	0
14	B	1	0	0	1	0
14	C	1	0	0	0	0
14	I	1	0	0	2	0
14	J	1	0	0	0	0
14	M	1	0	0	3	0
All	All	51069	0	51722	2518	20

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 25.

All (2518) 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)
2:B:378:TYR:CE1	2:B:388:GLU:CA	1.79	1.63
1:I:444:PRO:CG	9:U:50:THR:HG23	1.32	1.58
1:I:444:PRO:HG3	9:U:50:THR:CG2	1.09	1.56
2:J:378:TYR:CE1	2:J:388:GLU:HG3	1.38	1.56
3:C:194:GLU:HB2	3:C:196:TYR:CE2	1.41	1.55
2:J:394:VAL:HB	2:J:395:ARG:CG	1.08	1.54
3:C:161:VAL:CG2	3:C:199:VAL:HG23	1.06	1.53
3:M:148:ARG:CZ	3:M:162:GLU:HB2	1.39	1.51
2:B:378:TYR:CE1	2:B:388:GLU:N	1.69	1.48
2:J:107:MET:HB3	2:J:395:ARG:NH2	1.17	1.47
3:C:161:VAL:CG2	3:C:199:VAL:CG2	1.89	1.46
3:C:161:VAL:HG21	3:C:199:VAL:CG2	1.44	1.45
3:C:162:GLU:CA	3:C:196:TYR:HB2	1.45	1.44
1:I:6:LYS:HE3	2:J:1122:ARG:NH2	1.30	1.44
2:J:378:TYR:HH	2:J:388:GLU:N	0.95	1.43
2:B:378:TYR:CE1	2:B:388:GLU:HA	1.35	1.43
2:B:389:ASN:ND2	2:B:392:ARG:HD3	1.37	1.40
1:I:6:LYS:CE	2:J:1122:ARG:HH22	1.35	1.38
2:J:394:VAL:CB	2:J:395:ARG:HG3	1.54	1.38
1:I:666:PHE:H	2:J:729:LEU:CD1	1.37	1.37
2:J:63:PHE:HZ	2:J:388:GLU:CD	1.28	1.35
3:M:148:ARG:NH2	3:M:162:GLU:CB	1.86	1.35
3:M:148:ARG:NH2	3:M:162:GLU:HB2	1.05	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:394:VAL:CB	2:J:395:ARG:CG	2.05	1.33
2:J:63:PHE:CZ	2:J:388:GLU:CD	2.03	1.30
2:J:107:MET:CB	2:J:395:ARG:NH2	1.95	1.28
1:I:445:TYR:CE2	9:U:49:ILE:CG2	2.17	1.28
2:J:39:ASN:O	2:J:43:ASP:OD1	1.53	1.27
1:I:147:CYS:SG	1:I:152:ALA:HB2	1.73	1.27
2:J:1086:CYS:SG	2:J:1090:GLU:OE1	1.92	1.26
2:B:389:ASN:HD21	2:B:392:ARG:CD	1.48	1.26
2:B:378:TYR:CZ	2:B:388:GLU:HA	1.71	1.24
2:B:378:TYR:CD1	2:B:388:GLU:N	2.05	1.23
1:I:461:ASP:OD2	14:I:1201:HOH:O	1.55	1.23
2:J:107:MET:CB	2:J:395:ARG:CZ	2.08	1.21
2:J:378:TYR:OH	2:J:388:GLU:N	1.67	1.21
3:C:148:ARG:NE	3:C:163:ILE:HG12	1.56	1.20
3:M:165:PRO:HB3	3:M:195:GLY:CA	1.71	1.20
3:C:162:GLU:C	3:C:196:TYR:HB2	1.61	1.20
3:C:161:VAL:HG23	3:C:199:VAL:N	1.56	1.19
5:Q:9:ASP:OD2	6:R:3:GLY:HA2	1.40	1.19
2:J:63:PHE:HZ	2:J:388:GLU:CG	1.56	1.18
2:J:378:TYR:HE1	2:J:388:GLU:CA	1.56	1.18
3:C:148:ARG:HD2	3:C:163:ILE:CG1	1.70	1.18
1:I:100:CYS:SG	1:I:155:PHE:HZ	1.64	1.18
2:J:378:TYR:CE1	2:J:388:GLU:CG	2.26	1.18
2:J:378:TYR:CZ	2:J:388:GLU:N	2.11	1.18
5:E:92:MET:CE	5:E:127:PHE:CD2	2.28	1.17
1:A:100:CYS:SG	1:A:155:PHE:HZ	1.68	1.16
1:I:445:TYR:CE2	9:U:49:ILE:HG21	1.78	1.15
1:I:666:PHE:H	2:J:729:LEU:HD11	1.11	1.15
2:J:389:ASN:HA	2:J:390:ILE:HG23	1.16	1.14
1:I:445:TYR:CD2	9:U:49:ILE:HG21	1.83	1.13
5:E:1:MET:HE3	6:F:11:TYR:CD1	1.84	1.12
3:C:162:GLU:HA	3:C:196:TYR:HB2	1.21	1.11
1:I:666:PHE:N	2:J:729:LEU:CD1	2.11	1.11
2:B:389:ASN:ND2	2:B:392:ARG:CD	2.11	1.11
9:L:49:ILE:HD12	9:L:50:THR:H	1.11	1.11
1:A:666:PHE:O	2:B:729:LEU:HD13	1.51	1.10
5:E:9:ASP:OD2	6:F:3:GLY:HA2	1.51	1.10
1:A:666:PHE:O	2:B:729:LEU:CD1	1.98	1.10
1:I:445:TYR:CE2	9:U:49:ILE:HG23	1.86	1.09
2:J:378:TYR:CE1	2:J:388:GLU:CA	2.35	1.09
1:I:100:CYS:SG	1:I:155:PHE:CZ	2.45	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:444:PRO:HG3	9:U:50:THR:HG22	1.29	1.09
2:J:378:TYR:HE1	2:J:388:GLU:HA	1.16	1.08
2:J:107:MET:CB	2:J:395:ARG:HH22	1.58	1.08
2:J:1122:ARG:HG3	6:R:4:ARG:HH21	1.15	1.08
3:C:148:ARG:CD	3:C:163:ILE:CG1	2.31	1.07
3:C:194:GLU:CB	3:C:196:TYR:CE2	2.36	1.07
11:P:14:GLU:HG2	11:P:30:CYS:SG	1.94	1.07
1:A:150:CYS:O	1:A:152:ALA:N	1.86	1.07
2:B:378:TYR:CZ	2:B:388:GLU:CA	2.32	1.07
1:I:444:PRO:HG2	9:U:49:ILE:HB	1.31	1.07
5:Q:1:MET:HE3	6:R:11:TYR:CD1	1.90	1.07
2:J:1122:ARG:CD	5:Q:10:VAL:HG11	1.85	1.07
3:C:152:ILE:HG12	3:C:153:ASP:H	1.19	1.06
2:J:107:MET:HB3	2:J:395:ARG:CZ	1.61	1.06
1:I:666:PHE:N	2:J:729:LEU:HD11	1.67	1.06
2:J:391:GLN:O	2:J:392:ARG:HG3	1.55	1.06
2:B:393:PHE:O	2:B:394:VAL:HB	1.49	1.06
1:I:665:GLY:HA2	2:J:729:LEU:HD11	1.32	1.06
3:M:148:ARG:CZ	3:M:162:GLU:CB	2.24	1.05
2:J:1083:CYS:SG	2:J:1086:CYS:HB2	1.96	1.05
2:J:107:MET:HB2	2:J:395:ARG:CZ	1.86	1.05
1:I:6:LYS:HE3	2:J:1122:ARG:CZ	1.86	1.04
2:J:1122:ARG:CG	6:R:4:ARG:HH21	1.70	1.04
3:M:165:PRO:HB3	3:M:195:GLY:HA3	1.06	1.04
3:C:162:GLU:HA	3:C:196:TYR:CB	1.85	1.04
5:E:92:MET:CE	5:E:127:PHE:CE2	2.40	1.04
2:J:378:TYR:CE1	2:J:388:GLU:N	2.25	1.04
2:B:390:ILE:HD12	2:B:391:GLN:H	1.18	1.04
1:I:444:PRO:CG	9:U:50:THR:CG2	2.04	1.04
3:C:162:GLU:CA	3:C:196:TYR:CB	2.36	1.03
1:A:100:CYS:SG	1:A:155:PHE:CZ	2.51	1.03
1:A:758:LYS:O	1:A:761:ASN:OD1	1.76	1.03
2:J:38:TYR:O	2:J:41:PHE:HB3	1.59	1.03
5:E:92:MET:HE1	5:E:127:PHE:CD2	1.92	1.02
2:J:394:VAL:HB	2:J:395:ARG:HG2	1.08	1.02
1:I:103:CYS:SG	1:I:105:ARG:N	2.32	1.02
3:C:161:VAL:HG12	3:C:162:GLU:H	1.22	1.01
2:B:378:TYR:HE1	2:B:388:GLU:CA	1.35	1.01
1:A:531:MET:HB2	9:L:44:THR:CG2	1.91	1.01
11:P:14:GLU:CG	11:P:30:CYS:SG	2.49	1.01
3:M:151:THR:HG22	3:M:152:ILE:H	1.26	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:100:CYS:HB3	1:I:103:CYS:HB3	1.42	1.00
1:I:445:TYR:CZ	9:U:49:ILE:CG2	2.43	1.00
3:C:152:ILE:HG13	3:C:159:TYR:CE2	1.95	1.00
2:J:389:ASN:HA	2:J:390:ILE:CG2	1.92	1.00
2:J:393:PHE:O	2:J:394:VAL:HG22	1.60	0.99
2:B:729:LEU:HD23	2:B:731:TYR:HE1	1.21	0.99
2:B:744:LYS:NZ	9:L:53:ARG:NH2	2.09	0.99
3:C:162:GLU:C	3:C:196:TYR:CB	2.30	0.99
1:I:665:GLY:HA2	2:J:729:LEU:CD1	1.92	0.99
3:C:148:ARG:HD2	3:C:163:ILE:CB	1.91	0.99
1:I:6:LYS:HE2	2:J:1122:ARG:HH12	1.28	0.99
5:E:92:MET:HE3	5:E:127:PHE:CE2	1.96	0.98
2:B:389:ASN:HD21	2:B:392:ARG:HD3	0.84	0.98
3:C:194:GLU:HB2	3:C:196:TYR:CD2	1.98	0.98
3:C:148:ARG:HG2	3:C:149:GLU:HG3	1.41	0.98
3:C:161:VAL:HG22	3:C:199:VAL:CG2	1.92	0.98
5:Q:1:MET:HE3	6:R:11:TYR:HD1	1.21	0.97
11:W:27:CYS:HB3	11:W:30:CYS:SG	2.04	0.97
2:B:391:GLN:O	2:B:393:PHE:N	1.96	0.97
9:U:51:MET:HG2	9:U:53:ARG:HB2	1.46	0.97
2:B:744:LYS:HZ3	9:L:53:ARG:NH2	1.63	0.97
2:J:1122:ARG:HD3	5:Q:10:VAL:HG11	1.43	0.97
1:A:749:ILE:O	1:A:753:THR:HG22	1.65	0.97
2:J:394:VAL:CB	2:J:395:ARG:HG2	1.79	0.97
3:C:162:GLU:HG2	3:C:196:TYR:CD1	1.99	0.96
1:I:147:CYS:SG	1:I:152:ALA:CB	2.53	0.96
1:A:10:SER:HA	3:C:358:LEU:HD21	1.46	0.96
11:P:14:GLU:CD	11:P:30:CYS:SG	2.44	0.96
5:E:3:LYS:NZ	6:F:9:GLU:OE1	1.98	0.96
1:A:753:THR:HG23	1:A:754:GLY:H	1.26	0.96
2:J:378:TYR:CE1	2:J:388:GLU:HA	1.99	0.96
2:J:42:ILE:CG2	2:J:72:ILE:HD13	1.96	0.95
2:J:979:THR:HA	9:U:26:ASN:HD21	1.31	0.95
3:C:148:ARG:NH2	3:C:149:GLU:O	2.00	0.95
3:C:148:ARG:CD	3:C:163:ILE:HG12	1.94	0.95
2:B:744:LYS:HZ3	9:L:53:ARG:HH22	0.99	0.95
9:U:51:MET:HG2	9:U:53:ARG:CB	1.96	0.95
2:J:42:ILE:CG2	2:J:72:ILE:CD1	2.44	0.94
1:I:461:ASP:CG	14:I:1201:HOH:O	1.97	0.94
3:M:165:PRO:CB	3:M:195:GLY:HA3	1.96	0.94
5:Q:3:LYS:NZ	6:R:9:GLU:OE1	2.00	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:ARG:HB2	2:B:186:ARG:HH22	1.33	0.94
5:E:1:MET:HE1	6:F:11:TYR:HE1	1.29	0.94
1:I:665:GLY:CA	2:J:729:LEU:HD11	1.95	0.94
3:M:148:ARG:HH22	3:M:162:GLU:HB2	1.15	0.93
2:J:183:ARG:HB3	2:J:186:ARG:HH22	1.31	0.93
2:J:63:PHE:CZ	2:J:388:GLU:CG	2.46	0.93
2:B:510:ILE:HG22	2:B:513:ARG:HE	1.33	0.93
2:B:1063:TRP:NE1	2:B:1094:LYS:HE3	1.84	0.93
3:M:148:ARG:NH2	3:M:162:GLU:CG	2.31	0.92
2:B:378:TYR:CZ	2:B:388:GLU:N	2.37	0.92
5:Q:1:MET:CE	6:R:11:TYR:CD1	2.50	0.92
5:Q:9:ASP:OD2	6:R:3:GLY:CA	2.17	0.92
2:B:389:ASN:ND2	2:B:392:ARG:HB2	1.83	0.92
5:E:1:MET:HE3	6:F:11:TYR:HD1	1.25	0.92
3:C:148:ARG:NE	3:C:163:ILE:CG1	2.30	0.92
2:J:378:TYR:CZ	2:J:388:GLU:HG3	2.04	0.92
2:B:1063:TRP:CZ3	2:B:1074:GLU:CG	2.53	0.92
5:E:1:MET:CE	6:F:11:TYR:CE1	2.53	0.92
2:J:57:VAL:HG21	2:J:371:GLN:HA	1.52	0.92
3:C:161:VAL:HG23	3:C:199:VAL:HG23	1.47	0.91
5:E:1:MET:CE	6:F:11:TYR:CD1	2.52	0.91
3:C:194:GLU:CB	3:C:196:TYR:HE2	1.80	0.91
3:M:152:ILE:CG2	3:M:159:TYR:HA	2.01	0.91
2:B:57:VAL:HG21	2:B:371:GLN:HA	1.52	0.91
2:J:391:GLN:O	2:J:392:ARG:CG	2.19	0.91
1:I:6:LYS:CE	2:J:1122:ARG:HH12	1.84	0.91
1:A:531:MET:CB	9:L:44:THR:CG2	2.47	0.90
2:B:729:LEU:HD23	2:B:731:TYR:CE1	2.06	0.90
3:C:163:ILE:N	3:C:196:TYR:CB	2.35	0.90
3:C:161:VAL:CG2	3:C:199:VAL:CB	2.48	0.90
2:B:1063:TRP:CE2	2:B:1094:LYS:HE3	2.07	0.90
3:C:163:ILE:HD13	3:C:163:ILE:H	1.34	0.90
2:J:1086:CYS:SG	2:J:1090:GLU:CG	2.60	0.90
1:I:13:PHE:HE2	3:M:333:VAL:HG21	1.36	0.89
3:C:211:LEU:HA	3:C:214:ILE:CD1	2.02	0.89
1:I:40:TYR:H	1:I:41:PRO:HD3	1.37	0.89
5:E:1:MET:HE1	6:F:11:TYR:CE1	2.07	0.89
1:I:6:LYS:HE3	2:J:1122:ARG:HH22	0.75	0.89
2:J:116:GLN:CD	2:J:393:PHE:HD1	1.76	0.89
2:B:394:VAL:HG22	2:B:395:ARG:HG3	1.54	0.89
1:I:443:MET:HB3	9:U:49:ILE:HD12	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:393:PHE:O	2:J:394:VAL:CG2	2.20	0.89
3:C:148:ARG:HD2	3:C:163:ILE:HB	1.54	0.88
2:J:206:THR:HG1	2:J:218:THR:HG1	1.22	0.88
2:B:1063:TRP:CD1	2:B:1094:LYS:HG3	2.09	0.88
1:I:103:CYS:N	1:I:150:CYS:SG	2.47	0.88
3:M:21:LYS:HD3	7:S:71:GLY:HA3	1.54	0.88
3:C:216:GLU:O	3:C:220:LYS:HB3	1.72	0.88
11:P:30:CYS:SG	13:P:1501:ZN:ZN	1.62	0.88
2:J:1086:CYS:SG	2:J:1090:GLU:HG3	2.13	0.88
9:U:49:ILE:O	9:U:50:THR:OG1	1.92	0.88
2:J:63:PHE:CZ	2:J:388:GLU:OE1	2.27	0.88
2:J:41:PHE:O	2:J:45:GLY:O	1.92	0.87
2:B:391:GLN:OE1	2:B:393:PHE:CD2	2.27	0.87
3:C:163:ILE:N	3:C:196:TYR:HB2	1.89	0.87
1:I:126:ARG:NH2	7:S:40:LEU:O	2.07	0.87
5:Q:1:MET:CE	6:R:11:TYR:HD1	1.87	0.87
1:I:444:PRO:O	9:U:49:ILE:HD13	1.74	0.87
9:L:49:ILE:HD12	9:L:50:THR:N	1.90	0.87
9:L:92:ALA:O	9:L:94:GLU:N	2.06	0.87
3:M:182:LEU:HD23	3:M:185:SER:CB	2.05	0.87
3:C:148:ARG:CD	3:C:163:ILE:HG13	2.05	0.87
2:B:389:ASN:CG	2:B:392:ARG:HD3	1.95	0.86
3:C:163:ILE:HB	3:C:164:ASP:HA	1.56	0.86
10:N:62:TYR:O	10:N:63:LYS:NZ	2.09	0.86
2:B:1063:TRP:CZ3	2:B:1074:GLU:HG3	2.09	0.86
1:I:531:MET:HB2	9:U:44:THR:HG23	1.56	0.86
5:Q:7:VAL:HG13	6:R:5:LYS:O	1.75	0.86
2:J:398:ILE:O	2:J:398:ILE:HG22	1.75	0.85
3:C:21:LYS:HD3	7:H:71:GLY:HA3	1.58	0.85
2:B:1063:TRP:NE1	2:B:1094:LYS:HG3	1.90	0.85
2:J:1122:ARG:HD2	5:Q:10:VAL:HG11	1.55	0.85
2:B:286:PRO:HB2	2:B:289:TYR:HB2	1.58	0.85
3:C:194:GLU:HB2	3:C:196:TYR:HE2	1.09	0.85
1:I:444:PRO:CD	9:U:50:THR:HG23	2.06	0.85
1:I:666:PHE:H	2:J:729:LEU:HD12	1.41	0.85
2:J:286:PRO:HB2	2:J:289:TYR:HB2	1.58	0.85
1:I:666:PHE:N	2:J:729:LEU:HD12	1.92	0.84
3:M:187:LYS:HD2	3:M:202:PRO:HD2	1.58	0.84
5:E:92:MET:HE1	5:E:127:PHE:CE2	2.07	0.84
3:M:163:ILE:O	3:M:195:GLY:O	1.96	0.84
5:Q:1:MET:HE1	6:R:11:TYR:CE1	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:PHE:O	2:B:394:VAL:CB	2.25	0.84
3:C:216:GLU:O	3:C:220:LYS:CB	2.25	0.84
5:E:81:ASN:O	5:E:82:GLN:HG2	1.77	0.84
3:C:148:ARG:CZ	3:C:163:ILE:HG12	2.06	0.84
3:C:148:ARG:NH1	3:C:163:ILE:O	2.11	0.84
3:C:191:PHE:HB3	3:C:198:LEU:HB2	1.60	0.84
3:C:162:GLU:HA	3:C:196:TYR:CD1	2.13	0.83
3:C:148:ARG:CZ	3:C:149:GLU:O	2.26	0.83
2:J:46:LEU:HD12	2:J:46:LEU:O	1.78	0.83
3:C:212:ARG:HG3	3:C:213:LYS:N	1.91	0.83
2:J:1086:CYS:SG	2:J:1090:GLU:CD	2.57	0.83
1:A:666:PHE:O	2:B:729:LEU:HD12	1.76	0.83
2:J:63:PHE:CZ	2:J:388:GLU:HG2	2.12	0.83
9:U:49:ILE:HG22	9:U:50:THR:H	1.42	0.83
3:C:148:ARG:HD2	3:C:163:ILE:HG13	1.59	0.83
5:Q:1:MET:HE1	6:R:11:TYR:HE1	1.43	0.83
2:J:45:GLY:O	2:J:46:LEU:HB3	1.77	0.82
3:C:151:THR:HG22	3:C:152:ILE:H	1.44	0.82
3:C:163:ILE:CB	3:C:164:ASP:HA	2.09	0.82
1:I:6:LYS:NZ	2:J:1122:ARG:HH22	1.76	0.82
1:A:750:MET:HA	1:A:753:THR:CG2	2.09	0.82
3:C:153:ASP:OD2	3:C:157:MET:HB3	1.78	0.82
1:I:100:CYS:SG	1:I:103:CYS:HB2	2.20	0.82
3:M:148:ARG:NH1	3:M:162:GLU:HB2	1.94	0.82
4:D:2:VAL:HG11	9:L:85:VAL:HA	1.59	0.82
1:I:103:CYS:HB2	1:I:150:CYS:SG	2.20	0.82
1:I:531:MET:HB3	9:U:44:THR:OG1	1.79	0.82
2:B:1063:TRP:CZ2	2:B:1094:LYS:HE3	2.13	0.81
11:W:30:CYS:SG	11:W:32:SER:HB3	2.20	0.81
1:I:445:TYR:CZ	9:U:49:ILE:HG21	2.12	0.81
1:I:563:LEU:HB2	1:I:614:GLY:HA2	1.62	0.81
3:M:160:VAL:HG12	3:M:161:VAL:H	1.43	0.81
1:A:531:MET:CB	9:L:44:THR:HG21	2.10	0.81
2:J:394:VAL:CG2	2:J:395:ARG:HG3	2.11	0.81
1:A:563:LEU:HB2	1:A:614:GLY:HA2	1.63	0.81
2:B:390:ILE:CD1	2:B:391:GLN:H	1.93	0.81
5:E:7:VAL:HG13	6:F:5:LYS:O	1.80	0.81
2:J:395:ARG:O	2:J:397:SER:N	2.14	0.81
2:B:146:ILE:HG21	10:N:61:VAL:HG21	1.61	0.81
1:A:79:LEU:HA	1:A:252:ASN:HD21	1.46	0.80
1:I:100:CYS:HB3	1:I:103:CYS:CB	2.10	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:432:ARG:O	2:J:1043:HIS:ND1	2.15	0.80
3:C:162:GLU:HG2	3:C:196:TYR:CG	2.16	0.80
2:J:183:ARG:HG3	2:J:337:GLU:OE2	1.82	0.80
1:A:508:ILE:HG13	1:A:754:GLY:O	1.81	0.80
2:J:952:GLU:OE2	2:J:952:GLU:N	2.15	0.80
3:M:182:LEU:O	3:M:185:SER:HB2	1.82	0.80
2:B:378:TYR:OH	2:B:388:GLU:HA	1.80	0.80
2:J:1122:ARG:HG2	2:J:1122:ARG:HH11	1.47	0.80
3:M:148:ARG:HG2	3:M:149:GLU:HG3	1.63	0.80
1:A:531:MET:CB	9:L:44:THR:HG23	2.12	0.80
2:J:1122:ARG:NH2	5:Q:67:TYR:CE2	2.49	0.80
3:M:204:LYS:HG3	3:M:205:VAL:HG23	1.62	0.80
1:I:452:LEU:HB3	1:I:504:ILE:HD11	1.64	0.80
1:I:384:VAL:HG12	1:I:392:ILE:HB	1.65	0.79
7:S:41:PRO:HB2	7:S:77:ARG:HG2	1.63	0.79
3:C:152:ILE:HG12	3:C:153:ASP:N	1.97	0.79
8:K:34:ILE:HB	8:K:38:GLN:HG3	1.64	0.79
10:N:57:ASP:HA	10:N:60:MET:HE3	1.62	0.79
8:T:34:ILE:HB	8:T:38:GLN:HG3	1.64	0.79
2:J:1122:ARG:HG3	6:R:4:ARG:NH2	1.96	0.79
3:C:162:GLU:CB	3:C:196:TYR:HB2	2.13	0.79
1:I:6:LYS:CE	2:J:1122:ARG:NH1	2.45	0.79
1:I:531:MET:HB2	9:U:44:THR:CG2	2.12	0.79
5:E:9:ASP:OD2	6:F:3:GLY:CA	2.29	0.79
2:J:391:GLN:O	2:J:392:ARG:CB	2.31	0.79
5:Q:1:MET:CE	6:R:11:TYR:CE1	2.66	0.79
4:O:2:VAL:HG11	9:U:85:VAL:HA	1.63	0.79
1:I:6:LYS:CE	2:J:1122:ARG:NH2	2.11	0.78
1:I:103:CYS:SG	1:I:105:ARG:HB2	2.23	0.78
2:J:107:MET:HB3	2:J:395:ARG:HH22	0.76	0.78
1:A:834:ARG:HG3	3:C:80:THR:HG22	1.66	0.78
7:H:41:PRO:HB2	7:H:77:ARG:HG2	1.63	0.78
3:C:162:GLU:C	3:C:196:TYR:CA	2.52	0.78
1:I:79:LEU:HA	1:I:252:ASN:HD21	1.47	0.78
2:J:1122:ARG:CG	6:R:4:ARG:NH2	2.47	0.78
2:B:389:ASN:ND2	2:B:392:ARG:CB	2.45	0.78
5:E:8:LYS:HE3	6:F:5:LYS:HD2	1.64	0.78
2:J:979:THR:HA	9:U:26:ASN:ND2	1.99	0.78
3:C:153:ASP:HB2	3:C:158:GLU:O	1.84	0.78
3:M:187:LYS:O	3:M:188:SER:OG	2.02	0.78
10:N:58:GLN:O	10:N:61:VAL:HG12	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1122:ARG:HD2	5:Q:10:VAL:CG1	2.13	0.78
1:A:452:LEU:HB3	1:A:504:ILE:HD11	1.64	0.77
2:B:391:GLN:OE1	2:B:393:PHE:CE2	2.37	0.77
3:C:161:VAL:HG23	3:C:198:LEU:C	2.04	0.77
1:A:384:VAL:HG12	1:A:392:ILE:HB	1.65	0.77
2:J:63:PHE:HZ	2:J:388:GLU:HG2	1.43	0.77
3:M:182:LEU:CD2	3:M:185:SER:HB2	2.14	0.77
3:C:196:TYR:CE1	3:C:198:LEU:HD11	2.20	0.77
2:B:744:LYS:NZ	9:L:53:ARG:HH22	1.74	0.77
3:C:161:VAL:HG23	3:C:199:VAL:CG2	2.10	0.77
2:J:370:MET:SD	2:J:398:ILE:HG12	2.24	0.76
2:J:57:VAL:HB	2:J:58:PRO:HA	1.67	0.76
2:B:1063:TRP:HE1	2:B:1094:LYS:HE3	1.48	0.76
2:J:394:VAL:HB	2:J:395:ARG:HG3	0.77	0.76
3:M:152:ILE:HG23	3:M:159:TYR:HA	1.66	0.76
1:I:147:CYS:SG	1:I:152:ALA:CA	2.74	0.76
2:B:390:ILE:O	2:B:392:ARG:N	2.19	0.76
2:J:361:VAL:HG11	2:J:417:PRO:HG3	1.67	0.76
5:Q:3:LYS:NZ	6:R:9:GLU:CD	2.39	0.76
2:B:952:GLU:OE2	2:B:952:GLU:N	2.17	0.76
1:I:632:LYS:HZ2	1:I:634:LEU:H	1.30	0.76
2:B:390:ILE:HD12	2:B:391:GLN:N	1.99	0.76
1:A:531:MET:HB2	9:L:44:THR:HG21	1.66	0.75
3:C:161:VAL:HG23	3:C:199:VAL:CB	2.16	0.75
1:I:9:GLY:CA	2:J:1120:LYS:HB2	2.15	0.75
4:O:35:SER:HB2	4:O:141:LYS:HB3	1.68	0.75
9:L:46:GLU:OE2	9:L:56:ARG:HD2	1.85	0.75
2:B:361:VAL:HG11	2:B:417:PRO:HG3	1.67	0.75
2:J:1122:ARG:HG2	2:J:1122:ARG:NH1	2.01	0.75
2:B:749:ARG:NH2	4:D:147:GLN:OE1	2.20	0.75
1:I:480:GLU:HA	8:T:10:ALA:HB1	1.68	0.75
1:I:585:LEU:O	1:I:586:GLU:HB3	1.86	0.75
1:I:9:GLY:HA3	2:J:1120:LYS:HB2	1.67	0.75
3:C:194:GLU:OE1	3:C:196:TYR:HE2	1.69	0.75
4:D:35:SER:HB2	4:D:141:LYS:HB3	1.68	0.75
3:C:343:THR:O	3:C:347:PHE:HB3	1.87	0.75
2:J:735:ASN:HB3	2:J:741:ILE:HG13	1.69	0.75
3:M:67:VAL:O	3:M:71:SER:OG	2.05	0.75
2:J:683:TRP:CD1	2:J:686:PHE:HB3	2.22	0.74
2:B:683:TRP:CD1	2:B:686:PHE:HB3	2.22	0.74
2:B:183:ARG:HG2	2:B:337:GLU:OE1	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:735:ASN:HB3	2:B:741:ILE:HG13	1.69	0.74
2:J:394:VAL:CG1	2:J:395:ARG:HG2	2.17	0.74
1:A:16:LEU:HD11	2:B:1109:LYS:HG3	1.68	0.74
2:B:57:VAL:HB	2:B:58:PRO:HA	1.67	0.74
2:B:123:ILE:HG22	2:B:403:LEU:HD22	1.69	0.74
1:A:625:ALA:O	1:A:632:LYS:NZ	2.18	0.74
5:E:92:MET:HE1	5:E:127:PHE:HD2	1.51	0.74
7:H:13:VAL:HG22	7:H:14:LEU:HG	1.70	0.74
2:J:771:GLN:HB3	2:J:818:PRO:HG3	1.69	0.74
1:I:6:LYS:HE3	2:J:1122:ARG:NH1	2.02	0.74
2:B:286:PRO:HD2	2:B:290:ARG:HE	1.53	0.73
3:C:160:VAL:CG2	3:C:198:LEU:HG	2.18	0.73
3:C:67:VAL:O	3:C:71:SER:OG	2.05	0.73
2:B:239:THR:HB	2:B:242:GLU:HG2	1.70	0.73
2:B:389:ASN:HD22	2:B:392:ARG:HB2	1.52	0.73
2:B:771:GLN:HB3	2:B:818:PRO:HG3	1.69	0.73
3:C:212:ARG:HG3	3:C:213:LYS:H	1.49	0.73
3:C:345:HIS:O	3:C:348:ALA:N	2.20	0.73
2:J:123:ILE:HG22	2:J:403:LEU:HD22	1.69	0.73
2:J:996:ARG:HH22	2:J:1000:MET:HE3	1.53	0.73
2:J:286:PRO:HD2	2:J:290:ARG:HE	1.53	0.73
2:J:239:THR:HB	2:J:242:GLU:HG2	1.70	0.73
3:C:134:VAL:HG12	3:C:138:ILE:HD11	1.70	0.73
3:M:134:VAL:HG12	3:M:138:ILE:HD11	1.70	0.73
3:C:164:ASP:CG	3:C:165:PRO:HD2	2.09	0.73
1:I:304:LEU:HB3	2:J:1111:MET:HE2	1.71	0.73
1:A:444:PRO:CD	9:L:50:THR:HG22	2.19	0.72
2:B:744:LYS:HZ1	9:L:53:ARG:NH2	1.87	0.72
2:J:395:ARG:HB3	2:J:398:ILE:CD1	2.19	0.72
5:E:1:MET:CE	6:F:11:TYR:HD1	1.98	0.72
1:I:665:GLY:C	2:J:729:LEU:HD11	2.09	0.72
1:I:445:TYR:CG	9:U:49:ILE:HG21	2.24	0.72
2:J:42:ILE:HG21	2:J:72:ILE:HD13	1.71	0.72
1:A:671:ASP:OD1	2:B:969:SER:OG	2.07	0.72
2:J:939:LEU:HD11	2:J:966:PHE:HD2	1.54	0.72
11:W:27:CYS:CB	11:W:30:CYS:SG	2.77	0.72
1:A:666:PHE:C	2:B:729:LEU:HD13	2.10	0.72
2:B:939:LEU:HD11	2:B:966:PHE:HD2	1.54	0.72
1:I:74:PHE:HE1	1:I:222:PRO:HD3	1.54	0.72
7:S:13:VAL:HG22	7:S:14:LEU:HG	1.71	0.72
11:P:14:GLU:CD	11:P:30:CYS:HG	1.92	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:309:ASP:OD1	2:J:309:ASP:N	2.23	0.72
2:J:378:TYR:HE1	2:J:388:GLU:CB	2.01	0.72
2:J:904:THR:HG22	2:J:906:SER:H	1.55	0.72
1:I:666:PHE:H	2:J:729:LEU:CG	2.03	0.72
2:J:378:TYR:CZ	2:J:388:GLU:CG	2.70	0.72
2:J:1101:PHE:CG	3:M:367:ILE:HG13	2.25	0.72
3:M:153:ASP:CB	3:M:157:MET:HB2	2.20	0.72
2:J:395:ARG:HD3	2:J:398:ILE:HD11	1.72	0.72
2:B:309:ASP:OD1	2:B:309:ASP:N	2.23	0.71
3:C:186:PHE:C	3:C:187:LYS:HG2	2.10	0.71
2:J:42:ILE:HG23	2:J:72:ILE:HD11	1.72	0.71
2:B:904:THR:HG22	2:B:906:SER:H	1.56	0.71
2:B:63:PHE:CD1	2:B:392:ARG:NH2	2.58	0.71
2:B:996:ARG:HH22	2:B:1000:MET:HE3	1.53	0.71
9:L:48:PRO:O	9:L:49:ILE:HG23	1.89	0.71
1:I:13:PHE:CE2	3:M:333:VAL:HG21	2.25	0.71
2:J:392:ARG:O	2:J:394:VAL:N	2.22	0.71
3:M:152:ILE:HG23	3:M:160:VAL:H	1.54	0.71
3:C:163:ILE:HB	3:C:164:ASP:CA	2.20	0.71
2:B:981:ARG:NH2	9:L:30:GLU:OE2	2.22	0.71
2:B:432:TYR:HB2	2:B:682:GLY:HA2	1.73	0.71
3:C:151:THR:HG22	3:C:152:ILE:N	2.04	0.71
2:J:749:ARG:NH2	4:O:147:GLN:OE1	2.24	0.71
2:B:146:ILE:CG2	10:N:61:VAL:HG21	2.20	0.71
1:I:670:ILE:HD11	2:J:929:ILE:HG12	1.71	0.71
2:J:39:ASN:C	2:J:41:PHE:H	1.94	0.71
1:A:181:MET:SD	1:A:189:ARG:NH1	2.64	0.71
3:C:223:LEU:O	3:C:225:GLY:N	2.23	0.71
1:A:564:PRO:HD2	1:A:567:LEU:HD11	1.72	0.71
1:A:749:ILE:O	1:A:753:THR:CG2	2.39	0.71
9:L:25:ALA:HB1	9:L:43:TYR:CE2	2.26	0.71
2:J:1068:CYS:SG	2:J:1070:HIS:CD2	2.84	0.71
3:M:165:PRO:HB3	3:M:195:GLY:HA2	1.72	0.71
3:C:162:GLU:HA	3:C:196:TYR:CG	2.25	0.71
9:L:25:ALA:HB1	9:L:43:TYR:CD2	2.26	0.71
9:L:49:ILE:CD1	9:L:50:THR:H	1.98	0.71
1:I:449:ARG:CZ	9:U:49:ILE:HD11	2.21	0.71
3:M:145:ASN:OD1	3:M:145:ASN:N	2.24	0.71
5:Q:9:ASP:OD1	6:R:4:ARG:HG2	1.90	0.71
5:E:9:ASP:OD1	5:E:10:VAL:N	2.23	0.70
2:B:378:TYR:HE1	2:B:388:GLU:C	1.93	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:LEU:HD12	3:C:177:LYS:HZ2	1.55	0.70
1:A:531:MET:HB3	9:L:44:THR:CG2	2.20	0.70
1:I:822:MET:HG2	2:J:458:LEU:HB3	1.72	0.70
2:B:47:GLN:HE22	2:B:69:LYS:HA	1.56	0.70
2:B:275:ASP:O	2:B:279:ARG:HB2	1.91	0.70
2:J:432:TYR:HB2	2:J:682:GLY:HA2	1.73	0.70
1:A:60:CYS:SG	1:A:61:GLU:N	2.64	0.70
2:J:116:GLN:OE1	2:J:393:PHE:HD1	1.73	0.70
3:M:153:ASP:HB3	3:M:157:MET:HB2	1.73	0.70
1:A:74:PHE:HE1	1:A:222:PRO:HD3	1.57	0.70
1:I:181:MET:SD	1:I:189:ARG:NH1	2.64	0.70
1:I:840:TYR:OH	3:M:323:ARG:NH2	2.25	0.70
3:M:223:LEU:O	3:M:225:GLY:N	2.23	0.70
3:C:196:TYR:CD1	3:C:196:TYR:O	2.45	0.70
1:A:712:LYS:HD2	3:C:92:ILE:HB	1.74	0.70
1:I:476:GLU:OE1	8:T:11:ARG:NH1	2.23	0.70
2:J:41:PHE:CD1	2:J:42:ILE:HD13	2.27	0.70
1:A:863:PRO:HB3	3:C:360:GLY:HA2	1.75	0.69
3:M:120:LEU:O	3:M:125:ARG:NH1	2.26	0.69
3:M:152:ILE:O	3:M:160:VAL:HB	1.92	0.69
3:C:148:ARG:HG2	3:C:149:GLU:CG	2.18	0.69
1:I:564:PRO:HD2	1:I:567:LEU:HD11	1.72	0.69
2:J:378:TYR:CD1	2:J:388:GLU:HG3	2.22	0.69
3:C:342:THR:HB	3:C:345:HIS:HB2	1.73	0.69
2:B:390:ILE:C	2:B:392:ARG:H	1.93	0.69
1:I:60:CYS:SG	1:I:61:GLU:N	2.65	0.69
3:C:145:ASN:N	3:C:145:ASN:OD1	2.25	0.69
2:J:42:ILE:HG23	2:J:72:ILE:CD1	2.21	0.69
2:J:63:PHE:CE1	2:J:388:GLU:OE1	2.45	0.69
1:A:13:PHE:HE1	2:B:1115:PRO:HB3	1.57	0.69
1:A:894:ILE:HG13	3:C:29:ILE:HD12	1.75	0.69
2:B:730:SER:HA	2:B:735:ASN:HD21	1.58	0.69
3:C:120:LEU:O	3:C:125:ARG:NH1	2.26	0.69
5:E:3:LYS:NZ	6:F:9:GLU:CD	2.46	0.69
1:A:758:LYS:HG2	1:A:760:LEU:HD21	1.74	0.69
2:B:389:ASN:HD21	2:B:392:ARG:NE	1.88	0.69
3:C:211:LEU:HA	3:C:214:ILE:HD12	1.73	0.69
10:N:60:MET:O	10:N:62:TYR:N	2.23	0.69
1:I:447:THR:O	1:I:449:ARG:NH1	2.26	0.69
1:I:640:GLU:HG2	1:I:896:ARG:NH1	2.07	0.69
1:I:834:ARG:HH12	3:M:99:PRO:HD3	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:MET:HB3	9:L:44:THR:HG23	1.72	0.69
5:Q:8:LYS:HE3	6:R:5:LYS:HD2	1.73	0.69
10:N:57:ASP:HA	10:N:60:MET:CE	2.23	0.69
2:J:275:ASP:O	2:J:279:ARG:HB2	1.91	0.69
3:M:182:LEU:CD2	3:M:185:SER:CB	2.71	0.69
3:M:148:ARG:HH12	3:M:162:GLU:C	1.96	0.68
1:I:103:CYS:CA	1:I:150:CYS:SG	2.81	0.68
2:J:378:TYR:CE1	2:J:388:GLU:CB	2.74	0.68
2:J:730:SER:HA	2:J:735:ASN:HD21	1.57	0.68
3:M:153:ASP:OD2	3:M:160:VAL:HG21	1.93	0.68
1:A:872:TYR:CZ	3:C:64:VAL:HG11	2.28	0.68
2:B:719:PRO:HG3	10:N:53:VAL:HG11	1.76	0.68
2:J:395:ARG:HB3	2:J:398:ILE:HD11	1.76	0.68
3:C:161:VAL:HG12	3:C:162:GLU:N	2.03	0.68
3:M:64:VAL:HA	3:M:67:VAL:HG22	1.75	0.68
5:Q:9:ASP:OD1	5:Q:10:VAL:N	2.23	0.68
3:C:161:VAL:HG23	3:C:199:VAL:CA	2.23	0.68
3:C:162:GLU:C	3:C:196:TYR:HA	2.13	0.68
1:A:447:THR:O	1:A:449:ARG:NH1	2.25	0.68
1:A:894:ILE:O	1:A:897:THR:HG23	1.93	0.68
2:J:392:ARG:C	2:J:394:VAL:H	1.96	0.68
2:J:393:PHE:C	2:J:394:VAL:HG22	2.14	0.68
1:A:445:TYR:HB2	1:A:449:ARG:HH22	1.59	0.68
3:C:286:ILE:HD13	3:C:306:MET:HG2	1.76	0.68
1:I:671:ASP:OD1	2:J:969:SER:OG	2.11	0.68
3:M:160:VAL:HG12	3:M:161:VAL:N	2.09	0.68
1:A:63:CYS:HG	1:A:73:HIS:HE2	1.42	0.68
1:I:100:CYS:CB	1:I:103:CYS:HB3	2.20	0.68
3:C:358:LEU:HD12	3:C:359:ASN:H	1.59	0.67
3:M:148:ARG:NH1	3:M:162:GLU:C	2.47	0.67
3:C:64:VAL:HA	3:C:67:VAL:HG22	1.75	0.67
2:B:731:TYR:CE2	2:B:902:PRO:HG3	2.29	0.67
3:C:55:LYS:HE2	8:K:3:ARG:HH22	1.60	0.67
1:I:103:CYS:SG	1:I:105:ARG:CB	2.82	0.67
1:A:753:THR:HG23	1:A:754:GLY:N	2.05	0.67
4:D:6:ILE:HG13	4:D:14:ILE:HD11	1.77	0.67
1:I:775:ARG:HD3	2:J:453:PHE:HD2	1.60	0.67
2:J:42:ILE:CG2	2:J:72:ILE:HD11	2.22	0.67
2:J:56:VAL:HG12	2:J:367:VAL:HG13	1.77	0.67
1:I:94:ARG:HG3	1:I:138:HIS:CD2	2.30	0.67
2:J:211:LYS:HA	3:M:212:ARG:NH2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:VAL:HG11	3:C:311:MET:HG2	1.77	0.67
1:I:445:TYR:HB2	1:I:449:ARG:HH22	1.60	0.67
2:B:365:GLN:OE1	2:B:406:ARG:NH1	2.28	0.67
5:E:81:ASN:O	5:E:82:GLN:CG	2.43	0.67
3:M:286:ILE:HD13	3:M:306:MET:HG2	1.77	0.67
5:Q:41:ASP:OD2	6:R:1:MET:SD	2.53	0.67
1:A:94:ARG:HG3	1:A:138:HIS:CD2	2.30	0.67
2:B:389:ASN:ND2	2:B:389:ASN:O	2.27	0.67
4:D:56:ASP:HB3	11:P:46:VAL:HG21	1.75	0.67
2:J:41:PHE:CE1	2:J:42:ILE:HD13	2.30	0.67
4:O:6:ILE:HG13	4:O:14:ILE:HD11	1.77	0.67
2:J:378:TYR:HE1	2:J:388:GLU:HG3	1.34	0.67
9:U:51:MET:CG	9:U:53:ARG:HB2	2.24	0.67
1:A:556:LYS:HD2	1:A:616:LEU:HD22	1.77	0.66
2:J:729:LEU:HD23	2:J:730:SER:C	2.15	0.66
3:C:287:ASP:O	3:C:291:SER:OG	2.13	0.66
1:I:147:CYS:SG	1:I:152:ALA:N	2.68	0.66
1:A:850:GLN:OE1	2:B:1037:ARG:NH1	2.29	0.66
2:B:433:MET:HG3	2:B:656:LEU:HD11	1.78	0.66
2:B:856:VAL:HG12	11:P:35:LEU:HB2	1.77	0.66
3:M:287:ASP:O	3:M:291:SER:OG	2.13	0.66
1:I:16:LEU:HG	2:J:1114:ARG:HB3	1.77	0.66
2:J:365:GLN:OE1	2:J:406:ARG:NH1	2.28	0.66
2:J:1109:LYS:HD3	2:J:1115:PRO:HD2	1.78	0.66
9:U:51:MET:HA	9:U:52:ALA:C	2.15	0.66
1:A:508:ILE:HG21	1:A:754:GLY:CA	2.25	0.66
2:J:433:MET:HG3	2:J:656:LEU:HD11	1.78	0.66
1:A:750:MET:HA	1:A:753:THR:HG22	1.76	0.66
1:I:775:ARG:HD3	2:J:453:PHE:CD2	2.31	0.66
2:J:1065:CYS:HB3	2:J:1068:CYS:HB3	1.75	0.66
2:B:56:VAL:HG12	2:B:367:VAL:HG13	1.77	0.66
1:I:894:ILE:HG13	3:M:29:ILE:HD12	1.78	0.66
2:J:43:ASP:OD1	2:J:43:ASP:N	2.28	0.66
2:J:546:ARG:NH1	2:J:555:ILE:O	2.29	0.66
2:J:800:ILE:HD11	2:J:812:LEU:HA	1.77	0.66
9:L:25:ALA:CB	9:L:43:TYR:CE2	2.78	0.66
2:J:174:LEU:HD21	2:J:180:LEU:HD11	1.77	0.66
1:A:505:GLN:HB2	2:B:917:HIS:CD2	2.30	0.65
2:J:556:ASN:OD1	2:J:576:ARG:NH1	2.29	0.65
3:M:321:ILE:HA	3:M:326:ILE:HG13	1.78	0.65
2:B:959:LYS:HA	4:D:201:ARG:HH21	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:389:ASN:CA	2:J:390:ILE:HG23	2.11	0.65
2:J:820:ARG:O	2:J:837:ARG:NH1	2.28	0.65
4:O:226:THR:OG1	4:O:227:ASN:N	2.29	0.65
3:C:96:LEU:HB2	3:C:100:ARG:HB2	1.78	0.65
1:I:6:LYS:HE2	2:J:1122:ARG:NH1	2.04	0.65
3:M:96:LEU:HB2	3:M:100:ARG:HB2	1.78	0.65
4:O:162:SER:HA	4:O:188:GLU:HB3	1.78	0.65
1:A:712:LYS:HZ2	3:C:92:ILE:N	1.95	0.65
3:C:162:GLU:CG	3:C:196:TYR:CD1	2.77	0.65
2:B:546:ARG:NH1	2:B:555:ILE:O	2.29	0.65
2:B:556:ASN:OD1	2:B:576:ARG:NH1	2.30	0.65
3:C:203:LYS:HB2	3:C:203:LYS:HZ2	1.59	0.65
5:Q:100:ARG:CZ	6:R:43:VAL:HG13	2.26	0.65
2:B:174:LEU:HD21	2:B:180:LEU:HD11	1.78	0.65
2:B:759:THR:HB	2:B:869:THR:HG22	1.79	0.65
1:A:309:LYS:HB3	3:C:341:ILE:HG23	1.77	0.65
2:J:614:VAL:HG13	2:J:615:ILE:HG12	1.79	0.65
1:A:863:PRO:CB	3:C:360:GLY:HA2	2.27	0.65
2:B:800:ILE:HD11	2:B:812:LEU:HA	1.77	0.65
2:J:389:ASN:O	2:J:389:ASN:ND2	2.29	0.65
2:J:759:THR:HB	2:J:869:THR:HG22	1.79	0.65
2:J:793:HIS:HB3	2:J:800:ILE:HG23	1.79	0.65
4:D:162:SER:HA	4:D:188:GLU:HB3	1.78	0.65
2:J:198:ARG:HD3	2:J:304:PRO:HB2	1.78	0.65
1:A:248:ILE:HD11	1:A:282:TYR:HB2	1.79	0.65
2:B:45:GLY:O	2:B:47:GLN:N	2.30	0.65
3:C:194:GLU:OE1	3:C:196:TYR:CE2	2.48	0.65
1:I:40:TYR:H	1:I:41:PRO:CD	2.10	0.65
1:I:445:TYR:CD2	9:U:49:ILE:CG2	2.61	0.65
1:I:556:LYS:HD2	1:I:616:LEU:HD22	1.77	0.64
5:Q:14:PRO:HB3	5:Q:16:ARG:HH11	1.63	0.64
4:D:200:PRO:HB2	4:D:203:PHE:HD1	1.61	0.64
1:I:147:CYS:H	1:I:152:ALA:HB2	1.62	0.64
2:B:614:VAL:HG13	2:B:615:ILE:HG12	1.79	0.64
3:C:164:ASP:OD1	3:C:165:PRO:HD2	1.97	0.64
2:B:793:HIS:HB3	2:B:800:ILE:HG23	1.79	0.64
1:A:750:MET:CA	1:A:753:THR:HG22	2.26	0.64
3:C:113:THR:OG1	3:C:113:THR:O	2.15	0.64
3:M:148:ARG:NH2	3:M:162:GLU:HG2	2.11	0.64
3:M:151:THR:HG22	3:M:152:ILE:N	2.06	0.64
4:O:154:LYS:NZ	4:O:155:TYR:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:ARG:HD3	2:B:304:PRO:HB2	1.78	0.64
5:E:14:PRO:HB3	5:E:16:ARG:HH11	1.63	0.64
2:J:1122:ARG:CD	6:R:4:ARG:HH21	2.11	0.64
9:U:52:ALA:O	9:U:53:ARG:HB3	1.96	0.64
2:B:183:ARG:NH2	2:B:454:GLU:OE2	2.30	0.64
3:C:162:GLU:HA	3:C:196:TYR:HD1	1.59	0.64
9:L:93:ILE:O	9:L:94:GLU:HG3	1.97	0.64
1:I:248:ILE:HD11	1:I:282:TYR:HB2	1.79	0.64
2:J:25:TRP:CZ2	2:J:485:LEU:HB3	2.33	0.64
3:C:186:PHE:O	3:C:187:LYS:HG2	1.96	0.63
2:J:746:SER:HB3	2:J:751:LEU:HD12	1.80	0.63
2:J:969:SER:HB3	2:J:971:ARG:HG3	1.80	0.63
1:A:623:LYS:HB2	1:A:754:GLY:HA3	1.80	0.63
2:B:25:TRP:CZ2	2:B:485:LEU:HB3	2.33	0.63
3:C:157:MET:O	3:C:158:GLU:HB2	1.96	0.63
2:J:981:ARG:NH2	9:U:30:GLU:OE2	2.29	0.63
2:B:57:VAL:HG11	2:B:371:GLN:HG3	1.80	0.63
1:I:100:CYS:SG	1:I:103:CYS:CB	2.86	0.63
1:I:492:ILE:HA	1:I:499:PRO:HA	1.79	0.63
5:E:5:LEU:CD1	6:F:6:LYS:HD3	2.29	0.63
1:I:895:VAL:O	1:I:897:THR:N	2.31	0.63
3:M:229:VAL:HG21	3:M:245:THR:HG22	1.81	0.63
4:O:194:ILE:HA	4:O:221:VAL:HG21	1.79	0.63
3:C:321:ILE:HA	3:C:326:ILE:HG13	1.79	0.63
3:M:358:LEU:HD12	3:M:359:ASN:H	1.62	0.63
2:B:532:VAL:HG12	2:B:533:GLU:H	1.64	0.63
3:C:160:VAL:CG2	3:C:198:LEU:CG	2.77	0.63
5:E:41:ASP:OD2	6:F:1:MET:SD	2.56	0.63
2:J:57:VAL:HG11	2:J:371:GLN:HG3	1.79	0.63
3:M:182:LEU:HD22	3:M:185:SER:HB2	1.80	0.63
4:O:62:ARG:NH2	10:V:2:ILE:O	2.32	0.63
4:O:200:PRO:HB2	4:O:203:PHE:HD1	1.63	0.63
3:C:161:VAL:CG2	3:C:198:LEU:C	2.67	0.63
4:D:194:ILE:HA	4:D:221:VAL:HG21	1.79	0.63
2:J:42:ILE:HG22	2:J:72:ILE:HD13	1.80	0.63
4:D:154:LYS:NZ	4:D:155:TYR:O	2.32	0.63
1:A:656:LEU:HD13	1:A:659:TRP:HE1	1.64	0.62
2:B:161:ILE:HG21	2:B:412:ALA:HB2	1.81	0.62
3:C:55:LYS:HG2	8:K:3:ARG:HH21	1.65	0.62
2:J:1063:TRP:HE3	2:J:1092:ILE:HG22	1.64	0.62
1:A:897:THR:HG21	3:C:45:ILE:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:979:THR:HA	9:L:26:ASN:HD21	1.64	0.62
1:I:47:MET:O	1:I:49:LYS:N	2.32	0.62
7:S:17:GLU:HB2	7:S:64:LYS:HB2	1.81	0.62
2:B:969:SER:HB3	2:B:971:ARG:HG3	1.81	0.62
3:C:180:ARG:O	3:C:182:LEU:N	2.32	0.62
3:C:229:VAL:HG21	3:C:245:THR:HG22	1.81	0.62
2:J:11:THR:O	2:J:593:ARG:NH2	2.31	0.62
2:J:65:VAL:HG13	2:J:395:ARG:NH2	2.14	0.62
2:J:398:ILE:O	2:J:398:ILE:CG2	2.46	0.62
2:B:1109:LYS:HD3	2:B:1115:PRO:HD2	1.81	0.62
3:C:93:ASN:O	3:C:95:THR:N	2.33	0.62
1:A:806:ASN:N	1:A:806:ASN:OD1	2.32	0.62
2:B:522:VAL:HG22	2:B:568:VAL:HB	1.82	0.62
1:I:449:ARG:NH2	9:U:49:ILE:HD11	2.13	0.62
3:M:113:THR:O	3:M:113:THR:OG1	2.15	0.62
1:A:150:CYS:C	1:A:152:ALA:N	2.52	0.62
9:U:51:MET:HG2	9:U:53:ARG:HB3	1.77	0.62
9:U:51:MET:HA	9:U:52:ALA:HB3	1.81	0.62
3:C:211:LEU:HA	3:C:214:ILE:HD11	1.80	0.62
2:J:532:VAL:HG12	2:J:533:GLU:H	1.64	0.62
3:M:173:LEU:HB3	3:M:177:LYS:HZ3	1.65	0.62
5:Q:125:ARG:HE	5:Q:125:ARG:H	1.48	0.62
3:C:187:LYS:NZ	3:C:206:THR:HB	2.15	0.62
3:M:191:PHE:HB2	3:M:198:LEU:HB2	1.82	0.62
1:A:492:ILE:HA	1:A:499:PRO:HA	1.80	0.62
1:A:508:ILE:HG21	1:A:754:GLY:C	2.20	0.62
2:J:37:SER:O	2:J:41:PHE:HB2	1.99	0.62
2:B:11:THR:O	2:B:593:ARG:NH2	2.32	0.62
2:B:190:VAL:HG21	2:B:331:SER:HB3	1.82	0.62
9:U:44:THR:C	9:U:45:ILE:HG13	2.21	0.62
2:B:746:SER:HB3	2:B:751:LEU:HD12	1.81	0.61
3:C:163:ILE:N	3:C:196:TYR:HB3	2.15	0.61
7:H:50:VAL:HG13	7:H:55:ALA:HB3	1.81	0.61
1:I:665:GLY:CA	2:J:729:LEU:CD1	2.65	0.61
2:J:161:ILE:HG21	2:J:412:ALA:HB2	1.81	0.61
2:J:183:ARG:HG2	2:J:184:ASP:N	2.15	0.61
2:J:207:VAL:HG12	2:J:217:VAL:HG22	1.81	0.61
2:J:330:LEU:HD21	2:J:337:GLU:HG2	1.82	0.61
3:M:339:PHE:O	3:M:341:ILE:N	2.33	0.61
1:A:463:ASP:HA	2:B:890:GLY:HA2	1.81	0.61
2:B:330:LEU:HD21	2:B:337:GLU:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:931:ALA:HB1	2:B:990:GLY:HA3	1.81	0.61
3:C:331:ALA:H	3:C:336:ARG:HH12	1.46	0.61
6:F:116:ASP:HA	6:F:119:ARG:HE	1.65	0.61
2:J:93:ARG:HG3	2:J:160:ILE:HD13	1.82	0.61
5:Q:5:LEU:CD1	6:R:6:LYS:HD3	2.30	0.61
5:Q:99:ILE:HD13	5:Q:142:VAL:HG21	1.82	0.61
6:R:116:ASP:HA	6:R:119:ARG:HE	1.65	0.61
7:S:50:VAL:HG13	7:S:55:ALA:HB3	1.81	0.61
1:A:47:MET:O	1:A:49:LYS:N	2.33	0.61
2:B:979:THR:HA	9:L:26:ASN:ND2	2.16	0.61
7:H:17:GLU:HB2	7:H:64:LYS:HB2	1.81	0.61
3:M:182:LEU:O	3:M:185:SER:CB	2.48	0.61
2:B:276:TYR:O	2:B:279:ARG:HB3	2.01	0.61
3:C:143:LEU:HB2	3:C:222:ARG:HG3	1.81	0.61
2:J:165:GLU:OE1	2:J:429:ARG:NH1	2.33	0.61
2:J:818:PRO:HA	2:J:836:ARG:HB3	1.83	0.61
3:M:173:LEU:HD12	3:M:177:LYS:HZ2	1.64	0.61
3:M:279:GLU:OE1	7:S:65:ARG:NH1	2.34	0.61
5:E:39:ASP:HA	5:E:154:ARG:HH11	1.66	0.61
5:E:125:ARG:HE	5:E:125:ARG:H	1.48	0.61
1:I:656:LEU:HD13	1:I:659:TRP:HE1	1.64	0.61
2:J:116:GLN:OE1	2:J:393:PHE:CD1	2.53	0.61
2:J:190:VAL:HG21	2:J:331:SER:HB3	1.82	0.61
2:J:931:ALA:HB1	2:J:990:GLY:HA3	1.81	0.61
7:S:55:ALA:HB1	7:S:79:VAL:HG21	1.82	0.61
2:J:971:ARG:HB2	2:J:986:ASP:HB3	1.82	0.61
3:C:386:LEU:HD11	5:E:20:MET:C	2.21	0.61
1:I:103:CYS:HB2	1:I:150:CYS:HG	1.64	0.61
2:J:522:VAL:HG22	2:J:568:VAL:HB	1.81	0.61
2:B:411:LEU:HD12	2:B:416:TRP:HH2	1.66	0.60
5:E:49:LEU:N	5:E:73:ASN:O	2.33	0.60
2:J:803:GLU:O	11:W:44:ARG:NE	2.34	0.60
2:B:971:ARG:HB2	2:B:986:ASP:HB3	1.82	0.60
4:D:50:ASN:HD22	4:D:52:SER:H	1.48	0.60
2:J:233:ARG:NH2	2:J:240:ASP:OD1	2.35	0.60
5:Q:39:ASP:HA	5:Q:154:ARG:HH11	1.66	0.60
3:C:279:GLU:OE1	7:H:65:ARG:NH1	2.34	0.60
1:I:535:MET:HE1	1:I:652:GLN:HE22	1.66	0.60
3:M:378:VAL:HG21	8:T:8:GLU:HG2	1.83	0.60
4:O:50:ASN:HD22	4:O:52:SER:H	1.49	0.60
2:B:233:ARG:NH2	2:B:240:ASP:OD1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:470:GLU:OE2	2:B:482:ASN:ND2	2.35	0.60
3:C:160:VAL:HG21	3:C:198:LEU:CG	2.32	0.60
3:C:160:VAL:HG23	3:C:198:LEU:HB3	1.82	0.60
2:J:411:LEU:HD12	2:J:416:TRP:HH2	1.66	0.60
1:A:6:LYS:HG2	2:B:1094:LYS:O	2.02	0.60
1:A:630:ASP:N	1:A:630:ASP:OD1	2.34	0.60
2:B:207:VAL:HG12	2:B:217:VAL:HG22	1.82	0.60
2:B:758:ARG:HH11	2:B:844:ARG:HG3	1.66	0.60
2:B:818:PRO:HA	2:B:836:ARG:HB3	1.82	0.60
3:C:217:LYS:HA	3:C:221:HIS:HB2	1.83	0.60
7:H:55:ALA:HB1	7:H:79:VAL:HG21	1.82	0.60
1:I:806:ASN:N	1:I:806:ASN:OD1	2.32	0.60
4:O:62:ARG:HH12	10:V:2:ILE:HB	1.66	0.60
1:A:444:PRO:HD2	9:L:50:THR:HG23	1.82	0.60
2:B:165:GLU:OE1	2:B:429:ARG:NH1	2.34	0.60
1:I:11:ILE:HD12	3:M:358:LEU:CD2	2.32	0.60
1:A:62:THR:HG21	2:B:1078:ARG:HH11	1.66	0.60
1:A:666:PHE:H	2:B:729:LEU:HD13	1.66	0.60
5:E:5:LEU:HD11	6:F:6:LYS:HD3	1.83	0.60
7:H:43:ILE:N	7:H:78:LEU:O	2.29	0.60
2:J:276:TYR:O	2:J:279:ARG:HB3	2.01	0.60
2:J:378:TYR:CZ	2:J:388:GLU:OE2	2.55	0.60
5:Q:80:ARG:HG3	5:Q:83:GLU:HB2	1.84	0.60
1:A:95:VAL:HG22	1:A:201:LEU:HD23	1.84	0.60
2:B:1065:CYS:HB3	2:B:1068:CYS:HB2	1.83	0.60
2:J:391:GLN:O	2:J:392:ARG:HB2	2.02	0.60
1:A:444:PRO:HD2	9:L:50:THR:CG2	2.32	0.60
4:D:60:ALA:HB1	11:P:48:ALA:HB2	1.82	0.60
1:I:480:GLU:CD	2:J:1047:MET:HB2	2.22	0.60
2:J:39:ASN:C	2:J:41:PHE:N	2.55	0.60
9:U:59:VAL:HG21	9:U:71:LEU:HD21	1.83	0.60
2:B:146:ILE:CG2	10:N:61:VAL:CG2	2.80	0.60
5:E:92:MET:HE2	5:E:127:PHE:CD2	2.34	0.60
10:N:61:VAL:HG13	10:N:61:VAL:O	2.02	0.60
2:J:46:LEU:HD12	2:J:46:LEU:C	2.21	0.60
3:M:134:VAL:O	3:M:138:ILE:HG13	2.02	0.60
3:M:189:ALA:HB3	3:M:199:VAL:HA	1.83	0.60
10:V:7:CYS:SG	10:V:8:PHE:N	2.75	0.60
11:W:30:CYS:SG	11:W:32:SER:CB	2.90	0.60
3:C:134:VAL:O	3:C:138:ILE:HG13	2.02	0.59
9:L:59:VAL:HG21	9:L:71:LEU:HD21	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:756:ARG:HG3	2:J:917:HIS:HB3	1.83	0.59
2:J:758:ARG:HH11	2:J:844:ARG:HG3	1.66	0.59
1:A:63:CYS:O	2:B:1076:LYS:HB2	2.01	0.59
1:A:666:PHE:H	2:B:729:LEU:CD1	2.15	0.59
2:B:394:VAL:CG2	2:B:395:ARG:HG3	2.30	0.59
5:E:100:ARG:CZ	6:F:43:VAL:HG13	2.31	0.59
1:I:449:ARG:NE	9:U:49:ILE:HD11	2.17	0.59
2:J:205:ILE:HD11	2:J:303:LEU:H	1.67	0.59
2:J:1091:ARG:H	2:J:1091:ARG:HD3	1.67	0.59
5:Q:2:TYR:OH	6:R:44:SER:OG	2.17	0.59
1:A:758:LYS:HG2	1:A:760:LEU:CD2	2.33	0.59
2:B:93:ARG:HG3	2:B:160:ILE:HD13	1.83	0.59
2:B:789:LYS:HB3	2:B:792:ARG:HB2	1.84	0.59
3:C:161:VAL:O	3:C:162:GLU:HG3	2.01	0.59
1:I:63:CYS:HG	1:I:73:HIS:HE2	1.47	0.59
1:I:666:PHE:O	2:J:729:LEU:HG	2.03	0.59
2:J:1122:ARG:CG	2:J:1122:ARG:HH11	2.15	0.59
5:Q:5:LEU:HD11	6:R:6:LYS:HD3	1.83	0.59
2:B:20:VAL:O	2:B:23:SER:OG	2.18	0.59
5:E:99:ILE:HD13	5:E:142:VAL:HG21	1.83	0.59
1:I:690:ALA:HA	1:I:693:LYS:HD2	1.83	0.59
2:J:789:LYS:HB3	2:J:792:ARG:HB2	1.83	0.59
1:A:535:MET:HE1	1:A:652:GLN:HE22	1.67	0.59
1:A:583:GLU:CG	1:A:584:ALA:H	2.15	0.59
2:B:49:VAL:HG11	2:B:360:ARG:HA	1.84	0.59
2:B:702:VAL:HG23	10:N:53:VAL:HG12	1.84	0.59
3:M:313:THR:HG22	3:M:318:ILE:HG22	1.85	0.59
3:C:216:GLU:O	3:C:220:LYS:N	2.35	0.59
4:D:145:LYS:NZ	11:P:48:ALA:O	2.31	0.59
5:E:80:ARG:HG3	5:E:83:GLU:HB2	1.84	0.59
2:J:63:PHE:CZ	2:J:388:GLU:OE2	2.55	0.59
2:J:599:ILE:HD11	2:J:609:LEU:HD11	1.84	0.59
3:C:216:GLU:O	3:C:220:LYS:CA	2.51	0.59
4:D:151:VAL:HG22	4:D:224:VAL:HG22	1.84	0.59
5:E:46:LEU:HD22	6:F:21:LEU:HD21	1.84	0.59
1:A:444:PRO:CD	9:L:50:THR:CG2	2.80	0.59
2:B:599:ILE:HD11	2:B:609:LEU:HD11	1.84	0.59
3:C:148:ARG:H	3:C:148:ARG:HD3	1.68	0.59
9:U:43:TYR:HB2	9:U:56:ARG:O	2.03	0.59
2:B:389:ASN:ND2	2:B:392:ARG:CG	2.66	0.59
10:N:2:ILE:HD11	10:N:56:ILE:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:497:GLY:O	1:I:884:GLN:NE2	2.35	0.59
1:I:583:GLU:CG	1:I:584:ALA:H	2.16	0.59
2:J:20:VAL:O	2:J:23:SER:OG	2.18	0.59
3:C:160:VAL:HG21	3:C:198:LEU:HG	1.83	0.59
3:C:189:ALA:HB3	3:C:199:VAL:HA	1.84	0.59
1:I:444:PRO:HG3	9:U:50:THR:HG23	0.59	0.59
3:M:148:ARG:HH22	3:M:162:GLU:CB	1.82	0.59
1:A:150:CYS:C	1:A:152:ALA:H	2.06	0.58
1:A:690:ALA:HA	1:A:693:LYS:HD2	1.84	0.58
2:B:79:GLU:HG2	2:B:95:ARG:HH22	1.68	0.58
2:B:205:ILE:HD11	2:B:303:LEU:H	1.67	0.58
3:C:229:VAL:HG22	3:C:230:GLY:H	1.68	0.58
3:C:298:LEU:HD13	3:C:298:LEU:H	1.68	0.58
3:C:313:THR:HG22	3:C:318:ILE:HG22	1.85	0.58
10:N:7:CYS:SG	10:N:8:PHE:N	2.76	0.58
1:I:147:CYS:H	1:I:152:ALA:CB	2.16	0.58
2:J:395:ARG:CD	2:J:398:ILE:HD11	2.32	0.58
2:J:470:GLU:OE2	2:J:482:ASN:ND2	2.35	0.58
3:M:119:TYR:HD2	3:M:263:ARG:HD2	1.68	0.58
3:M:128:ARG:HG3	3:M:241:TYR:CE2	2.38	0.58
3:M:331:ALA:H	3:M:336:ARG:HH12	1.51	0.58
1:A:444:PRO:HD3	9:L:50:THR:HG22	1.83	0.58
2:B:1122:ARG:HG3	5:E:60:VAL:HG21	1.84	0.58
4:D:160:HIS:ND1	4:D:188:GLU:OE1	2.27	0.58
4:O:16:PHE:CE1	4:O:222:PHE:HB2	2.38	0.58
1:I:95:VAL:HG22	1:I:201:LEU:HD23	1.83	0.58
1:I:783:TYR:CE1	2:J:461:THR:HG22	2.38	0.58
2:J:801:PHE:HB2	11:W:40:PRO:HD3	1.84	0.58
4:O:145:LYS:NZ	11:W:48:ALA:O	2.35	0.58
3:C:191:PHE:HD2	3:C:198:LEU:HD13	1.68	0.58
1:I:100:CYS:CB	1:I:103:CYS:CB	2.80	0.58
1:I:163:THR:HB	1:I:276:GLN:HE21	1.69	0.58
1:I:870:PHE:CE2	7:S:76:TYR:HD2	2.21	0.58
3:M:143:LEU:HB2	3:M:222:ARG:HG3	1.84	0.58
3:M:358:LEU:CD1	14:M:401:HOH:O	2.51	0.58
1:A:875:ASP:HB3	7:H:70:ALA:HB2	1.85	0.58
2:J:45:GLY:O	2:J:46:LEU:CB	2.50	0.58
2:J:508:VAL:O	2:J:513:ARG:NH1	2.36	0.58
3:M:148:ARG:H	3:M:148:ARG:HD3	1.68	0.58
1:A:105:ARG:HH21	1:A:148:PRO:HB2	1.69	0.58
2:B:766:ARG:HG2	2:B:772:LYS:HG2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:343:THR:OG1	3:C:344:GLN:N	2.35	0.58
3:M:55:LYS:HE2	8:T:3:ARG:HH22	1.67	0.58
1:A:497:GLY:O	1:A:884:GLN:NE2	2.36	0.58
2:B:151:ASP:HB3	2:B:684:ALA:HB3	1.85	0.58
1:I:103:CYS:CB	1:I:150:CYS:SG	2.91	0.58
1:I:449:ARG:NH2	9:U:49:ILE:CD1	2.66	0.58
2:J:513:ARG:HG2	2:J:514:ARG:N	2.17	0.58
3:M:154:ILE:HD12	3:M:154:ILE:H	1.69	0.58
3:M:229:VAL:HG22	3:M:230:GLY:H	1.69	0.58
1:A:163:THR:HB	1:A:276:GLN:HE21	1.68	0.58
2:B:789:LYS:HD2	1:I:37:ASP:OD1	2.03	0.58
10:N:19:TYR:HD1	10:N:20:GLU:H	1.52	0.58
3:M:312:MET:HA	3:M:326:ILE:HD11	1.86	0.58
2:J:79:GLU:HG2	2:J:95:ARG:HH22	1.68	0.58
3:M:358:LEU:HD11	14:M:401:HOH:O	2.04	0.58
2:B:378:TYR:HE1	2:B:389:ASN:N	2.00	0.58
9:L:46:GLU:OE2	9:L:56:ARG:CD	2.51	0.58
3:C:157:MET:HA	3:C:157:MET:CE	2.33	0.57
3:M:147:ALA:O	3:M:167:ARG:NH2	2.37	0.57
4:O:151:VAL:HG22	4:O:224:VAL:HG22	1.84	0.57
10:V:19:TYR:HD1	10:V:20:GLU:H	1.52	0.57
1:A:13:PHE:CE1	2:B:1115:PRO:HB3	2.39	0.57
3:C:128:ARG:HG3	3:C:241:TYR:CE2	2.39	0.57
3:C:161:VAL:HB	3:C:198:LEU:CA	2.33	0.57
4:D:47:PHE:N	11:P:44:ARG:O	2.34	0.57
5:E:1:MET:HE3	6:F:11:TYR:CE1	2.24	0.57
10:V:2:ILE:HD11	10:V:56:ILE:HD12	1.85	0.57
2:B:803:GLU:OE2	2:B:871:ARG:NH2	2.36	0.57
3:C:177:LYS:HA	3:C:180:ARG:HB2	1.85	0.57
1:I:74:PHE:CE1	1:I:222:PRO:HD3	2.38	0.57
1:I:284:ASN:HB3	1:I:287:THR:HG23	1.86	0.57
3:M:182:LEU:HD23	3:M:185:SER:HB2	1.75	0.57
5:Q:48:ILE:HD13	5:Q:74:VAL:HG13	1.86	0.57
2:B:237:LEU:HD22	2:B:242:GLU:HB3	1.85	0.57
2:B:749:ARG:HE	4:D:144:ALA:HB1	1.68	0.57
3:C:147:ALA:O	3:C:167:ARG:NH2	2.37	0.57
3:C:216:GLU:HA	3:C:220:LYS:CB	2.33	0.57
4:D:226:THR:OG1	4:D:227:ASN:N	2.29	0.57
2:J:237:LEU:HD22	2:J:242:GLU:HB3	1.85	0.57
3:M:298:LEU:HD13	3:M:298:LEU:H	1.68	0.57
5:Q:49:LEU:N	5:Q:73:ASN:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:159:PHE:HB3	1:I:166:TRP:HE3	1.69	0.57
3:M:262:THR:HG22	7:S:12:HIS:CG	2.38	0.57
2:B:731:TYR:HE2	2:B:902:PRO:HG3	1.69	0.57
8:K:12:ILE:HD11	8:K:53:VAL:HG23	1.87	0.57
1:I:146:VAL:HA	1:I:152:ALA:HB3	1.86	0.57
1:I:156:PRO:HB3	1:I:169:ARG:HA	1.87	0.57
1:I:858:GLY:O	1:I:871:LYS:HA	2.05	0.57
2:J:38:TYR:C	2:J:41:PHE:HB3	2.23	0.57
2:J:151:ASP:HB3	2:J:684:ALA:HB3	1.86	0.57
3:M:217:LYS:HD2	3:M:217:LYS:N	2.19	0.57
2:B:378:TYR:OH	2:B:388:GLU:CA	2.48	0.57
3:C:161:VAL:HB	3:C:198:LEU:HA	1.87	0.57
1:I:105:ARG:HH21	1:I:148:PRO:HB2	1.69	0.57
1:I:326:PHE:N	2:J:1052:ARG:HH12	2.03	0.57
1:I:527:GLU:OE2	9:U:41:ALA:N	2.37	0.57
2:J:395:ARG:CB	2:J:398:ILE:CD1	2.83	0.57
2:J:803:GLU:OE2	2:J:871:ARG:NH2	2.36	0.57
2:J:816:THR:HB	2:J:836:ARG:HH21	1.70	0.57
8:T:12:ILE:HD11	8:T:53:VAL:HG23	1.87	0.57
10:N:56:ILE:O	10:N:60:MET:HG3	2.05	0.57
1:A:284:ASN:HB3	1:A:287:THR:HG23	1.86	0.57
1:A:640:GLU:HG2	1:A:896:ARG:HH12	1.68	0.57
1:A:709:LEU:HB2	1:A:717:THR:HG22	1.87	0.57
5:E:92:MET:CE	5:E:127:PHE:HD2	2.05	0.57
2:B:816:THR:HB	2:B:836:ARG:HH21	1.70	0.57
3:C:114:PRO:HG2	3:C:247:GLY:HA2	1.86	0.57
4:D:50:ASN:H	11:P:39:ARG:HD3	1.70	0.57
1:A:750:MET:HA	1:A:753:THR:HG21	1.87	0.56
1:A:885:GLY:HA2	3:C:303:ARG:HH12	1.70	0.56
1:I:445:TYR:CZ	9:U:49:ILE:HG22	2.40	0.56
1:I:635:ASP:O	1:I:639:ARG:HG3	2.05	0.56
1:I:709:LEU:HB2	1:I:717:THR:HG22	1.87	0.56
2:J:211:LYS:HA	3:M:212:ARG:HH21	1.70	0.56
1:A:858:GLY:O	1:A:871:LYS:HA	2.05	0.56
3:C:153:ASP:OD1	3:C:159:TYR:HA	2.05	0.56
1:I:105:ARG:NH2	1:I:148:PRO:HB2	2.20	0.56
1:I:356:PRO:HG3	1:I:473:GLN:HB3	1.87	0.56
1:I:624:LYS:O	1:I:632:LYS:HB3	2.05	0.56
2:J:688:ILE:HD11	10:V:62:TYR:CD1	2.40	0.56
2:J:747:ILE:HG23	2:J:876:PRO:HG2	1.88	0.56
4:O:119:PRO:HD2	10:V:15:ALA:HB1	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:864:LYS:HG3	11:P:25:VAL:HG11	1.88	0.56
3:C:92:ILE:HG13	3:C:93:ASN:H	1.70	0.56
4:D:28:ALA:HB1	4:D:243:LEU:HD21	1.87	0.56
2:J:58:PRO:HG2	2:J:60:ILE:O	2.05	0.56
2:J:766:ARG:HG2	2:J:772:LYS:HG2	1.87	0.56
2:J:1088:GLU:OE2	5:Q:40:ARG:HB2	2.05	0.56
3:M:214:ILE:C	3:M:216:GLU:H	2.08	0.56
10:V:22:LYS:NZ	10:V:54:GLU:HG2	2.21	0.56
1:A:74:PHE:CE1	1:A:222:PRO:HD3	2.40	0.56
1:A:769:LEU:HB2	1:A:804:VAL:HG21	1.87	0.56
2:B:58:PRO:HG2	2:B:60:ILE:O	2.05	0.56
2:B:899:GLU:OE1	2:B:899:GLU:N	2.32	0.56
3:C:119:TYR:CD2	3:C:263:ARG:HB3	2.41	0.56
3:C:119:TYR:HD2	3:C:263:ARG:HB3	1.70	0.56
3:C:162:GLU:O	3:C:196:TYR:HA	2.05	0.56
3:C:312:MET:HA	3:C:326:ILE:HD11	1.86	0.56
2:J:1063:TRP:NE1	2:J:1074:GLU:OE1	2.39	0.56
2:J:1122:ARG:HD2	6:R:4:ARG:NH2	2.21	0.56
1:A:150:CYS:SG	1:A:153:PRO:HD3	2.45	0.56
2:B:65:VAL:HG11	2:B:395:ARG:HH12	1.71	0.56
3:C:160:VAL:HG21	3:C:198:LEU:HD23	1.86	0.56
4:O:28:ALA:HB1	4:O:243:LEU:HD21	1.87	0.56
1:A:150:CYS:O	1:A:151:GLY:C	2.44	0.56
2:B:854:VAL:HG13	2:B:868:VAL:HG22	1.87	0.56
2:B:76:GLU:HG2	2:B:86:PRO:HA	1.88	0.56
2:B:747:ILE:HG23	2:B:876:PRO:HG2	1.88	0.56
3:C:153:ASP:HB2	3:C:158:GLU:C	2.26	0.56
1:I:112:GLU:O	1:I:116:TYR:HB2	2.06	0.56
1:I:309:LYS:HE3	3:M:347:PHE:HB2	1.88	0.56
1:I:513:LEU:HD13	1:I:664:LYS:HZ2	1.71	0.56
1:I:632:LYS:HD3	1:I:633:LEU:H	1.71	0.56
2:J:986:ASP:C	2:J:987:ILE:HD13	2.26	0.56
2:J:1042:GLY:O	3:M:70:GLN:NE2	2.35	0.56
3:M:55:LYS:HG2	8:T:3:ARG:HH21	1.70	0.56
1:A:112:GLU:O	1:A:116:TYR:HB2	2.05	0.56
1:A:387:PRO:HD3	1:A:410:TRP:CD1	2.41	0.56
2:B:959:LYS:HA	4:D:201:ARG:NH2	2.21	0.56
3:M:111:PRO:HG3	3:M:268:ASN:HA	1.88	0.56
1:A:159:PHE:HB3	1:A:166:TRP:HE3	1.69	0.56
2:B:206:THR:OG1	2:B:218:THR:OG1	2.19	0.56
2:B:683:TRP:HD1	2:B:683:TRP:O	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:22:LYS:NZ	10:N:54:GLU:HG2	2.21	0.56
2:J:521:ARG:H	2:J:531:THR:HG22	1.71	0.56
2:B:815:ARG:HD2	2:B:839:THR:HB	1.88	0.55
5:E:48:ILE:HD13	5:E:74:VAL:HG13	1.88	0.55
1:I:10:SER:HA	3:M:358:LEU:HD21	1.87	0.55
2:J:719:PRO:HG3	10:V:53:VAL:HG11	1.88	0.55
3:M:114:PRO:HG2	3:M:247:GLY:HA2	1.87	0.55
1:A:452:LEU:HD13	2:B:736:MET:SD	2.46	0.55
1:A:640:GLU:HG2	1:A:896:ARG:NH1	2.22	0.55
2:B:606:TRP:CZ2	2:B:615:ILE:HG21	2.41	0.55
3:C:181:LYS:HE3	3:C:188:SER:HB3	1.87	0.55
1:I:625:ALA:O	1:I:632:LYS:NZ	2.21	0.55
2:J:39:ASN:O	2:J:41:PHE:N	2.39	0.55
2:J:394:VAL:HG11	2:J:395:ARG:HE	1.72	0.55
2:B:227:LYS:HB2	2:B:230:TYR:CD2	2.42	0.55
2:B:967:LYS:HG3	2:B:969:SER:H	1.71	0.55
4:D:16:PHE:CE1	4:D:222:PHE:HB2	2.41	0.55
5:E:92:MET:HE3	5:E:127:PHE:CD2	2.23	0.55
2:J:854:VAL:HG13	2:J:868:VAL:HG22	1.87	0.55
5:Q:46:LEU:HD22	6:R:21:LEU:HD21	1.87	0.55
3:C:27:LYS:O	3:C:31:TYR:HB2	2.06	0.55
2:B:59:ASP:H	2:B:375:THR:HG22	1.72	0.55
2:B:449:ASP:N	2:B:449:ASP:OD1	2.39	0.55
3:C:119:TYR:HD2	3:C:263:ARG:HD2	1.70	0.55
1:I:769:LEU:HB2	1:I:804:VAL:HG21	1.87	0.55
1:I:844:ARG:NH2	3:M:106:ASP:OD2	2.39	0.55
2:J:227:LYS:HB2	2:J:230:TYR:CD2	2.42	0.55
2:J:967:LYS:HG3	2:J:969:SER:H	1.71	0.55
4:O:160:HIS:ND1	4:O:188:GLU:OE1	2.27	0.55
1:A:105:ARG:NH2	1:A:148:PRO:HB2	2.22	0.55
2:J:968:HIS:ND1	4:O:201:ARG:HG2	2.21	0.55
2:J:1063:TRP:CE2	2:J:1094:LYS:HG3	2.41	0.55
1:I:387:PRO:HD3	1:I:410:TRP:CD1	2.42	0.55
2:J:41:PHE:O	2:J:45:GLY:C	2.44	0.55
2:J:286:PRO:O	2:J:288:GLU:N	2.40	0.55
2:J:606:TRP:CZ2	2:J:615:ILE:HG21	2.42	0.55
2:J:1066:GLU:HG2	2:J:1119:LEU:HD13	1.89	0.55
1:A:106:ILE:HG23	1:A:108:LEU:HB2	1.89	0.55
1:A:513:LEU:HD13	1:A:664:LYS:HZ2	1.71	0.55
2:B:466:ILE:HG21	2:B:481:LYS:HD2	1.88	0.55
3:C:160:VAL:HG21	3:C:198:LEU:CD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:450:LEU:HD11	1:I:454:VAL:HB	1.89	0.55
1:I:640:GLU:HG2	1:I:896:ARG:HH12	1.72	0.55
2:J:449:ASP:OD1	2:J:449:ASP:N	2.39	0.55
2:J:513:ARG:HG2	2:J:514:ARG:H	1.70	0.55
2:J:815:ARG:HD2	2:J:839:THR:HB	1.89	0.55
3:M:151:THR:C	3:M:152:ILE:HG12	2.27	0.55
1:A:450:LEU:HD11	1:A:454:VAL:HB	1.89	0.55
1:A:635:ASP:O	1:A:639:ARG:HG3	2.05	0.55
2:B:878:LEU:HD23	2:B:892:ILE:HG22	1.89	0.55
1:I:856:TYR:CE1	8:T:55:ARG:HD3	2.41	0.55
2:B:95:ARG:CZ	11:P:33:LYS:HD3	2.36	0.55
2:J:76:GLU:HG2	2:J:86:PRO:HA	1.89	0.55
2:J:211:LYS:HG3	3:M:212:ARG:CZ	2.37	0.55
2:J:899:GLU:HG2	4:O:35:SER:HB3	1.89	0.55
3:M:75:PRO:HB3	3:M:298:LEU:HG	1.88	0.55
2:B:986:ASP:C	2:B:987:ILE:HD13	2.28	0.54
3:C:151:THR:CG2	3:C:152:ILE:H	2.18	0.54
1:I:783:TYR:HE1	2:J:461:THR:HG22	1.71	0.54
2:J:466:ILE:HG21	2:J:481:LYS:HD2	1.88	0.54
2:B:1063:TRP:NE1	2:B:1094:LYS:CG	2.69	0.54
1:I:585:LEU:O	1:I:586:GLU:CB	2.54	0.54
2:J:683:TRP:HD1	2:J:683:TRP:O	1.89	0.54
5:Q:8:LYS:HG3	6:R:7:LEU:HD22	1.89	0.54
7:S:43:ILE:N	7:S:78:LEU:O	2.28	0.54
2:B:183:ARG:NH1	2:B:337:GLU:OE1	2.40	0.54
3:C:181:LYS:C	3:C:183:THR:H	2.09	0.54
2:J:59:ASP:H	2:J:375:THR:HG22	1.72	0.54
2:J:183:ARG:HG3	2:J:337:GLU:CD	2.26	0.54
2:J:559:LEU:HD22	2:J:568:VAL:HG22	1.90	0.54
2:B:34:HIS:HB3	2:B:129:MET:HE1	1.88	0.54
3:C:380:LEU:HB2	5:E:59:ILE:HB	1.88	0.54
2:J:183:ARG:HB3	2:J:186:ARG:NH2	2.13	0.54
9:U:9:GLU:HB2	9:U:12:LEU:HD22	1.90	0.54
7:H:67:SER:N	7:H:71:GLY:O	2.28	0.54
2:J:42:ILE:HG22	2:J:72:ILE:CD1	2.36	0.54
2:J:1063:TRP:NE1	2:J:1094:LYS:HE3	2.23	0.54
9:U:45:ILE:HG12	9:U:55:PRO:HA	1.88	0.54
1:A:13:PHE:CE2	3:C:333:VAL:HG21	2.43	0.54
3:C:161:VAL:CG2	3:C:199:VAL:HB	2.36	0.54
1:I:106:ILE:HG23	1:I:108:LEU:HB2	1.89	0.54
1:I:578:GLU:HB3	1:I:579:PRO:HD2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:962:GLU:O	2:J:965:GLY:N	2.37	0.54
3:M:27:LYS:O	3:M:31:TYR:HB2	2.06	0.54
1:A:10:SER:HA	3:C:358:LEU:CD2	2.28	0.54
3:C:75:PRO:HB3	3:C:298:LEU:HG	1.88	0.54
4:D:50:ASN:N	11:P:39:ARG:HH11	2.05	0.54
2:J:959:LYS:HA	4:O:201:ARG:HH21	1.73	0.54
2:B:521:ARG:H	2:B:531:THR:HG22	1.72	0.54
2:B:939:LEU:HD11	2:B:966:PHE:CD2	2.39	0.54
2:B:1063:TRP:HE1	2:B:1094:LYS:CE	2.19	0.54
1:I:61:GLU:O	1:I:63:CYS:N	2.36	0.54
2:J:182:GLU:N	2:J:191:VAL:O	2.39	0.54
2:J:391:GLN:C	2:J:392:ARG:HG3	2.26	0.54
1:A:361:GLU:HG2	1:A:408:ILE:HD11	1.90	0.54
1:A:867:ILE:HD13	1:A:870:PHE:HE1	1.73	0.54
3:C:111:PRO:HG3	3:C:268:ASN:HA	1.89	0.54
1:I:609:VAL:HG13	1:I:619:GLY:HA3	1.90	0.54
1:I:842:GLN:NE2	3:M:70:GLN:HA	2.23	0.54
9:U:50:THR:O	9:U:51:MET:HB2	2.08	0.54
1:A:308:LEU:HD12	1:A:309:LYS:HG3	1.89	0.54
2:B:227:LYS:HB2	2:B:230:TYR:HD2	1.73	0.54
2:B:793:HIS:NE2	2:B:805:LYS:O	2.41	0.54
1:I:397:SER:OG	1:I:398:ASN:N	2.40	0.54
1:I:837:GLN:HB3	3:M:102:ILE:HD11	1.90	0.54
2:J:793:HIS:NE2	2:J:805:LYS:O	2.40	0.54
3:M:153:ASP:CG	3:M:157:MET:HB2	2.28	0.54
3:M:279:GLU:HG3	7:S:63:ILE:HG21	1.90	0.54
1:A:396:GLU:HB3	1:I:40:TYR:OH	2.08	0.53
9:L:9:GLU:HB2	9:L:12:LEU:HD22	1.90	0.53
1:I:326:PHE:HB2	2:J:1052:ARG:HH22	1.73	0.53
2:J:438:HIS:HD2	2:J:441:ARG:HE	1.55	0.53
3:M:262:THR:HG22	7:S:12:HIS:CD2	2.43	0.53
1:A:8:ILE:HD13	3:C:367:ILE:HD11	1.90	0.53
1:A:326:PHE:HA	2:B:1008:ARG:O	2.09	0.53
2:B:183:ARG:HB2	2:B:186:ARG:NH2	2.14	0.53
2:B:286:PRO:O	2:B:288:GLU:N	2.40	0.53
3:C:191:PHE:CD2	3:C:198:LEU:HD22	2.43	0.53
10:N:56:ILE:O	10:N:60:MET:HE3	2.08	0.53
1:A:397:SER:OG	1:A:398:ASN:N	2.41	0.53
2:B:1066:GLU:HG2	2:B:1119:LEU:HD13	1.91	0.53
2:J:878:LEU:HD23	2:J:892:ILE:HG22	1.90	0.53
2:J:1076:LYS:O	2:J:1078:ARG:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:266:THR:HG22	3:M:268:ASN:H	1.73	0.53
1:A:49:LYS:HG3	1:A:50:ARG:HH21	1.74	0.53
2:B:182:GLU:N	2:B:191:VAL:O	2.40	0.53
3:C:266:THR:HG22	3:C:268:ASN:H	1.73	0.53
3:C:369:GLN:HG3	3:C:370:PRO:HD2	1.90	0.53
11:P:11:CYS:SG	11:P:30:CYS:SG	3.05	0.53
2:J:800:ILE:HD11	2:J:812:LEU:HD23	1.90	0.53
1:A:667:THR:HG23	2:B:971:ARG:HH21	1.73	0.53
3:C:192:GLU:OE1	3:C:197:THR:HG23	2.09	0.53
3:C:194:GLU:C	3:C:196:TYR:H	2.11	0.53
11:W:47:LYS:HB3	11:W:49:ILE:HG13	1.90	0.53
1:A:8:ILE:HG13	2:B:1095:VAL:HG11	1.91	0.53
1:A:127:LYS:HB2	3:C:330:LYS:HB3	1.91	0.53
2:B:299:ASP:HB3	2:B:308:VAL:O	2.09	0.53
2:B:392:ARG:HG2	2:B:392:ARG:O	2.07	0.53
3:C:161:VAL:CG1	3:C:162:GLU:H	2.05	0.53
4:D:3:GLU:HG3	4:D:19:SER:HB2	1.91	0.53
4:D:143:HIS:NE2	11:P:49:ILE:O	2.41	0.53
1:I:462:PHE:O	1:I:464:GLY:N	2.42	0.53
2:J:227:LYS:HB2	2:J:230:TYR:HD2	1.73	0.53
2:J:939:LEU:HD11	2:J:966:PHE:CD2	2.39	0.53
2:J:1122:ARG:HH11	6:R:4:ARG:NH2	2.07	0.53
1:A:156:PRO:HG3	1:A:169:ARG:HG3	1.90	0.53
1:A:194:PRO:HB2	1:A:196:LYS:HD2	1.91	0.53
1:A:329:ARG:O	2:B:1005:MET:HA	2.08	0.53
1:A:609:VAL:HG13	1:A:619:GLY:HA3	1.91	0.53
2:B:65:VAL:HG21	2:B:395:ARG:HH12	1.74	0.53
3:M:375:THR:O	3:M:378:VAL:HG12	2.09	0.53
1:A:462:PHE:O	1:A:464:GLY:N	2.40	0.53
2:B:273:ALA:HA	2:B:276:TYR:CD2	2.44	0.53
2:B:438:HIS:HD2	2:B:441:ARG:HE	1.55	0.53
2:B:800:ILE:HD11	2:B:812:LEU:HD23	1.90	0.53
2:B:962:GLU:O	2:B:965:GLY:N	2.38	0.53
2:B:1054:LEU:HD22	2:B:1059:LYS:HE3	1.91	0.53
4:D:62:ARG:HH12	10:N:2:ILE:HD12	1.74	0.53
1:I:665:GLY:C	2:J:729:LEU:CD1	2.75	0.53
2:J:299:ASP:HB3	2:J:308:VAL:O	2.09	0.53
1:A:404:GLU:O	1:A:406:LEU:N	2.41	0.53
1:I:194:PRO:HB2	1:I:196:LYS:HD2	1.91	0.53
1:I:344:GLY:HA3	1:I:449:ARG:HB2	1.91	0.53
1:I:444:PRO:CD	9:U:50:THR:CG2	2.78	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:959:LYS:HA	4:O:201:ARG:NH2	2.24	0.53
2:J:968:HIS:CD2	2:J:968:HIS:C	2.82	0.53
2:J:1054:LEU:HD22	2:J:1059:LYS:HE3	1.91	0.53
2:B:390:ILE:C	2:B:392:ARG:N	2.60	0.53
3:C:348:ALA:O	3:C:351:GLU:HG2	2.08	0.53
9:L:52:ALA:C	9:L:54:LYS:H	2.13	0.53
2:J:273:ALA:HA	2:J:276:TYR:CD2	2.44	0.53
2:J:392:ARG:C	2:J:394:VAL:N	2.63	0.53
3:M:153:ASP:CB	3:M:157:MET:CB	2.87	0.53
3:M:216:GLU:O	3:M:221:HIS:N	2.42	0.53
3:C:262:THR:HG22	7:H:12:HIS:CG	2.44	0.52
1:I:361:GLU:HG2	1:I:408:ILE:HD11	1.90	0.52
2:J:116:GLN:CD	2:J:393:PHE:CD1	2.69	0.52
4:O:3:GLU:HG3	4:O:19:SER:HB2	1.91	0.52
1:A:264:PRO:HB2	1:A:267:ILE:HD13	1.91	0.52
1:A:753:THR:CG2	1:A:754:GLY:H	2.09	0.52
1:A:808:TYR:HE2	2:B:923:MET:SD	2.32	0.52
2:B:559:LEU:HD22	2:B:568:VAL:HG22	1.90	0.52
2:B:1063:TRP:CE3	2:B:1074:GLU:HG2	2.44	0.52
1:I:633:LEU:O	1:I:636:ILE:HG12	2.10	0.52
1:I:867:ILE:HD11	7:S:40:LEU:HD22	1.91	0.52
2:J:729:LEU:HD23	2:J:730:SER:N	2.24	0.52
2:J:749:ARG:HE	4:O:144:ALA:HB1	1.74	0.52
3:M:153:ASP:OD2	3:M:157:MET:HG3	2.09	0.52
3:M:156:ASN:O	3:M:158:GLU:HG2	2.09	0.52
1:A:156:PRO:HB3	1:A:169:ARG:HA	1.90	0.52
1:A:630:ASP:HB2	1:A:632:LYS:HE2	1.92	0.52
3:C:178:VAL:O	3:C:181:LYS:HB3	2.09	0.52
4:D:62:ARG:HH22	10:N:2:ILE:HB	1.73	0.52
1:A:344:GLY:HA3	1:A:449:ARG:HB2	1.91	0.52
1:I:264:PRO:HB2	1:I:267:ILE:HD13	1.91	0.52
3:M:369:GLN:HG3	3:M:370:PRO:HD2	1.92	0.52
4:O:163:LYS:HG2	4:O:168:TRP:CE2	2.44	0.52
5:Q:82:GLN:HB3	6:R:98:LYS:HG3	1.90	0.52
2:B:94:ILE:HG21	11:P:34:ILE:HG12	1.90	0.52
2:B:373:GLN:HG2	2:B:397:SER:HB2	1.91	0.52
3:C:73:GLY:O	3:C:76:SER:OG	2.27	0.52
3:C:192:GLU:HG3	3:C:197:THR:OG1	2.10	0.52
4:D:163:LYS:HG2	4:D:168:TRP:CE2	2.44	0.52
3:M:197:THR:HG22	3:M:198:LEU:N	2.24	0.52
3:M:322:GLY:O	3:M:324:HIS:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:62:ARG:HH22	10:V:2:ILE:HB	1.72	0.52
2:B:467:CYS:SG	2:B:470:GLU:HB2	2.49	0.52
2:B:702:VAL:HG23	10:N:53:VAL:CG1	2.40	0.52
2:B:1063:TRP:CE3	2:B:1074:GLU:CG	2.93	0.52
1:I:852:LEU:HD11	3:M:311:MET:HG3	1.91	0.52
2:J:373:GLN:CG	2:J:397:SER:HB2	2.40	0.52
2:J:462:HIS:HB3	2:J:466:ILE:HB	1.92	0.52
3:M:348:ALA:O	3:M:351:GLU:HG2	2.10	0.52
1:A:187:ARG:NE	1:A:211:GLU:O	2.42	0.52
1:A:872:TYR:CE1	3:C:64:VAL:HG11	2.45	0.52
3:C:148:ARG:HD3	3:C:148:ARG:N	2.25	0.52
3:C:160:VAL:HG22	3:C:198:LEU:HG	1.91	0.52
5:E:2:TYR:HH	6:F:44:SER:HG	1.54	0.52
1:I:156:PRO:HG3	1:I:169:ARG:HG3	1.92	0.52
1:I:842:GLN:HE21	3:M:70:GLN:HA	1.75	0.52
2:J:467:CYS:SG	2:J:470:GLU:HB2	2.50	0.52
2:J:962:GLU:HA	2:J:966:PHE:O	2.09	0.52
1:A:295:HIS:O	1:A:297:SER:N	2.43	0.52
2:B:557:VAL:HG22	2:B:570:ILE:HG23	1.92	0.52
2:B:782:ILE:HG22	2:B:783:GLN:H	1.74	0.52
2:B:888:GLN:NE2	2:B:918:GLY:O	2.43	0.52
3:C:104:ILE:HD13	3:C:289:ILE:HG12	1.92	0.52
3:C:161:VAL:H	3:C:199:VAL:H	1.56	0.52
1:I:431:HIS:HA	3:M:70:GLN:HB3	1.91	0.52
2:J:731:TYR:CE2	2:J:902:PRO:HG3	2.44	0.52
3:M:152:ILE:HG23	3:M:160:VAL:N	2.23	0.52
9:U:49:ILE:C	9:U:50:THR:HG1	2.00	0.52
2:B:395:ARG:O	2:B:397:SER:N	2.41	0.52
3:C:155:LEU:CD2	3:C:156:ASN:ND2	2.73	0.52
2:J:41:PHE:CE2	2:J:356:LYS:HG2	2.45	0.52
2:J:730:SER:HB3	2:J:915:ASN:ND2	2.25	0.52
2:B:808:GLY:O	2:B:843:VAL:HG12	2.10	0.52
2:B:968:HIS:CD2	2:B:968:HIS:C	2.82	0.52
3:C:196:TYR:O	3:C:198:LEU:HD12	2.10	0.52
3:C:322:GLY:O	3:C:324:HIS:N	2.42	0.52
1:I:834:ARG:HD2	3:M:98:LEU:HD13	1.92	0.52
2:J:469:THR:HG21	2:J:668:ASN:HB3	1.92	0.52
2:J:1122:ARG:CD	6:R:4:ARG:NH2	2.72	0.52
1:A:195:ASP:HB3	1:A:205:PRO:HB3	1.92	0.51
2:B:462:HIS:HB3	2:B:466:ILE:HB	1.91	0.51
2:B:467:CYS:SG	2:B:651:GLY:N	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:11:CYS:SG	11:P:14:GLU:OE2	2.68	0.51
1:I:150:CYS:HB3	1:I:153:PRO:HD3	1.92	0.51
1:I:445:TYR:HB2	1:I:449:ARG:NH2	2.25	0.51
2:J:107:MET:CA	2:J:395:ARG:HH22	2.20	0.51
2:J:557:VAL:HG22	2:J:570:ILE:HG23	1.92	0.51
2:J:888:GLN:NE2	2:J:918:GLY:O	2.43	0.51
1:A:508:ILE:HG21	1:A:754:GLY:O	2.10	0.51
2:B:1048:LEU:O	2:B:1051:GLU:HB3	2.10	0.51
3:C:160:VAL:CG2	3:C:198:LEU:CB	2.88	0.51
3:C:203:LYS:HB2	3:C:203:LYS:NZ	2.23	0.51
3:C:358:LEU:CD1	3:C:359:ASN:H	2.23	0.51
1:I:309:LYS:CE	3:M:347:PHE:HB2	2.40	0.51
1:I:849:LEU:O	3:M:65:GLY:HA3	2.09	0.51
2:J:361:VAL:O	2:J:365:GLN:HG2	2.10	0.51
3:M:104:ILE:HD13	3:M:289:ILE:HG12	1.92	0.51
7:S:67:SER:N	7:S:71:GLY:O	2.26	0.51
1:A:356:PRO:HG3	1:A:473:GLN:HB3	1.90	0.51
2:B:1063:TRP:O	2:B:1072:ALA:N	2.35	0.51
3:C:124:HIS:ND1	3:C:130:LYS:HB3	2.25	0.51
3:C:187:LYS:HD3	3:C:203:LYS:HZ2	1.74	0.51
2:J:789:LYS:HE2	2:J:792:ARG:HB2	1.93	0.51
2:J:982:ARG:HD3	4:O:155:TYR:CD2	2.45	0.51
3:M:119:TYR:CD2	3:M:263:ARG:HB3	2.45	0.51
7:S:61:ILE:HG22	7:S:63:ILE:HG13	1.93	0.51
1:A:101:ARG:O	1:A:102:GLU:HB2	2.10	0.51
2:B:361:VAL:O	2:B:365:GLN:HG2	2.11	0.51
2:B:390:ILE:HD12	2:B:391:GLN:HB2	1.92	0.51
2:B:962:GLU:HA	2:B:966:PHE:O	2.09	0.51
3:C:216:GLU:C	3:C:220:LYS:HB3	2.31	0.51
3:C:217:LYS:O	3:C:218:VAL:HB	2.10	0.51
5:E:9:ASP:OD1	6:F:4:ARG:HG2	2.09	0.51
2:J:414:GLY:O	2:J:422:GLY:N	2.44	0.51
2:J:782:ILE:HG22	2:J:783:GLN:H	1.74	0.51
3:M:124:HIS:ND1	3:M:130:LYS:HB3	2.25	0.51
1:A:99:THR:HG21	1:A:193:ILE:HD11	1.93	0.51
1:A:783:TYR:HE2	1:A:789:THR:HB	1.74	0.51
2:B:389:ASN:HD22	2:B:392:ARG:CB	2.19	0.51
3:C:216:GLU:HA	3:C:220:LYS:HB2	1.93	0.51
3:C:375:THR:O	3:C:378:VAL:HG12	2.10	0.51
5:E:81:ASN:C	5:E:82:GLN:HG2	2.31	0.51
7:H:61:ILE:HG22	7:H:63:ILE:HG13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:187:LYS:NZ	3:M:201:ARG:HB3	2.26	0.51
9:U:51:MET:CA	9:U:52:ALA:HB3	2.41	0.51
1:I:49:LYS:HG3	1:I:50:ARG:HH21	1.75	0.51
1:I:445:TYR:CE1	9:U:49:ILE:HG21	2.46	0.51
1:A:113:ILE:HG23	1:A:200:LEU:HD11	1.93	0.51
2:B:812:LEU:HD11	2:B:843:VAL:HG23	1.93	0.51
5:E:39:ASP:O	5:E:43:GLY:N	2.43	0.51
1:I:113:ILE:HG23	1:I:200:LEU:HD11	1.92	0.51
1:I:867:ILE:HD13	1:I:870:PHE:HE1	1.76	0.51
2:B:885:ARG:HD2	2:B:993:TYR:HB3	1.92	0.51
3:C:161:VAL:HG21	3:C:199:VAL:HG23	0.51	0.51
10:N:10:CYS:O	10:N:12:LYS:HG2	2.10	0.51
10:N:56:ILE:C	10:N:60:MET:HE3	2.31	0.51
2:J:885:ARG:HD2	2:J:993:TYR:HB3	1.92	0.51
3:M:119:TYR:HD2	3:M:263:ARG:HB3	1.76	0.51
2:B:899:GLU:HG2	4:D:35:SER:HB3	1.92	0.51
4:D:26:ALA:HB1	4:D:222:PHE:HZ	1.76	0.51
1:I:308:LEU:HD12	1:I:309:LYS:HG3	1.93	0.51
1:I:544:ASP:OD2	1:I:551:PRO:HB2	2.11	0.51
2:J:459:HIS:ND1	2:J:461:THR:HG23	2.26	0.51
3:M:186:PHE:O	3:M:187:LYS:HB3	2.11	0.51
4:O:26:ALA:HB1	4:O:222:PHE:HZ	1.74	0.51
5:E:42:GLU:HG3	6:F:2:ILE:HG12	1.92	0.51
1:I:531:MET:CB	9:U:44:THR:CG2	2.85	0.51
2:J:378:TYR:HE1	2:J:388:GLU:CG	1.93	0.51
2:J:899:GLU:OE1	2:J:899:GLU:N	2.32	0.51
7:S:25:GLU:O	7:S:29:LEU:HB2	2.11	0.51
10:V:2:ILE:HG12	10:V:56:ILE:HG21	1.93	0.51
1:A:21:ILE:HD11	2:B:1112:VAL:HG23	1.92	0.50
1:A:61:GLU:O	1:A:63:CYS:N	2.36	0.50
2:B:326:LYS:HD2	2:B:335:ARG:HE	1.76	0.50
2:B:554:VAL:HA	2:B:578:ARG:HH12	1.76	0.50
2:B:607:SER:O	2:B:610:ILE:HG13	2.12	0.50
2:B:789:LYS:HE2	2:B:792:ARG:HB2	1.92	0.50
3:C:279:GLU:HG3	7:H:63:ILE:HG21	1.93	0.50
4:D:171:LEU:HD21	4:D:200:PRO:HD2	1.93	0.50
5:E:6:LYS:O	6:F:7:LEU:HD23	2.10	0.50
5:E:8:LYS:HG3	6:F:7:LEU:HD22	1.93	0.50
1:I:101:ARG:O	1:I:102:GLU:HB2	2.11	0.50
2:J:352:GLY:O	2:J:356:LYS:HG3	2.12	0.50
3:M:148:ARG:HD3	3:M:148:ARG:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:ILE:HG12	2:B:105:LEU:HG	1.94	0.50
2:B:458:LEU:HD11	2:B:468:PRO:HA	1.93	0.50
2:B:1063:TRP:CZ2	2:B:1094:LYS:CE	2.89	0.50
1:I:83:VAL:HG13	1:I:276:GLN:OE1	2.10	0.50
2:J:70:ILE:HG12	2:J:105:LEU:HG	1.94	0.50
2:J:458:LEU:HD11	2:J:468:PRO:HA	1.92	0.50
3:M:337:ALA:HA	3:M:346:LEU:HB2	1.93	0.50
6:R:18:LYS:HD2	6:R:49:GLU:HA	1.94	0.50
1:A:578:GLU:HB3	1:A:579:PRO:HD2	1.92	0.50
1:A:755:ALA:HB1	2:B:917:HIS:CD2	2.46	0.50
2:B:429:ARG:HB3	2:B:683:TRP:HZ3	1.76	0.50
2:J:429:ARG:HB3	2:J:683:TRP:HZ3	1.76	0.50
2:J:1042:GLY:C	3:M:70:GLN:HE22	2.13	0.50
3:M:38:LYS:HG2	3:M:41:GLU:HG3	1.92	0.50
3:M:178:VAL:HB	3:M:190:GLU:OE2	2.10	0.50
2:B:63:PHE:CG	2:B:392:ARG:NH2	2.80	0.50
2:B:312:ASN:HD22	2:B:312:ASN:H	1.59	0.50
2:B:1087:GLY:O	2:B:1089:ASP:N	2.32	0.50
3:C:38:LYS:HG2	3:C:41:GLU:HG3	1.92	0.50
5:E:15:PRO:HB2	8:K:24:ALA:HB2	1.92	0.50
1:I:9:GLY:HA3	2:J:1120:LYS:CB	2.39	0.50
2:J:24:TYR:HB2	2:J:606:TRP:NE1	2.27	0.50
1:A:633:LEU:O	1:A:636:ILE:HG12	2.11	0.50
2:B:50:VAL:HG11	2:B:70:ILE:HG13	1.93	0.50
2:B:390:ILE:CG1	2:B:391:GLN:H	2.24	0.50
1:I:308:LEU:HD13	3:M:346:LEU:HD11	1.93	0.50
1:I:359:VAL:HG22	1:I:408:ILE:HA	1.94	0.50
2:J:192:ALA:HB3	2:J:207:VAL:HG23	1.94	0.50
2:J:373:GLN:HG2	2:J:397:SER:HB2	1.93	0.50
2:J:779:SER:O	2:J:781:ASN:N	2.44	0.50
4:O:171:LEU:HD21	4:O:200:PRO:HD2	1.94	0.50
1:A:63:CYS:O	1:A:65:ALA:N	2.45	0.50
1:A:81:ARG:HG3	1:A:82:PRO:HD2	1.94	0.50
2:B:464:GLY:HA3	2:B:579:ARG:HD3	1.94	0.50
2:B:708:ARG:H	2:B:947:THR:HG1	1.56	0.50
1:I:187:ARG:NE	1:I:211:GLU:O	2.42	0.50
1:I:505:GLN:OE1	2:J:737:GLU:N	2.40	0.50
2:J:724:PHE:CD1	2:J:994:TYR:HB2	2.47	0.50
2:J:808:GLY:O	2:J:843:VAL:HG12	2.10	0.50
2:B:378:TYR:OH	2:B:388:GLU:CB	2.60	0.50
2:B:803:GLU:O	11:P:44:ARG:NE	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1062:VAL:HG11	2:B:1071:LEU:HD13	1.94	0.50
1:I:204:HIS:ND1	1:I:205:PRO:HD2	2.27	0.50
2:J:312:ASN:HD22	2:J:312:ASN:H	1.60	0.50
2:B:469:THR:HG21	2:B:668:ASN:HB3	1.93	0.50
7:H:25:GLU:O	7:H:29:LEU:HB2	2.11	0.50
1:I:99:THR:HG21	1:I:193:ILE:HD11	1.93	0.50
1:I:195:ASP:HB3	1:I:205:PRO:HB3	1.92	0.50
1:I:238:GLU:HG2	1:I:242:THR:HB	1.94	0.50
2:J:368:LYS:O	2:J:371:GLN:HB3	2.12	0.50
2:J:464:GLY:HA3	2:J:579:ARG:HD3	1.94	0.50
2:J:856:VAL:HG22	2:J:866:VAL:HG22	1.94	0.50
2:J:1062:VAL:HG11	2:J:1071:LEU:HD13	1.93	0.50
5:Q:3:LYS:HD2	6:R:11:TYR:CE1	2.47	0.50
5:Q:146:ILE:HA	5:Q:163:MET:HG2	1.94	0.50
9:U:51:MET:HA	9:U:52:ALA:CB	2.41	0.50
2:B:24:TYR:HB2	2:B:606:TRP:NE1	2.27	0.50
2:B:111:VAL:O	2:B:114:ILE:HG12	2.11	0.50
3:C:121:ASP:OD1	3:C:123:GLU:HG2	2.12	0.50
3:C:162:GLU:HB3	3:C:163:ILE:HD13	1.94	0.50
1:I:891:ASP:OD1	1:I:891:ASP:N	2.42	0.50
2:J:326:LYS:HD2	2:J:335:ARG:HE	1.76	0.50
2:J:659:TYR:HB3	2:J:662:HIS:CD2	2.47	0.50
2:J:812:LEU:HD11	2:J:843:VAL:HG23	1.92	0.50
4:O:178:ARG:NH2	4:O:196:ALA:O	2.28	0.50
7:S:66:LYS:HG2	7:S:72:TYR:CE1	2.47	0.50
1:A:204:HIS:ND1	1:A:205:PRO:HD2	2.27	0.49
1:A:449:ARG:NH2	2:B:878:LEU:HD12	2.27	0.49
2:B:579:ARG:NH2	2:B:623:GLU:OE2	2.44	0.49
2:B:606:TRP:O	2:B:609:LEU:HB2	2.12	0.49
2:B:779:SER:O	2:B:781:ASN:N	2.44	0.49
2:B:856:VAL:HG22	2:B:866:VAL:HG22	1.94	0.49
1:I:9:GLY:N	2:J:1120:LYS:HB2	2.27	0.49
1:I:44:GLY:HA2	1:I:49:LYS:HG2	1.94	0.49
1:I:493:SER:HB3	1:I:500:LEU:HB2	1.94	0.49
1:I:867:ILE:HD13	1:I:870:PHE:CE1	2.47	0.49
2:J:34:HIS:HB3	2:J:129:MET:HE1	1.94	0.49
2:J:433:MET:HE1	2:J:652:ILE:HG12	1.93	0.49
2:J:606:TRP:HZ3	2:J:617:TYR:HH	1.58	0.49
2:J:1091:ARG:HD3	2:J:1091:ARG:N	2.27	0.49
1:A:891:ASP:O	1:A:895:VAL:HG23	2.12	0.49
2:B:659:TYR:HB3	2:B:662:HIS:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:158:GLU:C	3:C:159:TYR:CD1	2.86	0.49
1:I:694:VAL:HA	1:I:697:LEU:HD12	1.94	0.49
2:J:395:ARG:CB	2:J:398:ILE:HD11	2.40	0.49
2:J:554:VAL:HA	2:J:578:ARG:HH12	1.76	0.49
2:J:729:LEU:HD22	2:J:731:TYR:CD1	2.47	0.49
1:A:83:VAL:HG13	1:A:276:GLN:OE1	2.13	0.49
1:A:105:ARG:HA	1:A:197:ASP:OD2	2.13	0.49
2:B:57:VAL:HB	2:B:58:PRO:CA	2.35	0.49
1:I:524:TYR:HD1	1:I:524:TYR:H	1.59	0.49
2:J:41:PHE:CE2	2:J:356:LYS:CG	2.95	0.49
3:M:121:ASP:OD1	3:M:123:GLU:HG2	2.12	0.49
1:A:694:VAL:HA	1:A:697:LEU:HD12	1.94	0.49
1:A:867:ILE:HD13	1:A:870:PHE:CE1	2.47	0.49
3:C:159:TYR:O	3:C:160:VAL:HB	2.12	0.49
2:J:652:ILE:HG23	2:J:653:PRO:HD3	1.94	0.49
2:J:706:ASN:HB2	2:J:710:MET:SD	2.53	0.49
1:A:245:LEU:O	1:A:249:ILE:HG13	2.13	0.49
2:B:1082:TYR:HD1	2:B:1088:GLU:H	1.59	0.49
1:I:26:ALA:HB3	1:I:51:LEU:HD23	1.95	0.49
1:A:783:TYR:CE2	1:A:789:THR:HB	2.48	0.49
3:C:262:THR:HG22	7:H:12:HIS:CD2	2.48	0.49
7:H:63:ILE:O	7:H:74:TYR:HA	2.12	0.49
1:I:245:LEU:O	1:I:249:ILE:HG13	2.12	0.49
1:I:401:LEU:HA	1:I:404:GLU:CG	2.43	0.49
1:I:630:ASP:CG	1:I:631:GLY:H	2.16	0.49
1:I:666:PHE:O	2:J:729:LEU:HA	2.12	0.49
2:J:413:THR:HG23	2:J:415:SER:H	1.77	0.49
2:J:573:ASP:OD1	2:J:573:ASP:N	2.41	0.49
2:J:1078:ARG:HG3	2:J:1080:LYS:HG2	1.94	0.49
3:M:119:TYR:CD2	3:M:263:ARG:HD2	2.48	0.49
7:S:63:ILE:O	7:S:74:TYR:HA	2.12	0.49
1:A:531:MET:C	9:L:44:THR:HG21	2.33	0.49
2:B:65:VAL:HG11	2:B:395:ARG:NH1	2.28	0.49
2:B:192:ALA:HB3	2:B:207:VAL:HG23	1.94	0.49
2:B:459:HIS:ND1	2:B:461:THR:HG23	2.28	0.49
2:B:618:LEU:HD22	2:B:622:GLU:HG2	1.95	0.49
1:I:713:THR:O	1:I:717:THR:HG23	2.12	0.49
1:I:769:LEU:HB2	1:I:804:VAL:CG2	2.43	0.49
2:J:41:PHE:CD1	2:J:42:ILE:CD1	2.96	0.49
2:J:111:VAL:O	2:J:114:ILE:HG12	2.11	0.49
2:J:467:CYS:SG	2:J:651:GLY:N	2.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:812:LEU:HD21	2:J:843:VAL:HG23	1.94	0.49
3:M:76:SER:HA	3:M:79:MET:HE3	1.94	0.49
1:A:508:ILE:HG21	1:A:754:GLY:HA3	1.93	0.49
1:A:536:ASP:HA	1:A:540:LEU:HB2	1.93	0.49
1:A:669:ALA:HB2	2:B:971:ARG:NE	2.28	0.49
1:A:713:THR:O	1:A:717:THR:HG23	2.12	0.49
2:B:520:TYR:CZ	2:B:532:VAL:HB	2.48	0.49
2:B:885:ARG:HD2	2:B:993:TYR:HD2	1.78	0.49
2:B:982:ARG:HD3	4:D:155:TYR:CD2	2.48	0.49
2:B:1063:TRP:CZ3	2:B:1074:GLU:HG2	2.46	0.49
3:C:149:GLU:O	3:C:150:GLU:HG2	2.13	0.49
8:K:12:ILE:HG23	8:K:51:ILE:HB	1.95	0.49
1:I:105:ARG:HA	1:I:197:ASP:OD2	2.13	0.49
2:J:591:LEU:HG	2:J:614:VAL:HB	1.95	0.49
2:J:618:LEU:HD22	2:J:622:GLU:HG2	1.95	0.49
3:M:73:GLY:O	3:M:76:SER:OG	2.26	0.49
1:A:21:ILE:HD13	1:A:219:PRO:HD3	1.95	0.49
1:A:445:TYR:HB2	1:A:449:ARG:NH2	2.25	0.49
2:B:88:TYR:CD2	2:B:148:LEU:HD11	2.48	0.49
2:B:428:ASP:OD2	2:B:434:SER:OG	2.31	0.49
3:C:378:VAL:HG21	8:K:8:GLU:HG2	1.95	0.49
1:I:463:ASP:OD1	1:I:464:GLY:N	2.46	0.49
2:J:324:ALA:O	2:J:328:LEU:HG	2.13	0.49
1:A:33:ASP:HB3	1:A:43:GLU:OE1	2.12	0.49
2:B:429:ARG:HE	2:B:435:THR:HG21	1.78	0.49
2:B:433:MET:HE1	2:B:652:ILE:HG12	1.94	0.49
2:B:606:TRP:HZ3	2:B:617:TYR:HH	1.57	0.49
2:B:730:SER:HB3	2:B:915:ASN:ND2	2.27	0.49
2:B:753:ARG:HA	2:B:876:PRO:HD3	1.95	0.49
3:C:175:MET:O	3:C:178:VAL:HB	2.13	0.49
4:D:10:ARG:HB2	4:D:13:SER:OG	2.13	0.49
1:I:446:ARG:HH21	2:J:1002:ALA:HA	1.77	0.49
2:J:607:SER:O	2:J:610:ILE:HG13	2.12	0.49
2:J:730:SER:HA	2:J:735:ASN:ND2	2.26	0.49
3:M:21:LYS:HE3	3:M:21:LYS:HB3	1.48	0.49
8:T:12:ILE:HG23	8:T:51:ILE:HB	1.95	0.49
1:A:439:ARG:NH2	1:A:482:LYS:HE3	2.28	0.48
2:B:24:TYR:HB2	2:B:606:TRP:CE2	2.48	0.48
2:B:414:GLY:O	2:B:422:GLY:N	2.43	0.48
3:C:183:THR:O	3:C:183:THR:HG22	2.12	0.48
1:I:94:ARG:HG3	1:I:138:HIS:HD2	1.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:346:PRO:HB2	1:I:349:VAL:HG23	1.95	0.48
1:I:531:MET:C	9:U:44:THR:HG21	2.33	0.48
2:J:244:VAL:HG13	2:J:257:LEU:HD12	1.96	0.48
2:J:354:LEU:HD12	2:J:416:TRP:NE1	2.28	0.48
2:J:429:ARG:HE	2:J:435:THR:HG21	1.78	0.48
1:A:338:ILE:O	1:A:451:ASN:ND2	2.47	0.48
2:B:591:LEU:HG	2:B:614:VAL:HB	1.95	0.48
2:B:629:ALA:HB2	2:B:639:HIS:CG	2.49	0.48
2:B:652:ILE:HG23	2:B:653:PRO:HD3	1.95	0.48
3:C:196:TYR:CG	3:C:196:TYR:O	2.66	0.48
3:C:331:ALA:H	3:C:336:ARG:NH1	2.09	0.48
1:I:10:SER:C	2:J:1118:ARG:HB3	2.34	0.48
1:I:572:ARG:HD2	1:I:576:CYS:HB3	1.95	0.48
1:I:875:ASP:HB3	7:S:70:ALA:HB2	1.95	0.48
2:J:428:ASP:OD2	2:J:434:SER:OG	2.31	0.48
1:A:435:ILE:HB	2:B:1039:VAL:HG21	1.94	0.48
1:A:493:SER:HB3	1:A:500:LEU:HB2	1.94	0.48
1:A:572:ARG:HD2	1:A:576:CYS:HB3	1.95	0.48
2:B:207:VAL:HG21	2:B:323:MET:HB3	1.95	0.48
2:B:368:LYS:O	2:B:371:GLN:HB3	2.12	0.48
2:B:378:TYR:OH	2:B:388:GLU:HB2	2.13	0.48
2:B:812:LEU:HD21	2:B:843:VAL:HG23	1.94	0.48
6:F:18:LYS:HD2	6:F:49:GLU:HA	1.94	0.48
1:I:779:LEU:HD12	1:I:802:GLY:HA3	1.95	0.48
2:J:159:PHE:HE1	2:J:168:ILE:HG13	1.78	0.48
2:J:606:TRP:O	2:J:609:LEU:HB2	2.12	0.48
2:J:731:TYR:CZ	2:J:902:PRO:HG3	2.48	0.48
2:J:799:LEU:HG	2:J:813:VAL:HG22	1.95	0.48
3:M:122:GLU:HG2	3:M:125:ARG:NH2	2.29	0.48
1:A:463:ASP:OD1	1:A:464:GLY:N	2.46	0.48
2:B:724:PHE:CD1	2:B:994:TYR:HB2	2.47	0.48
10:N:2:ILE:HG12	10:N:56:ILE:HG21	1.94	0.48
1:I:6:LYS:NZ	2:J:1122:ARG:NH2	2.48	0.48
3:M:270:TRP:HA	3:M:318:ILE:HD11	1.95	0.48
4:O:201:ARG:HA	4:O:204:GLU:HG2	1.96	0.48
10:V:10:CYS:O	10:V:12:LYS:HG2	2.12	0.48
1:A:221:PRO:HG2	1:A:226:ARG:HE	1.78	0.48
1:A:769:LEU:HB2	1:A:804:VAL:CG2	2.43	0.48
2:B:191:VAL:HG13	2:B:208:GLU:HB3	1.96	0.48
2:B:536:ARG:HA	2:B:539:VAL:HG22	1.95	0.48
2:B:799:LEU:HG	2:B:813:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:42:ILE:HG22	1:I:47:MET:HB3	1.96	0.48
2:J:88:TYR:CD2	2:J:148:LEU:HD11	2.48	0.48
2:J:1122:ARG:CD	5:Q:10:VAL:CG1	2.69	0.48
3:M:191:PHE:N	3:M:197:THR:HG23	2.29	0.48
3:M:290:VAL:O	3:M:294:ARG:HG3	2.13	0.48
5:Q:6:LYS:O	6:R:7:LEU:HD23	2.13	0.48
5:Q:16:ARG:H	5:Q:16:ARG:HD2	1.79	0.48
1:A:346:PRO:HB2	1:A:349:VAL:HG23	1.96	0.48
2:B:785:TYR:CE2	2:B:787:GLY:HA2	2.49	0.48
3:C:270:TRP:HA	3:C:318:ILE:HD11	1.95	0.48
1:I:15:ILE:HD12	1:I:208:SER:HB2	1.96	0.48
1:I:21:ILE:HD13	1:I:219:PRO:HD3	1.96	0.48
2:J:24:TYR:HB2	2:J:606:TRP:CE2	2.48	0.48
2:J:191:VAL:HG13	2:J:208:GLU:HB3	1.96	0.48
2:J:289:TYR:O	2:J:293:ARG:HB2	2.14	0.48
2:J:579:ARG:NH2	2:J:623:GLU:OE2	2.46	0.48
2:B:159:PHE:HE1	2:B:168:ILE:HG13	1.78	0.48
2:B:413:THR:HG23	2:B:415:SER:H	1.77	0.48
2:B:794:LEU:HB3	2:B:798:GLY:HA2	1.95	0.48
1:I:11:ILE:HD12	3:M:358:LEU:HD22	1.96	0.48
1:I:63:CYS:O	1:I:65:ALA:N	2.46	0.48
1:I:81:ARG:HG3	1:I:82:PRO:HD2	1.95	0.48
1:I:378:TYR:HB2	1:I:379:PRO:HD3	1.95	0.48
1:I:783:TYR:HE2	1:I:789:THR:HB	1.79	0.48
2:J:885:ARG:HD2	2:J:993:TYR:HD2	1.79	0.48
3:M:321:ILE:O	3:M:327:VAL:HG23	2.14	0.48
1:A:163:THR:CB	1:A:276:GLN:HE21	2.27	0.48
1:A:443:MET:SD	1:A:449:ARG:HD3	2.53	0.48
1:A:535:MET:HB3	1:A:540:LEU:HD12	1.95	0.48
1:A:779:LEU:HD12	1:A:802:GLY:HA3	1.95	0.48
2:B:706:ASN:HB2	2:B:710:MET:SD	2.53	0.48
5:E:146:ILE:HA	5:E:163:MET:HG2	1.94	0.48
10:N:60:MET:C	10:N:62:TYR:H	2.15	0.48
1:I:444:PRO:CG	9:U:50:THR:HG22	2.10	0.48
1:I:874:GLU:HG3	7:S:67:SER:OG	2.13	0.48
3:M:176:GLU:O	3:M:179:VAL:N	2.47	0.48
4:O:10:ARG:HB2	4:O:13:SER:OG	2.13	0.48
1:A:10:SER:HB2	2:B:1118:ARG:HB3	1.94	0.48
2:B:759:THR:HA	2:B:869:THR:HA	1.95	0.48
3:C:122:GLU:HG2	3:C:125:ARG:NH2	2.29	0.48
3:C:160:VAL:HG23	3:C:198:LEU:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:LEU:HB3	3:C:177:LYS:NZ	2.28	0.48
3:C:196:TYR:CE1	3:C:198:LEU:CD1	2.94	0.48
1:I:535:MET:HB3	1:I:540:LEU:HD12	1.95	0.48
2:J:49:VAL:HG13	2:J:199:HIS:HE1	1.79	0.48
2:J:729:LEU:HD23	2:J:730:SER:O	2.13	0.48
5:Q:3:LYS:HZ2	6:R:9:GLU:CD	2.16	0.48
1:A:81:ARG:HG2	1:A:272:TRP:CD2	2.49	0.48
1:A:654:THR:OG1	1:A:655:LYS:N	2.46	0.48
2:B:354:LEU:HD12	2:B:416:TRP:NE1	2.28	0.48
3:C:290:VAL:O	3:C:294:ARG:HG3	2.13	0.48
1:I:163:THR:CB	1:I:276:GLN:HE21	2.27	0.48
1:I:439:ARG:NH2	1:I:482:LYS:HE3	2.28	0.48
1:I:837:GLN:HB3	3:M:102:ILE:CD1	2.44	0.48
2:J:1122:ARG:NH2	5:Q:67:TYR:HE2	2.08	0.48
3:M:152:ILE:CG2	3:M:159:TYR:CA	2.86	0.48
3:M:314:LEU:HD13	3:M:315:ASP:N	2.29	0.48
1:A:26:ALA:HB3	1:A:51:LEU:HD23	1.95	0.47
1:A:359:VAL:HG22	1:A:408:ILE:HA	1.95	0.47
2:B:244:VAL:HG13	2:B:257:LEU:HD12	1.96	0.47
3:C:155:LEU:CD2	3:C:156:ASN:HD22	2.27	0.47
3:C:187:LYS:HB3	3:C:201:ARG:HG2	1.96	0.47
3:M:148:ARG:HH21	3:M:162:GLU:CG	2.21	0.47
10:V:5:VAL:O	10:V:6:ARG:HB2	2.14	0.47
2:B:352:GLY:O	2:B:356:LYS:HG3	2.13	0.47
2:B:579:ARG:HH21	2:B:623:GLU:CD	2.18	0.47
2:B:766:ARG:NH1	2:B:862:GLY:O	2.47	0.47
3:C:119:TYR:CD2	3:C:263:ARG:HD2	2.48	0.47
3:C:314:LEU:HD13	3:C:315:ASP:N	2.29	0.47
1:I:221:PRO:HG2	1:I:226:ARG:HE	1.79	0.47
1:I:623:LYS:HB2	1:I:754:GLY:HA3	1.96	0.47
2:J:207:VAL:HG21	2:J:323:MET:HB3	1.95	0.47
2:J:451:PRO:HB2	2:J:453:PHE:CE1	2.49	0.47
2:J:591:LEU:HD13	2:J:595:HIS:CE1	2.49	0.47
2:J:766:ARG:NH1	2:J:862:GLY:O	2.47	0.47
2:J:794:LEU:HB3	2:J:798:GLY:HA2	1.96	0.47
3:M:325:GLY:O	3:M:329:GLU:HG2	2.15	0.47
8:T:30:VAL:HB	8:T:31:PRO:HD3	1.96	0.47
3:C:155:LEU:HD21	3:C:156:ASN:ND2	2.29	0.47
3:C:236:LYS:HE3	3:C:241:TYR:CE2	2.49	0.47
2:J:395:ARG:CB	2:J:398:ILE:HD12	2.44	0.47
2:J:536:ARG:HA	2:J:539:VAL:HG22	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1122:ARG:NE	5:Q:67:TYR:CD2	2.81	0.47
3:M:151:THR:O	3:M:152:ILE:HD13	2.13	0.47
3:M:163:ILE:HD12	3:M:197:THR:HB	1.95	0.47
3:M:236:LYS:HE3	3:M:241:TYR:CE2	2.49	0.47
3:M:380:LEU:HB2	5:Q:59:ILE:HB	1.95	0.47
4:O:55:PHE:HB2	4:O:58:ILE:HD12	1.95	0.47
1:A:378:TYR:HB2	1:A:379:PRO:HD3	1.95	0.47
1:A:524:TYR:H	1:A:524:TYR:HD1	1.58	0.47
1:A:893:VAL:HG11	3:C:49:THR:HA	1.96	0.47
3:C:207:LYS:HE3	3:C:210:ASP:OD1	2.14	0.47
3:C:337:ALA:HA	3:C:346:LEU:HB2	1.97	0.47
5:E:16:ARG:H	5:E:16:ARG:HD2	1.79	0.47
9:L:25:ALA:HB3	9:L:43:TYR:CE2	2.49	0.47
1:I:338:ILE:O	1:I:451:ASN:ND2	2.47	0.47
1:I:499:PRO:HD2	1:I:630:ASP:HB2	1.96	0.47
2:J:520:TYR:CZ	2:J:532:VAL:HB	2.48	0.47
2:J:1081:VAL:HG22	2:J:1092:ILE:HD13	1.95	0.47
3:M:93:ASN:HB3	3:M:94:VAL:HG22	1.94	0.47
9:U:30:GLU:HA	9:U:33:HIS:HD1	1.79	0.47
2:B:17:LEU:HD22	2:B:644:LEU:HA	1.97	0.47
2:B:591:LEU:HD13	2:B:595:HIS:CE1	2.49	0.47
2:B:768:LEU:O	2:J:380:ARG:NH2	2.47	0.47
3:C:161:VAL:HG22	3:C:199:VAL:CB	2.33	0.47
3:C:321:ILE:O	3:C:327:VAL:HG23	2.15	0.47
1:I:165:TYR:HB2	1:I:181:MET:HB3	1.97	0.47
1:I:352:GLU:OE2	2:J:1009:SER:HB3	2.14	0.47
2:J:591:LEU:HB3	2:J:595:HIS:CD2	2.50	0.47
2:J:629:ALA:HB2	2:J:639:HIS:CG	2.49	0.47
2:J:753:ARG:HA	2:J:876:PRO:HD3	1.95	0.47
2:J:759:THR:HA	2:J:869:THR:HA	1.96	0.47
2:J:785:TYR:CE2	2:J:787:GLY:HA2	2.49	0.47
2:J:962:GLU:OE1	4:O:201:ARG:NH1	2.48	0.47
3:M:180:ARG:O	3:M:180:ARG:HD3	2.15	0.47
3:M:220:LYS:C	3:M:222:ARG:H	2.17	0.47
1:A:15:ILE:HD12	1:A:208:SER:HB2	1.96	0.47
1:A:569:ILE:HG13	1:A:636:ILE:HD13	1.97	0.47
2:B:591:LEU:HB3	2:B:595:HIS:CD2	2.50	0.47
5:E:6:LYS:O	6:F:7:LEU:CD2	2.62	0.47
7:H:40:LEU:HB2	7:H:78:LEU:HD12	1.97	0.47
2:J:429:ARG:O	2:J:431:ASN:N	2.48	0.47
2:J:708:ARG:H	2:J:947:THR:HG1	1.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:729:LEU:HD22	2:J:731:TYR:CE1	2.49	0.47
1:A:165:TYR:HB2	1:A:181:MET:HB3	1.96	0.47
1:A:209:ARG:HB2	1:A:212:TRP:CD2	2.50	0.47
1:A:645:ARG:HB3	1:A:649:PHE:CE2	2.50	0.47
2:B:289:TYR:O	2:B:293:ARG:HB2	2.13	0.47
2:B:324:ALA:O	2:B:328:LEU:HG	2.15	0.47
2:B:429:ARG:O	2:B:431:ASN:N	2.48	0.47
2:B:744:LYS:HB3	2:B:897:PRO:HA	1.97	0.47
2:B:919:ILE:H	2:B:920:PRO:HD2	1.80	0.47
2:B:940:THR:O	10:N:32:GLY:HA3	2.14	0.47
7:H:29:LEU:HD11	7:H:76:TYR:CZ	2.49	0.47
8:K:30:VAL:HB	8:K:31:PRO:HD3	1.96	0.47
1:I:160:GLU:HA	1:I:164:ILE:O	2.15	0.47
2:J:57:VAL:HB	2:J:58:PRO:CA	2.35	0.47
2:J:681:LEU:HD13	2:J:696:LEU:HD23	1.97	0.47
3:M:187:LYS:HE3	3:M:201:ARG:HB3	1.96	0.47
9:U:6:ILE:HD11	9:U:16:TYR:CE2	2.50	0.47
10:V:8:PHE:HB2	10:V:47:ARG:HH22	1.80	0.47
1:A:758:LYS:HA	1:A:758:LYS:HE3	1.96	0.47
1:A:848:ALA:HB2	3:C:327:VAL:HG22	1.97	0.47
2:B:681:LEU:HD13	2:B:696:LEU:HD23	1.97	0.47
4:D:55:PHE:HB2	4:D:58:ILE:HD12	1.95	0.47
1:I:209:ARG:HB2	1:I:212:TRP:CD2	2.49	0.47
2:J:323:MET:O	2:J:327:VAL:HG23	2.14	0.47
2:J:856:VAL:HG12	11:W:35:LEU:HB2	1.95	0.47
3:M:358:LEU:CD1	3:M:359:ASN:H	2.25	0.47
7:S:29:LEU:HD11	7:S:76:TYR:CZ	2.49	0.47
9:U:50:THR:OG1	9:U:51:MET:N	2.46	0.47
11:W:17:LEU:HD22	11:W:28:PRO:HD2	1.97	0.47
1:A:632:LYS:N	1:A:632:LYS:HE3	2.30	0.47
2:B:395:ARG:HD3	2:B:398:ILE:HD11	1.96	0.47
3:C:161:VAL:HG22	3:C:199:VAL:HB	1.95	0.47
5:E:125:ARG:H	5:E:125:ARG:NE	2.12	0.47
10:N:8:PHE:HB2	10:N:47:ARG:HH22	1.80	0.47
1:I:443:MET:SD	1:I:449:ARG:HD3	2.55	0.47
1:I:476:GLU:HA	8:T:14:GLY:HA3	1.96	0.47
1:I:480:GLU:OE2	2:J:1047:MET:HB2	2.14	0.47
2:J:325:LEU:HD23	2:J:326:LYS:HG2	1.97	0.47
3:M:148:ARG:NH1	3:M:162:GLU:CB	2.66	0.47
5:Q:39:ASP:O	5:Q:43:GLY:N	2.43	0.47
6:R:117:GLU:O	6:R:119:ARG:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:LEU:O	1:A:586:GLU:HB3	2.15	0.47
2:B:31:VAL:CG2	2:B:155:PRO:HB2	2.45	0.47
2:B:323:MET:O	2:B:327:VAL:HG23	2.15	0.47
2:B:325:LEU:HD23	2:B:326:LYS:HG2	1.97	0.47
2:B:636:THR:H	2:B:639:HIS:HD2	1.63	0.47
3:C:181:LYS:O	3:C:183:THR:N	2.48	0.47
9:L:6:ILE:HD11	9:L:16:TYR:CE2	2.50	0.47
1:I:305:ALA:O	1:I:309:LYS:HD2	2.14	0.47
1:I:783:TYR:CE2	1:I:789:THR:HB	2.50	0.47
2:J:1122:ARG:HD2	6:R:4:ARG:HH21	1.77	0.47
3:M:160:VAL:HG11	3:M:198:LEU:HD12	1.96	0.47
3:M:266:THR:HB	3:M:272:ILE:HD11	1.97	0.47
2:B:373:GLN:CG	2:B:397:SER:HB2	2.45	0.46
2:B:925:VAL:HA	2:B:928:LEU:HD12	1.97	0.46
1:I:430:LEU:HD23	3:M:74:GLU:HG3	1.96	0.46
2:J:151:ASP:HB2	2:J:718:ARG:HH22	1.80	0.46
3:M:187:LYS:CE	3:M:201:ARG:HB3	2.45	0.46
3:M:323:ARG:H	3:M:327:VAL:HB	1.80	0.46
5:Q:6:LYS:O	6:R:7:LEU:CD2	2.63	0.46
9:U:28:LEU:HD23	9:U:57:PHE:HE2	1.79	0.46
2:B:342:HIS:HE1	2:B:620:ALA:HB1	1.81	0.46
2:B:574:ASP:OD1	14:B:1301:HOH:O	2.20	0.46
2:B:986:ASP:O	2:B:987:ILE:HD13	2.15	0.46
3:C:189:ALA:HB3	3:C:199:VAL:HG13	1.97	0.46
3:C:220:LYS:C	3:C:222:ARG:H	2.18	0.46
3:C:323:ARG:H	3:C:327:VAL:HB	1.79	0.46
3:C:325:GLY:O	3:C:329:GLU:HG2	2.14	0.46
3:C:330:LYS:H	3:C:330:LYS:HD3	1.80	0.46
4:D:201:ARG:HA	4:D:204:GLU:HG2	1.96	0.46
10:N:56:ILE:HG12	10:N:60:MET:CG	2.45	0.46
1:I:81:ARG:HG2	1:I:272:TRP:CD2	2.50	0.46
1:I:435:ILE:O	2:J:1043:HIS:CE1	2.68	0.46
3:M:128:ARG:HG3	3:M:241:TYR:HE2	1.77	0.46
3:M:187:LYS:O	3:M:187:LYS:HG3	2.15	0.46
4:O:178:ARG:HH12	4:O:197:PHE:HA	1.80	0.46
3:C:194:GLU:CG	3:C:196:TYR:HE2	2.29	0.46
10:N:57:ASP:CA	10:N:60:MET:HE3	2.38	0.46
1:I:645:ARG:HB3	1:I:649:PHE:CE2	2.50	0.46
2:J:513:ARG:HA	2:J:514:ARG:HH11	1.81	0.46
2:J:861:ASP:HB3	2:J:863:THR:HG23	1.98	0.46
5:Q:8:LYS:CG	6:R:7:LEU:HD22	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:GLU:N	2:B:1116:SER:O	2.29	0.46
1:A:426:ARG:HB2	1:A:467:MET:HE3	1.98	0.46
1:A:462:PHE:HB2	2:B:737:GLU:O	2.15	0.46
2:B:603:THR:HB	2:B:604:LEU:HD23	1.98	0.46
2:B:683:TRP:CD1	2:B:683:TRP:O	2.67	0.46
1:I:477:ALA:HA	2:J:1047:MET:HB3	1.97	0.46
2:J:342:HIS:HE1	2:J:620:ALA:HB1	1.81	0.46
2:J:744:LYS:HB3	2:J:897:PRO:HA	1.97	0.46
2:J:1083:CYS:HG	2:J:1086:CYS:HB2	1.76	0.46
3:M:116:MET:HE1	3:M:253:VAL:HG21	1.97	0.46
1:A:160:GLU:HA	1:A:164:ILE:O	2.15	0.46
2:B:205:ILE:CD1	2:B:303:LEU:H	2.29	0.46
2:B:269:THR:HB	2:B:270:GLN:H	1.55	0.46
2:B:904:THR:HG21	2:B:972:GLU:OE1	2.15	0.46
3:C:303:ARG:HA	3:C:306:MET:HE2	1.96	0.46
8:K:49:ILE:H	8:K:49:ILE:HG13	1.46	0.46
11:P:43:ALA:O	11:P:44:ARG:HD3	2.16	0.46
2:J:21:MET:SD	2:J:645:MET:HB3	2.55	0.46
2:J:636:THR:H	2:J:639:HIS:HD2	1.63	0.46
2:J:650:LEU:HB2	2:J:654:ALA:HB3	1.97	0.46
2:J:683:TRP:CD1	2:J:683:TRP:O	2.66	0.46
2:J:726:VAL:HG11	2:J:992:ILE:HG12	1.98	0.46
3:M:216:GLU:O	3:M:221:HIS:HB2	2.15	0.46
5:Q:27:LYS:HD3	5:Q:51:VAL:HG23	1.97	0.46
1:A:347:LEU:HD22	1:A:444:PRO:HA	1.97	0.46
1:A:405:LYS:HB2	1:A:405:LYS:HE3	1.72	0.46
2:B:861:ASP:HB3	2:B:863:THR:HG23	1.97	0.46
3:C:116:MET:HE1	3:C:253:VAL:HG21	1.98	0.46
3:C:128:ARG:HG3	3:C:241:TYR:HE2	1.78	0.46
3:C:342:THR:CB	3:C:345:HIS:HB2	2.43	0.46
4:D:200:PRO:HB2	4:D:203:PHE:CD1	2.48	0.46
1:I:569:ILE:HG13	1:I:636:ILE:HD13	1.97	0.46
2:J:17:LEU:HD22	2:J:644:LEU:HA	1.97	0.46
2:J:235:LEU:HD13	2:J:313:ARG:HB3	1.97	0.46
3:M:215:ALA:HA	3:M:219:LYS:HG3	1.98	0.46
9:U:28:LEU:HD23	9:U:57:PHE:CE2	2.51	0.46
2:B:766:ARG:HD3	2:B:772:LYS:HE2	1.98	0.46
3:C:187:LYS:HD3	3:C:203:LYS:NZ	2.30	0.46
10:N:5:VAL:O	10:N:6:ARG:HB2	2.15	0.46
1:I:654:THR:OG1	1:I:655:LYS:N	2.47	0.46
1:I:756:ARG:HH12	2:J:922:ARG:HH12	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:31:VAL:CG2	2:J:155:PRO:HB2	2.45	0.46
7:S:40:LEU:HB2	7:S:78:LEU:HD12	1.98	0.46
7:S:75:TYR:HD1	7:S:76:TYR:H	1.64	0.46
1:A:59:ARG:HH12	11:W:21:THR:HG21	1.81	0.46
1:A:94:ARG:HG3	1:A:138:HIS:HD2	1.75	0.46
1:A:580:GLU:H	1:A:580:GLU:HG3	1.63	0.46
1:A:624:LYS:O	1:A:632:LYS:HD3	2.14	0.46
1:A:666:PHE:N	2:B:729:LEU:HD13	2.30	0.46
2:B:432:TYR:O	2:B:435:THR:HG23	2.16	0.46
2:B:447:SER:HB2	2:B:450:GLN:HG2	1.98	0.46
2:B:451:PRO:HB2	2:B:453:PHE:CE1	2.50	0.46
2:B:730:SER:HA	2:B:735:ASN:ND2	2.27	0.46
2:B:731:TYR:OH	2:B:902:PRO:HG3	2.16	0.46
3:C:76:SER:HA	3:C:79:MET:HE3	1.98	0.46
4:D:29:LEU:O	4:D:33:ILE:HG13	2.16	0.46
1:I:103:CYS:SG	1:I:105:ARG:CA	3.03	0.46
1:I:670:ILE:HG21	2:J:932:ILE:HD11	1.97	0.46
1:I:750:MET:HE1	2:J:916:PRO:O	2.16	0.46
2:J:902:PRO:HB2	2:J:974:MET:CG	2.46	0.46
2:J:986:ASP:O	2:J:987:ILE:HD13	2.16	0.46
3:M:152:ILE:HG21	3:M:158:GLU:O	2.16	0.46
3:M:303:ARG:HA	3:M:306:MET:HE2	1.97	0.46
3:M:374:GLY:HA2	8:T:7:PHE:CE2	2.51	0.46
5:Q:125:ARG:H	5:Q:125:ARG:NE	2.12	0.46
1:A:336:PRO:HD2	2:B:734:TYR:CE1	2.51	0.46
1:A:584:ALA:O	1:A:605:TYR:OH	2.23	0.46
1:A:757:GLY:O	1:A:758:LYS:HD2	2.16	0.46
2:B:161:ILE:HD12	2:B:411:LEU:HB3	1.97	0.46
2:B:416:TRP:HB2	2:B:420:ARG:HG3	1.98	0.46
2:B:749:ARG:HE	4:D:144:ALA:CB	2.27	0.46
4:D:46:GLU:HA	11:P:45:ARG:HA	1.97	0.46
6:F:117:GLU:O	6:F:119:ARG:N	2.48	0.46
9:L:45:ILE:C	9:L:47:HIS:H	2.19	0.46
11:P:17:LEU:HD22	11:P:28:PRO:HD2	1.97	0.46
1:I:347:LEU:HD22	1:I:444:PRO:HA	1.97	0.46
1:I:446:ARG:HB3	2:J:1005:MET:SD	2.56	0.46
1:I:639:ARG:NH2	1:I:882:SER:O	2.48	0.46
2:J:429:ARG:HA	2:J:429:ARG:HD2	1.78	0.46
2:J:513:ARG:NH1	2:J:531:THR:OG1	2.48	0.46
2:J:968:HIS:HD2	2:J:969:SER:CA	2.29	0.46
1:A:670:ILE:HG21	2:B:958:ARG:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:MET:SD	2:B:645:MET:HB3	2.55	0.46
3:C:269:ILE:HG22	3:C:270:TRP:H	1.80	0.46
4:D:178:ARG:HH12	4:D:197:PHE:HA	1.80	0.46
1:I:542:GLU:H	1:I:542:GLU:HG2	1.49	0.46
2:J:228:PHE:CE1	2:J:320:LEU:HD22	2.51	0.46
3:M:100:ARG:HH21	3:M:288:GLU:HG2	1.81	0.46
3:M:286:ILE:O	3:M:290:VAL:HG23	2.16	0.46
4:O:127:GLN:HE21	10:V:63:LYS:HG2	1.81	0.46
10:V:56:ILE:HG12	10:V:60:MET:HG2	1.97	0.46
1:A:305:ALA:O	1:A:309:LYS:HD2	2.16	0.45
2:B:56:VAL:CG2	2:B:65:VAL:HB	2.46	0.45
2:B:744:LYS:HG3	2:B:895:ILE:HD11	1.98	0.45
3:C:155:LEU:HD23	3:C:156:ASN:HD22	1.81	0.45
3:C:266:THR:HB	3:C:272:ILE:HD11	1.97	0.45
1:I:426:ARG:HB2	1:I:467:MET:HE3	1.97	0.45
1:I:443:MET:CB	9:U:49:ILE:HD12	2.38	0.45
1:I:665:GLY:HA2	2:J:729:LEU:HD13	1.91	0.45
1:I:787:VAL:HG23	1:I:801:ARG:HH11	1.81	0.45
2:J:925:VAL:HA	2:J:928:LEU:HD12	1.97	0.45
2:J:1059:LYS:HE2	2:J:1096:GLU:HG2	1.98	0.45
2:J:1101:PHE:CD2	3:M:367:ILE:HG13	2.52	0.45
3:M:62:GLU:HG3	3:M:63:ALA:H	1.81	0.45
5:Q:100:ARG:NE	6:R:43:VAL:HG13	2.31	0.45
11:W:43:ALA:O	11:W:44:ARG:HD3	2.15	0.45
1:A:167:GLU:HG3	1:A:179:HIS:HB3	1.98	0.45
3:C:333:VAL:O	3:C:337:ALA:N	2.50	0.45
1:I:6:LYS:CE	2:J:1122:ARG:CZ	2.63	0.45
1:I:134:ILE:HD13	1:I:134:ILE:HA	1.82	0.45
1:I:507:HIS:NE2	1:I:654:THR:HB	2.32	0.45
2:J:205:ILE:CD1	2:J:303:LEU:H	2.29	0.45
2:J:211:LYS:HG3	3:M:212:ARG:NH2	2.31	0.45
2:J:358:LEU:HD23	2:J:416:TRP:CE2	2.51	0.45
2:J:603:THR:HB	2:J:604:LEU:HD23	1.99	0.45
2:J:904:THR:HG21	2:J:972:GLU:OE1	2.15	0.45
3:M:160:VAL:HG11	3:M:198:LEU:CD1	2.46	0.45
3:M:173:LEU:HB3	3:M:177:LYS:NZ	2.30	0.45
1:A:264:PRO:O	1:A:266:LEU:N	2.50	0.45
1:A:577:ASP:HA	1:A:581:ARG:HG3	1.97	0.45
2:B:126:LEU:HD12	2:B:127:PRO:HD2	1.99	0.45
2:B:378:TYR:HE1	2:B:388:GLU:HA	0.95	0.45
2:B:636:THR:N	2:B:639:HIS:HD2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1059:LYS:HE2	2:B:1096:GLU:HG2	1.98	0.45
5:E:5:LEU:HD13	6:F:6:LYS:CD	2.46	0.45
10:N:62:TYR:C	10:N:63:LYS:HZ2	2.10	0.45
1:I:750:MET:HA	1:I:753:THR:HG22	1.97	0.45
2:J:269:THR:HB	2:J:270:GLN:H	1.55	0.45
2:J:432:TYR:O	2:J:435:THR:HG23	2.16	0.45
2:J:579:ARG:HH21	2:J:623:GLU:CD	2.19	0.45
2:J:637:GLU:H	2:J:637:GLU:HG2	1.42	0.45
2:J:968:HIS:HD2	2:J:969:SER:N	2.15	0.45
3:M:104:ILE:HD12	3:M:288:GLU:HB3	1.98	0.45
4:O:226:THR:HB	4:O:235:ILE:HD11	1.99	0.45
1:A:150:CYS:O	1:A:153:PRO:HD3	2.16	0.45
1:A:639:ARG:NH2	1:A:882:SER:O	2.49	0.45
2:B:122:ARG:HE	2:B:400:PRO:HG3	1.82	0.45
2:B:389:ASN:OD1	2:B:392:ARG:HD3	2.15	0.45
2:B:902:PRO:HB2	2:B:974:MET:CG	2.46	0.45
2:B:942:ARG:CZ	2:B:942:ARG:HB2	2.47	0.45
3:C:62:GLU:HG3	3:C:63:ALA:H	1.81	0.45
3:C:194:GLU:CB	3:C:196:TYR:CD2	2.84	0.45
4:D:50:ASN:ND2	4:D:52:SER:H	2.13	0.45
6:F:112:ILE:O	6:F:116:ASP:N	2.49	0.45
2:J:25:TRP:HZ2	2:J:485:LEU:HB3	1.80	0.45
2:J:189:LYS:NZ	3:M:212:ARG:NH1	2.64	0.45
2:J:731:TYR:OH	2:J:902:PRO:HG3	2.17	0.45
2:J:919:ILE:H	2:J:920:PRO:HD2	1.80	0.45
3:M:331:ALA:H	3:M:336:ARG:NH1	2.15	0.45
2:B:228:PHE:CE1	2:B:320:LEU:HD22	2.51	0.45
2:B:778:PRO:HD3	2:B:814:GLY:HA3	1.99	0.45
9:L:46:GLU:C	9:L:47:HIS:CG	2.89	0.45
1:I:666:PHE:O	2:J:916:PRO:HG3	2.16	0.45
2:J:56:VAL:CG2	2:J:65:VAL:HB	2.46	0.45
2:J:485:LEU:HD12	2:J:648:ALA:HA	1.98	0.45
2:J:636:THR:N	2:J:639:HIS:HD2	2.14	0.45
2:J:766:ARG:HD3	2:J:772:LYS:HE2	1.99	0.45
3:M:177:LYS:C	3:M:179:VAL:H	2.19	0.45
3:M:330:LYS:H	3:M:330:LYS:HD3	1.82	0.45
1:A:632:LYS:HE3	1:A:632:LYS:H	1.81	0.45
1:A:783:TYR:OH	2:B:623:GLU:OE2	2.31	0.45
2:B:131:LYS:N	2:B:135:CYS:SG	2.90	0.45
2:B:231:VAL:O	2:B:235:LEU:HB2	2.17	0.45
2:B:235:LEU:HD13	2:B:313:ARG:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:609:LEU:HD22	2:B:614:VAL:HG11	1.97	0.45
2:B:726:VAL:HG11	2:B:992:ILE:HG12	1.98	0.45
3:C:286:ILE:O	3:C:290:VAL:HG23	2.17	0.45
3:C:386:LEU:HD12	3:C:386:LEU:HA	1.66	0.45
1:I:445:TYR:CD1	9:U:49:ILE:HG21	2.51	0.45
1:I:791:PHE:CE2	1:I:800:ALA:HA	2.52	0.45
2:J:67:PHE:CD1	2:J:107:MET:HG2	2.52	0.45
2:J:89:PRO:HG3	2:J:99:TYR:CE2	2.51	0.45
2:J:416:TRP:HB2	2:J:420:ARG:HG3	1.98	0.45
2:J:744:LYS:HG3	2:J:895:ILE:HD11	1.98	0.45
2:J:942:ARG:CZ	2:J:942:ARG:HB2	2.47	0.45
3:M:153:ASP:CG	3:M:157:MET:HG3	2.37	0.45
2:B:151:ASP:HB2	2:B:718:ARG:HH22	1.81	0.45
2:B:878:LEU:HD23	2:B:878:LEU:HA	1.74	0.45
2:B:939:LEU:HB2	2:B:964:LEU:HD13	1.99	0.45
5:E:5:LEU:HD13	6:F:6:LYS:HD3	1.98	0.45
5:E:42:GLU:O	5:E:78:GLU:HB2	2.17	0.45
1:I:167:GLU:HG3	1:I:179:HIS:HB3	1.99	0.45
2:J:1121:ASP:OD2	3:M:379:LYS:HE3	2.17	0.45
3:M:269:ILE:HG22	3:M:270:TRP:H	1.80	0.45
5:Q:5:LEU:HD13	6:R:6:LYS:CD	2.47	0.45
6:R:112:ILE:O	6:R:116:ASP:N	2.49	0.45
1:A:507:HIS:NE2	1:A:654:THR:HB	2.32	0.45
4:D:226:THR:HB	4:D:235:ILE:HD11	1.98	0.45
8:K:24:ALA:HA	8:K:25:PRO:HD2	1.84	0.45
1:I:870:PHE:HE2	7:S:75:TYR:HD1	1.64	0.45
2:J:161:ILE:HD12	2:J:411:LEU:HB3	1.97	0.45
2:J:231:VAL:O	2:J:235:LEU:HB2	2.16	0.45
2:J:239:THR:HG22	2:J:241:LYS:H	1.82	0.45
2:J:447:SER:HB2	2:J:450:GLN:HG2	1.98	0.45
4:O:29:LEU:O	4:O:33:ILE:HG13	2.16	0.45
1:A:147:CYS:HA	1:A:148:PRO:HD3	1.81	0.45
1:A:161:ARG:HA	1:A:162:PRO:C	2.38	0.45
1:A:187:ARG:O	1:A:191:GLU:HG3	2.17	0.45
1:A:543:PRO:O	1:A:544:ASP:HB2	2.15	0.45
2:B:67:PHE:CD1	2:B:107:MET:HG2	2.51	0.45
2:B:650:LEU:HB2	2:B:654:ALA:HB3	1.97	0.45
11:P:10:LYS:O	11:P:35:LEU:HA	2.17	0.45
1:I:180:ARG:NH1	1:I:182:MET:SD	2.89	0.45
2:J:63:PHE:HD1	2:J:111:VAL:HG13	1.82	0.45
2:J:107:MET:C	2:J:395:ARG:NH2	2.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:157:MET:O	3:M:158:GLU:HB2	2.17	0.45
4:O:50:ASN:ND2	4:O:52:SER:H	2.13	0.45
1:A:791:PHE:CE2	1:A:800:ALA:HA	2.52	0.45
1:A:895:VAL:O	1:A:897:THR:N	2.50	0.45
2:B:63:PHE:HD1	2:B:111:VAL:HG13	1.82	0.45
2:B:89:PRO:HG3	2:B:99:TYR:CE2	2.51	0.45
2:B:815:ARG:HG2	2:B:816:THR:H	1.82	0.45
5:E:27:LYS:HD3	5:E:51:VAL:HG23	1.98	0.45
1:I:103:CYS:SG	1:I:104:GLY:N	2.89	0.45
1:I:161:ARG:HA	1:I:162:PRO:C	2.38	0.45
2:J:41:PHE:HD1	2:J:42:ILE:HD13	1.79	0.45
2:J:503:MET:HA	2:J:507:VAL:HB	1.99	0.45
2:J:791:TYR:OH	2:J:838:GLU:OE2	2.25	0.45
3:M:281:ALA:O	3:M:285:ILE:HG12	2.17	0.45
2:B:773:ASP:OD2	2:B:815:ARG:NH1	2.44	0.44
3:C:104:ILE:HD12	3:C:288:GLU:HB3	1.98	0.44
4:D:27:ASN:HD22	4:D:27:ASN:HA	1.51	0.44
7:H:75:TYR:HD1	7:H:76:TYR:H	1.64	0.44
1:I:867:ILE:H	1:I:867:ILE:HG13	1.27	0.44
2:J:609:LEU:HD22	2:J:614:VAL:HG11	1.98	0.44
2:J:1080:LYS:HB3	5:Q:154:ARG:HD3	1.99	0.44
3:M:153:ASP:HB2	3:M:160:VAL:HG23	1.98	0.44
5:Q:42:GLU:O	5:Q:78:GLU:HB2	2.17	0.44
11:W:10:LYS:O	11:W:35:LEU:HA	2.17	0.44
2:B:968:HIS:HD2	2:B:969:SER:CA	2.30	0.44
3:C:107:ALA:HB1	3:C:270:TRP:CZ2	2.52	0.44
3:C:173:LEU:HB3	3:C:177:LYS:HZ3	1.81	0.44
3:C:385:PRO:HA	3:C:386:LEU:CD1	2.48	0.44
4:D:150:PHE:HD1	10:N:12:LYS:HZ1	1.65	0.44
4:D:201:ARG:H	4:D:201:ARG:HG3	1.18	0.44
10:N:56:ILE:HG23	10:N:60:MET:HE2	1.99	0.44
2:B:10:PRO:O	2:B:11:THR:OG1	2.24	0.44
2:B:357:ASP:HA	2:B:360:ARG:NH1	2.32	0.44
2:B:358:LEU:HD23	2:B:416:TRP:CE2	2.51	0.44
3:C:210:ASP:O	3:C:214:ILE:HG13	2.17	0.44
9:L:46:GLU:O	9:L:47:HIS:CG	2.71	0.44
1:I:187:ARG:O	1:I:191:GLU:HG3	2.17	0.44
1:I:404:GLU:O	1:I:406:LEU:HG	2.17	0.44
1:I:758:LYS:HB3	1:I:759:ILE:H	1.53	0.44
2:J:179:THR:HA	2:J:194:VAL:HG22	1.99	0.44
2:J:305:HIS:CE1	2:J:306:MET:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:45:ILE:HD13	9:U:53:ARG:NH1	2.32	0.44
1:A:632:LYS:HZ2	1:A:633:LEU:H	1.66	0.44
1:A:787:VAL:HG23	1:A:801:ARG:HH11	1.82	0.44
2:B:222:VAL:HA	2:B:223:PRO:HD2	1.79	0.44
2:B:286:PRO:HD2	2:B:290:ARG:NE	2.29	0.44
2:B:503:MET:HA	2:B:507:VAL:HB	2.00	0.44
2:B:853:LYS:HE2	2:B:869:THR:HG21	2.00	0.44
3:C:187:LYS:HZ1	3:C:206:THR:HB	1.83	0.44
3:C:348:ALA:O	3:C:352:ARG:HG2	2.16	0.44
4:D:181:PRO:HD3	4:D:194:ILE:HD13	1.99	0.44
9:L:52:ALA:O	9:L:53:ARG:HB2	2.17	0.44
1:I:309:LYS:HZ1	3:M:346:LEU:HG	1.82	0.44
1:I:588:LEU:C	1:I:588:LEU:CD2	2.86	0.44
3:M:154:ILE:HD12	3:M:154:ILE:N	2.32	0.44
5:Q:113:LEU:HD12	5:Q:118:VAL:HG11	2.00	0.44
7:S:42:GLN:HA	7:S:78:LEU:H	1.82	0.44
1:A:251:ILE:HD13	1:A:274:LEU:HD22	2.00	0.44
1:A:542:GLU:H	1:A:542:GLU:HG2	1.49	0.44
1:A:704:GLY:C	1:A:706:LEU:H	2.21	0.44
2:B:182:GLU:HG3	2:B:183:ARG:H	1.82	0.44
2:B:239:THR:HG22	2:B:241:LYS:H	1.82	0.44
2:B:485:LEU:HD12	2:B:648:ALA:HA	1.99	0.44
2:B:649:ILE:HD13	2:B:649:ILE:HA	1.80	0.44
5:E:8:LYS:CG	6:F:7:LEU:HD22	2.47	0.44
1:I:41:PRO:HB2	1:I:42:ILE:HD13	2.00	0.44
2:J:25:TRP:CH2	2:J:485:LEU:HD22	2.52	0.44
2:J:131:LYS:N	2:J:135:CYS:SG	2.89	0.44
2:J:729:LEU:HB3	2:J:731:TYR:HE1	1.82	0.44
2:J:809:LYS:H	2:J:809:LYS:HG2	1.52	0.44
2:J:1068:CYS:SG	2:J:1070:HIS:CG	3.11	0.44
4:O:50:ASN:ND2	4:O:52:SER:OG	2.42	0.44
1:A:180:ARG:NH1	1:A:182:MET:SD	2.90	0.44
1:A:743:MET:HA	1:A:748:VAL:HG11	2.00	0.44
2:B:25:TRP:CH2	2:B:485:LEU:HD22	2.53	0.44
2:B:703:PRO:HG3	2:B:715:PHE:HE2	1.83	0.44
2:B:745:ALA:HB1	2:B:749:ARG:CZ	2.48	0.44
2:B:902:PRO:HB2	2:B:974:MET:HG2	1.99	0.44
3:C:177:LYS:H	3:C:177:LYS:HG3	1.64	0.44
4:D:50:ASN:ND2	4:D:52:SER:OG	2.41	0.44
5:E:3:LYS:CE	6:F:9:GLU:OE1	2.64	0.44
1:I:152:ALA:HA	1:I:153:PRO:HD2	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:445:TYR:HD2	2:J:878:LEU:HD12	1.83	0.44
1:I:667:THR:HA	2:J:916:PRO:HB3	1.99	0.44
5:Q:112:GLN:HA	5:Q:166:ARG:HG3	2.00	0.44
7:S:37:ILE:H	7:S:37:ILE:HG12	1.31	0.44
10:V:6:ARG:HB3	10:V:7:CYS:H	1.44	0.44
1:A:891:ASP:OD1	1:A:891:ASP:N	2.42	0.44
3:C:204:LYS:C	3:C:206:THR:N	2.71	0.44
3:C:216:GLU:HA	3:C:220:LYS:HB3	2.00	0.44
4:D:199:LEU:HD21	4:D:211:ILE:HG21	1.99	0.44
5:E:112:GLN:HA	5:E:166:ARG:HG3	2.00	0.44
1:I:244:LYS:HE3	1:I:244:LYS:HB2	1.66	0.44
1:I:295:HIS:O	1:I:297:SER:N	2.49	0.44
2:J:35:LEU:CD2	2:J:132:SER:HA	2.48	0.44
2:J:122:ARG:HE	2:J:400:PRO:HG3	1.82	0.44
3:M:107:ALA:HB1	3:M:270:TRP:CZ2	2.52	0.44
3:M:364:ASN:O	3:M:367:ILE:HG22	2.18	0.44
1:A:93:HIS:CE1	1:A:160:GLU:HB2	2.53	0.44
2:B:573:ASP:OD1	2:B:576:ARG:NE	2.40	0.44
3:C:144:GLU:H	3:C:144:GLU:HG2	1.54	0.44
5:E:113:LEU:HD12	5:E:118:VAL:HG11	2.00	0.44
11:P:14:GLU:OE2	11:P:30:CYS:SG	2.75	0.44
1:I:74:PHE:CE1	1:I:221:PRO:HA	2.53	0.44
1:I:93:HIS:NE2	1:I:160:GLU:HB2	2.33	0.44
1:I:673:GLU:CB	1:I:809:LYS:HD2	2.48	0.44
1:I:704:GLY:C	1:I:706:LEU:H	2.21	0.44
1:I:756:ARG:NH2	2:J:922:ARG:HH22	2.16	0.44
2:J:41:PHE:HE2	2:J:356:LYS:CG	2.31	0.44
2:J:126:LEU:HD12	2:J:127:PRO:HD2	1.99	0.44
2:J:393:PHE:O	2:J:394:VAL:HG23	2.13	0.44
2:J:902:PRO:HB2	2:J:974:MET:HG2	2.00	0.44
3:M:384:LEU:O	5:Q:22:PRO:HG3	2.18	0.44
11:W:14:GLU:HB2	11:W:15:VAL:H	1.59	0.44
1:A:100:CYS:O	1:A:103:CYS:SG	2.75	0.44
1:A:104:GLY:O	1:A:194:PRO:HD2	2.17	0.44
1:A:852:LEU:HD11	3:C:311:MET:HG3	1.99	0.44
2:B:539:VAL:HG12	2:B:557:VAL:HG12	1.99	0.44
3:C:100:ARG:HH21	3:C:288:GLU:HG2	1.81	0.44
3:C:281:ALA:O	3:C:285:ILE:HG12	2.18	0.44
1:I:104:GLY:O	1:I:194:PRO:HD2	2.18	0.44
1:I:106:ILE:HD13	1:I:201:LEU:HD11	2.00	0.44
1:I:351:MET:HG2	1:I:415:HIS:ND1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:357:ASP:HA	2:J:360:ARG:NH1	2.32	0.44
2:J:778:PRO:HD3	2:J:814:GLY:HA3	1.99	0.44
2:J:1063:TRP:HE1	2:J:1094:LYS:HE3	1.82	0.44
3:M:160:VAL:CG1	3:M:161:VAL:H	2.21	0.44
4:O:54:LEU:HD11	10:V:2:ILE:HD12	1.98	0.44
5:Q:61:PRO:HA	8:T:11:ARG:NH2	2.33	0.44
7:S:41:PRO:HG2	7:S:75:TYR:CE1	2.53	0.44
9:U:35:ASN:ND2	9:U:73:GLU:OE1	2.51	0.44
1:A:93:HIS:NE2	1:A:160:GLU:HB2	2.33	0.43
1:A:172:GLU:OE1	1:A:173:GLU:N	2.51	0.43
1:A:867:ILE:H	1:A:867:ILE:HG13	1.28	0.43
2:B:365:GLN:HE21	2:B:365:GLN:HB3	1.56	0.43
2:B:688:ILE:HD11	10:N:62:TYR:CD1	2.52	0.43
2:B:968:HIS:HD2	2:B:969:SER:N	2.16	0.43
3:C:163:ILE:H	3:C:163:ILE:CD1	2.08	0.43
3:C:384:LEU:HD21	5:E:18:PHE:HA	2.00	0.43
7:H:42:GLN:HA	7:H:78:LEU:H	1.82	0.43
9:L:35:ASN:ND2	9:L:73:GLU:OE1	2.52	0.43
1:I:536:ASP:HA	1:I:540:LEU:HB2	2.00	0.43
1:I:852:LEU:HD13	3:M:307:LEU:HD21	1.99	0.43
2:J:182:GLU:HG3	2:J:183:ARG:H	1.82	0.43
2:J:222:VAL:HA	2:J:223:PRO:HD2	1.79	0.43
2:J:322:MET:HE1	2:J:523:TYR:HE2	1.83	0.43
2:J:491:THR:HB	2:J:492:GLY:H	1.58	0.43
2:J:992:ILE:HD11	2:J:994:TYR:CE1	2.53	0.43
3:M:269:ILE:H	3:M:269:ILE:HG13	1.57	0.43
3:M:288:GLU:O	3:M:292:THR:OG1	2.35	0.43
4:O:62:ARG:HH12	10:V:2:ILE:HD12	1.83	0.43
4:O:181:PRO:HD3	4:O:194:ILE:HD13	1.99	0.43
5:Q:167:GLN:HB2	5:Q:170:LEU:HD12	1.99	0.43
6:R:120:PRO:O	6:R:122:GLU:N	2.44	0.43
1:A:664:LYS:HG2	2:B:984:GLU:OE2	2.18	0.43
2:B:179:THR:HA	2:B:194:VAL:HG22	2.00	0.43
5:E:167:GLN:HB2	5:E:170:LEU:HD12	1.99	0.43
8:K:8:GLU:HB3	8:K:53:VAL:HG21	2.00	0.43
1:I:264:PRO:O	1:I:266:LEU:N	2.49	0.43
1:I:894:ILE:HD13	3:M:45:ILE:HD13	2.00	0.43
2:J:280:LEU:HD23	2:J:280:LEU:HA	1.89	0.43
2:J:745:ALA:HB1	2:J:749:ARG:CZ	2.48	0.43
2:J:925:VAL:O	2:J:929:ILE:HG13	2.18	0.43
4:O:199:LEU:HD21	4:O:211:ILE:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PHE:HA	1:A:156:PRO:HD2	1.75	0.43
1:A:163:THR:HB	1:A:276:GLN:NE2	2.33	0.43
1:A:673:GLU:CB	1:A:809:LYS:HD2	2.48	0.43
2:B:148:LEU:HA	2:B:148:LEU:HD13	1.63	0.43
2:B:391:GLN:HE22	2:B:393:PHE:HE2	1.65	0.43
2:B:574:ASP:OD1	2:B:574:ASP:N	2.51	0.43
4:D:119:PRO:HD2	10:N:15:ALA:HB1	2.00	0.43
5:E:3:LYS:HZ2	6:F:9:GLU:CD	2.21	0.43
5:E:174:GLU:HG3	5:E:175:TRP:N	2.33	0.43
1:I:765:MET:HG3	2:J:923:MET:HG2	1.99	0.43
2:J:391:GLN:HB3	2:J:392:ARG:H	1.67	0.43
2:J:539:VAL:HG12	2:J:557:VAL:HG12	1.99	0.43
2:J:853:LYS:HE2	2:J:869:THR:HG21	2.00	0.43
3:M:336:ARG:HB3	3:M:345:HIS:HB3	2.00	0.43
3:M:385:PRO:HA	5:Q:22:PRO:HD3	1.99	0.43
1:A:10:SER:CB	2:B:1118:ARG:HB3	2.48	0.43
1:A:527:GLU:HG3	9:L:40:PHE:CD1	2.53	0.43
4:D:92:GLU:HB2	4:D:130:THR:HG23	2.00	0.43
1:I:127:LYS:HB2	3:M:330:LYS:HB3	2.01	0.43
2:J:1040:LEU:O	2:J:1042:GLY:N	2.49	0.43
3:M:236:LYS:O	3:M:237:GLU:HB3	2.18	0.43
3:M:359:ASN:OD1	14:M:401:HOH:O	2.21	0.43
1:A:8:ILE:HB	3:C:369:GLN:OE1	2.19	0.43
1:A:757:GLY:O	1:A:758:LYS:HB2	2.17	0.43
2:B:25:TRP:HZ2	2:B:485:LEU:HB3	1.80	0.43
2:B:485:LEU:HD11	2:B:655:SER:OG	2.19	0.43
2:B:702:VAL:O	10:N:51:SER:HB2	2.19	0.43
2:B:992:ILE:HD11	2:B:994:TYR:CE1	2.53	0.43
3:C:152:ILE:HG13	3:C:159:TYR:CD2	2.48	0.43
9:L:91:ALA:C	9:L:94:GLU:OE1	2.57	0.43
1:I:444:PRO:O	9:U:49:ILE:CD1	2.58	0.43
2:J:749:ARG:HE	4:O:144:ALA:CB	2.30	0.43
1:A:351:MET:HG2	1:A:415:HIS:ND1	2.33	0.43
1:A:635:ASP:O	1:A:638:VAL:HG22	2.18	0.43
1:A:885:GLY:O	3:C:303:ARG:NH2	2.46	0.43
2:B:35:LEU:CD2	2:B:132:SER:HA	2.48	0.43
3:C:187:LYS:CE	3:C:206:THR:HB	2.48	0.43
1:I:93:HIS:CE1	1:I:160:GLU:HB2	2.53	0.43
2:J:46:LEU:O	2:J:50:VAL:HG12	2.19	0.43
5:Q:5:LEU:CD1	6:R:6:LYS:CD	2.96	0.43
7:S:43:ILE:HG22	7:S:44:LYS:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ILE:HD13	1:A:201:LEU:HD11	2.01	0.43
2:B:99:TYR:HB2	2:B:160:ILE:HB	2.01	0.43
2:B:305:HIS:CE1	2:B:306:MET:HG2	2.53	0.43
2:B:1066:GLU:HA	2:B:1119:LEU:HD22	2.00	0.43
7:H:41:PRO:HG2	7:H:75:TYR:CE1	2.54	0.43
1:I:436:MET:HB2	1:I:458:TYR:OH	2.19	0.43
1:I:834:ARG:NH1	3:M:99:PRO:HD3	2.30	0.43
3:M:333:VAL:O	3:M:337:ALA:N	2.51	0.43
4:O:225:GLU:OE2	10:V:42:ARG:NH2	2.51	0.43
1:A:684:HIS:O	1:A:688:ARG:HG3	2.19	0.43
2:B:516:ALA:HA	2:B:517:PRO:HA	1.72	0.43
2:B:698:HIS:HE1	2:B:873:LEU:HD21	1.84	0.43
2:B:749:ARG:NH1	4:D:150:PHE:HZ	2.17	0.43
1:I:150:CYS:CB	1:I:153:PRO:HD3	2.48	0.43
1:I:251:ILE:HD13	1:I:274:LEU:HD22	2.00	0.43
1:I:582:CYS:HB2	1:I:608:PHE:CE1	2.54	0.43
2:J:780:PRO:HA	2:J:785:TYR:CZ	2.54	0.43
3:M:100:ARG:O	3:M:104:ILE:HG22	2.19	0.43
8:T:38:GLN:H	8:T:38:GLN:HG2	1.37	0.43
1:A:103:CYS:SG	1:A:104:GLY:N	2.91	0.43
3:C:13:LYS:HE2	3:C:13:LYS:HB2	1.82	0.43
1:I:370:ARG:HD3	1:I:379:PRO:O	2.19	0.43
1:I:447:THR:HG22	2:J:1001:VAL:HG21	2.00	0.43
1:I:543:PRO:O	1:I:544:ASP:HB2	2.18	0.43
1:I:632:LYS:NZ	1:I:634:LEU:H	2.08	0.43
1:I:808:TYR:HE2	2:J:923:MET:SD	2.42	0.43
2:J:378:TYR:C	2:J:380:ARG:H	2.22	0.43
2:J:429:ARG:HG3	2:J:683:TRP:CZ3	2.54	0.43
3:M:100:ARG:NH2	3:M:267:ASN:O	2.52	0.43
3:M:177:LYS:C	3:M:179:VAL:N	2.72	0.43
4:O:92:GLU:HB2	4:O:130:THR:HG23	1.99	0.43
10:V:22:LYS:HZ3	10:V:54:GLU:HG2	1.82	0.43
2:B:780:PRO:HA	2:B:785:TYR:CZ	2.54	0.43
5:E:100:ARG:NE	6:F:43:VAL:HG13	2.34	0.43
1:I:564:PRO:HB2	1:I:567:LEU:HD21	2.01	0.43
1:I:743:MET:HA	1:I:748:VAL:HG11	2.00	0.43
2:J:41:PHE:HD1	2:J:42:ILE:CD1	2.32	0.43
3:M:205:VAL:O	3:M:205:VAL:HG12	2.19	0.43
7:S:43:ILE:HG22	7:S:44:LYS:H	1.84	0.43
7:S:56:LYS:O	7:S:58:GLY:N	2.51	0.43
1:A:150:CYS:SG	1:A:153:PRO:CD	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ARG:HD3	1:A:379:PRO:O	2.19	0.42
2:B:17:LEU:HB3	2:B:644:LEU:O	2.19	0.42
2:B:393:PHE:O	2:B:394:VAL:CG1	2.67	0.42
2:B:591:LEU:HD22	2:B:595:HIS:NE2	2.34	0.42
2:B:1087:GLY:C	2:B:1089:ASP:H	2.18	0.42
3:C:179:VAL:HG22	3:C:190:GLU:OE2	2.19	0.42
3:C:385:PRO:HA	3:C:386:LEU:HD13	2.01	0.42
4:D:45:VAL:O	11:P:46:VAL:N	2.47	0.42
4:D:98:MET:HG2	4:D:100:TYR:HE1	1.84	0.42
7:H:13:VAL:HG13	7:H:14:LEU:H	1.84	0.42
7:H:56:LYS:O	7:H:58:GLY:N	2.51	0.42
10:N:62:TYR:O	10:N:63:LYS:HG3	2.20	0.42
1:I:17:SER:HB3	1:I:20:GLU:HG3	2.00	0.42
1:I:159:PHE:HD1	1:I:159:PHE:HA	1.78	0.42
1:I:626:TYR:HA	1:I:632:LYS:NZ	2.34	0.42
2:J:165:GLU:OE2	2:J:689:ARG:NH2	2.52	0.42
2:J:220:PRO:HD2	2:J:301:ASN:HB3	2.01	0.42
2:J:591:LEU:HD22	2:J:595:HIS:NE2	2.34	0.42
2:J:703:PRO:HG3	2:J:715:PHE:HE2	1.83	0.42
2:J:939:LEU:HB2	2:J:964:LEU:HD13	1.99	0.42
2:J:1066:GLU:HA	2:J:1119:LEU:HD22	2.00	0.42
2:J:1101:PHE:CD1	3:M:367:ILE:HG13	2.54	0.42
3:M:178:VAL:O	3:M:190:GLU:OE1	2.37	0.42
8:T:8:GLU:HB3	8:T:53:VAL:HG21	2.00	0.42
1:A:120:PHE:CD2	1:A:133:LEU:HD11	2.54	0.42
1:A:221:PRO:O	1:A:226:ARG:NH2	2.49	0.42
2:B:41:PHE:HD1	2:B:356:LYS:HG2	1.83	0.42
2:B:429:ARG:HG3	2:B:683:TRP:CZ3	2.54	0.42
3:C:100:ARG:O	3:C:104:ILE:HG22	2.19	0.42
3:C:214:ILE:HG22	3:C:218:VAL:HB	2.01	0.42
3:C:364:ASN:O	3:C:367:ILE:HG22	2.19	0.42
9:L:28:LEU:HD23	9:L:57:PHE:HE2	1.84	0.42
1:I:444:PRO:CB	9:U:50:THR:HG22	2.48	0.42
2:J:573:ASP:OD1	2:J:576:ARG:NE	2.40	0.42
2:J:649:ILE:HD13	2:J:649:ILE:HA	1.79	0.42
2:J:815:ARG:HG2	2:J:816:THR:H	1.83	0.42
3:M:262:THR:HA	7:S:12:HIS:HB3	2.01	0.42
4:O:50:ASN:HD22	4:O:50:ASN:C	2.22	0.42
5:Q:174:GLU:HG3	5:Q:175:TRP:N	2.33	0.42
6:R:38:PHE:CD2	6:R:40:GLU:HG2	2.54	0.42
2:B:573:ASP:HB2	2:B:574:ASP:H	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:160:VAL:CG2	3:C:198:LEU:HB3	2.47	0.42
7:H:65:ARG:NH1	7:H:75:TYR:HD2	2.18	0.42
10:N:56:ILE:C	10:N:58:GLN:H	2.23	0.42
1:I:495:ARG:HG2	3:M:300:VAL:HG23	2.02	0.42
1:I:684:HIS:O	1:I:688:ARG:HG3	2.19	0.42
1:I:889:ASP:O	1:I:893:VAL:HG23	2.20	0.42
2:J:99:TYR:HB2	2:J:160:ILE:HB	2.01	0.42
2:J:498:VAL:O	2:J:502:LEU:HG	2.19	0.42
2:J:749:ARG:HH21	4:O:144:ALA:HB1	1.83	0.42
2:J:903:TRP:HE1	4:O:153:TYR:H	1.67	0.42
1:A:9:GLY:O	3:C:358:LEU:HD11	2.19	0.42
1:A:17:SER:HB3	1:A:20:GLU:HG3	2.01	0.42
2:B:220:PRO:HD2	2:B:301:ASN:HB3	2.01	0.42
7:H:43:ILE:HG22	7:H:44:LYS:H	1.84	0.42
10:N:52:HIS:CE1	10:N:54:GLU:H	2.38	0.42
1:I:31:VAL:HA	1:I:32:PRO:HD3	1.86	0.42
1:I:364:TYR:OH	1:I:406:LEU:HB3	2.19	0.42
1:I:878:ASP:HA	1:I:879:PRO:HD2	1.85	0.42
2:J:365:GLN:HG2	2:J:365:GLN:H	1.66	0.42
2:J:510:ILE:HA	2:J:513:ARG:NH2	2.34	0.42
3:M:182:LEU:HA	3:M:185:SER:OG	2.19	0.42
4:O:60:ALA:HB1	11:W:48:ALA:HB2	2.00	0.42
5:Q:145:ARG:NH2	6:R:94:VAL:HG23	2.35	0.42
5:Q:174:GLU:O	5:Q:178:LYS:HB2	2.19	0.42
8:T:49:ILE:H	8:T:49:ILE:HG13	1.46	0.42
10:V:56:ILE:C	10:V:58:GLN:H	2.23	0.42
1:A:750:MET:C	1:A:753:THR:HG22	2.40	0.42
2:B:378:TYR:CE1	2:B:389:ASN:N	2.83	0.42
2:B:925:VAL:O	2:B:929:ILE:HG13	2.20	0.42
3:C:187:LYS:O	3:C:188:SER:HB2	2.20	0.42
6:F:38:PHE:CD2	6:F:40:GLU:HG2	2.54	0.42
9:L:28:LEU:HD23	9:L:57:PHE:CE2	2.55	0.42
1:I:456:PRO:HB3	1:I:628:ARG:NH1	2.35	0.42
1:I:712:LYS:HD2	3:M:93:ASN:OD1	2.20	0.42
3:M:130:LYS:O	3:M:134:VAL:HG23	2.19	0.42
3:M:160:VAL:CG1	3:M:161:VAL:N	2.79	0.42
3:M:213:LYS:O	3:M:216:GLU:HG3	2.18	0.42
2:B:58:PRO:HG3	2:B:63:PHE:HB2	2.02	0.42
2:B:498:VAL:O	2:B:502:LEU:HG	2.19	0.42
4:D:161:VAL:HG11	4:D:171:LEU:HD12	2.01	0.42
5:E:174:GLU:O	5:E:178:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:404:GLU:H	1:I:404:GLU:HG2	1.69	0.42
3:M:109:LYS:HA	3:M:270:TRP:CD1	2.55	0.42
3:M:343:THR:OG1	3:M:344:GLN:OE1	2.34	0.42
9:U:49:ILE:HG22	9:U:50:THR:N	2.21	0.42
1:A:456:PRO:HB3	1:A:628:ARG:NH1	2.35	0.42
1:A:462:PHE:CD2	2:B:737:GLU:HB2	2.55	0.42
2:B:378:TYR:C	2:B:380:ARG:H	2.22	0.42
2:B:554:VAL:HA	2:B:578:ARG:NH1	2.35	0.42
1:I:9:GLY:HA3	2:J:1120:LYS:CG	2.50	0.42
1:I:44:GLY:HA2	1:I:49:LYS:HD3	2.01	0.42
1:I:120:PHE:CD2	1:I:133:LEU:HD11	2.54	0.42
1:I:370:ARG:HH21	1:I:417:GLU:CD	2.22	0.42
1:I:439:ARG:NH1	1:I:486:GLU:OE2	2.52	0.42
1:I:635:ASP:O	1:I:638:VAL:HG22	2.18	0.42
1:I:658:ILE:HD13	2:J:733:GLY:HA3	2.02	0.42
1:I:756:ARG:NH1	2:J:922:ARG:HH12	2.17	0.42
7:S:65:ARG:NH1	7:S:75:TYR:HD2	2.17	0.42
1:A:863:PRO:HB2	3:C:360:GLY:HA2	2.02	0.42
2:B:31:VAL:HG21	2:B:155:PRO:HB2	2.02	0.42
2:B:77:PHE:HD1	2:B:77:PHE:HA	1.67	0.42
2:B:189:LYS:HB3	2:B:190:VAL:H	1.60	0.42
2:B:681:LEU:O	2:B:718:ARG:HB3	2.20	0.42
3:C:72:ILE:HD12	3:C:72:ILE:HA	1.89	0.42
1:I:368:LYS:O	1:I:372:LEU:HB2	2.20	0.42
1:I:781:ARG:HH22	2:J:341:ASP:HB2	1.84	0.42
2:J:645:MET:HA	2:J:646:PRO:HD2	1.95	0.42
3:M:214:ILE:C	3:M:216:GLU:N	2.73	0.42
3:M:348:ALA:O	3:M:352:ARG:HG2	2.18	0.42
4:O:24:PRO:HB3	9:U:30:GLU:OE1	2.19	0.42
5:Q:48:ILE:HA	5:Q:74:VAL:HG13	2.01	0.42
2:B:63:PHE:HB3	2:B:392:ARG:NH2	2.34	0.42
2:B:365:GLN:HG2	2:B:365:GLN:H	1.67	0.42
3:C:120:LEU:C	3:C:260:ASP:HB2	2.40	0.42
3:C:163:ILE:HG22	3:C:165:PRO:HD3	2.02	0.42
1:I:147:CYS:SG	1:I:152:ALA:HA	2.58	0.42
1:I:587:LYS:HB2	1:I:588:LEU:H	1.72	0.42
1:I:656:LEU:O	1:I:660:VAL:HG23	2.20	0.42
2:J:17:LEU:HB3	2:J:644:LEU:O	2.19	0.42
2:J:485:LEU:HD11	2:J:655:SER:OG	2.19	0.42
2:J:898:GLN:O	2:J:901:MET:HB2	2.20	0.42
8:T:16:ARG:HG2	8:T:49:ILE:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:CYS:O	1:A:152:ALA:CA	2.65	0.42
1:A:370:ARG:HH21	1:A:417:GLU:CD	2.22	0.42
1:A:439:ARG:NH1	1:A:486:GLU:OE2	2.52	0.42
1:A:521:PHE:N	1:A:521:PHE:CD1	2.88	0.42
1:A:772:GLN:HB2	1:A:779:LEU:HD11	2.02	0.42
2:B:366:LEU:HD21	2:B:398:ILE:O	2.20	0.42
3:C:109:LYS:HA	3:C:270:TRP:CD1	2.55	0.42
3:C:177:LYS:HE2	3:C:178:VAL:N	2.34	0.42
4:D:50:ASN:HD22	4:D:50:ASN:C	2.23	0.42
7:H:43:ILE:HG22	7:H:44:LYS:N	2.34	0.42
1:I:432:ARG:O	1:I:434:SER:N	2.53	0.42
1:I:553:TRP:HB3	1:I:558:ILE:HD11	2.01	0.42
2:J:31:VAL:HG21	2:J:155:PRO:HB2	2.02	0.42
2:J:758:ARG:NH1	2:J:844:ARG:HG3	2.34	0.42
3:M:120:LEU:C	3:M:260:ASP:HB2	2.40	0.42
9:U:44:THR:C	9:U:45:ILE:CG1	2.88	0.42
1:A:463:ASP:HA	2:B:890:GLY:CA	2.49	0.41
1:A:656:LEU:O	1:A:660:VAL:HG23	2.20	0.41
2:B:510:ILE:HA	2:B:513:ARG:HG3	2.01	0.41
2:B:801:PHE:O	2:B:804:SER:OG	2.36	0.41
3:C:165:PRO:HG2	3:C:166:GLU:OE2	2.20	0.41
4:D:23:VAL:HA	4:D:220:PHE:HE2	1.85	0.41
1:I:782:GLY:O	2:J:459:HIS:HE1	2.03	0.41
2:J:681:LEU:O	2:J:718:ARG:HB3	2.20	0.41
3:M:153:ASP:CG	3:M:157:MET:CB	2.87	0.41
4:O:61:HIS:O	4:O:65:MET:HG2	2.20	0.41
1:A:756:ARG:HB3	2:B:921:SER:HB3	2.01	0.41
2:B:130:LEU:HD22	2:B:158:TYR:CZ	2.55	0.41
2:B:165:GLU:OE2	2:B:689:ARG:NH2	2.52	0.41
2:B:731:TYR:HE2	2:B:902:PRO:CG	2.31	0.41
2:B:809:LYS:H	2:B:809:LYS:HG2	1.52	0.41
3:C:288:GLU:O	3:C:292:THR:OG1	2.35	0.41
7:H:66:LYS:HG2	7:H:72:TYR:CE1	2.55	0.41
1:I:63:CYS:SG	1:I:73:HIS:NE2	2.77	0.41
2:J:148:LEU:HA	2:J:148:LEU:HD13	1.63	0.41
2:J:286:PRO:HD2	2:J:290:ARG:NE	2.28	0.41
2:J:498:VAL:HG12	2:J:502:LEU:HD11	2.02	0.41
2:J:554:VAL:HA	2:J:578:ARG:NH1	2.35	0.41
2:J:749:ARG:NH1	4:O:150:PHE:HZ	2.18	0.41
4:O:112:LYS:HE2	4:O:112:LYS:HB3	1.89	0.41
1:A:309:LYS:HZ1	3:C:343:THR:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ARG:O	1:A:443:MET:HG3	2.20	0.41
1:A:553:TRP:HB3	1:A:558:ILE:HD11	2.02	0.41
1:A:854:VAL:CG2	3:C:62:GLU:HB3	2.50	0.41
2:B:940:THR:OG1	2:B:964:LEU:HD11	2.20	0.41
3:C:21:LYS:HE3	3:C:21:LYS:HB3	1.41	0.41
3:C:100:ARG:NH2	3:C:267:ASN:O	2.52	0.41
5:E:3:LYS:HD2	6:F:11:TYR:CE1	2.55	0.41
5:E:48:ILE:HA	5:E:74:VAL:HG13	2.03	0.41
1:I:31:VAL:HG11	1:I:43:GLU:OE1	2.20	0.41
1:I:521:PHE:N	1:I:521:PHE:CD1	2.88	0.41
1:I:536:ASP:O	1:I:537:VAL:C	2.59	0.41
2:J:940:THR:OG1	2:J:964:LEU:HD11	2.20	0.41
4:O:161:VAL:HG11	4:O:171:LEU:HD12	2.01	0.41
1:A:244:LYS:O	1:A:248:ILE:HG13	2.21	0.41
1:A:331:VAL:HG23	2:B:1001:VAL:HG23	2.01	0.41
1:A:368:LYS:O	1:A:372:LEU:HB2	2.20	0.41
1:A:635:ASP:OD1	1:A:639:ARG:NE	2.50	0.41
1:A:878:ASP:HA	1:A:879:PRO:HD2	1.85	0.41
1:A:889:ASP:O	1:A:893:VAL:HG23	2.20	0.41
3:C:215:ALA:O	3:C:220:LYS:HB2	2.19	0.41
4:D:61:HIS:O	4:D:65:MET:HG2	2.20	0.41
4:D:201:ARG:HA	4:D:204:GLU:CG	2.50	0.41
1:I:709:LEU:H	1:I:717:THR:HG21	1.85	0.41
2:J:508:VAL:HA	2:J:509:PRO:HD2	1.88	0.41
2:J:592:THR:HB	2:J:593:ARG:H	1.64	0.41
2:J:801:PHE:O	2:J:804:SER:OG	2.37	0.41
3:M:55:LYS:HG2	8:T:3:ARG:NH2	2.35	0.41
3:M:143:LEU:HA	3:M:146:LEU:HB2	2.03	0.41
1:A:238:GLU:HG2	1:A:239:ASP:N	2.35	0.41
1:A:679:ALA:O	1:A:683:ILE:HG12	2.21	0.41
1:A:854:VAL:HG22	3:C:64:VAL:HG23	2.03	0.41
2:B:274:LEU:HD12	2:B:274:LEU:HA	1.89	0.41
2:B:670:TYR:O	2:B:674:MET:HB2	2.20	0.41
2:B:983:LEU:H	2:B:983:LEU:HG	1.65	0.41
2:B:1083:CYS:HB2	2:B:1084:PRO:HD2	2.02	0.41
3:C:55:LYS:HG2	8:K:3:ARG:NH2	2.33	0.41
3:C:130:LYS:O	3:C:134:VAL:HG23	2.19	0.41
5:E:2:TYR:OH	6:F:44:SER:OG	2.27	0.41
1:I:13:PHE:HB2	3:M:355:VAL:O	2.20	0.41
1:I:209:ARG:HB2	1:I:212:TRP:CE2	2.56	0.41
1:I:635:ASP:OD1	1:I:639:ARG:NE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:160:VAL:C	3:M:161:VAL:HG23	2.40	0.41
3:M:385:PRO:HA	5:Q:22:PRO:CD	2.50	0.41
4:O:41:ALA:HB3	4:O:146:TRP:CD1	2.56	0.41
4:O:201:ARG:HA	4:O:204:GLU:CG	2.50	0.41
5:Q:5:LEU:HD13	6:R:6:LYS:HD3	2.02	0.41
5:Q:27:LYS:HD2	5:Q:50:ASP:HA	2.03	0.41
7:S:13:VAL:HG13	7:S:14:LEU:H	1.84	0.41
10:V:52:HIS:CE1	10:V:54:GLU:H	2.38	0.41
1:A:307:ARG:C	1:A:309:LYS:H	2.23	0.41
1:A:456:PRO:HB3	1:A:628:ARG:HH11	1.85	0.41
1:A:472:PRO:HG2	1:A:478:GLN:HG2	2.03	0.41
1:A:709:LEU:H	1:A:717:THR:HG21	1.85	0.41
2:B:193:LYS:HE3	2:B:204:LEU:HD11	2.03	0.41
3:C:189:ALA:HB2	3:C:200:VAL:O	2.21	0.41
1:I:244:LYS:O	1:I:248:ILE:HG13	2.21	0.41
1:I:456:PRO:HB3	1:I:628:ARG:HH11	1.86	0.41
2:J:912:LEU:HD23	2:J:912:LEU:HA	1.89	0.41
3:M:191:PHE:HD1	3:M:191:PHE:HA	1.69	0.41
1:A:74:PHE:CE1	1:A:221:PRO:HA	2.55	0.41
1:A:867:ILE:HD12	7:H:40:LEU:HA	2.03	0.41
2:B:116:GLN:HE21	2:B:117:GLU:HB3	1.86	0.41
2:B:591:LEU:HD13	2:B:595:HIS:ND1	2.35	0.41
2:B:678:SER:OG	2:B:995:GLN:OE1	2.29	0.41
2:B:731:TYR:C	2:B:733:GLY:H	2.23	0.41
6:F:121:LEU:HD23	6:F:121:LEU:HA	1.91	0.41
9:L:43:TYR:O	9:L:44:THR:HG22	2.21	0.41
10:N:7:CYS:HB2	10:N:14:LEU:HD12	2.03	0.41
2:J:16:GLU:HA	2:J:19:LEU:HD12	2.03	0.41
2:J:174:LEU:HD11	2:J:340:LYS:HB2	2.02	0.41
2:J:189:LYS:HZ2	3:M:212:ARG:NH1	2.19	0.41
2:J:373:GLN:HE21	2:J:397:SER:HA	1.84	0.41
1:A:62:THR:HA	2:B:1077:ARG:HH11	1.85	0.41
1:A:244:LYS:HB2	1:A:244:LYS:HE3	1.66	0.41
1:A:848:ALA:HB2	3:C:327:VAL:CG2	2.51	0.41
2:B:691:ASP:O	2:B:759:THR:HG23	2.21	0.41
2:B:898:GLN:O	2:B:901:MET:HB2	2.20	0.41
2:B:1082:TYR:HD1	2:B:1088:GLU:N	2.18	0.41
9:L:4:GLU:HB2	9:L:16:TYR:HB2	2.03	0.41
1:I:472:PRO:HG2	1:I:478:GLN:HG2	2.02	0.41
1:I:772:GLN:HB2	1:I:779:LEU:HD11	2.01	0.41
2:J:135:CYS:O	2:J:137:LEU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:773:ASP:OD2	2:J:815:ARG:NH1	2.44	0.41
3:M:72:ILE:HD12	3:M:72:ILE:HA	1.88	0.41
3:M:144:GLU:H	3:M:144:GLU:HG2	1.56	0.41
3:M:157:MET:HB3	3:M:160:VAL:CG2	2.51	0.41
4:O:219:SER:C	4:O:220:PHE:HD1	2.24	0.41
1:A:22:ARG:HA	1:A:76:HIS:ND1	2.36	0.41
1:A:159:PHE:HD1	1:A:159:PHE:HA	1.78	0.41
1:A:285:ASN:ND2	1:A:301:LEU:O	2.43	0.41
1:A:479:ALA:O	1:A:483:ILE:HG12	2.21	0.41
1:A:542:GLU:HA	1:A:543:PRO:HA	1.90	0.41
1:A:564:PRO:HB2	1:A:567:LEU:HD21	2.02	0.41
1:A:583:GLU:HG3	1:A:584:ALA:H	1.86	0.41
2:B:16:GLU:HA	2:B:19:LEU:HD12	2.03	0.41
2:B:135:CYS:O	2:B:137:LEU:N	2.54	0.41
2:B:498:VAL:HG12	2:B:502:LEU:HD11	2.02	0.41
2:B:731:TYR:CZ	2:B:902:PRO:HG3	2.55	0.41
2:B:903:TRP:HZ3	2:B:977:GLY:HA2	1.86	0.41
3:C:187:LYS:HB2	3:C:188:SER:H	1.73	0.41
3:C:194:GLU:CD	3:C:196:TYR:HE2	2.22	0.41
8:K:38:GLN:H	8:K:38:GLN:HG2	1.37	0.41
9:L:43:TYR:C	9:L:44:THR:CG2	2.89	0.41
10:N:61:VAL:O	10:N:61:VAL:HG22	2.21	0.41
1:I:24:MET:HA	2:J:1084:PRO:CB	2.50	0.41
1:I:230:THR:HG22	1:I:236:ARG:HD3	2.03	0.41
1:I:441:ARG:O	1:I:443:MET:HG3	2.20	0.41
1:I:479:ALA:O	1:I:483:ILE:HG12	2.21	0.41
1:I:679:ALA:O	1:I:683:ILE:HG12	2.21	0.41
2:J:116:GLN:HE21	2:J:117:GLU:HB3	1.86	0.41
2:J:520:TYR:OH	2:J:535:GLY:HA2	2.21	0.41
2:J:691:ASP:O	2:J:759:THR:HG23	2.21	0.41
2:J:698:HIS:HE1	2:J:873:LEU:HD21	1.84	0.41
2:J:980:GLY:HA3	4:O:23:VAL:HG13	2.03	0.41
2:J:1054:LEU:O	2:J:1056:GLU:N	2.54	0.41
3:M:157:MET:C	3:M:159:TYR:H	2.24	0.41
4:O:23:VAL:HA	4:O:220:PHE:HE2	1.85	0.41
4:O:225:GLU:HG3	10:V:12:LYS:NZ	2.36	0.41
1:A:209:ARG:HB2	1:A:212:TRP:CE2	2.56	0.41
1:A:856:TYR:HE2	3:C:377:ILE:O	2.04	0.41
2:B:47:GLN:HE21	2:B:51:ASN:ND2	2.19	0.41
2:B:204:LEU:HD23	2:B:205:ILE:N	2.36	0.41
2:B:520:TYR:OH	2:B:535:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:968:HIS:CD2	2:B:969:SER:N	2.89	0.41
8:K:16:ARG:HG2	8:K:49:ILE:HG22	2.02	0.41
11:P:17:LEU:HD11	11:P:27:CYS:HA	2.03	0.41
1:I:86:VAL:HG11	1:I:287:THR:HG21	2.03	0.41
1:I:307:ARG:C	1:I:309:LYS:H	2.24	0.41
1:I:493:SER:HA	1:I:494:PRO:HD3	1.92	0.41
1:I:789:THR:HG21	2:J:623:GLU:OE2	2.21	0.41
2:J:109:PRO:HG2	2:J:116:GLN:OE1	2.21	0.41
2:J:189:LYS:NZ	3:M:212:ARG:HH12	2.19	0.41
2:J:1050:ILE:HD11	3:M:370:PRO:CA	2.50	0.41
3:M:148:ARG:CZ	3:M:162:GLU:HB3	2.38	0.41
3:M:217:LYS:C	3:M:218:VAL:HG23	2.41	0.41
1:A:362:PHE:HD2	8:K:34:ILE:O	2.03	0.40
3:C:96:LEU:CB	3:C:100:ARG:HB2	2.49	0.40
3:C:107:ALA:HB1	3:C:270:TRP:HZ2	1.86	0.40
5:E:3:LYS:CE	6:F:9:GLU:CD	2.90	0.40
5:E:27:LYS:HD2	5:E:50:ASP:HA	2.03	0.40
10:N:60:MET:C	10:N:62:TYR:N	2.73	0.40
1:I:147:CYS:HA	1:I:148:PRO:HD3	1.83	0.40
1:I:622:ASP:OD1	1:I:624:LYS:HB2	2.21	0.40
1:I:662:THR:HG23	2:J:731:TYR:HA	2.03	0.40
2:J:130:LEU:HD22	2:J:158:TYR:CZ	2.55	0.40
2:J:520:TYR:CZ	2:J:535:GLY:HA2	2.56	0.40
2:J:521:ARG:N	2:J:531:THR:HG22	2.36	0.40
2:J:968:HIS:CD2	2:J:969:SER:N	2.89	0.40
2:J:1122:ARG:NE	2:J:1122:ARG:C	2.75	0.40
3:M:183:THR:C	3:M:185:SER:N	2.75	0.40
3:M:183:THR:O	3:M:185:SER:N	2.53	0.40
10:V:7:CYS:HB2	10:V:14:LEU:HD12	2.03	0.40
1:A:55:ASP:O	1:A:57:GLY:N	2.52	0.40
1:A:628:ARG:O	1:A:630:ASP:N	2.46	0.40
1:A:831:THR:HA	3:C:80:THR:HG21	2.03	0.40
5:E:156:ILE:H	5:E:156:ILE:HG13	1.68	0.40
7:H:43:ILE:O	7:H:80:VAL:N	2.53	0.40
10:N:1:MET:H1	10:N:55:LEU:N	2.18	0.40
1:I:841:MET:O	1:I:845:LEU:HG	2.22	0.40
2:J:58:PRO:HG3	2:J:63:PHE:HB2	2.02	0.40
2:J:309:ASP:HB2	2:J:312:ASN:ND2	2.37	0.40
2:J:670:TYR:O	2:J:674:MET:HB2	2.20	0.40
4:O:157:THR:HG22	4:O:215:ILE:HA	2.03	0.40
1:A:187:ARG:HD2	1:A:214:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:MET:HB2	1:A:458:TYR:OH	2.21	0.40
2:B:95:ARG:NH2	11:P:33:LYS:HD3	2.37	0.40
2:B:114:ILE:HG12	2:B:114:ILE:H	1.79	0.40
2:B:153:LYS:HD2	2:B:153:LYS:HA	1.86	0.40
2:B:429:ARG:HA	2:B:429:ARG:HD2	1.78	0.40
3:C:320:PRO:O	3:C:325:GLY:HA3	2.22	0.40
4:D:41:ALA:HB3	4:D:146:TRP:CD1	2.56	0.40
5:E:24:GLU:O	5:E:28:ILE:HG13	2.22	0.40
6:F:117:GLU:C	6:F:119:ARG:H	2.24	0.40
1:I:362:PHE:CZ	8:T:26:VAL:HG21	2.57	0.40
3:M:107:ALA:HB1	3:M:270:TRP:HZ2	1.87	0.40
3:M:320:PRO:O	3:M:325:GLY:HA3	2.21	0.40
3:M:334:LEU:HA	3:M:337:ALA:HB3	2.03	0.40
4:O:219:SER:O	4:O:220:PHE:HD1	2.05	0.40
3:C:55:LYS:HE2	8:K:3:ARG:NH2	2.32	0.40
10:N:12:LYS:HE3	10:N:12:LYS:HB3	1.65	0.40
1:I:419:GLY:N	1:I:440:VAL:O	2.52	0.40
1:I:526:VAL:HG21	1:I:553:TRP:CD1	2.57	0.40
1:I:709:LEU:HD12	1:I:717:THR:HA	2.04	0.40
2:J:121:VAL:HG12	2:J:122:ARG:O	2.21	0.40
2:J:193:LYS:HE2	2:J:195:PHE:CE2	2.56	0.40
2:J:509:PRO:C	2:J:511:GLU:H	2.24	0.40
2:J:591:LEU:HD13	2:J:595:HIS:ND1	2.35	0.40
3:M:13:LYS:HE2	3:M:13:LYS:HB2	1.83	0.40
3:M:160:VAL:HG13	3:M:199:VAL:H	1.86	0.40
4:O:118:ILE:HG23	10:V:15:ALA:HB3	2.04	0.40
4:O:141:LYS:HE3	4:O:141:LYS:HB2	1.96	0.40
6:R:117:GLU:C	6:R:119:ARG:H	2.24	0.40
2:B:193:LYS:HE2	2:B:195:PHE:CE2	2.56	0.40
3:C:204:LYS:HG3	3:C:205:VAL:N	2.36	0.40
9:L:43:TYR:C	9:L:44:THR:HG23	2.41	0.40
1:I:28:GLU:HB2	1:I:76:HIS:HE2	1.87	0.40
2:J:10:PRO:O	2:J:11:THR:OG1	2.24	0.40
2:J:459:HIS:CE1	2:J:461:THR:HG23	2.57	0.40
2:J:516:ALA:HA	2:J:517:PRO:HA	1.72	0.40

All (20) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:98:LYS:NZ	5:Q:82:GLN:NE2[3_445]	1.00	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:PRO:C	6:F:31:GLU:OE1[1_655]	1.06	1.14
2:B:61:PRO:O	6:F:31:GLU:OE1[1_655]	1.11	1.09
2:B:61:PRO:CB	6:F:31:GLU:CD[1_655]	1.35	0.85
2:B:61:PRO:CA	6:F:31:GLU:OE1[1_655]	1.41	0.79
2:B:61:PRO:CA	6:F:31:GLU:CD[1_655]	1.59	0.61
2:B:61:PRO:CB	6:F:31:GLU:OE2[1_655]	1.66	0.54
11:P:29:TYR:CD2	6:R:122:GLU:CD[1_655]	1.66	0.54
2:B:61:PRO:CA	6:F:31:GLU:OE2[1_655]	1.70	0.50
11:P:29:TYR:CD2	6:R:122:GLU:OE1[1_655]	1.73	0.47
11:P:29:TYR:CD2	6:R:122:GLU:OE2[1_655]	1.75	0.45
11:P:29:TYR:CG	6:R:122:GLU:OE1[1_655]	1.77	0.43
6:F:98:LYS:NZ	5:Q:82:GLN:CD[3_445]	1.86	0.34
2:B:61:PRO:CB	6:F:31:GLU:OE1[1_655]	1.97	0.23
6:F:97:ALA:O	5:Q:81:ASN:ND2[3_445]	2.05	0.15
2:B:61:PRO:CB	6:F:31:GLU:CG[1_655]	2.08	0.12
5:E:81:ASN:ND2	6:R:97:ALA:O[3_445]	2.08	0.12
5:E:82:GLN:OE1	6:R:98:LYS:CD[3_445]	2.08	0.12
11:P:29:TYR:CB	6:R:122:GLU:OE1[1_655]	2.08	0.12
2:B:284:GLY:N	1:I:150:CYS:O[3_545]	2.17	0.03

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	855/906 (94%)	689 (81%)	116 (14%)	50 (6%)	1	13
1	I	853/906 (94%)	692 (81%)	110 (13%)	51 (6%)	1	13
2	B	1061/1123 (94%)	872 (82%)	141 (13%)	48 (4%)	2	18
2	J	1061/1123 (94%)	864 (81%)	143 (14%)	54 (5%)	1	16
3	C	365/391 (93%)	258 (71%)	73 (20%)	34 (9%)	0	7
3	M	365/391 (93%)	266 (73%)	75 (20%)	24 (7%)	1	11
4	D	256/259 (99%)	241 (94%)	12 (5%)	3 (1%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	O	256/259 (99%)	242 (94%)	11 (4%)	3 (1%)	11	43
5	E	179/190 (94%)	161 (90%)	18 (10%)	0	100	100
5	Q	179/190 (94%)	161 (90%)	18 (10%)	0	100	100
6	F	120/122 (98%)	108 (90%)	8 (7%)	4 (3%)	3	25
6	R	120/122 (98%)	108 (90%)	8 (7%)	4 (3%)	3	25
7	H	74/82 (90%)	59 (80%)	10 (14%)	5 (7%)	1	11
7	S	74/82 (90%)	60 (81%)	10 (14%)	4 (5%)	1	14
8	K	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1	9
8	T	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1	9
9	L	92/100 (92%)	74 (80%)	12 (13%)	6 (6%)	1	12
9	U	92/100 (92%)	75 (82%)	10 (11%)	7 (8%)	1	9
10	N	61/65 (94%)	44 (72%)	11 (18%)	6 (10%)	0	6
10	V	61/65 (94%)	44 (72%)	11 (18%)	6 (10%)	0	6
11	P	40/49 (82%)	24 (60%)	10 (25%)	6 (15%)	0	2
11	W	40/49 (82%)	22 (55%)	11 (28%)	7 (18%)	0	2
All	All	6312/6688 (94%)	5150 (82%)	832 (13%)	330 (5%)	1	15

All (330) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	151	GLY
1	A	153	PRO
1	A	154	GLN
1	A	398	ASN
1	A	400	GLU
1	A	430	LEU
1	A	463	ASP
1	A	537	VAL
1	A	583	GLU
1	A	630	ASP
2	B	57	VAL
2	B	183	ARG
2	B	286	PRO
2	B	287	LYS
2	B	391	GLN
2	B	392	ARG

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Mol	Chain	Res	Type
2	B	394	VAL
2	B	430	THR
2	B	513	ARG
2	B	515	PRO
2	B	521	ARG
2	B	845	PRO
3	C	161	VAL
3	C	162	GLU
3	C	165	PRO
3	C	181	LYS
3	C	224	LYS
4	D	209	LYS
7	H	9	ILE
7	H	11	ASP
8	K	28	ILE
8	K	30	VAL
9	L	49	ILE
9	L	93	ILE
10	N	2	ILE
10	N	61	VAL
11	P	19	LEU
11	P	20	ALA
1	I	40	TYR
1	I	41	PRO
1	I	48	ASP
1	I	154	GLN
1	I	395	MET
1	I	397	SER
1	I	398	ASN
1	I	400	GLU
1	I	430	LEU
1	I	463	ASP
1	I	537	VAL
1	I	583	GLU
1	I	587	LYS
1	I	642	GLY
1	I	643	VAL
2	J	43	ASP
2	J	57	VAL
2	J	183	ARG
2	J	286	PRO
2	J	287	LYS

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Mol	Chain	Res	Type
2	J	392	ARG
2	J	393	PHE
2	J	394	VAL
2	J	396	ASN
2	J	430	THR
2	J	515	PRO
2	J	521	ARG
2	J	845	PRO
3	M	152	ILE
3	M	205	VAL
3	M	224	LYS
3	M	237	GLU
3	M	340	GLU
4	O	209	LYS
7	S	11	ASP
8	T	28	ILE
8	T	30	VAL
9	U	93	ILE
10	V	2	ILE
1	A	64	GLY
1	A	65	ALA
1	A	296	LYS
1	A	297	SER
1	A	405	LYS
1	A	578	GLU
1	A	585	LEU
1	A	608	PHE
1	A	758	LYS
2	B	56	VAL
2	B	79	GLU
2	B	138	TYR
2	B	390	ILE
2	B	944	VAL
2	B	1055	GLU
2	B	1057	SER
2	B	1082	TYR
3	C	94	VAL
3	C	160	VAL
3	C	209	SER
3	C	323	ARG
3	C	342	THR
3	C	343	THR

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Mol	Chain	Res	Type
3	C	346	LEU
3	C	357	PRO
3	C	358	LEU
3	C	361	VAL
3	C	385	PRO
10	N	11	GLY
11	P	13	LYS
11	P	14	GLU
1	I	35	TYR
1	I	64	GLY
1	I	65	ALA
1	I	103	CYS
1	I	174	GLY
1	I	297	SER
1	I	585	LEU
1	I	586	GLU
1	I	608	PHE
2	J	40	ALA
2	J	56	VAL
2	J	79	GLU
2	J	138	TYR
2	J	944	VAL
2	J	1055	GLU
2	J	1057	SER
2	J	1077	ARG
3	M	93	ASN
3	M	323	ARG
3	M	357	PRO
3	M	358	LEU
3	M	361	VAL
7	S	7	PHE
9	U	48	PRO
10	V	11	GLY
11	W	13	LYS
11	W	14	GLU
1	A	172	GLU
1	A	173	GLU
1	A	261	ALA
1	A	378	TYR
1	A	395	MET
1	A	397	SER
1	A	404	GLU

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Mol	Chain	Res	Type
1	A	548	ASN
1	A	710	PRO
1	A	754	GLY
1	A	896	ARG
2	B	136	ARG
2	B	212	ASP
2	B	222	VAL
2	B	591	LEU
2	B	780	PRO
2	B	819	PRO
3	C	35	TYR
3	C	36	LYS
3	C	108	ARG
3	C	140	GLY
3	C	158	GLU
3	C	182	LEU
3	C	188	SER
3	C	191	PHE
3	C	221	HIS
9	L	23	THR
9	L	50	THR
1	I	261	ALA
1	I	378	TYR
1	I	396	GLU
1	I	433	MET
1	I	578	GLU
1	I	710	PRO
2	J	136	ARG
2	J	212	ASP
2	J	222	VAL
2	J	397	SER
2	J	591	LEU
2	J	780	PRO
2	J	1042	GLY
2	J	1076	LYS
3	M	35	TYR
3	M	36	LYS
3	M	108	ARG
3	M	140	GLY
3	M	208	LEU
3	M	215	ALA
3	M	218	VAL

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Mol	Chain	Res	Type
3	M	221	HIS
9	U	23	THR
9	U	50	THR
1	A	69	GLU
1	A	152	ALA
1	A	161	ARG
1	A	265	GLN
1	A	433	MET
1	A	544	ASP
1	A	767	ALA
1	A	871	LYS
2	B	82	GLY
2	B	188	ASN
2	B	223	PRO
2	B	236	GLY
2	B	269	THR
2	B	379	GLN
2	B	774	ASN
2	B	919	ILE
2	B	923	MET
3	C	107	ALA
3	C	121	ASP
3	C	142	THR
3	C	163	ILE
3	C	344	GLN
6	F	28	GLY
6	F	31	GLU
6	F	118	TYR
7	H	57	PRO
11	P	24	GLU
1	I	69	GLU
1	I	161	ARG
1	I	265	GLN
1	I	405	LYS
1	I	538	ASN
1	I	588	LEU
1	I	632	LYS
1	I	767	ALA
2	J	46	LEU
2	J	82	GLY
2	J	188	ASN
2	J	223	PRO

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Mol	Chain	Res	Type
2	J	236	GLY
2	J	269	THR
2	J	379	GLN
2	J	774	ASN
2	J	919	ILE
3	M	107	ALA
3	M	121	ASP
3	M	142	THR
3	M	187	LYS
6	R	28	GLY
6	R	31	GLU
6	R	118	TYR
7	S	57	PRO
11	W	21	THR
11	W	24	GLU
1	A	535	MET
1	A	540	LEU
1	A	542	GLU
1	A	632	LYS
1	A	756	ARG
1	A	867	ILE
1	A	888	VAL
2	B	11	THR
2	B	32	ARG
2	B	224	LYS
2	B	445	PRO
2	B	498	VAL
2	B	516	ALA
2	B	837	ARG
2	B	876	PRO
2	B	1072	ALA
3	C	187	LYS
3	C	341	ILE
3	C	384	LEU
4	D	11	PRO
7	H	10	PHE
9	L	48	PRO
10	N	41	GLU
11	P	42	VAL
1	I	44	GLY
1	I	152	ALA
1	I	296	LYS

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Mol	Chain	Res	Type
1	I	540	LEU
1	I	542	GLU
1	I	544	ASP
1	I	867	ILE
1	I	871	LYS
1	I	888	VAL
2	J	11	THR
2	J	32	ARG
2	J	224	LYS
2	J	399	ARG
2	J	498	VAL
2	J	516	ALA
2	J	837	ARG
2	J	876	PRO
2	J	1046	ALA
2	J	1072	ALA
3	M	203	LYS
4	O	11	PRO
10	V	41	GLU
11	W	19	LEU
11	W	42	VAL
1	A	36	ASP
1	A	464	GLY
2	B	46	LEU
2	B	1112	VAL
7	H	80	VAL
8	K	24	ALA
9	L	46	GLU
10	N	3	VAL
10	N	4	PRO
1	I	464	GLY
1	I	535	MET
1	I	633	LEU
2	J	445	PRO
2	J	1041	ILE
2	J	1112	VAL
3	M	95	THR
7	S	80	VAL
8	T	24	ALA
9	U	51	MET
9	U	53	ARG
10	V	3	VAL

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Mol	Chain	Res	Type
10	V	4	PRO
11	W	20	ALA
2	B	705	VAL
4	D	21	VAL
2	J	705	VAL
4	O	21	VAL
9	U	49	ILE
10	V	61	VAL
1	A	543	PRO
2	B	517	PRO
3	C	205	VAL
6	F	33	PRO
1	I	543	PRO
2	J	517	PRO
6	R	33	PRO
1	A	41	PRO
8	K	33	GLY
2	J	390	ILE
8	T	33	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	743/779 (95%)	639 (86%)	104 (14%)	3	16
1	I	740/779 (95%)	636 (86%)	104 (14%)	3	16
2	B	923/969 (95%)	788 (85%)	135 (15%)	2	15
2	J	923/969 (95%)	787 (85%)	136 (15%)	2	15
3	C	314/334 (94%)	252 (80%)	62 (20%)	1	6
3	M	313/334 (94%)	250 (80%)	63 (20%)	1	5
4	D	227/228 (100%)	218 (96%)	9 (4%)	27	56
4	O	227/228 (100%)	218 (96%)	9 (4%)	27	56
5	E	160/167 (96%)	144 (90%)	16 (10%)	6	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Q	160/167 (96%)	145 (91%)	15 (9%)	7	29
6	F	107/107 (100%)	99 (92%)	8 (8%)	11	35
6	R	107/107 (100%)	99 (92%)	8 (8%)	11	35
7	H	68/72 (94%)	51 (75%)	17 (25%)	0	3
7	S	68/72 (94%)	50 (74%)	18 (26%)	0	2
8	K	45/46 (98%)	38 (84%)	7 (16%)	2	13
8	T	45/46 (98%)	38 (84%)	7 (16%)	2	13
9	L	81/87 (93%)	77 (95%)	4 (5%)	21	50
9	U	81/87 (93%)	76 (94%)	5 (6%)	15	42
10	N	57/59 (97%)	50 (88%)	7 (12%)	4	20
10	V	57/59 (97%)	51 (90%)	6 (10%)	5	25
11	P	35/40 (88%)	30 (86%)	5 (14%)	2	16
11	W	35/40 (88%)	31 (89%)	4 (11%)	4	22
All	All	5516/5776 (96%)	4767 (86%)	749 (14%)	3	17

All (749) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	33	ASP
1	A	34	THR
1	A	36	ASP
1	A	38	ASP
1	A	40	TYR
1	A	42	ILE
1	A	46	LEU
1	A	47	MET
1	A	51	LEU
1	A	58	LEU
1	A	74	PHE
1	A	76	HIS
1	A	81	ARG
1	A	105	ARG
1	A	106	ILE
1	A	108	LEU
1	A	116	TYR
1	A	123	MET

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Mol	Chain	Res	Type
1	A	133	LEU
1	A	149	HIS
1	A	158	LYS
1	A	159	PHE
1	A	161	ARG
1	A	170	LYS
1	A	176	GLU
1	A	180	ARG
1	A	188	ASP
1	A	196	LYS
1	A	204	HIS
1	A	242	THR
1	A	255	LEU
1	A	287	THR
1	A	288	SER
1	A	335	ASP
1	A	337	MET
1	A	359	VAL
1	A	362	PHE
1	A	364	TYR
1	A	372	LEU
1	A	384	VAL
1	A	388	GLU
1	A	393	ARG
1	A	395	MET
1	A	399	ARG
1	A	408	ILE
1	A	412	VAL
1	A	422	VAL
1	A	423	LEU
1	A	424	PHE
1	A	426	ARG
1	A	431	HIS
1	A	435	ILE
1	A	469	LEU
1	A	484	LEU
1	A	504	ILE
1	A	505	GLN
1	A	516	ARG
1	A	523	ARG
1	A	524	TYR
1	A	530	LEU

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Mol	Chain	Res	Type
1	A	532	PHE
1	A	536	ASP
1	A	538	ASN
1	A	540	LEU
1	A	542	GLU
1	A	557	THR
1	A	561	LEU
1	A	567	LEU
1	A	569	ILE
1	A	572	ARG
1	A	575	LEU
1	A	577	ASP
1	A	580	GLU
1	A	583	GLU
1	A	585	LEU
1	A	602	LYS
1	A	603	LEU
1	A	612	GLN
1	A	632	LYS
1	A	637	ILE
1	A	641	TYR
1	A	647	ARG
1	A	654	THR
1	A	656	LEU
1	A	668	THR
1	A	706	LEU
1	A	712	LYS
1	A	728	GLU
1	A	743	MET
1	A	758	LYS
1	A	806	ASN
1	A	825	ARG
1	A	851	ASP
1	A	853	LYS
1	A	854	VAL
1	A	855	ASP
1	A	862	ASP
1	A	864	THR
1	A	867	ILE
1	A	868	VAL
1	A	883	TRP
1	A	884	GLN

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Mol	Chain	Res	Type
1	A	891	ASP
2	B	46	LEU
2	B	50	VAL
2	B	55	GLU
2	B	56	VAL
2	B	57	VAL
2	B	59	ASP
2	B	66	LYS
2	B	77	PHE
2	B	81	GLN
2	B	84	ARG
2	B	94	ILE
2	B	105	LEU
2	B	108	ILE
2	B	111	VAL
2	B	114	ILE
2	B	125	GLU
2	B	133	LYS
2	B	142	ASP
2	B	143	GLU
2	B	148	LEU
2	B	161	ILE
2	B	166	ARG
2	B	168	ILE
2	B	170	SER
2	B	179	THR
2	B	184	ASP
2	B	190	VAL
2	B	199	HIS
2	B	207	VAL
2	B	210	LYS
2	B	218	THR
2	B	235	LEU
2	B	259	ASP
2	B	263	ASP
2	B	269	THR
2	B	270	GLN
2	B	279	ARG
2	B	292	ARG
2	B	293	ARG
2	B	308	VAL
2	B	309	ASP

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Mol	Chain	Res	Type
2	B	320	LEU
2	B	322	MET
2	B	325	LEU
2	B	346	LYS
2	B	347	ARG
2	B	353	ASP
2	B	358	LEU
2	B	365	GLN
2	B	366	LEU
2	B	370	MET
2	B	377	THR
2	B	388	GLU
2	B	389	ASN
2	B	394	VAL
2	B	395	ARG
2	B	409	HIS
2	B	416	TRP
2	B	429	ARG
2	B	431	ASN
2	B	435	THR
2	B	448	ARG
2	B	458	LEU
2	B	469	THR
2	B	470	GLU
2	B	480	VAL
2	B	491	THR
2	B	497	GLU
2	B	510	ILE
2	B	520	TYR
2	B	521	ARG
2	B	524	LEU
2	B	536	ARG
2	B	537	LYS
2	B	545	ASP
2	B	554	VAL
2	B	559	LEU
2	B	578	ARG
2	B	599	ILE
2	B	603	THR
2	B	604	LEU
2	B	610	ILE
2	B	630	THR

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Mol	Chain	Res	Type
2	B	637	GLU
2	B	644	LEU
2	B	650	LEU
2	B	656	LEU
2	B	681	LEU
2	B	683	TRP
2	B	687	ARG
2	B	688	ILE
2	B	695	HIS
2	B	725	VAL
2	B	726	VAL
2	B	740	VAL
2	B	751	LEU
2	B	759	THR
2	B	765	LYS
2	B	776	GLU
2	B	782	ILE
2	B	786	LEU
2	B	793	HIS
2	B	796	GLU
2	B	800	ILE
2	B	801	PHE
2	B	809	LYS
2	B	816	THR
2	B	842	THR
2	B	843	VAL
2	B	848	LYS
2	B	850	VAL
2	B	855	ILE
2	B	861	ASP
2	B	873	LEU
2	B	878	LEU
2	B	896	VAL
2	B	908	ILE
2	B	942	ARG
2	B	952	GLU
2	B	967	LYS
2	B	968	HIS
2	B	971	ARG
2	B	981	ARG
2	B	983	LEU
2	B	984	GLU

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Mol	Chain	Res	Type
2	B	989	ILE
2	B	992	ILE
2	B	1055	GLU
2	B	1062	VAL
2	B	1067	SER
2	B	1089	ASP
2	B	1091	ARG
2	B	1112	VAL
2	B	1118	ARG
2	B	1121	ASP
3	C	7	ILE
3	C	9	SER
3	C	12	SER
3	C	15	GLU
3	C	21	LYS
3	C	23	GLU
3	C	25	TYR
3	C	29	ILE
3	C	31	TYR
3	C	37	LEU
3	C	38	LYS
3	C	40	ASP
3	C	43	GLN
3	C	64	VAL
3	C	71	SER
3	C	94	VAL
3	C	113	THR
3	C	129	ASP
3	C	141	THR
3	C	144	GLU
3	C	145	ASN
3	C	148	ARG
3	C	149	GLU
3	C	157	MET
3	C	163	ILE
3	C	166	GLU
3	C	167	ARG
3	C	170	LYS
3	C	176	GLU
3	C	177	LYS
3	C	180	ARG
3	C	181	LYS

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Mol	Chain	Res	Type
3	C	182	LEU
3	C	186	PHE
3	C	187	LYS
3	C	216	GLU
3	C	219	LYS
3	C	223	LEU
3	C	236	LYS
3	C	240	GLU
3	C	244	TYR
3	C	246	GLU
3	C	269	ILE
3	C	291	SER
3	C	292	THR
3	C	298	LEU
3	C	302	VAL
3	C	311	MET
3	C	315	ASP
3	C	326	ILE
3	C	330	LYS
3	C	339	PHE
3	C	340	GLU
3	C	342	THR
3	C	346	LEU
3	C	347	PHE
3	C	355	VAL
3	C	358	LEU
3	C	362	VAL
3	C	369	GLN
3	C	373	VAL
3	C	384	LEU
4	D	14	ILE
4	D	16	PHE
4	D	27	ASN
4	D	50	ASN
4	D	188	GLU
4	D	193	THR
4	D	194	ILE
4	D	198	TYR
4	D	201	ARG
5	E	1	MET
5	E	5	LEU
5	E	16	ARG

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Mol	Chain	Res	Type
5	E	46	LEU
5	E	59	ILE
5	E	74	VAL
5	E	91	GLU
5	E	93	MET
5	E	110	ILE
5	E	119	VAL
5	E	125	ARG
5	E	138	LEU
5	E	153	SER
5	E	165	MET
5	E	174	GLU
5	E	177	GLU
6	F	7	LEU
6	F	40	GLU
6	F	50	ARG
6	F	55	LYS
6	F	71	ASP
6	F	90	LEU
6	F	100	GLU
6	F	121	LEU
7	H	6	GLU
7	H	9	ILE
7	H	10	PHE
7	H	29	LEU
7	H	37	ILE
7	H	38	SER
7	H	40	LEU
7	H	44	LYS
7	H	50	VAL
7	H	51	VAL
7	H	53	LEU
7	H	62	GLU
7	H	69	THR
7	H	74	TYR
7	H	75	TYR
7	H	78	LEU
7	H	81	GLU
8	K	3	ARG
8	K	35	THR
8	K	38	GLN
8	K	41	LEU

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Mol	Chain	Res	Type
8	K	46	LYS
8	K	49	ILE
8	K	57	SER
9	L	43	TYR
9	L	46	GLU
9	L	50	THR
9	L	93	ILE
10	N	3	VAL
10	N	12	LYS
10	N	19	TYR
10	N	48	THR
10	N	54	GLU
10	N	60	MET
10	N	63	LYS
11	P	14	GLU
11	P	15	VAL
11	P	21	THR
11	P	23	ARG
11	P	44	ARG
1	I	10	SER
1	I	33	ASP
1	I	34	THR
1	I	37	ASP
1	I	38	ASP
1	I	42	ILE
1	I	46	LEU
1	I	47	MET
1	I	51	LEU
1	I	58	LEU
1	I	74	PHE
1	I	76	HIS
1	I	81	ARG
1	I	105	ARG
1	I	106	ILE
1	I	108	LEU
1	I	116	TYR
1	I	123	MET
1	I	133	LEU
1	I	149	HIS
1	I	158	LYS
1	I	159	PHE
1	I	161	ARG

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Mol	Chain	Res	Type
1	I	169	ARG
1	I	170	LYS
1	I	176	GLU
1	I	180	ARG
1	I	188	ASP
1	I	196	LYS
1	I	204	HIS
1	I	242	THR
1	I	255	LEU
1	I	287	THR
1	I	288	SER
1	I	335	ASP
1	I	337	MET
1	I	359	VAL
1	I	362	PHE
1	I	364	TYR
1	I	372	LEU
1	I	384	VAL
1	I	388	GLU
1	I	393	ARG
1	I	395	MET
1	I	399	ARG
1	I	408	ILE
1	I	412	VAL
1	I	422	VAL
1	I	423	LEU
1	I	424	PHE
1	I	426	ARG
1	I	431	HIS
1	I	435	ILE
1	I	469	LEU
1	I	484	LEU
1	I	504	ILE
1	I	505	GLN
1	I	516	ARG
1	I	523	ARG
1	I	524	TYR
1	I	530	LEU
1	I	532	PHE
1	I	536	ASP
1	I	538	ASN
1	I	540	LEU

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Mol	Chain	Res	Type
1	I	542	GLU
1	I	547	GLU
1	I	557	THR
1	I	561	LEU
1	I	567	LEU
1	I	569	ILE
1	I	572	ARG
1	I	575	LEU
1	I	577	ASP
1	I	585	LEU
1	I	588	LEU
1	I	602	LYS
1	I	603	LEU
1	I	612	GLN
1	I	632	LYS
1	I	637	ILE
1	I	641	TYR
1	I	647	ARG
1	I	654	THR
1	I	656	LEU
1	I	668	THR
1	I	706	LEU
1	I	712	LYS
1	I	728	GLU
1	I	743	MET
1	I	806	ASN
1	I	825	ARG
1	I	851	ASP
1	I	853	LYS
1	I	854	VAL
1	I	855	ASP
1	I	862	ASP
1	I	864	THR
1	I	867	ILE
1	I	868	VAL
1	I	883	TRP
1	I	884	GLN
1	I	891	ASP
1	I	897	THR
2	J	43	ASP
2	J	46	LEU
2	J	55	GLU

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Mol	Chain	Res	Type
2	J	56	VAL
2	J	57	VAL
2	J	59	ASP
2	J	66	LYS
2	J	77	PHE
2	J	81	GLN
2	J	84	ARG
2	J	94	ILE
2	J	105	LEU
2	J	108	ILE
2	J	111	VAL
2	J	114	ILE
2	J	125	GLU
2	J	133	LYS
2	J	142	ASP
2	J	143	GLU
2	J	148	LEU
2	J	161	ILE
2	J	166	ARG
2	J	168	ILE
2	J	170	SER
2	J	179	THR
2	J	184	ASP
2	J	190	VAL
2	J	199	HIS
2	J	207	VAL
2	J	210	LYS
2	J	218	THR
2	J	235	LEU
2	J	259	ASP
2	J	263	ASP
2	J	269	THR
2	J	270	GLN
2	J	279	ARG
2	J	292	ARG
2	J	293	ARG
2	J	308	VAL
2	J	309	ASP
2	J	320	LEU
2	J	322	MET
2	J	325	LEU
2	J	346	LYS

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Mol	Chain	Res	Type
2	J	347	ARG
2	J	353	ASP
2	J	358	LEU
2	J	365	GLN
2	J	366	LEU
2	J	370	MET
2	J	377	THR
2	J	388	GLU
2	J	389	ASN
2	J	409	HIS
2	J	416	TRP
2	J	429	ARG
2	J	431	ASN
2	J	435	THR
2	J	448	ARG
2	J	458	LEU
2	J	469	THR
2	J	470	GLU
2	J	480	VAL
2	J	491	THR
2	J	497	GLU
2	J	503	MET
2	J	510	ILE
2	J	513	ARG
2	J	520	TYR
2	J	524	LEU
2	J	536	ARG
2	J	537	LYS
2	J	545	ASP
2	J	554	VAL
2	J	559	LEU
2	J	578	ARG
2	J	599	ILE
2	J	603	THR
2	J	604	LEU
2	J	610	ILE
2	J	637	GLU
2	J	644	LEU
2	J	650	LEU
2	J	656	LEU
2	J	681	LEU
2	J	683	TRP

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Mol	Chain	Res	Type
2	J	687	ARG
2	J	688	ILE
2	J	695	HIS
2	J	725	VAL
2	J	726	VAL
2	J	740	VAL
2	J	751	LEU
2	J	759	THR
2	J	765	LYS
2	J	776	GLU
2	J	782	ILE
2	J	786	LEU
2	J	793	HIS
2	J	796	GLU
2	J	800	ILE
2	J	801	PHE
2	J	809	LYS
2	J	816	THR
2	J	820	ARG
2	J	842	THR
2	J	848	LYS
2	J	850	VAL
2	J	855	ILE
2	J	861	ASP
2	J	873	LEU
2	J	878	LEU
2	J	896	VAL
2	J	908	ILE
2	J	928	LEU
2	J	942	ARG
2	J	952	GLU
2	J	967	LYS
2	J	968	HIS
2	J	971	ARG
2	J	981	ARG
2	J	983	LEU
2	J	984	GLU
2	J	989	ILE
2	J	992	ILE
2	J	1032	PHE
2	J	1039	VAL
2	J	1055	GLU

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Mol	Chain	Res	Type
2	J	1062	VAL
2	J	1067	SER
2	J	1080	LYS
2	J	1091	ARG
2	J	1112	VAL
2	J	1118	ARG
2	J	1122	ARG
3	M	7	ILE
3	M	9	SER
3	M	12	SER
3	M	15	GLU
3	M	21	LYS
3	M	23	GLU
3	M	25	TYR
3	M	29	ILE
3	M	31	TYR
3	M	37	LEU
3	M	38	LYS
3	M	40	ASP
3	M	43	GLN
3	M	64	VAL
3	M	71	SER
3	M	93	ASN
3	M	94	VAL
3	M	113	THR
3	M	129	ASP
3	M	141	THR
3	M	144	GLU
3	M	145	ASN
3	M	148	ARG
3	M	153	ASP
3	M	154	ILE
3	M	155	LEU
3	M	166	GLU
3	M	167	ARG
3	M	170	LYS
3	M	176	GLU
3	M	177	LYS
3	M	180	ARG
3	M	181	LYS
3	M	182	LEU
3	M	191	PHE

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Mol	Chain	Res	Type
3	M	192	GLU
3	M	208	LEU
3	M	210	ASP
3	M	212	ARG
3	M	219	LYS
3	M	223	LEU
3	M	236	LYS
3	M	237	GLU
3	M	240	GLU
3	M	244	TYR
3	M	246	GLU
3	M	291	SER
3	M	292	THR
3	M	298	LEU
3	M	302	VAL
3	M	311	MET
3	M	315	ASP
3	M	326	ILE
3	M	330	LYS
3	M	342	THR
3	M	346	LEU
3	M	347	PHE
3	M	355	VAL
3	M	358	LEU
3	M	362	VAL
3	M	369	GLN
3	M	373	VAL
3	M	384	LEU
4	O	14	ILE
4	O	16	PHE
4	O	27	ASN
4	O	50	ASN
4	O	188	GLU
4	O	193	THR
4	O	194	ILE
4	O	198	TYR
4	O	201	ARG
5	Q	5	LEU
5	Q	16	ARG
5	Q	46	LEU
5	Q	59	ILE
5	Q	74	VAL

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Mol	Chain	Res	Type
5	Q	91	GLU
5	Q	93	MET
5	Q	110	ILE
5	Q	119	VAL
5	Q	125	ARG
5	Q	138	LEU
5	Q	153	SER
5	Q	165	MET
5	Q	174	GLU
5	Q	177	GLU
6	R	7	LEU
6	R	40	GLU
6	R	50	ARG
6	R	55	LYS
6	R	71	ASP
6	R	90	LEU
6	R	100	GLU
6	R	121	LEU
7	S	6	GLU
7	S	7	PHE
7	S	9	ILE
7	S	10	PHE
7	S	29	LEU
7	S	37	ILE
7	S	38	SER
7	S	40	LEU
7	S	44	LYS
7	S	50	VAL
7	S	51	VAL
7	S	53	LEU
7	S	62	GLU
7	S	69	THR
7	S	74	TYR
7	S	75	TYR
7	S	78	LEU
7	S	81	GLU
8	T	3	ARG
8	T	35	THR
8	T	38	GLN
8	T	41	LEU
8	T	46	LYS
8	T	49	ILE

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Mol	Chain	Res	Type
8	T	57	SER
9	U	44	THR
9	U	46	GLU
9	U	49	ILE
9	U	53	ARG
9	U	54	LYS
10	V	3	VAL
10	V	12	LYS
10	V	19	TYR
10	V	48	THR
10	V	54	GLU
10	V	60	MET
11	W	14	GLU
11	W	15	VAL
11	W	23	ARG
11	W	44	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	252	ASN
1	A	648	GLN
1	A	884	GLN
2	B	47	GLN
2	B	312	ASN
2	B	389	ASN
2	B	391	GLN
2	B	639	HIS
2	B	968	HIS
3	C	43	GLN
3	C	156	ASN
4	D	27	ASN
4	D	50	ASN
5	E	68	HIS
9	L	26	ASN
10	N	52	HIS
1	I	138	HIS
1	I	252	ASN
1	I	648	GLN
1	I	842	GLN
1	I	884	GLN

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Mol	Chain	Res	Type
2	J	51	ASN
2	J	312	ASN
2	J	639	HIS
2	J	1070	HIS
3	M	43	GLN
4	O	27	ASN
4	O	50	ASN
5	Q	68	HIS
10	V	52	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 14 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	896:ARG	C	897:THR	N	3.01

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

**Warning:** The R factor obtained from EDS is 0.3325, which does not match the depositor's R factor of 0.2766. Please interpret the results in this section carefully.

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	863/906 (95%)	-0.61	1 (0%) 92 89	41, 157, 264, 370	0
1	I	862/906 (95%)	-0.55	3 (0%) 90 82	54, 163, 263, 381	0
2	B	1069/1123 (95%)	-0.60	1 (0%) 92 89	46, 149, 253, 402	0
2	J	1069/1123 (95%)	-0.59	2 (0%) 92 86	39, 139, 248, 360	0
3	C	369/391 (94%)	-0.57	0 100 100	68, 192, 319, 372	0
3	M	369/391 (94%)	-0.58	1 (0%) 90 82	71, 193, 327, 419	0
4	D	258/259 (99%)	-0.69	1 (0%) 89 79	71, 143, 235, 295	0
4	O	258/259 (99%)	-0.70	1 (0%) 89 79	63, 136, 226, 319	0
5	E	181/190 (95%)	-0.69	0 100 100	69, 158, 250, 398	0
5	Q	181/190 (95%)	-0.77	0 100 100	90, 163, 244, 317	0
6	F	122/122 (100%)	-0.64	0 100 100	133, 164, 244, 447	0
6	R	122/122 (100%)	-0.66	0 100 100	142, 184, 257, 324	0
7	H	76/82 (92%)	-0.69	0 100 100	105, 157, 228, 268	0
7	S	76/82 (92%)	-0.72	0 100 100	114, 166, 248, 293	0
8	K	56/57 (98%)	-0.72	0 100 100	88, 131, 196, 288	0
8	T	56/57 (98%)	-0.70	0 100 100	62, 119, 227, 330	0
9	L	94/100 (94%)	-0.61	0 100 100	78, 142, 221, 331	0
9	U	94/100 (94%)	-0.65	1 (1%) 77 59	83, 149, 223, 474	0
10	N	63/65 (96%)	-0.65	0 100 100	81, 141, 218, 281	0
10	V	63/65 (96%)	-0.57	0 100 100	69, 131, 196, 232	0
11	P	42/49 (85%)	-0.59	0 100 100	125, 173, 254, 294	0
11	W	42/49 (85%)	-0.66	0 100 100	90, 147, 201, 253	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	6385/6688 (95%)	-0.61	11 (0%) 92 86	39, 156, 270, 474	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	626	TYR	2.6
1	I	626	TYR	2.6
2	J	1044	GLY	2.4
1	I	541	PRO	2.3
2	B	731	TYR	2.3
9	U	48	PRO	2.2
3	M	18	ASP	2.1
1	I	670	ILE	2.1
4	O	152	TYR	2.1
2	J	1048	LEU	2.1
4	D	77	LEU	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 monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
13	ZN	P	1501	1/1	0.68	0.09	354,354,354,354	0
12	MG	I	1101	1/1	0.83	0.08	175,175,175,175	0
12	MG	I	1104	1/1	0.90	0.13	54,54,54,54	0
13	ZN	B	1201	1/1	0.91	0.09	364,364,364,364	0
13	ZN	A	1003	1/1	0.92	0.11	488,488,488,488	0
13	ZN	I	1103	1/1	0.93	0.10	527,527,527,527	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
13	ZN	J	1301	1/1	0.93	0.09	521,521,521,521	0
13	ZN	V	1601	1/1	0.94	0.06	210,210,210,210	0
13	ZN	I	1102	1/1	0.95	0.04	147,147,147,147	0
13	ZN	A	1002	1/1	0.95	0.05	137,137,137,137	0
13	ZN	N	1401	1/1	0.95	0.06	127,127,127,127	0
12	MG	A	1004	1/1	0.95	0.08	58,58,58,58	0
12	MG	A	1001	1/1	0.97	0.08	52,52,52,52	0
13	ZN	W	1701	1/1	0.99	0.02	94,94,94,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.