



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:45 PM UTC

PDB ID : 3HOW / pdb\_00003how  
Title : Complete RNA polymerase II elongation complex III with a T-U mismatch and a frayed RNA 3'-uridine  
Authors : Sydow, J.F.; Brueckner, F.; Cheung, A.C.M.; Damsma, G.E.; Dengl, S.; Lehmann, E.; Vassylyev, D.; Cramer, P.  
Deposited on : 2009-06-03  
Resolution : 3.60 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

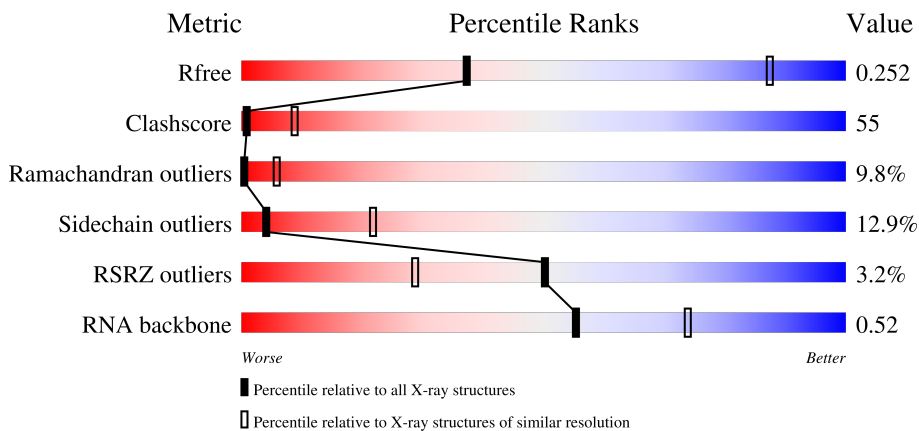
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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))
$R_{free}$	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 25%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 42%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 13%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 18%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 25% 42% 13% • 18%</p>
2	B	1224	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 25%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 47%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 17%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">4% 25% 47% 17% • 9%</p>
3	C	347	<div style="display: flex; align-items: center;"> <div style="width: 18%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 41%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 15%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 23%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">18% 41% 15% • 23%</p>
4	D	221	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 21%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 40%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 15%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 19%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">4% 21% 40% 15% • 19%</p>

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Mol	Chain	Length	Quality of chain
5	E	215	<p>22% 60% 15%</p>
6	F	155	<p>15% 30% 11% 44%</p>
7	G	171	<p>37% 50% 11%</p>
8	H	146	<p>5% 18% 51% 19% 8%</p>
9	I	122	<p>2% 28% 45% 19% 7%</p>
10	J	70	<p>16% 53% 20% 7%</p>
11	K	120	<p>30% 52% 13% 5%</p>
12	L	70	<p>9% 13% 36% 13% 37%</p>
13	2	12	<p>8% 8% 50% 42%</p>
14	1	26	<p>12% 27% 35% 12% 27%</p>
15	3	18	<p>6% 22% 22% 11% 6% 39%</p>

## 2 Entry composition i

There are 17 unique types of molecules in this entry. The entry contains 31876 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1416	11143	7021	1949	2111	62	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1112	8838	5594	1550	1639	55	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	266	2095	1317	348	417	13	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-28	MET	-	expression tag	UNP P16370
C	-27	GLY	-	expression tag	UNP P16370
C	-26	SER	-	expression tag	UNP P16370
C	-25	HIS	-	expression tag	UNP P16370
C	-24	HIS	-	expression tag	UNP P16370
C	-23	HIS	-	expression tag	UNP P16370
C	-22	HIS	-	expression tag	UNP P16370
C	-21	HIS	-	expression tag	UNP P16370
C	-20	HIS	-	expression tag	UNP P16370
C	-19	SER	-	expression tag	UNP P16370
C	-18	ASN	-	expression tag	UNP P16370
C	-17	SER	-	expression tag	UNP P16370
C	-16	GLY	-	expression tag	UNP P16370
C	-15	LEU	-	expression tag	UNP P16370

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	ASN	-	expression tag	UNP P16370
C	-13	ASP	-	expression tag	UNP P16370
C	-12	ILE	-	expression tag	UNP P16370
C	-11	PHE	-	expression tag	UNP P16370
C	-10	GLU	-	expression tag	UNP P16370
C	-9	ALA	-	expression tag	UNP P16370
C	-8	GLN	-	expression tag	UNP P16370
C	-7	LYS	-	expression tag	UNP P16370
C	-6	ILE	-	expression tag	UNP P16370
C	-5	GLU	-	expression tag	UNP P16370
C	-4	TRP	-	expression tag	UNP P16370
C	-3	HIS	-	expression tag	UNP P16370
C	-2	GLU	-	expression tag	UNP P16370
C	-1	ASP	-	expression tag	UNP P16370
C	0	THR	-	expression tag	UNP P16370
C	1	GLY	-	expression tag	UNP P16370

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	87	705	451	119	132	3	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	134	1076	677	182	213	4	0	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	114	927	571	168	178	10	0	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	114	919	590	156	171	2	0	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	44	351	217	70	60	4	0	0	0

- Molecule 13 is a DNA chain called 5'-D(\*AP\*CP\*TP\*AP\*CP\*TP\*TP\*GP\*AP\*GP\*CP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
13	2	7	137	68	22	41	6	0	0	0

- Molecule 14 is a DNA chain called 5'-D(\*AP\*GP\*CP\*TP\*C\*AP\*AP\*GP\*TP\*AP\*GP\*TP\*TP\*AP\*TP\*GP\*CP\*CP\*(BRU)P\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	Br	C	N	O				P
14	1	19	389	1	186	71	113	18	0	0	0

- Molecule 15 is a RNA chain called 5'-R(\*UP\*GP\*CP\*AP\*UP\*UP\*U\*CP\*AP\*AP\*CP\*CP

\*AP\*GP\*GP\*CP\*UP\*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
15	3	11	229	104	41	74	10	0	0	0

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

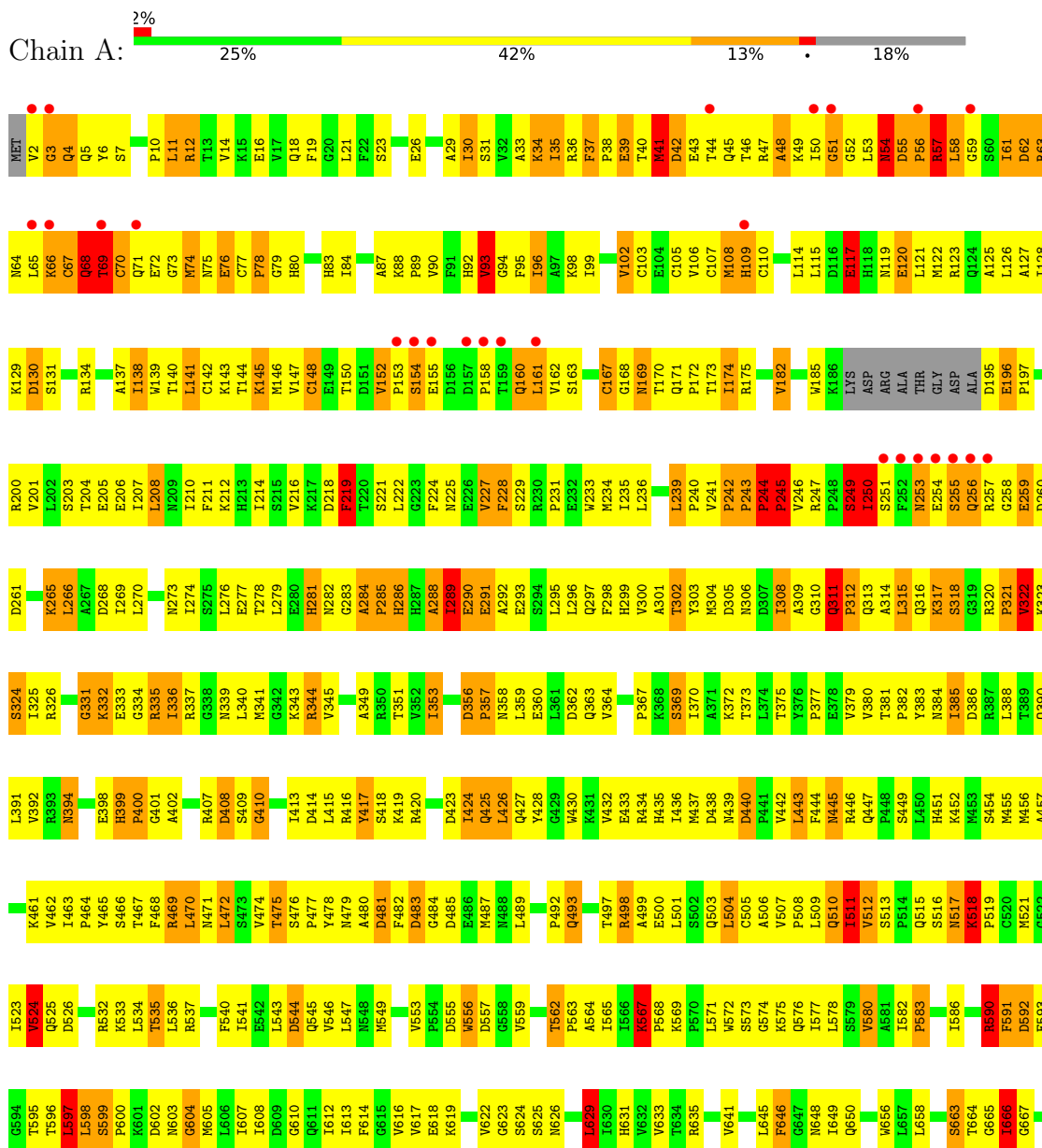
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

### 3 Residue-property plots

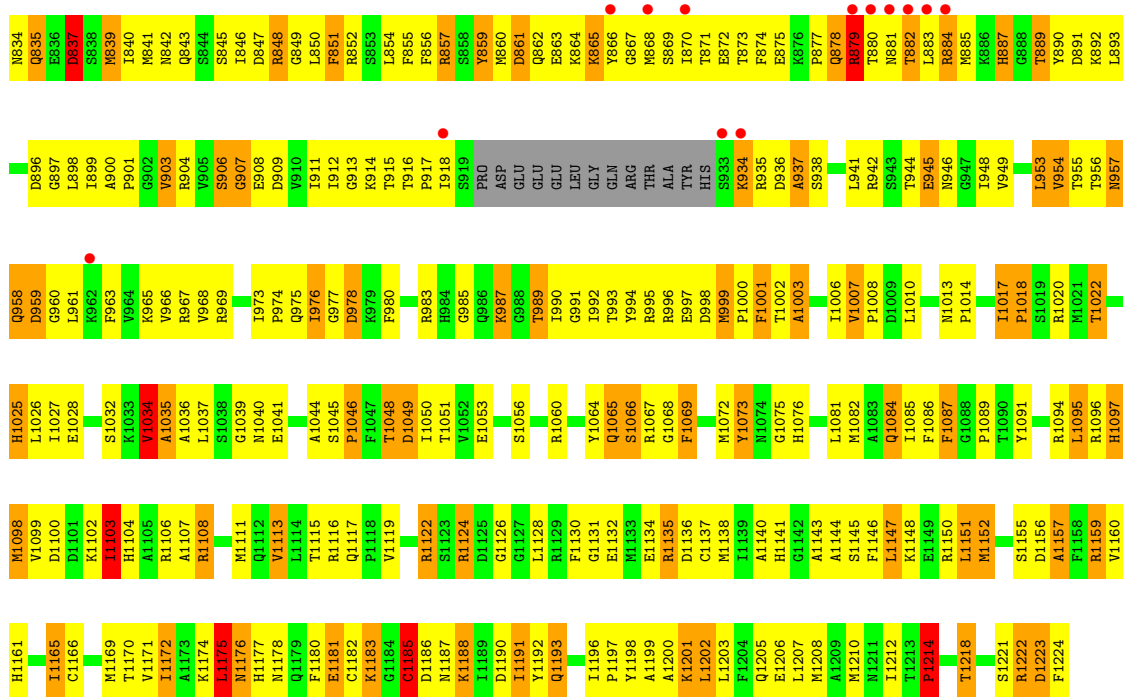
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

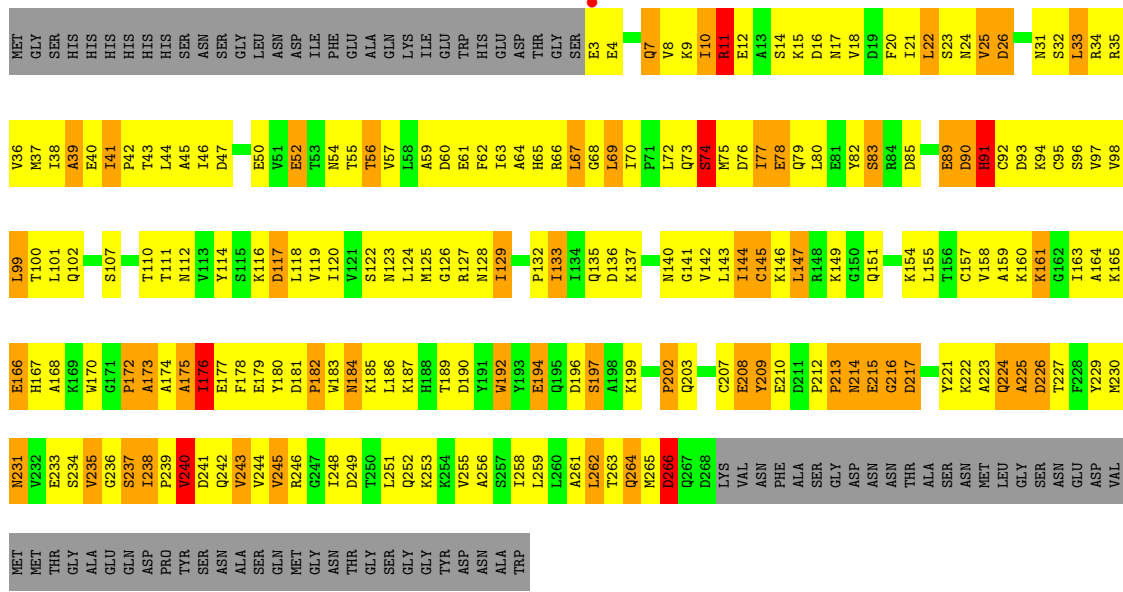
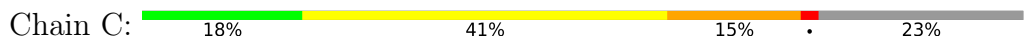




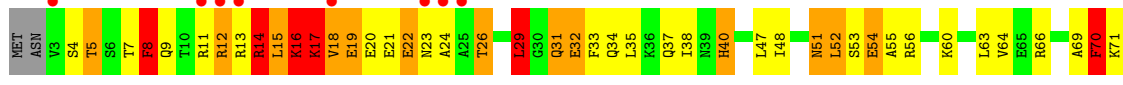
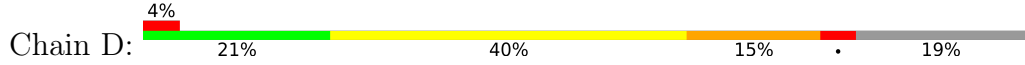




• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



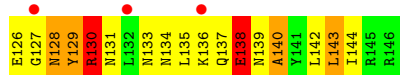
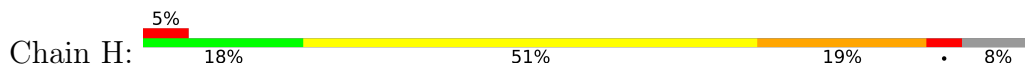
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



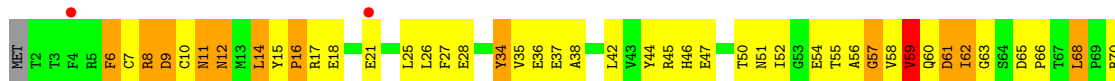




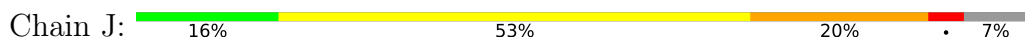
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



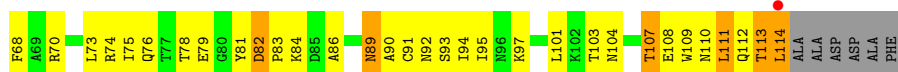
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



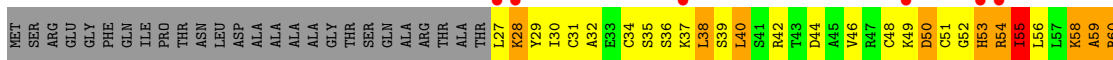
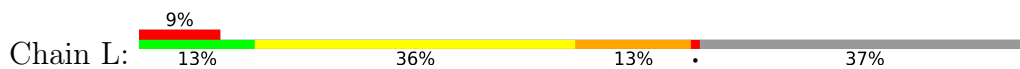
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



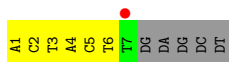
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



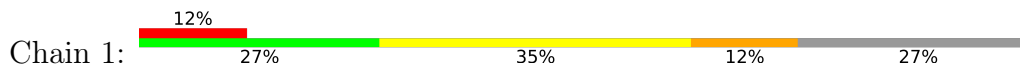
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



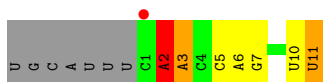
- Molecule 13: 5'-D(\*AP\*CP\*TP\*AP\*CP\*TP\*TP\*GP\*AP\*GP\*CP\*T)-3'



- Molecule 14: 5'-D(\*AP\*GP\*CP\*TP\*C\*AP\*AP\*GP\*TP\*AP\*GP\*TP\*TP\*AP\*TP\*GP\*CP\*C P\*(BRU)P\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'



- Molecule 15: 5'-R(\*UP\*GP\*CP\*AP\*UP\*UP\*U\*CP\*AP\*AP\*CP\*CP\*AP\*GP\*GP\*CP\*UP\*U)-3'



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	222.65Å 395.96Å 283.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 50.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.60) 99.9 (50.00-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 3.57Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.214 , 0.254 0.215 , 0.252	Depositor DCC
$R_{free}$ test set	2843 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	91.4	Xtrriage
Anisotropy	0.061	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 100.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.011 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.018 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	31876	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: BRU, 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	0.68	4/11342 (0.0%)	1.19	113/15337 (0.7%)
2	B	0.63	0/9009	1.12	67/12146 (0.6%)
3	C	0.67	0/2133	1.18	18/2891 (0.6%)
4	D	0.59	0/1444	1.22	19/1935 (1.0%)
5	E	0.58	0/1788	1.11	15/2406 (0.6%)
6	F	0.80	0/717	1.28	4/967 (0.4%)
7	G	0.64	0/1368	1.25	16/1844 (0.9%)
8	H	0.54	0/1094	1.10	10/1481 (0.7%)
9	I	0.53	0/945	1.14	12/1273 (0.9%)
10	J	0.64	0/541	1.18	6/727 (0.8%)
11	K	0.65	0/937	1.03	4/1265 (0.3%)
12	L	0.56	0/353	1.04	2/468 (0.4%)
13	2	0.41	0/152	0.83	0/232
14	1	0.39	0/413	0.84	0/634
15	3	0.47	0/255	0.96	2/395 (0.5%)
All	All	0.64	4/32491 (0.0%)	1.15	288/44001 (0.7%)

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
3	C	0	1
14	1	0	3
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	ASP	CA-C	-6.84	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	ASN	CA-C	6.02	1.60	1.52
1	A	250	ILE	CA-CB	5.64	1.62	1.54
1	A	437	MET	SD-CE	5.47	1.93	1.79

All (288) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	PRO	N-CA-C	-15.66	96.28	114.92
4	D	26	THR	N-CA-C	-14.78	94.56	112.59
7	G	62	LEU	CA-C-N	-12.44	104.29	119.84
7	G	62	LEU	C-N-CA	-12.44	104.29	119.84
2	B	296	GLU	N-CA-C	-11.94	99.19	113.88
2	B	1185	CYS	N-CA-C	-11.88	98.77	113.97
6	F	71	GLU	N-CA-C	-11.47	98.72	113.17
5	E	5	ASN	N-CA-C	-11.15	99.69	113.97
4	D	72	ARG	N-CA-C	-10.60	100.48	113.41
2	B	427	ASP	N-CA-C	-10.43	102.73	114.62
3	C	39	ALA	N-CA-C	10.21	126.51	112.93
1	A	158	PRO	N-CA-C	-9.63	101.27	114.27
1	A	466	SER	N-CA-C	9.37	123.42	112.93
2	B	363	HIS	N-CA-C	-9.35	98.47	110.53
1	A	511	ILE	N-CA-C	9.34	119.94	110.23
4	D	169	SER	N-CA-C	-9.15	103.22	114.75
1	A	1174	PHE	N-CA-C	-9.09	104.26	114.62
5	E	149	LEU	CA-C-N	-8.77	116.64	122.60
5	E	149	LEU	C-N-CA	-8.77	116.64	122.60
2	B	976	ILE	N-CA-C	8.63	118.64	110.53
1	A	1311	VAL	N-CA-C	8.46	120.52	108.17
5	E	63	ASN	N-CA-C	8.38	121.62	108.55
2	B	428	ILE	N-CA-C	-8.29	102.35	110.72
5	E	150	VAL	N-CA-C	8.24	115.06	107.56
1	A	440	ASP	N-CA-C	-8.14	99.39	109.65
1	A	281	HIS	N-CA-C	-8.14	102.39	113.30
11	K	55	LYS	N-CA-C	-8.13	103.26	113.02
8	H	34	ASP	N-CA-C	-8.11	104.37	112.97
1	A	143	LYS	N-CA-C	-8.03	102.12	112.23
2	B	681	TRP	N-CA-C	-7.92	101.74	111.40
1	A	1310	GLY	N-CA-C	-7.91	101.16	111.37
2	B	934	LYS	N-CA-C	7.89	122.53	108.24
1	A	710	LEU	N-CA-C	-7.86	102.03	111.69
2	B	542	MET	N-CA-C	7.85	120.53	111.11
1	A	311	GLN	N-CA-C	7.84	127.14	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1155	ASP	CA-C-N	7.70	127.34	119.56
1	A	1155	ASP	C-N-CA	7.70	127.34	119.56
2	B	555	ILE	N-CA-C	-7.69	103.74	110.74
2	B	1177	HIS	N-CA-C	-7.67	104.39	113.21
7	G	65	ASP	N-CA-C	-7.67	98.58	110.17
4	D	70	PHE	N-CA-C	-7.64	104.38	112.93
1	A	861	GLY	N-CA-C	-7.63	104.75	114.37
5	E	171	LYS	N-CA-C	-7.63	97.88	109.79
2	B	851	PHE	N-CA-C	7.60	121.93	111.90
1	A	117	GLU	N-CA-C	-7.48	104.13	113.18
1	A	243	PRO	CA-C-N	7.40	128.00	120.38
1	A	243	PRO	C-N-CA	7.40	128.00	120.38
2	B	805	THR	N-CA-C	7.36	119.24	108.86
1	A	1241	ARG	N-CA-C	7.35	122.12	112.72
6	F	74	ILE	CA-C-N	7.28	127.31	119.89
6	F	74	ILE	C-N-CA	7.28	127.31	119.89
9	I	112	SER	N-CA-C	-7.27	102.68	112.94
1	A	515	GLN	N-CA-C	-7.26	103.30	111.07
3	C	264	GLN	N-CA-C	-7.25	104.31	113.01
2	B	543	SER	N-CA-C	7.23	119.64	110.24
2	B	645	SER	N-CA-C	-7.20	104.62	113.19
2	B	606	LYS	N-CA-C	-7.18	104.50	113.55
4	D	31	GLN	N-CA-C	-7.17	103.46	111.71
2	B	66	ASP	N-CA-C	-7.12	104.16	112.92
4	D	188	ALA	N-CA-C	-7.12	103.69	112.38
10	J	3	VAL	N-CA-C	7.09	116.69	108.96
2	B	473	MET	N-CA-C	-7.08	104.38	113.16
2	B	127	GLY	N-CA-C	7.07	119.63	111.36
3	C	40	GLU	N-CA-C	7.06	120.77	112.72
8	H	110	ASP	N-CA-C	-7.01	103.40	113.21
1	A	886	ILE	N-CA-C	6.98	117.12	110.42
2	B	825	VAL	N-CA-C	6.96	118.63	108.53
4	D	209	ARG	N-CA-C	-6.93	103.33	111.03
2	B	99	LYS	CA-C-N	6.92	128.49	119.84
2	B	99	LYS	C-N-CA	6.92	128.49	119.84
1	A	242	PRO	CA-C-N	6.90	127.48	120.38
1	A	242	PRO	C-N-CA	6.90	127.48	120.38
2	B	628	THR	N-CA-C	-6.88	103.25	112.94
1	A	174	ILE	N-CA-C	6.87	119.98	109.12
7	G	115	MET	CA-C-N	-6.86	113.44	120.85
7	G	115	MET	C-N-CA	-6.86	113.44	120.85
8	H	130	ARG	N-CA-C	-6.85	102.17	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1207	LEU	N-CA-C	6.77	119.62	108.99
7	G	52	ASP	N-CA-C	6.73	118.31	110.97
1	A	663	SER	N-CA-C	6.73	116.87	108.19
1	A	602	ASP	N-CA-C	-6.72	102.62	111.02
1	A	513	SER	CA-C-N	6.69	127.54	120.12
1	A	513	SER	C-N-CA	6.69	127.54	120.12
1	A	356	ASP	CA-C-N	6.67	128.17	119.84
1	A	356	ASP	C-N-CA	6.67	128.17	119.84
4	D	8	PHE	N-CA-C	6.65	124.97	110.80
1	A	524	VAL	N-CA-C	6.64	116.64	108.53
10	J	5	VAL	N-CA-C	-6.60	100.23	109.21
1	A	291	GLU	N-CA-C	-6.57	104.29	112.90
6	F	127	GLU	N-CA-C	-6.55	103.61	112.26
1	A	513	SER	N-CA-C	6.54	119.33	110.31
1	A	3	GLY	N-CA-C	-6.51	106.33	115.32
1	A	1163	ILE	CA-C-N	6.51	126.27	119.05
1	A	1163	ILE	C-N-CA	6.51	126.27	119.05
1	A	320	ARG	CA-C-N	6.50	127.96	119.84
1	A	320	ARG	C-N-CA	6.50	127.96	119.84
1	A	582	ILE	CA-C-N	6.48	127.94	119.84
1	A	582	ILE	C-N-CA	6.48	127.94	119.84
1	A	108	MET	N-CA-C	-6.47	102.45	110.41
3	C	38	ILE	CB-CA-C	-6.46	103.42	112.14
4	D	142	LYS	N-CA-C	-6.42	102.96	111.24
4	D	54	GLU	N-CA-C	-6.40	104.02	112.34
2	B	1135	ARG	N-CA-C	-6.39	103.94	111.03
2	B	172	ILE	N-CA-C	6.38	117.11	108.17
3	C	41	ILE	CA-C-N	6.38	126.33	119.76
3	C	41	ILE	C-N-CA	6.38	126.33	119.76
2	B	748	ILE	N-CA-C	-6.35	102.93	111.44
9	I	18	GLU	N-CA-C	6.33	119.78	109.59
1	A	472	LEU	N-CA-C	6.33	118.99	111.71
10	J	44	TYR	N-CA-C	6.32	120.56	112.34
1	A	1422	ARG	N-CA-C	-6.31	105.52	113.72
1	A	55	ASP	N-CA-CB	6.26	121.52	110.37
2	B	763	GLN	N-CA-C	-6.26	100.38	109.59
2	B	1201	LYS	N-CA-C	-6.25	104.46	111.28
2	B	837	ASP	N-CA-C	6.25	120.86	113.23
2	B	803	LEU	N-CA-C	-6.24	104.41	111.14
1	A	480	ALA	N-CA-C	6.23	120.43	109.96
3	C	194	GLU	N-CA-C	-6.20	104.43	112.68
2	B	292	ILE	N-CA-C	6.18	122.24	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	567	LYS	CA-C-N	-6.18	112.12	119.84
1	A	567	LYS	C-N-CA	-6.18	112.12	119.84
2	B	1075	GLY	N-CA-C	6.17	121.32	113.24
1	A	1406	VAL	N-CA-C	6.16	116.91	110.62
8	H	35	GLN	N-CA-C	-6.16	106.40	114.04
2	B	882	THR	N-CA-C	6.15	121.45	111.37
2	B	1147	LEU	N-CA-C	-6.14	104.21	111.03
1	A	1258	HIS	N-CA-C	-6.13	105.28	112.89
1	A	1169	ILE	N-CA-C	6.13	122.10	109.34
4	D	18	VAL	N-CA-C	6.12	116.68	107.75
1	A	266	LEU	N-CA-C	-6.10	103.95	111.40
3	C	144	ILE	N-CA-C	6.10	116.28	110.42
4	D	38	ILE	N-CA-C	6.09	117.56	108.23
2	B	335	GLY	N-CA-C	-6.09	98.74	113.18
2	B	1113	VAL	CB-CA-C	-6.06	103.98	111.92
1	A	1121	GLU	CA-C-N	6.04	127.39	119.84
1	A	1121	GLU	C-N-CA	6.04	127.39	119.84
1	A	251	SER	N-CA-C	6.03	118.55	110.35
1	A	324	SER	N-CA-C	-6.02	102.43	110.55
4	D	199	ASN	N-CA-C	6.02	123.62	110.80
10	J	64	ASN	N-CA-C	5.97	123.00	109.81
7	G	133	SER	N-CA-C	-5.96	103.95	111.11
1	A	436	ILE	N-CA-C	-5.94	101.87	109.30
1	A	236	LEU	N-CA-C	5.94	119.07	110.28
4	D	12	ARG	N-CA-C	5.93	118.96	110.24
3	C	91	HIS	N-CA-C	5.93	117.53	108.52
1	A	950	GLY	N-CA-C	-5.92	106.91	114.37
2	B	1013	ASN	N-CA-C	5.92	117.11	109.65
2	B	1066	SER	N-CA-C	5.92	118.68	111.82
10	J	10	CYS	N-CA-C	5.91	120.61	113.17
3	C	96	SER	N-CA-C	5.90	117.81	108.79
2	B	832	GLY	N-CA-C	-5.88	106.65	114.95
2	B	476	ARG	N-CA-C	5.88	118.06	110.65
5	E	177	ARG	N-CA-C	5.85	118.45	110.55
1	A	239	LEU	N-CA-C	5.84	119.20	108.69
4	D	51	ASN	N-CA-C	-5.84	101.03	110.32
1	A	1237	ILE	N-CA-C	5.84	116.77	108.42
1	A	4	GLN	N-CA-C	5.79	123.14	110.80
9	I	85	PHE	N-CA-C	5.78	118.97	110.59
7	G	76	ALA	N-CA-C	5.76	117.55	108.96
2	B	978	ASP	N-CA-C	5.75	118.79	110.28
1	A	289	ILE	N-CA-C	-5.72	105.54	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	GLU	N-CA-C	-5.71	103.16	110.53
8	H	26	ILE	N-CA-C	5.71	117.57	108.89
5	E	201	LYS	N-CA-C	-5.71	103.39	110.41
1	A	518	LYS	CA-C-N	5.69	125.45	119.76
1	A	518	LYS	C-N-CA	5.69	125.45	119.76
3	C	163	ILE	N-CA-C	5.64	115.70	108.82
2	B	232	SER	CA-C-N	-5.64	114.00	119.87
2	B	232	SER	C-N-CA	-5.64	114.00	119.87
1	A	987	VAL	N-CA-C	5.63	116.28	110.36
2	B	523	CYS	CA-C-N	5.63	125.16	119.19
2	B	523	CYS	C-N-CA	5.63	125.16	119.19
2	B	330	ALA	N-CA-C	-5.62	104.84	110.97
1	A	1005	GLU	N-CA-C	5.61	117.85	111.11
2	B	732	SER	N-CA-C	5.61	117.06	108.42
1	A	1445	ILE	CB-CA-C	-5.61	104.52	111.08
1	A	102	VAL	N-CA-C	-5.59	105.28	110.53
7	G	46	LEU	N-CA-C	5.58	120.07	112.04
1	A	288	ALA	N-CA-C	-5.54	99.01	110.80
1	A	1293	SER	N-CA-C	-5.54	102.09	110.39
1	A	432	VAL	CB-CA-C	-5.53	104.95	111.09
1	A	228	PHE	N-CA-C	5.53	120.16	113.41
5	E	55	ARG	N-CA-C	5.53	118.07	111.71
2	B	492	LEU	N-CA-C	-5.51	104.96	110.97
12	L	58	LYS	N-CA-C	5.51	119.25	112.03
2	B	1113	VAL	N-CA-C	5.50	116.57	111.45
9	I	61	ASP	N-CA-C	-5.49	105.94	113.30
2	B	861	ASP	N-CA-C	5.49	116.80	108.07
5	E	3	GLN	CB-CA-C	-5.48	109.27	115.79
1	A	590	ARG	N-CA-C	5.47	122.46	110.80
1	A	1038	THR	N-CA-C	-5.47	100.49	109.80
1	A	321	PRO	N-CA-C	5.47	123.74	112.47
9	I	14	LEU	N-CA-C	5.45	117.40	108.52
1	A	1376	THR	N-CA-C	5.44	120.05	113.41
15	3	10	U	N1-C1'-C2'	5.44	120.16	112.00
2	B	903	VAL	N-CA-C	5.44	117.29	109.51
7	G	138	THR	N-CA-C	5.43	116.40	108.14
7	G	139	ILE	N-CA-C	5.43	120.64	109.34
1	A	335	ARG	N-CA-C	-5.42	105.01	111.03
12	L	68	GLU	N-CA-C	-5.40	102.28	110.28
1	A	945	GLU	N-CA-C	-5.40	106.82	113.41
1	A	244	PRO	N-CA-C	5.39	117.28	110.70
1	A	362	ASP	N-CA-C	5.39	119.57	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	535	LEU	N-CA-C	-5.39	107.07	113.97
1	A	30	ILE	CB-CA-C	-5.38	104.88	112.14
2	B	213	ILE	N-CA-C	5.38	115.99	108.89
3	C	11	ARG	N-CA-C	-5.38	99.34	110.80
1	A	998	LEU	N-CA-C	5.38	118.31	109.76
7	G	129	SER	N-CA-C	5.38	115.49	108.07
9	I	109	ILE	N-CA-C	5.37	116.11	107.73
2	B	829	CYS	N-CA-C	-5.37	100.50	109.24
7	G	114	LEU	N-CA-C	-5.36	106.11	113.30
8	H	138	GLU	N-CA-C	-5.36	105.60	111.82
3	C	52	GLU	N-CA-C	-5.36	105.80	112.93
1	A	54	ASN	CA-C-N	5.36	134.87	121.80
1	A	54	ASN	C-N-CA	5.36	134.87	121.80
1	A	564	ALA	N-CA-C	-5.35	105.49	112.23
2	B	750	GLY	N-CA-C	-5.35	102.94	111.18
1	A	1262	LYS	N-CA-C	-5.34	105.50	112.23
1	A	927	VAL	N-CA-C	-5.34	105.64	110.82
1	A	227	VAL	N-CA-C	5.32	116.73	111.67
1	A	227	VAL	CB-CA-C	-5.32	105.52	111.80
3	C	135	GLN	N-CA-C	-5.32	105.49	113.89
1	A	1192	LEU	N-CA-C	5.32	118.15	109.59
8	H	16	ASP	N-CA-C	5.30	118.69	108.45
2	B	526	GLU	N-CA-C	5.29	116.87	108.67
1	A	279	LEU	N-CA-C	-5.29	105.54	113.89
1	A	83	HIS	N-CA-C	5.28	116.02	108.74
2	B	552	MET	N-CA-C	5.27	121.47	109.81
1	A	865	GLN	N-CA-C	-5.27	100.44	109.24
2	B	395	GLN	N-CA-C	-5.26	103.19	110.35
2	B	663	ALA	N-CA-C	-5.25	105.47	111.14
3	C	144	ILE	CB-CA-C	-5.25	105.26	111.97
15	3	2	A	C2'-C3'-O3'	5.24	121.56	113.70
1	A	467	THR	N-CA-C	5.24	117.94	109.40
1	A	781	ASP	N-CA-C	5.24	118.67	111.54
1	A	454	SER	N-CA-C	-5.23	106.74	113.02
8	H	36	CYS	N-CA-C	5.23	117.00	108.63
5	E	33	GLU	N-CA-C	-5.23	105.03	111.40
1	A	580	VAL	N-CA-C	-5.21	105.26	112.50
1	A	860	LEU	N-CA-C	-5.20	107.31	113.97
4	D	17	LYS	N-CA-C	5.20	121.88	110.80
2	B	1025	HIS	N-CA-C	-5.19	105.31	110.97
1	A	629	LEU	N-CA-C	-5.19	105.05	111.33
2	B	748	ILE	CB-CA-C	-5.18	103.71	112.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	165	GLN	N-CA-C	-5.18	105.52	111.07
1	A	1366	ARG	N-CA-C	5.18	117.60	111.33
8	H	23	VAL	N-CA-C	5.17	115.17	108.35
1	A	31	SER	N-CA-C	5.17	117.83	110.24
2	B	1130	PHE	N-CA-C	-5.15	98.47	107.73
11	K	82	ASP	CA-C-N	5.14	124.76	119.05
11	K	82	ASP	C-N-CA	5.14	124.76	119.05
2	B	208	SER	N-CA-C	5.14	117.75	110.50
1	A	1101	LEU	N-CA-C	-5.14	105.68	111.28
10	J	2	ILE	N-CA-C	5.13	120.02	109.34
11	K	20	LYS	N-CA-C	-5.13	99.75	108.26
1	A	847	ASP	N-CA-C	5.13	121.72	110.80
1	A	553	VAL	CA-C-N	5.13	126.25	119.84
1	A	553	VAL	C-N-CA	5.13	126.25	119.84
1	A	1359	ASP	N-CA-C	-5.12	106.98	113.18
9	I	83	ASN	N-CA-C	5.12	116.97	109.24
1	A	646	PHE	N-CA-C	-5.12	105.70	111.28
7	G	134	GLU	N-CA-C	5.12	119.48	112.68
7	G	131	GLN	N-CA-C	5.11	117.22	108.90
2	B	1208	MET	N-CA-C	-5.10	105.90	111.82
8	H	103	LYS	N-CA-C	5.10	117.87	109.72
1	A	1404	GLU	N-CA-C	5.08	121.62	110.80
3	C	225	ALA	N-CA-C	5.08	116.33	107.49
9	I	16	PRO	N-CA-C	5.07	119.17	110.95
7	G	40	GLY	N-CA-C	-5.07	106.58	113.37
1	A	483	ASP	N-CA-C	-5.07	107.12	113.15
9	I	68	LEU	CA-C-N	5.06	125.51	120.14
9	I	68	LEU	C-N-CA	5.06	125.51	120.14
1	A	78	PRO	N-CA-C	-5.05	102.06	112.47
5	E	63	ASN	CA-C-N	5.05	126.15	119.84
5	E	63	ASN	C-N-CA	5.05	126.15	119.84
1	A	1420	ASP	N-CA-C	5.05	117.68	111.82
2	B	1191	ILE	N-CA-C	5.05	115.54	108.17
3	C	7	GLN	N-CA-C	5.04	117.92	110.46
2	B	223	VAL	N-CA-C	5.04	115.84	108.58
4	D	147	TYR	N-CA-C	-5.03	104.88	111.02
3	C	266	ASP	N-CA-C	-5.03	105.51	111.69
2	B	807	ARG	N-CA-C	-5.02	105.94	111.71
4	D	29	LEU	N-CA-C	-5.01	103.04	110.46
9	I	15	TYR	CA-C-N	5.01	125.79	119.98
9	I	15	TYR	C-N-CA	5.01	125.79	119.98
5	E	95	THR	CA-C-N	5.00	127.74	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	95	THR	C-N-CA	5.00	127.74	120.79

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	1	18	DA	Sidechain
14	1	20	DG	Sidechain
14	1	21	DC	Sidechain
3	C	229	TYR	Sidechain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11143	0	11217	1206	0
2	B	8838	0	8870	1113	0
3	C	2095	0	2051	280	0
4	D	1434	0	1460	186	0
5	E	1752	0	1776	197	0
6	F	705	0	731	75	0
7	G	1340	0	1357	152	0
8	H	1076	0	1046	159	0
9	I	927	0	882	130	0
10	J	532	0	542	102	0
11	K	919	0	929	104	0
12	L	351	0	376	59	0
13	2	137	0	82	12	0
14	1	389	0	214	15	0
15	3	229	0	121	12	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31876	0	31654	3508	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 55.

All (3508) 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:882:THR:HG21	2:B:935:ARG:HA	1.24	1.19
1:A:53:LEU:HD23	1:A:54:ASN:N	1.59	1.18
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.26	1.16
1:A:353:ILE:HD12	1:A:487:MET:HE2	1.18	1.16
4:D:71:LYS:HA	4:D:74:GLN:HB2	1.23	1.13
7:G:26:LEU:HD12	7:G:56:ILE:HD11	1.22	1.11
1:A:567:LYS:CD	1:A:568:PRO:HD2	1.80	1.11
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.19	1.11
1:A:225:ASN:ND2	1:A:228:PHE:H	1.48	1.10
4:D:14:ARG:HB3	4:D:14:ARG:HH11	1.13	1.10
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.32	1.09
2:B:744:HIS:HD2	2:B:745:PRO:HD2	1.10	1.08
2:B:559:SER:HA	2:B:563:MET:HB3	1.11	1.07
4:D:220:LEU:HD23	4:D:221:TYR:H	1.17	1.07
1:A:855:THR:HG21	1:A:857:ARG:HE	1.20	1.06
7:G:112:LYS:HA	7:G:115:MET:HE3	1.33	1.06
5:E:117:THR:HG22	5:E:119:SER:H	1.19	1.06
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.37	1.04
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.36	1.04
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.40	1.03
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.34	1.03
2:B:806:THR:HG22	2:B:808:ALA:H	1.18	1.03
1:A:1116:LEU:HB3	1:A:1308:THR:HG21	1.37	1.03
1:A:41:MET:HB3	1:A:49:LYS:HA	1.40	1.02
1:A:53:LEU:CD2	1:A:54:ASN:H	1.69	1.02
2:B:850:LEU:HD12	2:B:851:PHE:N	1.74	1.02
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.40	1.02
2:B:510:LYS:HB3	2:B:511:PRO:HD3	1.42	1.02
1:A:567:LYS:HB3	8:H:96:VAL:H	1.21	1.02
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.22	1.02
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.40	1.02
8:H:4:THR:HA	8:H:60:ALA:HB2	1.41	1.01
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.38	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:40:LEU:HD13	12:L:44:ASP:HB3	1.37	1.01
10:J:1:MET:H1	10:J:57:ILE:H	1.06	1.00
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.42	1.00
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.40	1.00
1:A:1116:LEU:HB3	1:A:1308:THR:CG2	1.92	0.99
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.43	0.99
1:A:913:LEU:HD12	1:A:914:GLU:H	1.24	0.99
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.27	0.99
1:A:858:ASN:ND2	1:A:860:LEU:H	1.60	0.99
2:B:430:ARG:HB3	2:B:430:ARG:HH11	1.25	0.98
3:C:66:ARG:HH12	10:J:2:ILE:CG2	1.76	0.98
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.45	0.98
2:B:737:THR:HG21	9:I:66:PRO:HA	1.45	0.98
1:A:321:PRO:O	1:A:322:VAL:HB	1.64	0.97
1:A:315:LEU:HD23	1:A:315:LEU:H	1.30	0.97
2:B:168:GLY:H	2:B:450:ALA:HB1	1.30	0.96
2:B:744:HIS:CD2	2:B:745:PRO:HD2	2.00	0.96
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.30	0.95
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.46	0.95
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.47	0.95
1:A:901:LEU:H	1:A:926:GLN:NE2	1.65	0.95
9:I:111:THR:HG22	9:I:112:SER:H	1.31	0.95
2:B:589:VAL:HG12	2:B:590:HIS:H	1.30	0.95
1:A:61:ILE:HG22	1:A:62:ASP:H	1.29	0.95
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.46	0.95
1:A:1364:ASN:OD1	1:A:1366:ARG:HG2	1.66	0.95
2:B:839:MET:HE3	2:B:1010:LEU:HD23	1.47	0.94
6:F:82:THR:HG22	6:F:84:TYR:H	1.30	0.94
9:I:34:TYR:HD2	9:I:35:VAL:N	1.63	0.94
2:B:244:LEU:HD11	2:B:366:GLN:NE2	1.81	0.94
2:B:559:SER:HA	2:B:563:MET:CB	1.96	0.94
1:A:567:LYS:CG	1:A:568:PRO:HD2	1.98	0.94
1:A:738:LYS:H	1:A:738:LYS:HD3	1.33	0.94
2:B:429:PHE:HA	2:B:432:MET:HE3	1.50	0.94
1:A:1127:ASP:OD2	1:A:1130:GLN:HB2	1.68	0.94
2:B:708:GLU:HG3	2:B:709:ASP:H	1.30	0.94
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.51	0.93
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.03	0.93
2:B:130:VAL:HG23	2:B:167:ILE:HD13	1.49	0.93
1:A:21:LEU:HD12	1:A:229:SER:HB2	1.48	0.93
6:F:77:ASP:O	6:F:78:GLN:HB2	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.49	0.92
2:B:1065:GLN:HE21	2:B:1067:ARG:H	0.98	0.92
8:H:130:ARG:NH1	8:H:130:ARG:HB2	1.84	0.92
1:A:567:LYS:HB3	8:H:96:VAL:N	1.84	0.92
2:B:34:ILE:HG12	2:B:542:MET:HE1	1.51	0.92
2:B:995:ARG:HH12	3:C:165:LYS:HG2	1.33	0.92
8:H:40:LEU:HD13	8:H:123:MET:HE3	1.52	0.92
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.50	0.92
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	1.85	0.91
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.35	0.91
2:B:879:ARG:H	2:B:879:ARG:CD	1.84	0.90
8:H:81:PRO:HB2	8:H:82:PRO:HD2	1.51	0.90
3:C:56:THR:HG21	3:C:145:CYS:SG	2.12	0.90
1:A:567:LYS:HD3	8:H:95:TYR:CD2	2.05	0.90
1:A:858:ASN:C	1:A:858:ASN:HD22	1.78	0.90
1:A:1308:THR:HG23	1:A:1309:ASP:N	1.87	0.90
3:C:252:GLN:HE21	11:K:95:ILE:HG23	1.36	0.90
2:B:842:ASN:HD22	2:B:845:SER:H	1.19	0.90
4:D:220:LEU:CD2	4:D:221:TYR:H	1.83	0.90
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.52	0.90
2:B:345:LYS:HG2	2:B:346:GLU:H	1.35	0.90
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.53	0.89
2:B:638:PHE:HB3	2:B:651:LEU:HD21	1.52	0.89
2:B:810:GLU:HB2	2:B:815:ARG:HH22	1.35	0.89
1:A:53:LEU:HD23	1:A:54:ASN:H	0.77	0.89
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.71	0.89
1:A:122:MET:HE3	1:A:126:LEU:HD21	1.52	0.89
2:B:879:ARG:H	2:B:879:ARG:HD2	1.35	0.89
9:I:6:PHE:HB3	9:I:12:ASN:O	1.72	0.89
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.55	0.89
8:H:84:ALA:HB1	8:H:87:ARG:HB3	1.55	0.89
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.08	0.89
1:A:629:LEU:O	1:A:633:VAL:HG23	1.72	0.89
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.07	0.89
5:E:56:LYS:HE2	5:E:84:ASP:HB2	1.54	0.89
3:C:177:GLU:HG3	3:C:231:ASN:HD22	1.38	0.89
3:C:69:LEU:H	3:C:69:LEU:HD12	1.38	0.88
2:B:307:ASP:OD2	2:B:310:MET:HB2	1.74	0.88
2:B:805:THR:HG22	2:B:806:THR:H	1.35	0.88
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.08	0.88
2:B:549:THR:HG22	2:B:550:ASP:H	1.36	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:850:LEU:HD12	2:B:851:PHE:H	1.34	0.88
1:A:14:VAL:H	1:A:1432:GLN:HE22	0.91	0.88
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.55	0.88
3:C:33:LEU:HG	3:C:37:MET:HE2	1.55	0.88
1:A:41:MET:CB	1:A:49:LYS:HA	2.04	0.88
4:D:130:LEU:HD13	4:D:142:LYS:HD3	1.56	0.87
2:B:766:ARG:NH1	2:B:1020:ARG:HD2	1.89	0.87
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.57	0.87
1:A:416:ARG:HH11	1:A:417:TYR:HE2	1.23	0.86
4:D:155:ARG:HG2	4:D:219:THR:HG21	1.55	0.86
1:A:323:LYS:H	1:A:323:LYS:HD2	1.41	0.86
7:G:1:MET:SD	7:G:79:PHE:HD1	1.98	0.86
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.58	0.86
11:K:65:HIS:HD2	11:K:67:PHE:H	1.19	0.86
4:D:66:ARG:HD2	4:D:133:THR:HB	1.57	0.86
10:J:1:MET:N	10:J:57:ILE:H	1.73	0.86
11:K:65:HIS:CD2	11:K:67:PHE:H	1.92	0.86
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.05	0.86
9:I:34:TYR:CD2	9:I:35:VAL:N	2.43	0.86
1:A:107:CYS:HA	1:A:171:GLN:NE2	1.90	0.86
8:H:42:ILE:HG23	8:H:95:TYR:HE1	1.38	0.86
2:B:473:MET:HE3	2:B:474:SER:HA	1.58	0.85
3:C:66:ARG:HH12	10:J:2:ILE:HG21	1.37	0.85
1:A:11:LEU:O	1:A:11:LEU:HD23	1.76	0.85
2:B:890:TYR:O	2:B:893:LEU:HB2	1.76	0.85
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.58	0.85
1:A:225:ASN:HD22	1:A:228:PHE:H	1.18	0.85
2:B:291:ILE:HD13	2:B:300:HIS:NE2	1.91	0.85
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.58	0.85
2:B:999:MET:HA	2:B:999:MET:HE3	1.56	0.85
4:D:156:ASP:HB2	4:D:159:THR:HG23	1.58	0.85
6:F:103:MET:HE1	7:G:66:GLY:H	1.40	0.85
2:B:102:VAL:CG2	2:B:112:LEU:HD22	2.06	0.85
2:B:842:ASN:ND2	2:B:845:SER:H	1.75	0.85
2:B:345:LYS:HA	2:B:348:ARG:HE	1.38	0.85
2:B:863:GLU:OE2	2:B:873:THR:HA	1.77	0.85
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.12	0.85
2:B:944:THR:HG21	2:B:1122:ARG:NH2	1.92	0.85
2:B:603:LEU:HD13	2:B:608:ASP:HB2	1.59	0.84
2:B:1124:ARG:HB3	2:B:1124:ARG:NH1	1.92	0.84
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1312:ASN:HD21	1:A:1315:GLU:HG3	1.40	0.84
3:C:244:VAL:O	3:C:248:ILE:HG13	1.76	0.84
1:A:705:LYS:HB2	1:A:708:MET:HE3	1.58	0.84
2:B:289:LEU:HD13	2:B:375:ALA:HB2	1.58	0.84
2:B:806:THR:HG22	2:B:808:ALA:N	1.91	0.84
4:D:154:PHE:CD1	4:D:163:VAL:HG21	2.13	0.84
4:D:159:THR:O	4:D:163:VAL:HG23	1.77	0.84
1:A:853:ASP:OD1	1:A:855:THR:HB	1.78	0.84
7:G:138:THR:HG22	7:G:139:ILE:N	1.92	0.83
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	1.78	0.83
7:G:126:ASN:HD22	7:G:127:PRO:HA	1.42	0.83
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.61	0.83
1:A:1107:VAL:HG12	1:A:1107:VAL:O	1.78	0.83
7:G:34:VAL:HG11	7:G:74:TYR:HE1	1.43	0.83
3:C:242:GLN:HA	3:C:245:VAL:HG23	1.60	0.83
10:J:64:ASN:HB3	10:J:65:PRO:CD	2.08	0.83
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.58	0.83
1:A:107:CYS:HB2	1:A:114:LEU:HD21	1.60	0.83
2:B:1138:MET:HE2	2:B:1146:PHE:CD2	2.13	0.83
3:C:83:SER:OG	3:C:160:LYS:HD3	1.79	0.83
2:B:345:LYS:HG2	2:B:346:GLU:N	1.94	0.83
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.60	0.83
8:H:130:ARG:HB2	8:H:130:ARG:HH11	1.40	0.83
12:L:49:LYS:O	12:L:50:ASP:HB2	1.77	0.83
1:A:942:PHE:HZ	5:E:207:ARG:HG3	1.42	0.82
2:B:126:SER:OG	2:B:172:ILE:HD11	1.78	0.82
2:B:862:GLN:HG2	2:B:963:PHE:HD1	1.44	0.82
1:A:55:ASP:N	1:A:56:PRO:HD3	1.93	0.82
1:A:567:LYS:CB	8:H:95:TYR:HA	2.09	0.82
1:A:1409:LEU:HD13	2:B:1207:LEU:HD11	1.61	0.82
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.08	0.82
5:E:114:ASN:O	5:E:115:ASN:HB3	1.78	0.82
7:G:1:MET:SD	7:G:79:PHE:CD1	2.72	0.82
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.44	0.82
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.60	0.82
1:A:503:GLN:NE2	6:F:90:ARG:NH2	2.28	0.82
2:B:654:ARG:HH11	2:B:654:ARG:HG3	1.45	0.82
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.19	0.82
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.77	0.82
2:B:542:MET:HG2	2:B:747:MET:HE3	1.60	0.82
2:B:865:LYS:HG2	2:B:961:LEU:HD21	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LYS:HA	1:A:145:LYS:HE3	1.60	0.82
1:A:866:PHE:O	1:A:867:ILE:HD12	1.78	0.82
1:A:1170:ILE:H	1:A:1170:ILE:HD12	1.41	0.82
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.77	0.82
1:A:839:ARG:HG2	1:A:839:ARG:HH11	1.42	0.82
10:J:23:ASN:C	10:J:25:LEU:H	1.87	0.82
1:A:381:THR:HG22	1:A:383:TYR:H	1.43	0.81
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.14	0.81
1:A:901:LEU:H	1:A:926:GLN:HE21	1.26	0.81
2:B:261:ARG:HH11	2:B:261:ARG:HB3	1.44	0.81
5:E:79:TRP:HE1	5:E:81:GLU:HB2	1.43	0.81
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.61	0.81
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.62	0.81
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.77	0.81
8:H:89:LEU:C	8:H:91:ASP:H	1.86	0.81
1:A:858:ASN:HD22	1:A:860:LEU:H	1.24	0.81
1:A:288:ALA:HA	1:A:291:GLU:OE1	1.80	0.81
1:A:40:THR:HG22	1:A:41:MET:HG3	1.61	0.81
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.61	0.81
1:A:1116:LEU:N	1:A:1308:THR:HG22	1.95	0.81
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.63	0.81
2:B:800:GLN:HB3	10:J:52:THR:HG22	1.61	0.81
3:C:32:SER:O	3:C:36:VAL:HG23	1.80	0.81
7:G:30:LEU:HD22	7:G:72:VAL:HG11	1.62	0.81
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.63	0.81
2:B:589:VAL:HG12	2:B:590:HIS:N	1.96	0.81
15:3:11:U:H4'	15:3:11:U:OP1	1.80	0.81
1:A:534:LEU:O	1:A:574:GLY:HA3	1.81	0.80
1:A:714:PHE:HB2	9:I:97:MET:HE1	1.63	0.80
1:A:1214:GLU:O	1:A:1218:GLN:HG2	1.81	0.80
1:A:244:PRO:HB2	1:A:245:PRO:CD	2.11	0.80
11:K:57:LEU:HB2	11:K:76:GLN:HG2	1.61	0.80
1:A:754:SER:H	1:A:757:ASN:HD22	1.28	0.80
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.62	0.80
12:L:32:ALA:CB	12:L:55:ILE:HG13	2.11	0.80
10:J:1:MET:H1	10:J:57:ILE:N	1.79	0.80
1:A:98:LYS:O	1:A:102:VAL:HG23	1.82	0.80
1:A:534:LEU:O	1:A:534:LEU:HG	1.79	0.80
1:A:1445:ILE:H	1:A:1445:ILE:HD12	1.45	0.79
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.17	0.79
12:L:32:ALA:HB2	12:L:55:ILE:HG13	1.61	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:705:MET:HA	2:B:705:MET:HE3	1.62	0.79
8:H:95:TYR:HE2	8:H:97:MET:HG3	1.47	0.79
2:B:232:SER:HA	14:1:11:DA:OP1	1.82	0.79
1:A:115:LEU:HD12	1:A:142:CYS:HB3	1.65	0.79
1:A:353:ILE:CD1	1:A:487:MET:HE2	2.08	0.79
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.63	0.79
2:B:778:MET:HE1	2:B:1094:ARG:HD3	1.63	0.79
11:K:46:ILE:O	11:K:50:LEU:HB2	1.82	0.79
1:A:35:ILE:HG22	1:A:35:ILE:O	1.83	0.79
12:L:61:THR:HG22	12:L:63:ARG:HG3	1.64	0.79
1:A:117:GLU:H	1:A:117:GLU:CD	1.90	0.79
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.65	0.79
2:B:613:VAL:HG13	2:B:627:PHE:O	1.82	0.79
2:B:549:THR:HG22	2:B:550:ASP:N	1.98	0.79
4:D:47:LEU:HD13	4:D:48:ILE:N	1.98	0.78
4:D:126:ILE:HD13	4:D:145:MET:HE3	1.64	0.78
1:A:69:THR:HG21	2:B:1174:LYS:NZ	1.97	0.78
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.65	0.78
12:L:30:ILE:O	12:L:56:LEU:HA	1.82	0.78
1:A:69:THR:O	1:A:71:GLN:N	2.16	0.78
2:B:796:LEU:HD21	2:B:821:GLN:HE21	1.48	0.78
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.19	0.78
1:A:855:THR:CG2	1:A:857:ARG:HE	1.96	0.78
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.45	0.78
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.18	0.78
2:B:944:THR:HG21	2:B:1122:ARG:HH21	1.47	0.78
2:B:1165:ILE:HG22	4:D:15:LEU:HA	1.65	0.78
3:C:112:ASN:HB3	3:C:114:TYR:CE1	2.19	0.78
11:K:107:THR:HG22	11:K:108:GLU:N	1.97	0.78
1:A:855:THR:HG21	1:A:857:ARG:NE	1.99	0.78
4:D:220:LEU:HD23	4:D:221:TYR:N	1.97	0.78
1:A:353:ILE:HD12	1:A:487:MET:CE	2.06	0.78
5:E:112:TYR:O	5:E:137:GLU:HG3	1.84	0.78
7:G:14:HIS:CD2	7:G:16:SER:H	2.02	0.78
1:A:754:SER:N	1:A:757:ASN:HD22	1.82	0.77
2:B:798:TYR:HE2	3:C:62:PHE:CZ	2.02	0.77
1:A:55:ASP:C	1:A:57:ARG:H	1.91	0.77
4:D:155:ARG:CG	4:D:219:THR:HG21	2.15	0.77
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.20	0.77
1:A:1135:ARG:HG2	1:A:1136:SER:N	1.98	0.77
1:A:1329:THR:HG22	1:A:1331:SER:H	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:816:GLU:O	2:B:817:LEU:HD23	1.85	0.77
1:A:470:LEU:HD23	1:A:470:LEU:H	1.50	0.77
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.00	0.77
15:3:5:C:O2'	15:3:6:A:H5'	1.84	0.77
1:A:903:ASN:HD22	1:A:904:THR:N	1.82	0.77
5:E:117:THR:HG22	5:E:119:SER:N	1.99	0.77
1:A:49:LYS:HZ1	1:A:61:ILE:N	1.83	0.77
2:B:1187:ASN:O	2:B:1188:LYS:HB2	1.84	0.77
1:A:873:MET:C	1:A:1058:VAL:HG23	2.10	0.77
2:B:469:GLN:O	2:B:472:ALA:HB3	1.85	0.77
6:F:89:GLU:O	6:F:93:ILE:HD12	1.85	0.77
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.15	0.77
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.67	0.77
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.67	0.77
2:B:914:LYS:HG2	2:B:937:ALA:HB3	1.67	0.77
2:B:995:ARG:NH1	3:C:165:LYS:HG2	1.99	0.77
1:A:503:GLN:HE21	6:F:90:ARG:NH2	1.83	0.76
5:E:5:ASN:O	5:E:9:ILE:HG13	1.84	0.76
1:A:42:ASP:O	1:A:44:THR:N	2.18	0.76
2:B:658:ILE:HG22	2:B:662:MET:HE2	1.67	0.76
2:B:1020:ARG:HG2	2:B:1020:ARG:HH11	1.48	0.76
1:A:425:GLN:N	1:A:425:GLN:CD	2.43	0.76
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.67	0.76
2:B:1084:GLN:N	2:B:1084:GLN:NE2	2.32	0.76
1:A:535:THR:HG21	1:A:616:VAL:HA	1.68	0.76
3:C:89:GLU:O	3:C:90:ASP:HB3	1.85	0.76
12:L:60:ARG:HG2	12:L:61:THR:H	1.50	0.76
1:A:250:ILE:O	1:A:250:ILE:HG22	1.83	0.76
2:B:294:ASP:O	2:B:296:GLU:N	2.18	0.76
8:H:42:ILE:HG23	8:H:95:TYR:CE1	2.21	0.76
2:B:278:GLN:HG2	2:B:279:ASP:N	2.00	0.76
2:B:227:LYS:HG3	2:B:395:GLN:HG3	1.68	0.76
3:C:128:ASN:O	3:C:129:ILE:HG13	1.85	0.76
3:C:249:ASP:O	3:C:252:GLN:HB3	1.86	0.76
8:H:30:SER:HB2	8:H:36:CYS:HB3	1.68	0.76
10:J:53:HIS:HD2	10:J:54:VAL:N	1.84	0.76
2:B:193:LYS:NZ	12:L:32:ALA:HB1	2.01	0.76
2:B:401:PHE:HA	2:B:404:LYS:HG3	1.68	0.76
1:A:709:THR:HG22	1:A:710:LEU:H	1.51	0.76
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.26	0.75
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	1.99	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:706:GLN:HB2	2:B:709:ASP:HB3	1.68	0.75
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	1.86	0.75
1:A:62:ASP:O	1:A:63:ARG:C	2.28	0.75
2:B:278:GLN:HG2	2:B:279:ASP:H	1.51	0.75
2:B:996:ARG:HH12	3:C:174:ALA:HA	1.49	0.75
2:B:1072:MET:HE3	2:B:1085:ILE:CB	2.13	0.75
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.16	0.75
2:B:577:ALA:CB	2:B:589:VAL:HG11	2.15	0.75
2:B:806:THR:HB	2:B:809:MET:HG3	1.67	0.75
1:A:1130:GLN:O	1:A:1134:ILE:HG13	1.86	0.75
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.68	0.75
2:B:806:THR:N	2:B:809:MET:HE3	2.01	0.75
1:A:316:GLN:HE21	1:A:317:LYS:HD2	1.52	0.75
1:A:1279:ILE:HD11	1:A:1316:VAL:HG21	1.69	0.75
1:A:63:ARG:HA	1:A:74:MET:HE2	1.68	0.75
1:A:523:ILE:HG13	1:A:622:VAL:HG22	1.69	0.75
2:B:288:ALA:HB1	2:B:331:LEU:HD12	1.66	0.75
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.68	0.75
1:A:694:THR:O	1:A:698:GLN:HG3	1.87	0.75
1:A:167:CYS:HB2	1:A:169:ASN:ND2	2.01	0.74
2:B:815:ARG:HB2	2:B:815:ARG:HH11	1.52	0.74
1:A:34:LYS:NZ	1:A:57:ARG:NH2	2.35	0.74
1:A:343:LYS:HZ2	2:B:1151:LEU:HG	1.52	0.74
1:A:590:ARG:HG2	1:A:590:ARG:HH11	1.50	0.74
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.03	0.74
2:B:637:LEU:HB2	2:B:693:ILE:HD11	1.67	0.74
2:B:803:LEU:HD12	2:B:1032:SER:HB3	1.69	0.74
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.68	0.74
3:C:221:TYR:CE1	3:C:222:LYS:HG3	2.23	0.74
4:D:14:ARG:HB3	4:D:14:ARG:NH1	1.97	0.74
8:H:26:ILE:HD11	8:H:49:VAL:HG11	1.70	0.74
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.51	0.74
7:G:7:LEU:HB2	7:G:74:TYR:HE2	1.51	0.74
8:H:59:ILE:HG22	8:H:60:ALA:N	2.00	0.74
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.69	0.74
2:B:1175:LEU:O	2:B:1176:ASN:HB2	1.85	0.74
8:H:58:THR:HG22	8:H:59:ILE:H	1.52	0.74
1:A:767:GLN:NE2	1:A:774:ARG:HB3	2.02	0.74
2:B:244:LEU:HD11	2:B:366:GLN:HE22	1.49	0.74
3:C:43:THR:HG22	3:C:44:LEU:N	2.00	0.74
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.18	0.74
8:H:11:GLN:HA	8:H:53:ASP:O	1.88	0.74
2:B:957:ASN:O	2:B:959:ASP:N	2.21	0.74
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.80	0.74
3:C:208:GLU:O	3:C:210:GLU:N	2.20	0.74
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.03	0.74
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.70	0.74
1:A:50:ILE:C	1:A:52:GLY:H	1.96	0.73
1:A:388:LEU:O	1:A:392:VAL:HG23	1.88	0.73
2:B:345:LYS:O	2:B:347:LYS:HG2	1.88	0.73
6:F:99:LEU:HG	6:F:103:MET:HE3	1.69	0.73
2:B:1001:PHE:HE2	3:C:34:ARG:NE	1.86	0.73
8:H:40:LEU:HD12	8:H:123:MET:HB2	1.70	0.73
10:J:53:HIS:C	10:J:53:HIS:CD2	2.66	0.73
12:L:61:THR:CG2	12:L:63:ARG:HG3	2.17	0.73
1:A:399:HIS:O	1:A:401:GLY:N	2.21	0.73
2:B:516:ASN:HD22	2:B:516:ASN:N	1.84	0.73
1:A:722:LEU:H	1:A:722:LEU:HD12	1.51	0.73
1:A:946:VAL:HG12	1:A:947:PHE:CD2	2.24	0.73
2:B:879:ARG:HH22	2:B:885:MET:HE2	1.52	0.73
1:A:70:CYS:O	1:A:72:GLU:HG2	1.88	0.73
1:A:1161:THR:HG21	1:A:1163:ILE:HD12	1.69	0.73
8:H:130:ARG:HD3	8:H:130:ARG:N	2.03	0.73
10:J:14:VAL:CG1	10:J:50:ILE:HD11	2.19	0.73
2:B:873:THR:O	2:B:914:LYS:HA	1.87	0.73
3:C:147:LEU:N	3:C:147:LEU:HD23	2.04	0.73
5:E:2:ASP:O	5:E:3:GLN:HG2	1.87	0.73
11:K:47:ARG:HB3	11:K:47:ARG:NH1	2.03	0.73
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.69	0.73
12:L:58:LYS:O	12:L:59:ALA:O	2.06	0.73
1:A:443:LEU:HD12	2:B:1146:PHE:CE2	2.24	0.73
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.24	0.73
6:F:103:MET:HE1	7:G:66:GLY:N	2.03	0.73
11:K:113:THR:O	11:K:114:LEU:HB2	1.87	0.73
5:E:99:HIS:HE1	5:E:103:LYS:HD2	1.54	0.73
1:A:134:ARG:HD2	1:A:221:SER:O	1.89	0.72
5:E:22:MET:HE3	5:E:26:ARG:HE	1.54	0.72
2:B:705:MET:HB3	2:B:706:GLN:OE1	1.89	0.72
2:B:1182:CYS:O	2:B:1182:CYS:SG	2.47	0.72
9:I:111:THR:HG22	9:I:112:SER:N	2.02	0.72
1:A:482:PHE:O	2:B:989:THR:HG23	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.05	0.72
1:A:1422:ARG:HD3	2:B:1224:PHE:CZ	2.24	0.72
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.29	0.72
1:A:129:LYS:O	1:A:130:ASP:HB2	1.89	0.72
1:A:857:ARG:HD3	1:A:861:GLY:O	1.88	0.72
2:B:345:LYS:CG	2:B:346:GLU:H	2.01	0.72
1:A:590:ARG:O	1:A:591:PHE:HB2	1.89	0.72
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.71	0.72
12:L:55:ILE:HG12	12:L:56:LEU:H	1.53	0.72
8:H:130:ARG:HH11	8:H:130:ARG:CB	2.03	0.72
1:A:1436:ILE:O	1:A:1437:GLY:C	2.33	0.72
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.25	0.72
2:B:1122:ARG:HB3	14:1:22:DC:OP1	1.90	0.72
3:C:133:ILE:HD12	3:C:237:SER:N	2.04	0.72
6:F:86:THR:HG23	6:F:89:GLU:OE1	1.90	0.72
1:A:512:VAL:HA	1:A:519:PRO:HA	1.70	0.72
2:B:1183:LYS:N	2:B:1183:LYS:HE3	2.05	0.72
3:C:144:ILE:HG22	3:C:145:CYS:HB3	1.72	0.72
4:D:153:ARG:HB3	4:D:154:PHE:CE2	2.24	0.72
5:E:213:ILE:HG12	5:E:214:CYS:H	1.53	0.72
1:A:913:LEU:CD1	1:A:914:GLU:H	2.00	0.72
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.72	0.72
2:B:805:THR:HG22	2:B:806:THR:N	2.04	0.72
7:G:126:ASN:HD22	7:G:127:PRO:CA	2.03	0.72
15:3:2:A:H2'	15:3:3:A:H8	1.54	0.72
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.20	0.71
1:A:341:MET:HE1	2:B:1135:ARG:NH1	2.05	0.71
1:A:446:ARG:HB2	1:A:487:MET:SD	2.30	0.71
8:H:127:GLY:O	8:H:128:ASN:HB2	1.89	0.71
1:A:1397:LEU:HB2	1:A:1426:GLU:OE1	1.91	0.71
2:B:351:TYR:O	2:B:355:ILE:HG13	1.90	0.71
2:B:705:MET:N	2:B:710:LEU:HD12	2.04	0.71
2:B:810:GLU:CB	2:B:815:ARG:HH22	2.03	0.71
1:A:470:LEU:HD23	1:A:470:LEU:N	2.04	0.71
1:A:709:THR:HG22	1:A:710:LEU:N	2.05	0.71
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.21	0.71
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.05	0.71
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.19	0.71
9:I:50:THR:HG22	9:I:51:ASN:H	1.56	0.71
11:K:65:HIS:HD2	11:K:67:PHE:N	1.87	0.71
6:F:119:ARG:HG3	6:F:119:ARG:NH1	2.03	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:82:PRO:C	8:H:84:ALA:H	1.98	0.71
1:A:369:SER:HB3	11:K:2:ASN:HD21	1.56	0.71
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.72	0.71
2:B:299:GLU:HB3	2:B:571:PRO:HG3	1.72	0.71
1:A:830:LYS:O	1:A:834:THR:HB	1.91	0.71
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.26	0.71
2:B:172:ILE:HD13	2:B:178:ASN:HD22	1.54	0.71
2:B:1095:LEU:H	2:B:1095:LEU:HD12	1.53	0.71
4:D:4:SER:O	4:D:5:THR:HB	1.90	0.71
5:E:23:VAL:O	5:E:28:TYR:HB2	1.90	0.71
5:E:84:ASP:O	5:E:86:PRO:HD3	1.89	0.71
1:A:714:PHE:CB	9:I:97:MET:HE1	2.20	0.71
1:A:1094:VAL:HG22	1:A:1113:THR:HG21	1.71	0.71
2:B:227:LYS:H	2:B:395:GLN:NE2	1.89	0.71
2:B:745:PRO:O	2:B:747:MET:N	2.24	0.71
2:B:999:MET:HA	2:B:999:MET:CE	2.20	0.71
7:G:158:HIS:HD2	7:G:159:ALA:H	1.36	0.71
9:I:61:ASP:C	9:I:63:GLY:H	1.99	0.71
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.71	0.71
1:A:903:ASN:HD22	1:A:903:ASN:C	1.98	0.71
2:B:622:LYS:HE2	9:I:59:VAL:CG2	2.11	0.71
2:B:918:ILE:HD12	2:B:935:ARG:NH1	2.06	0.71
3:C:46:ILE:HD12	3:C:67:LEU:HB3	1.73	0.71
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.26	0.71
1:A:56:PRO:O	1:A:57:ARG:HG3	1.91	0.70
1:A:384:ASN:OD1	1:A:388:LEU:HD12	1.91	0.70
2:B:307:ASP:OD2	2:B:310:MET:HE3	1.91	0.70
4:D:130:LEU:C	4:D:132:GLN:H	1.99	0.70
9:I:44:TYR:CD1	9:I:45:ARG:N	2.59	0.70
1:A:1076:ALA:HA	1:A:1079:MET:HE2	1.73	0.70
2:B:601:ARG:O	2:B:605:ARG:HG3	1.91	0.70
2:B:642:ASP:HA	2:B:649:LYS:HA	1.72	0.70
7:G:128:PRO:O	7:G:138:THR:HG23	1.91	0.70
9:I:34:TYR:HE2	9:I:36:GLU:HB3	1.56	0.70
1:A:908:LEU:HD12	1:A:983:ILE:HD11	1.72	0.70
2:B:359:GLU:O	2:B:362:PRO:HD3	1.91	0.70
1:A:34:LYS:HZ2	1:A:57:ARG:NH2	1.89	0.70
1:A:866:PHE:C	1:A:867:ILE:HD12	2.16	0.70
2:B:364:ILE:HG13	2:B:585:VAL:HG13	1.73	0.70
2:B:882:THR:HG22	2:B:884:ARG:H	1.54	0.70
2:B:1001:PHE:HE2	3:C:34:ARG:CZ	2.02	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:203:GLN:HG3	3:C:207:CYS:SG	2.31	0.70
4:D:123:LEU:O	4:D:123:LEU:HD13	1.91	0.70
8:H:59:ILE:HG22	8:H:60:ALA:H	1.56	0.70
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.74	0.70
2:B:745:PRO:C	2:B:747:MET:H	1.99	0.70
3:C:145:CYS:HA	10:J:2:ILE:HD12	1.73	0.70
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.72	0.70
1:A:335:ARG:NH1	2:B:1206:GLU:OE1	2.24	0.70
1:A:535:THR:CG2	1:A:616:VAL:HA	2.22	0.70
2:B:955:THR:HG22	2:B:956:THR:N	2.05	0.70
5:E:48:ASP:CG	5:E:49:SER:H	1.98	0.70
15:3:2:A:H2'	15:3:3:A:C8	2.27	0.70
2:B:170:LEU:HD23	2:B:170:LEU:O	1.91	0.70
2:B:469:GLN:HG2	2:B:470:LYS:H	1.57	0.70
2:B:483:LEU:HD11	2:B:491:THR:CG2	2.21	0.70
8:H:101:ALA:HB2	8:H:116:TYR:HE2	1.57	0.70
9:I:50:THR:HG22	9:I:51:ASN:N	2.07	0.70
12:L:55:ILE:HD13	12:L:55:ILE:H	1.57	0.70
1:A:249:SER:O	1:A:250:ILE:HG13	1.91	0.70
3:C:66:ARG:NH1	10:J:2:ILE:HG21	2.05	0.70
9:I:98:VAL:HG13	9:I:100:PHE:HE1	1.57	0.70
1:A:549:MET:SD	1:A:577:ILE:HD11	2.32	0.70
3:C:3:GLU:HG2	3:C:4:GLU:HG3	1.72	0.70
1:A:69:THR:HG21	2:B:1174:LYS:HZ2	1.57	0.69
1:A:335:ARG:HD3	1:A:339:ASN:HD22	1.54	0.69
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.26	0.69
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.26	0.69
2:B:798:TYR:HE2	3:C:62:PHE:CE2	2.10	0.69
2:B:1002:THR:HG22	2:B:1072:MET:HG2	1.74	0.69
1:A:718:VAL:O	1:A:721:PHE:HB2	1.92	0.69
2:B:258:LEU:HG	2:B:258:LEU:O	1.92	0.69
2:B:313:MET:HE2	2:B:390:LEU:HD21	1.74	0.69
7:G:34:VAL:HG11	7:G:74:TYR:CE1	2.25	0.69
1:A:182:VAL:HG22	1:A:201:VAL:HA	1.74	0.69
1:A:208:LEU:HD21	1:A:212:LYS:HE3	1.74	0.69
1:A:982:THR:C	1:A:984:LYS:H	1.98	0.69
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.72	0.69
4:D:144:THR:O	4:D:148:LEU:HB2	1.91	0.69
1:A:591:PHE:HA	1:A:595:THR:HG21	1.75	0.69
2:B:637:LEU:HD12	2:B:693:ILE:HD11	1.74	0.69
3:C:183:TRP:O	3:C:185:LYS:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:12:DG:H2''	14:1:13:DT:H5'	1.75	0.69
2:B:542:MET:HE2	2:B:747:MET:HE2	1.74	0.69
4:D:13:ARG:C	4:D:15:LEU:H	1.99	0.69
1:A:66:LYS:NZ	1:A:68:GLN:H	1.90	0.69
2:B:1138:MET:HE2	2:B:1146:PHE:HD2	1.56	0.69
3:C:221:TYR:CD1	3:C:222:LYS:HG3	2.28	0.69
2:B:562:GLY:HA3	2:B:590:HIS:ND1	2.07	0.69
2:B:847:ASP:C	2:B:849:GLY:H	1.99	0.69
3:C:184:ASN:OD1	3:C:187:LYS:HA	1.92	0.69
4:D:12:ARG:HH12	4:D:14:ARG:HA	1.57	0.69
4:D:60:LYS:HE3	4:D:126:ILE:HD11	1.73	0.69
7:G:1:MET:SD	7:G:1:MET:C	2.76	0.69
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.22	0.69
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.75	0.69
2:B:559:SER:CA	2:B:563:MET:HB3	2.06	0.69
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.91	0.69
2:B:1084:GLN:N	2:B:1084:GLN:HE21	1.89	0.69
6:F:111:LEU:O	6:F:113:GLY:N	2.25	0.69
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.57	0.69
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.74	0.69
2:B:549:THR:HB	2:B:628:THR:OG1	1.93	0.69
5:E:171:LYS:HG2	5:E:174:GLN:HG3	1.75	0.69
9:I:8:ARG:HG3	9:I:9:ASP:OD1	1.92	0.69
2:B:806:THR:H	2:B:809:MET:HE3	1.57	0.68
1:A:265:LYS:O	1:A:269:ILE:HG13	1.92	0.68
4:D:12:ARG:HG2	4:D:12:ARG:HH11	1.58	0.68
1:A:134:ARG:HG2	1:A:138:ILE:HD11	1.75	0.68
1:A:913:LEU:HD12	1:A:914:GLU:N	2.05	0.68
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.08	0.68
1:A:1370:LEU:O	1:A:1374:VAL:HG23	1.93	0.68
2:B:39:ARG:HH21	2:B:665:GLU:CG	2.06	0.68
2:B:102:VAL:HG23	2:B:112:LEU:HD22	1.74	0.68
5:E:22:MET:HE3	5:E:26:ARG:HH21	1.56	0.68
6:F:109:VAL:HG12	6:F:110:ASP:N	2.08	0.68
2:B:810:GLU:HB2	2:B:815:ARG:NH2	2.07	0.68
5:E:22:MET:CE	5:E:26:ARG:HH21	2.07	0.68
11:K:101:LEU:O	11:K:101:LEU:HD23	1.94	0.68
2:B:39:ARG:HH21	2:B:665:GLU:HG2	1.58	0.68
2:B:53:GLN:HG2	2:B:547:VAL:CG2	2.23	0.68
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.57	0.68
7:G:1:MET:SD	7:G:2:PHE:N	2.67	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:14:GLU:HG2	8:H:15:VAL:N	2.09	0.68
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.20	0.68
14:1:18:DA:H3'	14:1:18:DA:OP1	1.93	0.68
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.74	0.68
2:B:427:ASP:HA	2:B:430:ARG:HG3	1.75	0.68
5:E:127:ILE:O	5:E:127:ILE:HG13	1.94	0.68
6:F:111:LEU:HD12	6:F:111:LEU:N	2.09	0.68
7:G:165:GLU:HB2	7:G:168:LEU:HD12	1.75	0.68
8:H:63:LEU:HD23	8:H:90:ALA:HB3	1.76	0.68
1:A:443:LEU:HD22	1:A:455:MET:HE2	1.76	0.68
1:A:860:LEU:HA	1:A:1422:ARG:NH2	2.09	0.68
1:A:942:PHE:CZ	5:E:207:ARG:HG3	2.28	0.68
2:B:25:ILE:CG2	2:B:658:ILE:HD12	2.24	0.68
2:B:363:HIS:O	2:B:364:ILE:HB	1.92	0.68
2:B:865:LYS:HB2	2:B:961:LEU:HD11	1.76	0.68
2:B:914:LYS:HE2	2:B:937:ALA:HB1	1.75	0.68
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.75	0.68
5:E:19:VAL:O	5:E:23:VAL:HG23	1.93	0.68
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.75	0.68
12:L:30:ILE:HG22	12:L:31:CYS:N	2.08	0.68
1:A:934:LYS:O	1:A:937:VAL:HG12	1.94	0.68
2:B:1099:VAL:HG13	2:B:1100:ASP:N	2.09	0.68
1:A:1353:TYR:HD2	1:A:1353:TYR:C	2.02	0.68
1:A:1348:LEU:O	1:A:1352:VAL:HG23	1.94	0.67
2:B:664:THR:HA	2:B:667:GLN:HE21	1.59	0.67
2:B:1187:ASN:O	2:B:1188:LYS:CB	2.43	0.67
3:C:242:GLN:C	3:C:244:VAL:H	2.01	0.67
1:A:66:LYS:HD3	1:A:67:CYS:N	2.09	0.67
1:A:332:LYS:C	1:A:334:GLY:H	2.00	0.67
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.29	0.67
3:C:98:VAL:C	3:C:99:LEU:HD22	2.20	0.67
3:C:243:VAL:O	3:C:243:VAL:HG12	1.94	0.67
4:D:66:ARG:O	4:D:70:PHE:HB2	1.94	0.67
4:D:139:LYS:HG2	4:D:143:ASN:ND2	2.09	0.67
8:H:89:LEU:HB2	8:H:91:ASP:OD1	1.95	0.67
1:A:108:MET:HA	1:A:210:ILE:HD13	1.75	0.67
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.75	0.67
1:A:283:GLY:O	1:A:285:PRO:HD2	1.93	0.67
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.76	0.67
8:H:143:LEU:HD12	8:H:143:LEU:N	2.09	0.67
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:97:ARG:O	6:F:101:ILE:HG13	1.93	0.67
7:G:138:THR:O	7:G:140:LYS:N	2.27	0.67
2:B:705:MET:H	2:B:710:LEU:HD12	1.59	0.67
2:B:707:PRO:HG2	2:B:708:GLU:H	1.59	0.67
2:B:1176:ASN:C	2:B:1178:ASN:H	2.02	0.67
3:C:112:ASN:CB	3:C:114:TYR:HE1	2.07	0.67
4:D:52:LEU:HD12	4:D:182:SER:HB2	1.74	0.67
12:L:34:CYS:O	12:L:34:CYS:SG	2.53	0.67
1:A:315:LEU:HD23	1:A:315:LEU:N	2.08	0.67
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.77	0.67
2:B:792:MET:HE2	2:B:857:ARG:NH2	2.09	0.67
2:B:882:THR:HG22	2:B:884:ARG:N	2.10	0.67
1:A:219:PHE:O	1:A:222:LEU:HB2	1.94	0.67
2:B:505:ASP:CG	13:2:1:DA:H8	2.03	0.67
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.30	0.67
10:J:16:ASP:OD1	10:J:17:LYS:HD2	1.95	0.67
1:A:57:ARG:O	1:A:68:GLN:HG2	1.95	0.67
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.76	0.67
1:A:1444:MET:CG	7:G:60:ARG:HA	2.24	0.67
2:B:637:LEU:HD21	2:B:742:GLU:HA	1.76	0.67
2:B:807:ARG:HG2	2:B:1045:SER:OG	1.95	0.67
2:B:1221:SER:O	2:B:1223:ASP:N	2.26	0.67
3:C:145:CYS:HA	10:J:2:ILE:CD1	2.25	0.67
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.77	0.67
3:C:252:GLN:NE2	11:K:95:ILE:HG23	2.07	0.67
4:D:14:ARG:HH11	4:D:14:ARG:CB	2.01	0.67
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.29	0.67
7:G:115:MET:HB3	7:G:116:PRO:HD2	1.76	0.67
1:A:23:SER:HA	1:A:233:TRP:NE1	2.09	0.67
1:A:34:LYS:HB3	1:A:36:ARG:NH1	2.09	0.67
5:E:77:SER:O	5:E:105:PHE:HB3	1.94	0.67
7:G:51:TYR:O	7:G:54:ILE:HG13	1.94	0.67
7:G:59:GLY:HA3	7:G:70:PHE:CD2	2.30	0.67
1:A:323:LYS:HD2	1:A:323:LYS:N	2.09	0.66
1:A:626:ASN:O	1:A:631:HIS:HD2	1.77	0.66
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.30	0.66
3:C:123:ASN:CG	3:C:125:MET:H	2.03	0.66
3:C:189:THR:HG22	3:C:190:ASP:N	2.08	0.66
2:B:955:THR:CG2	2:B:956:THR:N	2.58	0.66
11:K:40:HIS:ND1	11:K:61:TYR:OH	2.25	0.66
1:A:225:ASN:ND2	1:A:228:PHE:N	2.33	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:778:MET:HE2	2:B:1094:ARG:HG2	1.76	0.66
3:C:33:LEU:CG	3:C:37:MET:HE2	2.25	0.66
1:A:88:LYS:HG3	1:A:276:LEU:HD21	1.76	0.66
2:B:510:LYS:CB	2:B:511:PRO:HD3	2.23	0.66
11:K:63:VAL:HG23	11:K:63:VAL:O	1.94	0.66
1:A:40:THR:HB	1:A:41:MET:HE2	1.77	0.66
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.61	0.66
2:B:408:LEU:HD12	2:B:408:LEU:N	2.10	0.66
3:C:184:ASN:ND2	3:C:189:THR:HB	2.11	0.66
7:G:14:HIS:HD2	7:G:16:SER:H	1.43	0.66
1:A:1161:THR:C	1:A:1163:ILE:H	2.01	0.66
2:B:64:CYS:HA	2:B:67:SER:OG	1.95	0.66
8:H:15:VAL:HG22	8:H:26:ILE:CG1	2.25	0.66
8:H:84:ALA:HB2	8:H:87:ARG:CZ	2.26	0.66
1:A:134:ARG:HH11	1:A:221:SER:HA	1.61	0.66
1:A:596:THR:O	1:A:598:LEU:N	2.29	0.66
2:B:597:MET:HA	2:B:597:MET:CE	2.26	0.66
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.61	0.66
2:B:294:ASP:H	9:I:12:ASN:ND2	1.94	0.66
4:D:208:GLU:O	4:D:212:LYS:HG3	1.95	0.66
1:A:265:LYS:HD3	1:A:302:THR:CG2	2.25	0.66
2:B:25:ILE:HG21	2:B:658:ILE:HD12	1.76	0.66
2:B:686:ASN:C	2:B:688:GLY:H	2.03	0.66
1:A:62:ASP:O	1:A:64:ASN:HB2	1.96	0.66
1:A:30:ILE:HG23	2:B:1170:THR:HG23	1.78	0.65
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.30	0.65
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.76	0.65
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.77	0.65
2:B:216:GLU:OE1	2:B:537:LYS:HE3	1.96	0.65
2:B:464:GLY:O	2:B:477:ALA:HA	1.96	0.65
5:E:180:ARG:HB2	5:E:215:MET:OXT	1.95	0.65
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.30	0.65
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.62	0.65
1:A:1258:HIS:O	1:A:1262:LYS:HE3	1.97	0.65
1:A:1353:TYR:C	1:A:1353:TYR:CD2	2.74	0.65
2:B:847:ASP:HB3	3:C:167:HIS:NE2	2.12	0.65
4:D:118:THR:HB	4:D:121:LYS:HB2	1.78	0.65
4:D:123:LEU:O	4:D:127:ASP:HB2	1.97	0.65
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.78	0.65
2:B:891:ASP:O	2:B:893:LEU:N	2.29	0.65
8:H:104:PHE:HZ	8:H:136:LYS:HA	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:SER:HB3	1:A:206:GLU:HB2	1.79	0.65
1:A:424:ILE:HG22	1:A:425:GLN:N	2.11	0.65
1:A:745:GLN:HA	1:A:748:MET:HE3	1.78	0.65
2:B:247:GLY:C	2:B:249:ARG:H	2.04	0.65
4:D:124:GLU:HA	4:D:127:ASP:HB2	1.77	0.65
8:H:89:LEU:C	8:H:91:ASP:N	2.52	0.65
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.32	0.65
4:D:8:PHE:CE1	4:D:37:GLN:HB2	2.32	0.65
5:E:176:PRO:O	5:E:212:ARG:HA	1.96	0.65
6:F:85:MET:HE2	6:F:93:ILE:HD13	1.79	0.65
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.79	0.65
1:A:106:VAL:HG12	1:A:107:CYS:N	2.11	0.65
1:A:666:ILE:HD12	1:A:666:ILE:N	2.12	0.65
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.26	0.65
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.11	0.65
2:B:773:MET:SD	2:B:987:LYS:HD3	2.37	0.65
2:B:875:GLU:O	2:B:877:PRO:HD3	1.97	0.65
2:B:1001:PHE:CE2	3:C:34:ARG:NE	2.64	0.65
3:C:10:ILE:HG22	3:C:11:ARG:O	1.97	0.65
4:D:29:LEU:HD22	4:D:29:LEU:N	2.12	0.65
7:G:122:ASN:ND2	7:G:125:SER:HB3	2.11	0.65
8:H:44:VAL:O	8:H:44:VAL:HG12	1.97	0.65
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.25	0.65
1:A:288:ALA:HA	1:A:291:GLU:CD	2.22	0.65
1:A:344:ARG:HB3	1:A:344:ARG:HH11	1.62	0.65
1:A:1445:ILE:HD12	1:A:1445:ILE:N	2.12	0.65
2:B:282:ILE:HG21	2:B:382:ILE:HD11	1.78	0.65
2:B:976:ILE:O	2:B:990:ILE:HB	1.97	0.65
2:B:1001:PHE:CD1	2:B:1001:PHE:C	2.74	0.65
9:I:102:VAL:HG22	9:I:109:ILE:HG12	1.78	0.65
2:B:815:ARG:HD3	2:B:1041:GLU:OE2	1.97	0.65
3:C:165:LYS:O	11:K:6:ARG:NH1	2.29	0.65
4:D:7:THR:O	4:D:9:GLN:N	2.29	0.65
2:B:955:THR:HG22	2:B:956:THR:O	1.97	0.65
2:B:1174:LYS:O	2:B:1175:LEU:C	2.40	0.65
7:G:88:ASP:HB3	7:G:144:ARG:HA	1.77	0.65
1:A:19:PHE:O	1:A:1416:ALA:HA	1.96	0.65
1:A:481:ASP:OD1	1:A:485:ASP:OD2	2.15	0.65
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.97	0.65
2:B:497:ARG:NH2	2:B:775:LYS:NZ	2.45	0.65
2:B:773:MET:C	2:B:775:LYS:H	2.04	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:839:MET:HE3	2:B:1010:LEU:CD2	2.24	0.65
2:B:1001:PHE:C	2:B:1001:PHE:HD1	2.05	0.65
4:D:154:PHE:HE1	4:D:163:VAL:HG11	1.62	0.65
5:E:178:ILE:HG22	5:E:213:ILE:O	1.96	0.65
1:A:626:ASN:O	1:A:631:HIS:CD2	2.50	0.64
2:B:465:ASN:HD22	2:B:465:ASN:N	1.93	0.64
2:B:497:ARG:HH21	2:B:775:LYS:HZ3	1.44	0.64
6:F:135:ARG:HG2	6:F:137:TYR:CE1	2.32	0.64
10:J:53:HIS:CD2	10:J:54:VAL:N	2.66	0.64
1:A:567:LYS:CB	8:H:96:VAL:H	2.03	0.64
2:B:473:MET:HE3	2:B:474:SER:CA	2.26	0.64
2:B:705:MET:H	2:B:710:LEU:CD1	2.11	0.64
2:B:796:LEU:HD12	2:B:852:ARG:O	1.96	0.64
2:B:801:LYS:O	10:J:52:THR:HG23	1.96	0.64
5:E:22:MET:HE3	5:E:26:ARG:NE	2.12	0.64
7:G:116:PRO:HG2	7:G:119:LEU:HB3	1.78	0.64
1:A:154:SER:HB3	1:A:162:VAL:CG2	2.27	0.64
1:A:255:SER:OG	2:B:918:ILE:HD13	1.96	0.64
1:A:567:LYS:HD2	1:A:568:PRO:CD	2.21	0.64
1:A:853:ASP:OD1	1:A:855:THR:CB	2.45	0.64
2:B:168:GLY:HA2	2:B:450:ALA:O	1.96	0.64
3:C:33:LEU:CD1	3:C:37:MET:HE2	2.27	0.64
7:G:138:THR:HG22	7:G:139:ILE:H	1.62	0.64
10:J:24:LEU:O	10:J:30:LEU:HB2	1.97	0.64
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.32	0.64
1:A:590:ARG:HG2	1:A:590:ARG:NH1	2.10	0.64
2:B:387:LEU:H	2:B:387:LEU:HD12	1.63	0.64
2:B:430:ARG:HH11	2:B:430:ARG:CB	2.07	0.64
2:B:708:GLU:HG3	2:B:709:ASP:N	2.10	0.64
3:C:238:ILE:HD11	3:C:246:ARG:NH1	2.13	0.64
1:A:108:MET:HB3	1:A:210:ILE:HD11	1.78	0.64
1:A:225:ASN:ND2	1:A:227:VAL:H	1.95	0.64
1:A:768:GLN:CG	1:A:816:HIS:HA	2.26	0.64
1:A:1076:ALA:HA	1:A:1079:MET:CE	2.27	0.64
2:B:181:LEU:HD22	2:B:189:LEU:CD2	2.27	0.64
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.61	0.64
2:B:770:GLN:CD	2:B:983:ARG:HA	2.22	0.64
2:B:916:THR:HB	2:B:935:ARG:HD2	1.79	0.64
1:A:33:ALA:HA	1:A:57:ARG:NH1	2.12	0.64
1:A:195:ASP:O	1:A:196:GLU:HB3	1.97	0.64
1:A:332:LYS:O	1:A:333:GLU:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:MET:HE2	1:A:607:ILE:CG1	2.27	0.64
1:A:1230:GLU:O	1:A:1232:ASN:N	2.30	0.64
2:B:364:ILE:O	2:B:365:THR:HB	1.97	0.64
2:B:1001:PHE:CE2	3:C:34:ARG:CZ	2.80	0.64
3:C:236:GLY:O	3:C:238:ILE:N	2.30	0.64
7:G:120:THR:HG22	7:G:131:GLN:O	1.97	0.64
2:B:284:ILE:HD13	2:B:333:PHE:HD2	1.63	0.64
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.79	0.64
3:C:43:THR:CG2	3:C:44:LEU:N	2.60	0.64
3:C:112:ASN:CB	3:C:114:TYR:CE1	2.80	0.64
5:E:15:ALA:O	5:E:19:VAL:HG23	1.96	0.64
1:A:114:LEU:O	1:A:115:LEU:HG	1.98	0.64
1:A:567:LYS:CB	1:A:568:PRO:CD	2.75	0.64
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.33	0.64
1:A:1205:LYS:O	1:A:1207:LEU:HG	1.97	0.64
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.80	0.64
2:B:211:VAL:O	2:B:480:SER:HA	1.97	0.64
2:B:333:PHE:O	2:B:334:ILE:HG13	1.98	0.64
2:B:525:ALA:O	2:B:768:THR:HG23	1.97	0.64
2:B:589:VAL:CG1	2:B:590:HIS:H	2.09	0.64
2:B:987:LYS:HE3	15:3:11:U:O2'	1.98	0.64
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.13	0.64
2:B:1124:ARG:HB3	2:B:1124:ARG:HH11	1.62	0.64
5:E:179:GLN:HB2	5:E:182:ASP:HB2	1.80	0.64
7:G:158:HIS:CD2	7:G:159:ALA:H	2.15	0.64
8:H:8:ASP:OD2	8:H:9:ILE:N	2.27	0.64
1:A:67:CYS:C	1:A:68:GLN:HG3	2.22	0.64
1:A:390:GLN:O	1:A:394:ASN:HB2	1.98	0.64
2:B:30:SER:HB3	2:B:743:ILE:O	1.98	0.64
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.80	0.64
2:B:597:MET:HA	2:B:597:MET:HE3	1.78	0.64
2:B:996:ARG:NH2	3:C:175:ALA:H	1.96	0.64
3:C:11:ARG:HD3	3:C:21:ILE:HD11	1.80	0.64
4:D:18:VAL:O	4:D:19:GLU:HB2	1.95	0.64
8:H:100:THR:HG23	8:H:138:GLU:HG2	1.79	0.64
1:A:316:GLN:HG2	1:A:317:LYS:N	2.13	0.63
2:B:842:ASN:HD22	2:B:845:SER:N	1.93	0.63
3:C:91:HIS:HD2	3:C:91:HIS:O	1.80	0.63
4:D:35:LEU:HD12	4:D:35:LEU:N	2.13	0.63
4:D:119:ARG:HD3	4:D:221:TYR:CE2	2.32	0.63
5:E:29:PHE:O	5:E:30:ILE:HG13	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:99:HIS:CE1	5:E:103:LYS:HD2	2.34	0.63
12:L:28:LYS:HE3	12:L:39:SER:OG	1.97	0.63
1:A:427:GLN:HG3	1:A:430:TRP:CE2	2.33	0.63
1:A:571:LEU:HD22	8:H:46:LEU:HD11	1.80	0.63
2:B:60:GLN:O	2:B:63:ILE:HG22	1.98	0.63
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.79	0.63
3:C:39:ALA:O	3:C:164:ALA:HB3	1.98	0.63
2:B:582:VAL:HG22	2:B:626:ILE:CG2	2.29	0.63
2:B:953:LEU:HD23	2:B:953:LEU:O	1.98	0.63
3:C:248:ILE:HD13	11:K:101:LEU:HD22	1.80	0.63
7:G:138:THR:CG2	7:G:139:ILE:N	2.59	0.63
9:I:105:SER:O	9:I:106:CYS:HB3	1.98	0.63
1:A:343:LYS:NZ	2:B:1151:LEU:HG	2.13	0.63
2:B:549:THR:CG2	2:B:550:ASP:H	2.08	0.63
3:C:221:TYR:HE1	3:C:222:LYS:HE3	1.63	0.63
4:D:29:LEU:HB3	7:G:82:PHE:CE2	2.34	0.63
1:A:37:PHE:N	1:A:37:PHE:CD1	2.66	0.63
1:A:65:LEU:O	1:A:66:LYS:C	2.41	0.63
2:B:34:ILE:HG12	2:B:542:MET:CE	2.28	0.63
2:B:345:LYS:HB2	2:B:348:ARG:HH21	1.64	0.63
2:B:797:TYR:O	10:J:1:MET:HG2	1.99	0.63
3:C:22:LEU:HD22	3:C:230:MET:HE1	1.79	0.63
3:C:253:LYS:O	3:C:256:ALA:HB3	1.98	0.63
5:E:202:SER:OG	5:E:204:THR:HG22	1.99	0.63
8:H:40:LEU:CD1	8:H:123:MET:HE3	2.28	0.63
7:G:116:PRO:HG2	7:G:119:LEU:CB	2.28	0.63
8:H:26:ILE:CD1	8:H:49:VAL:HG11	2.28	0.63
1:A:481:ASP:OD1	1:A:483:ASP:OD2	2.17	0.63
1:A:698:GLN:HA	9:I:97:MET:O	1.97	0.63
4:D:64:VAL:C	4:D:66:ARG:H	2.07	0.63
4:D:154:PHE:CE1	4:D:163:VAL:HG21	2.34	0.63
5:E:69:ILE:N	5:E:69:ILE:HD12	2.13	0.63
8:H:84:ALA:O	8:H:85:GLY:C	2.41	0.63
1:A:472:LEU:O	1:A:475:THR:HB	1.98	0.63
5:E:22:MET:HE3	5:E:26:ARG:NH2	2.13	0.63
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.81	0.62
6:F:119:ARG:HH11	6:F:119:ARG:CG	2.05	0.62
7:G:91:VAL:HG12	7:G:92:VAL:N	2.12	0.62
7:G:129:SER:CB	7:G:138:THR:OG1	2.47	0.62
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.34	0.62
8:H:130:ARG:HD3	8:H:130:ARG:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ILE:HG22	1:A:290:GLU:N	2.14	0.62
1:A:380:VAL:HG12	1:A:428:TYR:HA	1.80	0.62
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.80	0.62
2:B:847:ASP:C	2:B:849:GLY:N	2.57	0.62
2:B:1221:SER:C	2:B:1223:ASP:H	2.08	0.62
5:E:69:ILE:HD12	5:E:69:ILE:H	1.64	0.62
5:E:94:LYS:CE	5:E:98:ILE:HD11	2.22	0.62
7:G:115:MET:HE1	7:G:130:TYR:CE2	2.33	0.62
9:I:58:VAL:HG13	9:I:62:ILE:HD13	1.81	0.62
12:L:40:LEU:HD22	12:L:44:ASP:CG	2.25	0.62
1:A:57:ARG:HB2	1:A:57:ARG:HH11	1.64	0.62
1:A:308:ILE:HG22	1:A:309:ALA:H	1.63	0.62
1:A:1107:VAL:O	1:A:1107:VAL:CG1	2.47	0.62
2:B:542:MET:HE2	2:B:747:MET:HG3	1.81	0.62
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.80	0.62
2:B:282:ILE:HD11	2:B:317:CYS:SG	2.40	0.62
4:D:14:ARG:NH1	4:D:16:LYS:HD2	2.15	0.62
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.80	0.62
1:A:34:LYS:NZ	1:A:57:ARG:HH21	1.98	0.62
1:A:425:GLN:N	1:A:425:GLN:OE1	2.33	0.62
2:B:134:LYS:HZ1	2:B:164:LYS:HE2	1.63	0.62
2:B:345:LYS:CG	2:B:346:GLU:N	2.62	0.62
3:C:258:ILE:HD11	11:K:42:LEU:HD21	1.82	0.62
5:E:207:ARG:HB3	5:E:207:ARG:HH11	1.64	0.62
12:L:53:HIS:HB3	12:L:55:ILE:CD1	2.28	0.62
1:A:1095:THR:HG21	1:A:1112:LYS:HD2	1.80	0.62
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.31	0.62
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.80	0.62
5:E:7:ARG:HD2	5:E:7:ARG:C	2.25	0.62
5:E:46:TYR:CE2	5:E:58:MET:HA	2.35	0.62
5:E:117:THR:HB	5:E:120:ALA:HB2	1.81	0.62
6:F:89:GLU:OE2	6:F:134:ILE:HG21	1.99	0.62
1:A:351:THR:CG2	2:B:1103:ILE:HA	2.21	0.62
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.82	0.62
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.34	0.62
1:A:1308:THR:CG2	1:A:1309:ASP:N	2.59	0.62
4:D:12:ARG:NH1	4:D:14:ARG:HA	2.13	0.62
6:F:69:LEU:HB3	6:F:71:GLU:CD	2.25	0.62
11:K:13:GLY:O	11:K:16:GLU:HG3	2.00	0.62
1:A:172:PRO:HD3	1:A:185:TRP:NE1	2.14	0.62
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:615:MET:HG2	2:B:626:ILE:HG12	1.81	0.62
2:B:1095:LEU:HD12	2:B:1095:LEU:N	2.14	0.62
3:C:82:TYR:O	3:C:83:SER:C	2.42	0.62
3:C:183:TRP:O	3:C:184:ASN:C	2.42	0.62
1:A:55:ASP:O	1:A:55:ASP:CG	2.42	0.62
1:A:305:ASP:OD1	1:A:306:ASN:N	2.32	0.62
2:B:547:VAL:HG12	2:B:612:GLU:OE2	1.99	0.62
2:B:642:ASP:O	2:B:644:GLU:N	2.30	0.62
2:B:882:THR:HB	2:B:934:LYS:O	2.00	0.62
2:B:1102:LYS:O	2:B:1103:ILE:C	2.42	0.62
8:H:123:MET:HE1	8:H:142:LEU:HD11	1.82	0.62
1:A:216:VAL:O	1:A:219:PHE:HB2	2.00	0.62
1:A:369:SER:HB3	11:K:2:ASN:ND2	2.14	0.62
2:B:294:ASP:C	2:B:296:GLU:H	2.07	0.62
2:B:852:ARG:HH22	12:L:70:ARG:C	2.06	0.62
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.24	0.62
7:G:129:SER:HB3	7:G:138:THR:OG1	2.00	0.62
9:I:8:ARG:HG3	9:I:9:ASP:N	2.15	0.62
11:K:68:PHE:HD1	11:K:70:ARG:HH12	1.47	0.62
1:A:73:GLY:O	1:A:75:ASN:N	2.33	0.61
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.29	0.61
2:B:868:MET:O	2:B:870:ILE:HG13	2.00	0.61
4:D:153:ARG:HB3	4:D:154:PHE:CD2	2.34	0.61
5:E:207:ARG:HB3	5:E:207:ARG:NH1	2.15	0.61
8:H:76:THR:O	8:H:77:ARG:HB2	2.00	0.61
1:A:66:LYS:HZ2	1:A:68:GLN:H	1.48	0.61
2:B:983:ARG:NH1	2:B:1028:GLU:OE1	2.33	0.61
3:C:124:LEU:O	3:C:127:ARG:HG2	2.00	0.61
3:C:189:THR:HG22	3:C:190:ASP:H	1.64	0.61
1:A:7:SER:HB3	2:B:1193:GLN:HE22	1.65	0.61
1:A:51:GLY:C	1:A:56:PRO:HB3	2.26	0.61
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.00	0.61
2:B:226:PHE:HA	2:B:395:GLN:HG2	1.83	0.61
3:C:76:ASP:OD2	3:C:128:ASN:N	2.32	0.61
1:A:1036:ARG:HG2	1:A:1036:ARG:HH11	1.64	0.61
2:B:261:ARG:HB3	2:B:261:ARG:NH1	2.13	0.61
2:B:290:GLY:O	2:B:292:ILE:HG13	1.99	0.61
6:F:69:LEU:HD22	6:F:71:GLU:OE2	1.99	0.61
1:A:1450:LEU:O	1:A:1450:LEU:HG	1.99	0.61
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.82	0.61
2:B:1159:ARG:HB3	2:B:1159:ARG:NH1	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:THR:HG22	2:B:1103:ILE:CA	2.21	0.61
1:A:353:ILE:HG13	1:A:470:LEU:HD21	1.82	0.61
1:A:456:MET:HE1	1:A:474:VAL:HG23	1.81	0.61
2:B:63:ILE:HD12	2:B:421:PHE:CE2	2.35	0.61
2:B:277:LYS:HE2	2:B:336:ARG:HD3	1.82	0.61
2:B:879:ARG:NH2	2:B:885:MET:HE2	2.15	0.61
2:B:1084:GLN:HE21	2:B:1084:GLN:H	1.47	0.61
4:D:51:ASN:O	4:D:52:LEU:O	2.19	0.61
8:H:87:ARG:HG2	8:H:88:SER:N	2.16	0.61
12:L:42:ARG:HH11	12:L:42:ARG:HG3	1.65	0.61
1:A:105:CYS:SG	1:A:139:TRP:HA	2.41	0.61
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.15	0.61
2:B:644:GLU:C	2:B:646:LEU:H	2.08	0.61
4:D:153:ARG:NH2	4:D:184:ALA:HA	2.15	0.61
7:G:26:LEU:HD12	7:G:56:ILE:CD1	2.15	0.61
1:A:2:VAL:HG11	2:B:1157:ALA:HB1	1.82	0.61
1:A:207:ILE:O	1:A:208:LEU:C	2.42	0.61
1:A:1141:THR:CG2	1:A:1205:LYS:HD3	2.30	0.61
2:B:289:LEU:HD13	2:B:375:ALA:CB	2.29	0.61
2:B:469:GLN:HG2	2:B:470:LYS:N	2.16	0.61
5:E:56:LYS:HZ3	5:E:84:ASP:H	1.49	0.61
5:E:136:ASN:OD1	5:E:137:GLU:N	2.34	0.61
8:H:15:VAL:HG22	8:H:26:ILE:HG13	1.82	0.61
8:H:139:ASN:O	8:H:140:ALA:CB	2.48	0.61
9:I:85:PHE:H	9:I:85:PHE:HD2	1.47	0.61
1:A:886:ILE:HD12	1:A:943:LEU:HB3	1.83	0.61
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.63	0.61
2:B:95:ILE:HB	2:B:130:VAL:HG13	1.82	0.61
2:B:278:GLN:CG	2:B:279:ASP:H	2.13	0.61
2:B:332:ASP:O	2:B:334:ILE:N	2.32	0.61
4:D:124:GLU:HA	4:D:127:ASP:CB	2.31	0.61
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.27	0.61
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.35	0.61
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.83	0.61
1:A:979:SER:OG	1:A:980:ASP:N	2.33	0.61
1:A:1395:GLY:HA3	1:A:1419:ASP:OD2	1.99	0.61
2:B:175:ARG:HB2	2:B:200:GLY:HA3	1.82	0.61
2:B:193:LYS:HZ1	12:L:32:ALA:HB1	1.66	0.61
9:I:111:THR:HG21	9:I:113:ASP:HB2	1.83	0.61
1:A:597:LEU:HD12	1:A:597:LEU:N	2.16	0.60
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	2.89	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:ARG:NH1	2:B:398:ARG:HB2	2.16	0.60
3:C:112:ASN:HB2	3:C:114:TYR:HE1	1.66	0.60
8:H:4:THR:HG22	8:H:5:LEU:N	2.16	0.60
9:I:85:PHE:HD1	9:I:99:LEU:HD22	1.65	0.60
1:A:63:ARG:CA	1:A:74:MET:HE2	2.31	0.60
1:A:225:ASN:HD22	1:A:228:PHE:N	1.94	0.60
1:A:317:LYS:O	1:A:318:SER:HB3	1.99	0.60
1:A:665:GLY:HA2	2:B:1026:LEU:CD2	2.31	0.60
2:B:510:LYS:HB3	2:B:511:PRO:CD	2.27	0.60
2:B:516:ASN:N	2:B:516:ASN:ND2	2.49	0.60
6:F:103:MET:O	6:F:104:ASN:HB2	2.01	0.60
8:H:31:THR:O	8:H:31:THR:HG22	1.99	0.60
1:A:35:ILE:HA	1:A:52:GLY:O	2.01	0.60
2:B:288:ALA:CB	2:B:331:LEU:HD12	2.30	0.60
2:B:583:ASN:ND2	2:B:628:THR:HG22	2.16	0.60
4:D:154:PHE:CD2	4:D:154:PHE:N	2.68	0.60
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.67	0.60
1:A:335:ARG:NH1	2:B:1202:LEU:HD13	2.16	0.60
1:A:399:HIS:O	1:A:400:PRO:C	2.44	0.60
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.31	0.60
2:B:871:THR:HG22	2:B:872:GLU:O	2.01	0.60
3:C:16:ASP:C	3:C:240:VAL:HG11	2.26	0.60
3:C:101:LEU:HB2	3:C:118:LEU:HD23	1.83	0.60
3:C:236:GLY:O	3:C:237:SER:C	2.44	0.60
4:D:138:ASN:HD21	7:G:35:GLU:HB3	1.64	0.60
5:E:42:PHE:CZ	5:E:58:MET:HE3	2.37	0.60
7:G:26:LEU:CD1	7:G:56:ILE:HD11	2.15	0.60
1:A:794:PRO:HG2	1:A:795:GLU:OE2	2.01	0.60
1:A:1095:THR:CG2	1:A:1112:LYS:HD2	2.32	0.60
2:B:883:LEU:O	2:B:885:MET:N	2.34	0.60
2:B:1202:LEU:HD22	2:B:1206:GLU:CD	2.26	0.60
3:C:261:ALA:HA	3:C:264:GLN:OE1	2.01	0.60
4:D:153:ARG:C	4:D:154:PHE:CD2	2.79	0.60
5:E:117:THR:HB	5:E:120:ALA:CB	2.32	0.60
8:H:23:VAL:HG22	8:H:42:ILE:O	2.01	0.60
10:J:7:CYS:SG	10:J:49:MET:HE3	2.41	0.60
11:K:21:ILE:HG12	11:K:33:ILE:HG23	1.82	0.60
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.84	0.60
2:B:811:TYR:N	2:B:811:TYR:CD1	2.70	0.60
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.00	0.60
5:E:89:GLY:C	5:E:91:LYS:H	2.08	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.01	0.60
1:A:1027:ALA:O	1:A:1031:VAL:HG23	2.00	0.60
2:B:759:PRO:C	2:B:761:HIS:H	2.10	0.60
3:C:7:GLN:HG3	11:K:104:ASN:HD22	1.67	0.60
3:C:258:ILE:O	3:C:262:LEU:HB2	2.01	0.60
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.83	0.60
2:B:65:GLU:OE1	2:B:418:LYS:HE3	2.01	0.60
2:B:1156:ASP:O	2:B:1157:ALA:O	2.20	0.60
5:E:44:ALA:O	5:E:45:LYS:HB2	1.99	0.60
1:A:284:ALA:O	1:A:286:HIS:N	2.35	0.60
1:A:853:ASP:O	1:A:854:ASN:HB2	1.99	0.60
2:B:652:LYS:HB3	2:B:689:LEU:CD2	2.31	0.60
2:B:734:HIS:O	2:B:735:ALA:HB2	2.02	0.60
2:B:1095:LEU:H	2:B:1095:LEU:CD1	2.12	0.60
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.66	0.60
8:H:87:ARG:HG2	8:H:88:SER:H	1.67	0.60
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.84	0.60
2:B:505:ASP:HA	13:2:1:DA:C8	2.36	0.60
2:B:553:PRO:O	2:B:557:PHE:HB2	2.02	0.60
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.82	0.60
3:C:17:ASN:N	3:C:240:VAL:HG11	2.16	0.60
4:D:185:CYS:O	4:D:211:LEU:HD22	2.01	0.60
1:A:709:THR:HB	1:A:712:GLU:H	1.67	0.59
1:A:839:ARG:HG2	1:A:839:ARG:NH1	2.12	0.59
2:B:189:LEU:HD13	2:B:196:PRO:HA	1.83	0.59
2:B:235:SER:OG	2:B:236:HIS:HD2	1.85	0.59
2:B:1096:ARG:HG2	2:B:1097:HIS:ND1	2.16	0.59
3:C:161:LYS:O	3:C:170:TRP:NE1	2.34	0.59
9:I:105:SER:O	9:I:106:CYS:CB	2.50	0.59
1:A:266:LEU:HD21	1:A:303:TYR:CZ	2.37	0.59
1:A:438:ASP:O	1:A:439:ASN:HB2	2.02	0.59
1:A:741:ASN:HD22	1:A:744:LYS:H	1.48	0.59
1:A:850:VAL:HG12	1:A:850:VAL:O	2.03	0.59
2:B:36:ALA:HA	2:B:39:ARG:HD2	1.84	0.59
2:B:882:THR:HG21	2:B:935:ARG:CA	2.16	0.59
4:D:14:ARG:HH12	4:D:16:LYS:HD2	1.67	0.59
4:D:134:THR:HG22	4:D:135:GLY:N	2.17	0.59
12:L:38:LEU:HD11	12:L:49:LYS:HE2	1.84	0.59
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.84	0.59
1:A:1042:PHE:CE2	1:A:1046:LEU:HD11	2.37	0.59
1:A:1202:MET:HE1	1:A:1212:VAL:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:891:ASP:C	2:B:893:LEU:H	2.09	0.59
2:B:1147:LEU:CD2	2:B:1151:LEU:HD22	2.32	0.59
3:C:66:ARG:NH1	10:J:2:ILE:CG2	2.57	0.59
1:A:67:CYS:O	1:A:70:CYS:HB3	2.01	0.59
2:B:35:SER:HA	2:B:811:TYR:HE2	1.68	0.59
2:B:687:GLU:O	2:B:689:LEU:HG	2.02	0.59
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.37	0.59
4:D:155:ARG:NE	4:D:221:TYR:CE1	2.68	0.59
5:E:79:TRP:NE1	5:E:81:GLU:HB2	2.15	0.59
10:J:3:VAL:HA	10:J:53:HIS:CE1	2.37	0.59
10:J:27:GLU:O	10:J:29:GLU:N	2.35	0.59
12:L:38:LEU:CD1	12:L:49:LYS:HE2	2.32	0.59
1:A:567:LYS:HB3	8:H:95:TYR:CA	2.32	0.59
2:B:637:LEU:HD22	2:B:741:CYS:O	2.02	0.59
2:B:847:ASP:O	2:B:849:GLY:N	2.35	0.59
3:C:91:HIS:C	3:C:91:HIS:CD2	2.80	0.59
1:A:146:MET:O	1:A:147:VAL:HG23	2.03	0.59
1:A:869:GLY:O	5:E:204:THR:HG21	2.02	0.59
1:A:1153:TYR:CD2	1:A:1163:ILE:HD11	2.37	0.59
7:G:119:LEU:HD11	7:G:130:TYR:HB3	1.84	0.59
1:A:596:THR:C	1:A:597:LEU:HD12	2.27	0.59
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.83	0.59
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.33	0.59
2:B:273:LEU:O	2:B:276:ILE:HB	2.03	0.59
2:B:418:LYS:HG2	2:B:422:LYS:HE3	1.85	0.59
2:B:460:ALA:O	2:B:462:ALA:N	2.35	0.59
2:B:583:ASN:HD21	2:B:628:THR:CG2	2.14	0.59
2:B:864:LYS:HG3	2:B:872:GLU:OE1	2.02	0.59
4:D:8:PHE:HE1	4:D:37:GLN:HB2	1.66	0.59
4:D:64:VAL:C	4:D:66:ARG:N	2.57	0.59
6:F:109:VAL:HG12	6:F:110:ASP:H	1.65	0.59
9:I:82:GLU:HB3	9:I:104:LEU:HG	1.83	0.59
11:K:61:TYR:C	11:K:61:TYR:CD2	2.81	0.59
1:A:61:ILE:HG22	1:A:62:ASP:N	2.08	0.59
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.36	0.59
1:A:1048:ASN:O	1:A:1049:ILE:C	2.44	0.59
1:A:1316:VAL:O	1:A:1316:VAL:HG12	2.02	0.59
2:B:57:TYR:CD1	2:B:57:TYR:N	2.71	0.59
4:D:139:LYS:HG2	4:D:143:ASN:HD22	1.67	0.59
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.84	0.59
2:B:519:TRP:C	2:B:519:TRP:CD1	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:198:LEU:O	4:D:200:ASN:N	2.35	0.59
1:A:10:PRO:HG2	2:B:1192:TYR:HD2	1.68	0.59
1:A:676:MET:O	1:A:679:ILE:HB	2.03	0.59
1:A:964:ILE:O	1:A:967:ALA:HB3	2.02	0.59
2:B:241:ARG:HG2	2:B:253:THR:HG22	1.85	0.59
2:B:770:GLN:HG2	2:B:983:ARG:O	2.03	0.59
8:H:30:SER:CB	8:H:36:CYS:HB3	2.32	0.59
1:A:107:CYS:HB2	1:A:114:LEU:CD2	2.30	0.58
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.85	0.58
2:B:622:LYS:HZ3	9:I:59:VAL:HG13	1.68	0.58
3:C:73:GLN:HE21	3:C:75:MET:H	1.51	0.58
1:A:331:GLY:O	1:A:332:LYS:O	2.21	0.58
2:B:90:ILE:HD12	2:B:432:MET:SD	2.44	0.58
2:B:102:VAL:HG21	2:B:112:LEU:HD22	1.85	0.58
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.33	0.58
2:B:282:ILE:CG2	2:B:382:ILE:HD11	2.32	0.58
2:B:637:LEU:CD2	2:B:742:GLU:HA	2.33	0.58
2:B:638:PHE:HD2	2:B:690:VAL:HG22	1.68	0.58
2:B:756:ILE:O	2:B:759:PRO:HD3	2.02	0.58
2:B:936:ASP:OD1	2:B:937:ALA:N	2.36	0.58
3:C:164:ALA:HA	3:C:167:HIS:O	2.02	0.58
5:E:48:ASP:HB3	5:E:54:GLN:NE2	2.19	0.58
1:A:1241:ARG:O	1:A:1242:VAL:HG23	2.03	0.58
2:B:20:ASP:O	2:B:22:SER:N	2.33	0.58
2:B:787:VAL:O	2:B:787:VAL:HG12	2.03	0.58
2:B:882:THR:CG2	2:B:884:ARG:H	2.15	0.58
7:G:13:LEU:CD2	7:G:17:PHE:HB2	2.32	0.58
7:G:111:THR:HG22	7:G:114:LEU:HD22	1.85	0.58
7:G:122:ASN:HB2	7:G:131:GLN:HE21	1.69	0.58
7:G:138:THR:CG2	7:G:139:ILE:H	2.16	0.58
10:J:23:ASN:O	10:J:25:LEU:N	2.36	0.58
1:A:50:ILE:O	1:A:52:GLY:N	2.36	0.58
1:A:129:LYS:O	1:A:130:ASP:CB	2.51	0.58
1:A:577:ILE:HA	1:A:580:VAL:HG23	1.86	0.58
1:A:786:HIS:CE1	2:B:705:MET:HE1	2.39	0.58
1:A:1129:GLU:OE1	1:A:1132:LYS:HD2	2.03	0.58
2:B:918:ILE:HG21	2:B:935:ARG:NH2	2.17	0.58
4:D:24:ALA:HB3	4:D:26:THR:HG23	1.85	0.58
6:F:82:THR:HG22	6:F:84:TYR:N	2.11	0.58
10:J:27:GLU:C	10:J:29:GLU:H	2.12	0.58
1:A:2:VAL:HG11	2:B:1157:ALA:CB	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:GLY:O	1:A:312:PRO:HD2	2.03	0.58
1:A:372:LYS:HA	1:A:435:HIS:HD1	1.67	0.58
1:A:623:GLY:C	1:A:625:SER:H	2.12	0.58
1:A:673:GLY:O	1:A:676:MET:HB2	2.02	0.58
2:B:418:LYS:HE2	2:B:422:LYS:NZ	2.18	0.58
2:B:999:MET:HE3	2:B:999:MET:CA	2.31	0.58
3:C:52:GLU:OE1	3:C:154:LYS:HE3	2.03	0.58
4:D:130:LEU:O	4:D:132:GLN:N	2.34	0.58
2:B:100:PRO:HB2	2:B:180:TYR:HE1	1.67	0.58
2:B:629:ASP:HB3	2:B:632:ARG:HD3	1.85	0.58
5:E:35:VAL:C	5:E:37:LEU:H	2.11	0.58
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.86	0.58
8:H:4:THR:HA	8:H:60:ALA:CB	2.27	0.58
9:I:7:CYS:SG	9:I:8:ARG:O	2.61	0.58
1:A:535:THR:HG23	1:A:575:LYS:HE2	1.85	0.58
2:B:604:ARG:NH2	2:B:614:SER:HA	2.19	0.58
2:B:891:ASP:C	2:B:893:LEU:N	2.59	0.58
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.51	0.58
3:C:196:ASP:HB3	3:C:199:LYS:HD2	1.85	0.58
4:D:29:LEU:HD12	7:G:82:PHE:CE2	2.38	0.58
5:E:56:LYS:NZ	5:E:84:ASP:H	2.00	0.58
5:E:98:ILE:HG22	5:E:102:GLU:HG3	1.84	0.58
5:E:182:ASP:HB3	5:E:185:ALA:HB2	1.85	0.58
1:A:317:LYS:O	1:A:318:SER:CB	2.52	0.58
1:A:511:ILE:HG22	1:A:512:VAL:N	2.18	0.58
1:A:993:LEU:HD12	1:A:993:LEU:O	2.04	0.58
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.86	0.58
2:B:246:LYS:HA	2:B:249:ARG:HE	1.69	0.58
2:B:509:ALA:O	2:B:510:LYS:C	2.47	0.58
2:B:798:TYR:CE2	3:C:62:PHE:CE2	2.91	0.58
2:B:906:SER:O	2:B:907:GLY:C	2.46	0.58
3:C:124:LEU:HD12	3:C:124:LEU:N	2.18	0.58
5:E:3:GLN:NE2	5:E:52:ARG:HH22	2.02	0.58
5:E:94:LYS:HE2	5:E:98:ILE:CD1	2.23	0.58
5:E:144:ILE:HG13	5:E:145:THR:N	2.17	0.58
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.86	0.58
7:G:12:THR:HG23	7:G:67:SER:HB3	1.85	0.58
10:J:2:ILE:CG2	10:J:3:VAL:N	2.65	0.58
1:A:675:THR:O	1:A:679:ILE:HG13	2.04	0.58
2:B:1115:THR:HG22	2:B:1117:GLN:H	1.69	0.58
3:C:117:ASP:N	3:C:117:ASP:OD1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:ILE:HD13	1:A:801:GLU:CG	2.32	0.58
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.86	0.58
2:B:192:LEU:O	2:B:193:LYS:HB2	2.04	0.58
2:B:639:ILE:HG22	2:B:641:GLU:HG2	1.86	0.58
3:C:186:LEU:HD21	3:C:225:ALA:HB2	1.84	0.58
9:I:73:ARG:HD2	9:I:101:PHE:CE2	2.38	0.58
1:A:332:LYS:O	1:A:333:GLU:CB	2.52	0.57
1:A:369:SER:CB	11:K:2:ASN:HD21	2.16	0.57
1:A:903:ASN:ND2	1:A:905:ASP:H	2.02	0.57
1:A:1241:ARG:O	1:A:1242:VAL:CB	2.51	0.57
2:B:189:LEU:O	2:B:192:LEU:N	2.36	0.57
2:B:211:VAL:CG2	2:B:483:LEU:HB2	2.34	0.57
2:B:637:LEU:HD12	2:B:693:ILE:CD1	2.34	0.57
2:B:966:VAL:HG12	2:B:967:ARG:N	2.18	0.57
4:D:17:LYS:HD2	4:D:17:LYS:C	2.29	0.57
4:D:29:LEU:HD12	7:G:82:PHE:CZ	2.39	0.57
4:D:118:THR:HG22	4:D:118:THR:O	2.03	0.57
4:D:196:PRO:O	4:D:198:LEU:N	2.36	0.57
8:H:84:ALA:HB2	8:H:87:ARG:NE	2.19	0.57
1:A:982:THR:C	1:A:984:LYS:N	2.57	0.57
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.04	0.57
1:A:1317:MET:HE1	1:A:1339:LEU:HD21	1.86	0.57
2:B:287:ARG:NH1	2:B:324:ILE:O	2.37	0.57
1:A:1021:LEU:O	1:A:1024:SER:HB3	2.04	0.57
2:B:357:GLN:O	2:B:366:GLN:HA	2.03	0.57
2:B:458:LYS:O	2:B:459:TYR:C	2.46	0.57
3:C:186:LEU:N	3:C:186:LEU:HD12	2.19	0.57
7:G:81:PRO:HG3	7:G:106:MET:SD	2.44	0.57
10:J:2:ILE:C	10:J:53:HIS:HE1	2.12	0.57
2:B:505:ASP:CG	13:2:1:DA:C8	2.82	0.57
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.87	0.57
6:F:96:THR:O	6:F:100:GLN:HG3	2.04	0.57
7:G:53:ASN:HD22	7:G:53:ASN:N	2.01	0.57
1:A:23:SER:HA	1:A:233:TRP:CD1	2.39	0.57
1:A:481:ASP:CG	15:3:11:U:H5"	2.30	0.57
1:A:549:MET:SD	1:A:577:ILE:CD1	2.92	0.57
2:B:1197:PRO:O	2:B:1200:ALA:N	2.36	0.57
3:C:263:THR:O	3:C:266:ASP:HB2	2.04	0.57
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.69	0.57
1:A:95:PHE:O	1:A:96:ILE:C	2.46	0.57
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:SER:C	2:B:236:HIS:HD2	2.12	0.57
2:B:638:PHE:CD2	2:B:690:VAL:HG22	2.40	0.57
2:B:1166:CYS:SG	2:B:1166:CYS:O	2.62	0.57
9:I:50:THR:HG22	9:I:52:ILE:H	1.69	0.57
1:A:66:LYS:O	1:A:67:CYS:HB2	2.03	0.57
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.05	0.57
1:A:1127:ASP:CG	1:A:1130:GLN:HB2	2.29	0.57
2:B:241:ARG:HG2	2:B:253:THR:CG2	2.35	0.57
2:B:737:THR:O	2:B:739:THR:HG23	2.05	0.57
2:B:830:TYR:O	2:B:831:SER:C	2.45	0.57
2:B:954:VAL:O	12:L:55:ILE:O	2.21	0.57
3:C:181:ASP:OD1	3:C:185:LYS:HB2	2.05	0.57
4:D:155:ARG:HE	4:D:221:TYR:HE1	1.47	0.57
4:D:217:LEU:O	4:D:219:THR:N	2.38	0.57
8:H:127:GLY:O	8:H:128:ASN:CB	2.52	0.57
1:A:75:ASN:O	1:A:76:GLU:CB	2.52	0.57
1:A:1120:LEU:O	1:A:1120:LEU:HD12	2.03	0.57
2:B:222:ILE:H	2:B:240:ILE:CD1	2.18	0.57
2:B:309:GLN:OE1	9:I:52:ILE:HD11	2.05	0.57
2:B:497:ARG:NH2	2:B:775:LYS:HZ3	2.03	0.57
2:B:975:GLN:HG2	2:B:976:ILE:H	1.69	0.57
2:B:1037:LEU:HD21	2:B:1064:TYR:HE1	1.69	0.57
4:D:203:SER:OG	4:D:206:GLU:HB2	2.05	0.57
1:A:316:GLN:HG2	1:A:317:LYS:HD2	1.87	0.57
1:A:399:HIS:CB	1:A:400:PRO:CD	2.79	0.57
1:A:524:VAL:HG12	1:A:525:GLN:H	1.68	0.57
1:A:786:HIS:N	1:A:786:HIS:CD2	2.68	0.57
1:A:861:GLY:HA3	5:E:174:GLN:HE22	1.70	0.57
1:A:1203:ASN:O	1:A:1204:ASP:C	2.47	0.57
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.19	0.57
1:A:1286:LYS:HD2	1:A:1304:TRP:CZ2	2.40	0.57
2:B:578:THR:C	2:B:589:VAL:HG13	2.29	0.57
2:B:622:LYS:NZ	9:I:59:VAL:HG13	2.19	0.57
2:B:805:THR:HA	2:B:809:MET:CE	2.33	0.57
5:E:195:VAL:HG22	5:E:213:ILE:HG13	1.87	0.57
7:G:116:PRO:HD2	7:G:119:LEU:HD23	1.87	0.57
13:2:5:DC:H2"	13:2:6:DT:OP2	2.03	0.57
1:A:49:LYS:NZ	1:A:61:ILE:HG13	2.20	0.57
1:A:1161:THR:CG2	1:A:1163:ILE:HD12	2.33	0.57
1:A:1312:ASN:HD21	1:A:1315:GLU:CG	2.16	0.57
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1445:ILE:H	1:A:1445:ILE:CD1	2.07	0.57
2:B:916:THR:HB	2:B:935:ARG:CG	2.34	0.57
2:B:916:THR:O	2:B:935:ARG:HG2	2.05	0.57
2:B:1222:ARG:O	2:B:1222:ARG:HG2	2.05	0.57
3:C:43:THR:CG2	3:C:44:LEU:H	2.17	0.57
10:J:1:MET:O	10:J:2:ILE:O	2.23	0.57
1:A:168:GLY:O	1:A:169:ASN:C	2.48	0.56
1:A:335:ARG:HH12	2:B:1206:GLU:CD	2.13	0.56
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.70	0.56
1:A:1161:THR:C	1:A:1163:ILE:N	2.63	0.56
1:A:1261:LYS:O	1:A:1264:GLU:HB3	2.05	0.56
1:A:1305:VAL:HG12	1:A:1306:LEU:N	2.19	0.56
2:B:298:LEU:N	2:B:298:LEU:CD2	2.67	0.56
2:B:737:THR:CG2	9:I:66:PRO:HA	2.26	0.56
2:B:955:THR:CG2	2:B:956:THR:H	2.18	0.56
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.87	0.56
2:B:1115:THR:O	2:B:1116:ARG:HB2	2.05	0.56
2:B:1172:ILE:HG22	2:B:1172:ILE:O	2.05	0.56
3:C:208:GLU:C	3:C:210:GLU:H	2.11	0.56
8:H:82:PRO:O	8:H:84:ALA:N	2.34	0.56
1:A:780:VAL:O	1:A:782:ARG:HG2	2.05	0.56
1:A:845:LEU:HD22	1:A:1374:VAL:HG21	1.85	0.56
1:A:861:GLY:HA3	5:E:174:GLN:NE2	2.20	0.56
2:B:241:ARG:HA	2:B:253:THR:HG22	1.86	0.56
2:B:840:ILE:HG21	2:B:994:TYR:HD1	1.71	0.56
3:C:43:THR:HG22	3:C:44:LEU:H	1.70	0.56
3:C:196:ASP:CB	3:C:199:LYS:HD2	2.35	0.56
1:A:265:LYS:HD3	1:A:302:THR:HG23	1.87	0.56
1:A:879:GLU:O	1:A:955:PRO:HA	2.04	0.56
2:B:46:GLN:HE21	2:B:539:LEU:HD12	1.70	0.56
2:B:293:PRO:O	2:B:294:ASP:O	2.24	0.56
2:B:557:PHE:CZ	2:B:603:LEU:HD11	2.41	0.56
2:B:557:PHE:HD2	2:B:557:PHE:O	1.88	0.56
2:B:846:ILE:CG2	2:B:974:PRO:HG2	2.34	0.56
2:B:1048:THR:OG1	2:B:1050:ILE:HG13	2.05	0.56
5:E:56:LYS:CE	5:E:84:ASP:HB2	2.32	0.56
8:H:63:LEU:CD2	8:H:90:ALA:HB3	2.35	0.56
1:A:777:PHE:CD1	1:A:781:ASP:HA	2.39	0.56
1:A:1256:GLU:O	1:A:1259:MET:HB3	2.05	0.56
2:B:235:SER:OG	2:B:236:HIS:CD2	2.59	0.56
4:D:12:ARG:HG2	4:D:12:ARG:NH1	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:83:GLN:C	8:H:85:GLY:H	2.14	0.56
10:J:2:ILE:C	10:J:53:HIS:CE1	2.84	0.56
11:K:53:ASP:HB3	11:K:56:VAL:HG23	1.87	0.56
1:A:919:ILE:HD13	1:A:983:ILE:HD12	1.88	0.56
2:B:361:LEU:O	2:B:363:HIS:O	2.22	0.56
2:B:1050:ILE:HG22	2:B:1051:THR:N	2.20	0.56
2:B:1106:ARG:HH11	2:B:1126:GLY:HA2	1.70	0.56
4:D:13:ARG:C	4:D:15:LEU:N	2.63	0.56
10:J:1:MET:N	10:J:56:LEU:N	2.53	0.56
10:J:3:VAL:N	10:J:53:HIS:HE1	2.03	0.56
1:A:225:ASN:HD21	1:A:228:PHE:H	1.45	0.56
1:A:648:ASN:O	1:A:649:ILE:C	2.49	0.56
1:A:908:LEU:CD1	1:A:983:ILE:HD11	2.36	0.56
2:B:897:GLY:O	2:B:898:LEU:HD23	2.06	0.56
3:C:186:LEU:HD21	3:C:224:GLN:O	2.05	0.56
9:I:88:SER:C	9:I:90:GLN:H	2.12	0.56
14:1:10:DA:H2''	14:1:11:DA:C8	2.41	0.56
1:A:41:MET:HB2	1:A:48:ALA:O	2.06	0.56
1:A:1242:VAL:CG1	1:A:1243:VAL:N	2.68	0.56
2:B:874:PHE:HA	2:B:913:GLY:O	2.04	0.56
2:B:906:SER:O	2:B:907:GLY:O	2.24	0.56
4:D:9:GLN:HG3	4:D:9:GLN:O	2.05	0.56
4:D:156:ASP:O	4:D:158:GLU:N	2.39	0.56
5:E:182:ASP:HB3	5:E:185:ALA:CB	2.36	0.56
7:G:106:MET:HE3	7:G:108:VAL:CG2	2.36	0.56
1:A:1092:LYS:O	1:A:1094:VAL:HG23	2.06	0.56
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.70	0.56
2:B:652:LYS:HB3	2:B:689:LEU:HD23	1.88	0.56
2:B:918:ILE:HD12	2:B:935:ARG:CZ	2.36	0.56
2:B:1183:LYS:HE3	2:B:1183:LYS:O	2.06	0.56
4:D:8:PHE:HD2	7:G:6:ASP:O	1.88	0.56
4:D:148:LEU:O	4:D:152:SER:OG	2.22	0.56
9:I:111:THR:HG22	9:I:113:ASP:H	1.69	0.56
10:J:3:VAL:HA	10:J:53:HIS:ND1	2.20	0.56
10:J:53:HIS:HD2	10:J:53:HIS:C	2.12	0.56
1:A:2:VAL:HG22	1:A:3:GLY:N	2.21	0.56
1:A:11:LEU:HB2	2:B:1193:GLN:HG2	1.88	0.56
1:A:21:LEU:CD1	1:A:1414:ALA:HA	2.36	0.56
1:A:68:GLN:OE1	1:A:68:GLN:O	2.23	0.56
2:B:22:SER:O	2:B:654:ARG:HD2	2.06	0.56
2:B:657:HIS:CE1	2:B:689:LEU:HD11	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:139:ASN:O	8:H:140:ALA:HB2	2.04	0.56
9:I:111:THR:CG2	9:I:112:SER:H	2.12	0.56
11:K:23:PRO:HA	11:K:31:VAL:HG13	1.88	0.56
1:A:695:LYS:C	1:A:697:ALA:H	2.14	0.56
1:A:830:LYS:HE3	1:A:1081:LEU:HD12	1.88	0.56
1:A:1155:ASP:OD2	1:A:1161:THR:HA	2.06	0.56
2:B:39:ARG:CZ	2:B:665:GLU:HG2	2.36	0.56
2:B:405:ARG:NE	2:B:632:ARG:HG2	2.21	0.56
2:B:766:ARG:HH12	2:B:1020:ARG:HD2	1.66	0.56
3:C:93:ASP:OD1	3:C:122:SER:HB2	2.05	0.56
7:G:153:GLN:HG3	7:G:154:VAL:HG23	1.87	0.56
1:A:456:MET:HE1	1:A:474:VAL:CG2	2.35	0.55
1:A:540:PHE:HZ	8:H:121:LEU:HD11	1.71	0.55
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.36	0.55
1:A:1029:ARG:HH11	1:A:1029:ARG:HG3	1.71	0.55
1:A:1229:SER:HB2	1:A:1233:ASP:OD2	2.06	0.55
1:A:1313:LEU:O	1:A:1315:GLU:N	2.38	0.55
2:B:641:GLU:C	2:B:643:ASP:H	2.13	0.55
4:D:138:ASN:HB3	4:D:141:LEU:HB3	1.86	0.55
8:H:4:THR:HG22	8:H:5:LEU:H	1.72	0.55
10:J:53:HIS:HD2	10:J:54:VAL:C	2.14	0.55
11:K:107:THR:O	11:K:111:LEU:HG	2.05	0.55
12:L:36:SER:O	12:L:37:LYS:C	2.49	0.55
1:A:108:MET:O	1:A:109:HIS:CB	2.52	0.55
1:A:472:LEU:HD11	2:B:835:GLN:NE2	2.21	0.55
1:A:738:LYS:H	1:A:738:LYS:CD	2.09	0.55
2:B:186:GLU:CG	10:J:62:ARG:HH22	2.18	0.55
2:B:278:GLN:CG	2:B:279:ASP:N	2.68	0.55
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.41	0.55
2:B:363:HIS:O	2:B:364:ILE:CB	2.54	0.55
2:B:430:ARG:HB3	2:B:430:ARG:NH1	2.09	0.55
2:B:696:GLU:O	2:B:699:GLU:HB2	2.06	0.55
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.46	0.55
3:C:258:ILE:HD12	3:C:258:ILE:N	2.22	0.55
5:E:213:ILE:HG12	5:E:214:CYS:N	2.20	0.55
1:A:1322:ILE:O	1:A:1324:PRO:HD3	2.07	0.55
2:B:615:MET:HB3	2:B:626:ILE:HG12	1.89	0.55
8:H:91:ASP:O	8:H:93:TYR:N	2.36	0.55
9:I:17:ARG:HG3	9:I:28:GLU:CD	2.31	0.55
1:A:335:ARG:HD3	1:A:339:ASN:ND2	2.22	0.55
1:A:883:LEU:HD11	1:A:1017:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:ASP:OD1	2:B:658:ILE:HG21	2.05	0.55
2:B:50:SER:OG	2:B:411:PRO:HD3	2.07	0.55
2:B:172:ILE:HD13	2:B:178:ASN:ND2	2.21	0.55
2:B:235:SER:C	2:B:236:HIS:CD2	2.84	0.55
2:B:750:GLY:O	2:B:751:VAL:C	2.49	0.55
4:D:119:ARG:HD3	4:D:221:TYR:CD2	2.41	0.55
5:E:22:MET:CE	5:E:26:ARG:NH2	2.70	0.55
1:A:316:GLN:NE2	1:A:317:LYS:HD2	2.19	0.55
1:A:427:GLN:O	1:A:428:TYR:C	2.50	0.55
1:A:557:ASP:OD2	1:A:559:VAL:HB	2.06	0.55
1:A:1241:ARG:O	1:A:1242:VAL:HB	2.06	0.55
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.71	0.55
2:B:616:ILE:HD12	2:B:616:ILE:N	2.21	0.55
2:B:773:MET:C	2:B:775:LYS:N	2.63	0.55
2:B:1020:ARG:HG2	2:B:1020:ARG:NH1	2.14	0.55
3:C:186:LEU:CD2	3:C:225:ALA:HB2	2.37	0.55
4:D:4:SER:O	4:D:5:THR:CB	2.54	0.55
1:A:40:THR:HB	1:A:41:MET:CE	2.37	0.55
1:A:442:VAL:CG2	1:A:489:LEU:HD11	2.37	0.55
1:A:544:ASP:CG	1:A:545:GLN:N	2.64	0.55
2:B:222:ILE:N	2:B:240:ILE:CD1	2.70	0.55
2:B:378:LEU:HD12	2:B:378:LEU:O	2.07	0.55
3:C:69:LEU:HB3	10:J:6:ARG:HD3	1.88	0.55
1:A:666:ILE:HD11	2:B:1067:ARG:O	2.07	0.55
1:A:1376:THR:O	1:A:1377:THR:C	2.49	0.55
2:B:408:LEU:O	2:B:411:PRO:HD2	2.05	0.55
2:B:785:TYR:CD1	2:B:786:ASN:N	2.74	0.55
2:B:893:LEU:HD21	2:B:897:GLY:C	2.32	0.55
3:C:80:LEU:HD11	3:C:95:CYS:C	2.31	0.55
12:L:30:ILE:HG22	12:L:31:CYS:H	1.71	0.55
1:A:89:PRO:C	1:A:204:THR:HG21	2.32	0.55
1:A:547:LEU:HD22	11:K:58:PHE:CE1	2.42	0.55
2:B:315:LYS:N	2:B:316:PRO:HD2	2.21	0.55
2:B:542:MET:HG2	2:B:747:MET:CE	2.35	0.55
2:B:773:MET:CE	2:B:985:GLY:HA2	2.36	0.55
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.34	0.55
2:B:1124:ARG:HB3	2:B:1124:ARG:CZ	2.37	0.55
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.31	0.55
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.89	0.55
8:H:128:ASN:ND2	8:H:131:ASN:OD1	2.39	0.55
9:I:55:THR:HG22	9:I:58:VAL:CG2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.36	0.55
1:A:756:ILE:O	1:A:759:ALA:HB3	2.06	0.55
1:A:1199:ARG:HG2	1:A:1236:LEU:HD11	1.89	0.55
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.37	0.55
2:B:185:THR:O	2:B:186:GLU:C	2.50	0.55
12:L:38:LEU:O	12:L:39:SER:HB3	2.07	0.55
1:A:69:THR:HB	2:B:1174:LYS:HE2	1.89	0.55
1:A:402:ALA:CB	1:A:434:ARG:HA	2.37	0.55
1:A:717:ASN:HA	1:A:720:ARG:NH2	2.23	0.55
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.87	0.55
2:B:311:LEU:O	2:B:314:LEU:N	2.35	0.55
2:B:773:MET:HE2	2:B:985:GLY:HA2	1.89	0.55
2:B:1182:CYS:O	2:B:1183:LYS:C	2.50	0.55
3:C:100:THR:HG21	3:C:102:GLN:HE21	1.71	0.55
5:E:124:VAL:N	5:E:125:PRO:HD2	2.22	0.55
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.89	0.55
9:I:101:PHE:N	9:I:101:PHE:CD1	2.72	0.55
1:A:311:GLN:O	1:A:312:PRO:C	2.49	0.54
1:A:518:LYS:HE2	1:A:624:SER:O	2.06	0.54
1:A:1437:GLY:O	1:A:1439:GLY:N	2.40	0.54
2:B:37:PHE:CD1	2:B:37:PHE:C	2.85	0.54
2:B:326:ASP:OD2	2:B:328:GLU:HB3	2.07	0.54
2:B:554:ILE:O	2:B:558:LEU:HG	2.08	0.54
2:B:555:ILE:O	2:B:558:LEU:HB2	2.06	0.54
2:B:744:HIS:HD2	2:B:745:PRO:CD	2.02	0.54
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.18	0.54
6:F:94:LEU:HD21	6:F:122:MET:HA	1.89	0.54
6:F:119:ARG:NH1	6:F:119:ARG:CG	2.65	0.54
10:J:36:LEU:HB2	10:J:47:ARG:HH12	1.72	0.54
1:A:65:LEU:O	1:A:66:LYS:O	2.25	0.54
1:A:664:THR:HG22	2:B:1014:PRO:HB3	1.89	0.54
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.89	0.54
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.91	0.54
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.42	0.54
2:B:165:VAL:HG11	2:B:448:ILE:HD13	1.89	0.54
2:B:637:LEU:CB	2:B:693:ILE:HD11	2.37	0.54
3:C:215:GLU:O	3:C:216:GLY:C	2.49	0.54
6:F:86:THR:OG1	6:F:89:GLU:HG3	2.06	0.54
1:A:482:PHE:C	1:A:484:GLY:H	2.14	0.54
1:A:500:GLU:O	1:A:504:LEU:HB2	2.07	0.54
1:A:794:PRO:C	1:A:796:SER:H	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.33	0.54
2:B:39:ARG:NH2	2:B:665:GLU:CG	2.67	0.54
2:B:199:MET:HE2	2:B:492:LEU:HD23	1.90	0.54
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.88	0.54
2:B:899:ILE:HG22	2:B:900:ALA:N	2.21	0.54
3:C:242:GLN:C	3:C:244:VAL:N	2.63	0.54
5:E:154:ILE:HG22	5:E:155:ARG:O	2.08	0.54
8:H:38:LEU:HD12	8:H:39:THR:H	1.71	0.54
9:I:93:LYS:HD3	9:I:93:LYS:N	2.22	0.54
15:3:2:A:O2'	15:3:3:A:O5'	2.18	0.54
1:A:35:ILE:CD1	1:A:241:VAL:HG11	2.37	0.54
1:A:224:PHE:CE2	1:A:234:MET:HE2	2.42	0.54
1:A:1158:PRO:HG2	1:A:1159:ARG:HD2	1.89	0.54
1:A:1280:GLU:O	1:A:1281:ARG:C	2.50	0.54
2:B:55:VAL:HG13	2:B:97:VAL:HG21	1.89	0.54
2:B:303:TYR:CD2	2:B:303:TYR:N	2.74	0.54
2:B:467:GLY:CA	2:B:475:SER:HB3	2.38	0.54
4:D:7:THR:O	4:D:7:THR:HG23	2.06	0.54
5:E:28:TYR:C	5:E:65:THR:HG22	2.32	0.54
7:G:51:TYR:C	7:G:51:TYR:CD2	2.85	0.54
8:H:89:LEU:O	8:H:91:ASP:N	2.41	0.54
1:A:87:ALA:HB1	1:A:276:LEU:HD23	1.87	0.54
1:A:106:VAL:HG12	1:A:107:CYS:H	1.73	0.54
1:A:250:ILE:O	1:A:250:ILE:CG2	2.52	0.54
1:A:730:GLY:O	1:A:732:LEU:N	2.41	0.54
2:B:25:ILE:HD13	2:B:653:VAL:HG12	1.89	0.54
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.38	0.54
2:B:482:VAL:O	2:B:483:LEU:C	2.49	0.54
2:B:710:LEU:O	2:B:711:GLU:HG2	2.06	0.54
2:B:893:LEU:CD2	2:B:897:GLY:C	2.80	0.54
4:D:207:LEU:HD12	4:D:207:LEU:O	2.07	0.54
7:G:111:THR:CG2	7:G:114:LEU:HB2	2.38	0.54
12:L:46:VAL:O	12:L:46:VAL:HG12	2.08	0.54
1:A:41:MET:O	1:A:42:ASP:C	2.51	0.54
1:A:598:LEU:O	1:A:599:SER:C	2.50	0.54
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.21	0.54
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.42	0.54
3:C:8:VAL:HG12	3:C:9:LYS:N	2.22	0.54
4:D:14:ARG:HH12	4:D:16:LYS:CD	2.20	0.54
5:E:82:PHE:O	5:E:83:CYS:HB2	2.08	0.54
1:A:424:ILE:HG22	1:A:425:GLN:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.40	0.54
1:A:1237:ILE:HG22	1:A:1238:ILE:N	2.22	0.54
2:B:57:TYR:N	2:B:57:TYR:HD1	2.06	0.54
2:B:504:ARG:C	2:B:506:GLY:H	2.15	0.54
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.43	0.54
2:B:1182:CYS:C	2:B:1183:LYS:HE3	2.32	0.54
3:C:209:TYR:HD1	3:C:209:TYR:H	1.55	0.54
4:D:35:LEU:HD12	4:D:35:LEU:H	1.73	0.54
9:I:78:CYS:SG	9:I:105:SER:O	2.66	0.54
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.33	0.54
1:A:567:LYS:CD	8:H:95:TYR:HA	2.38	0.54
1:A:567:LYS:CG	1:A:568:PRO:CD	2.81	0.54
2:B:110:HIS:HB3	12:L:54:ARG:HH22	1.71	0.54
2:B:526:GLU:OE1	2:B:752:ALA:HB3	2.08	0.54
1:A:471:ASN:O	1:A:474:VAL:HG12	2.08	0.54
2:B:582:VAL:O	2:B:582:VAL:HG12	2.08	0.54
2:B:916:THR:HB	2:B:935:ARG:CD	2.38	0.54
3:C:226:ASP:O	3:C:227:THR:HB	2.08	0.54
4:D:52:LEU:O	4:D:54:GLU:N	2.40	0.54
4:D:145:MET:O	4:D:149:THR:HB	2.08	0.54
7:G:120:THR:OG1	7:G:121:PHE:N	2.38	0.54
8:H:12:VAL:HA	8:H:28:ALA:HB2	1.88	0.54
1:A:55:ASP:C	1:A:57:ARG:N	2.62	0.54
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.43	0.54
1:A:332:LYS:C	1:A:334:GLY:N	2.66	0.54
1:A:535:THR:HG21	1:A:617:VAL:H	1.73	0.54
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.71	0.54
1:A:1046:LEU:N	1:A:1046:LEU:HD23	2.23	0.54
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.43	0.54
2:B:423:LYS:O	2:B:427:ASP:HB2	2.08	0.54
2:B:640:VAL:O	2:B:641:GLU:C	2.50	0.54
2:B:642:ASP:C	2:B:644:GLU:H	2.14	0.54
7:G:146:LYS:HB2	7:G:168:LEU:HD11	1.90	0.54
9:I:71:SER:OG	9:I:83:ASN:HB2	2.08	0.54
12:L:52:GLY:O	12:L:53:HIS:C	2.50	0.54
1:A:818:MET:HE3	2:B:514:LEU:O	2.07	0.53
1:A:879:GLU:OE1	1:A:962:ARG:NH2	2.40	0.53
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.43	0.53
1:A:903:ASN:C	1:A:903:ASN:ND2	2.66	0.53
2:B:805:THR:HA	2:B:809:MET:HE3	1.90	0.53
8:H:128:ASN:C	8:H:128:ASN:HD22	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.89	0.53
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.08	0.53
2:B:871:THR:HG22	2:B:872:GLU:N	2.23	0.53
3:C:34:ARG:HA	3:C:37:MET:HE3	1.91	0.53
8:H:94:ASP:O	8:H:95:TYR:HB2	2.09	0.53
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.73	0.53
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.38	0.53
1:A:95:PHE:O	1:A:98:LYS:N	2.39	0.53
1:A:102:VAL:HB	1:A:211:PHE:CZ	2.43	0.53
1:A:447:GLN:NE2	14:1:20:DG:H4'	2.23	0.53
1:A:946:VAL:HG22	5:E:201:LYS:HB3	1.90	0.53
1:A:1366:ARG:HG2	1:A:1366:ARG:HH11	1.72	0.53
2:B:282:ILE:HG21	2:B:382:ILE:CD1	2.38	0.53
2:B:377:PHE:C	2:B:379:GLY:N	2.64	0.53
2:B:505:ASP:OD2	13:2:1:DA:H5''	2.09	0.53
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.91	0.53
3:C:114:TYR:CD2	3:C:140:ASN:CB	2.91	0.53
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.43	0.53
3:C:235:VAL:HG13	10:J:13:VAL:HG22	1.90	0.53
5:E:143:ASN:HD22	5:E:146:HIS:CE1	2.26	0.53
9:I:68:LEU:HB3	9:I:84:VAL:HG23	1.91	0.53
11:K:42:LEU:HD11	11:K:46:ILE:HD11	1.91	0.53
11:K:45:LEU:HG	11:K:94:ILE:CD1	2.36	0.53
12:L:40:LEU:HD13	12:L:44:ASP:CB	2.27	0.53
1:A:506:ALA:O	1:A:507:VAL:C	2.51	0.53
1:A:603:ASN:O	1:A:604:GLY:C	2.50	0.53
1:A:973:ILE:HD13	1:A:1037:LEU:HA	1.91	0.53
1:A:1104:ILE:O	1:A:1106:ASN:N	2.41	0.53
2:B:110:HIS:CB	12:L:54:ARG:HH22	2.22	0.53
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.40	0.53
3:C:66:ARG:HA	3:C:69:LEU:CD1	2.38	0.53
7:G:132:SER:O	7:G:133:SER:C	2.52	0.53
12:L:49:LYS:O	12:L:50:ASP:CB	2.54	0.53
12:L:55:ILE:HG12	12:L:56:LEU:N	2.22	0.53
1:A:46:THR:O	1:A:47:ARG:C	2.52	0.53
1:A:90:VAL:HG11	1:A:297:GLN:HA	1.91	0.53
1:A:705:LYS:CB	1:A:708:MET:HE3	2.35	0.53
1:A:1006:ILE:HD12	5:E:163:GLU:HG3	1.90	0.53
2:B:654:ARG:HH11	2:B:654:ARG:CG	2.19	0.53
2:B:661:LEU:HD23	2:B:679:TYR:O	2.08	0.53
4:D:154:PHE:HB3	4:D:159:THR:OG1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:53:HIS:NE2	10:J:55:ASP:HA	2.23	0.53
1:A:322:VAL:O	1:A:322:VAL:HG12	2.06	0.53
5:E:17:ARG:O	5:E:20:LYS:HB2	2.08	0.53
5:E:191:LYS:O	5:E:192:ARG:C	2.50	0.53
1:A:418:SER:C	1:A:420:ARG:H	2.16	0.53
1:A:714:PHE:O	1:A:718:VAL:HG23	2.09	0.53
1:A:874:ASP:N	1:A:1058:VAL:HG23	2.23	0.53
1:A:973:ILE:HD11	1:A:1041:ALA:HB2	1.91	0.53
1:A:1120:LEU:HD12	1:A:1120:LEU:C	2.33	0.53
1:A:1277:GLU:C	1:A:1279:ILE:H	2.16	0.53
1:A:1278:ASN:O	1:A:1310:GLY:HA3	2.08	0.53
2:B:287:ARG:HG3	2:B:292:ILE:HA	1.91	0.53
2:B:570:VAL:CG2	2:B:573:GLN:HB3	2.38	0.53
2:B:805:THR:CG2	2:B:806:THR:H	2.14	0.53
5:E:180:ARG:O	5:E:186:LEU:HD21	2.09	0.53
1:A:71:GLN:O	1:A:73:GLY:N	2.36	0.53
1:A:332:LYS:HG2	1:A:333:GLU:HG2	1.91	0.53
1:A:364:VAL:O	1:A:364:VAL:HG13	2.08	0.53
1:A:720:ARG:O	1:A:724:GLU:HB2	2.09	0.53
2:B:333:PHE:O	2:B:334:ILE:CG1	2.56	0.53
2:B:842:ASN:HD22	2:B:845:SER:CB	2.21	0.53
2:B:893:LEU:HD22	2:B:897:GLY:HA2	1.91	0.53
4:D:128:VAL:C	4:D:130:LEU:N	2.66	0.53
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.38	0.53
1:A:117:GLU:CD	1:A:117:GLU:N	2.65	0.53
1:A:117:GLU:HA	1:A:123:ARG:HG3	1.90	0.53
1:A:134:ARG:HG2	1:A:138:ILE:CD1	2.39	0.53
1:A:367:PRO:HG2	1:A:370:ILE:HD12	1.89	0.53
1:A:517:ASN:ND2	1:A:1364:ASN:HB2	2.24	0.53
1:A:696:GLU:O	1:A:696:GLU:HG2	2.09	0.53
1:A:715:GLU:O	1:A:716:ASP:C	2.52	0.53
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.38	0.53
2:B:377:PHE:O	2:B:380:TYR:N	2.42	0.53
2:B:515:HIS:O	2:B:518:HIS:HB2	2.08	0.53
2:B:603:LEU:CD1	2:B:608:ASP:HB2	2.36	0.53
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.89	0.53
4:D:53:SER:HA	4:D:56:ARG:HB3	1.91	0.53
8:H:27:GLU:HA	8:H:38:LEU:O	2.09	0.53
9:I:34:TYR:CD2	9:I:34:TYR:C	2.87	0.53
11:K:53:ASP:OD1	11:K:55:LYS:HB2	2.09	0.53
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:622:LYS:CE	9:I:59:VAL:HG22	2.13	0.53
2:B:1135:ARG:O	2:B:1136:ASP:C	2.52	0.53
3:C:179:GLU:HG2	3:C:180:TYR:N	2.24	0.53
4:D:15:LEU:O	4:D:15:LEU:HD12	2.09	0.53
11:K:13:GLY:O	11:K:14:GLU:C	2.53	0.53
1:A:829:VAL:HG22	2:B:507:LYS:HD2	1.91	0.52
1:A:1081:LEU:HD11	1:A:1098:VAL:HG23	1.90	0.52
1:A:1094:VAL:HG13	1:A:1113:THR:HG21	1.91	0.52
5:E:212:ARG:HH11	5:E:212:ARG:HG3	1.73	0.52
7:G:61:ILE:HG22	7:G:62:LEU:O	2.09	0.52
7:G:90:THR:HG22	7:G:91:VAL:N	2.23	0.52
8:H:82:PRO:C	8:H:84:ALA:N	2.67	0.52
1:A:2:VAL:HG22	1:A:3:GLY:H	1.74	0.52
1:A:50:ILE:C	1:A:52:GLY:N	2.62	0.52
1:A:144:THR:O	1:A:146:MET:HG3	2.07	0.52
1:A:567:LYS:HB2	8:H:95:TYR:HA	1.90	0.52
1:A:901:LEU:N	1:A:926:GLN:NE2	2.46	0.52
2:B:26:THR:O	2:B:29:ASP:HB2	2.09	0.52
2:B:298:LEU:N	2:B:298:LEU:HD22	2.23	0.52
2:B:309:GLN:CD	9:I:52:ILE:HD11	2.34	0.52
2:B:449:ASN:C	2:B:451:LYS:H	2.18	0.52
2:B:936:ASP:CG	2:B:937:ALA:N	2.66	0.52
2:B:941:LEU:O	2:B:942:ARG:C	2.52	0.52
3:C:263:THR:C	3:C:265:MET:H	2.17	0.52
5:E:68:SER:HB3	5:E:75:MET:CE	2.39	0.52
7:G:34:VAL:HG13	7:G:45:ILE:HG21	1.92	0.52
9:I:50:THR:CG2	9:I:51:ASN:H	2.22	0.52
11:K:12:LEU:HD11	11:K:18:LYS:HE2	1.91	0.52
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.90	0.52
1:A:1081:LEU:HD11	1:A:1098:VAL:H	1.73	0.52
1:A:1264:GLU:OE2	9:I:46:HIS:HD2	1.92	0.52
2:B:39:ARG:HH21	2:B:665:GLU:CD	2.17	0.52
2:B:233:PRO:CD	14:1:11:DA:OP1	2.57	0.52
2:B:427:ASP:CA	2:B:430:ARG:HG3	2.37	0.52
2:B:521:LEU:HB3	2:B:633:VAL:CG1	2.39	0.52
2:B:879:ARG:CD	2:B:879:ARG:N	2.61	0.52
2:B:969:ARG:CD	3:C:61:GLU:OE2	2.58	0.52
2:B:1034:VAL:O	2:B:1036:ALA:N	2.42	0.52
3:C:18:VAL:HG12	3:C:18:VAL:O	2.09	0.52
5:E:48:ASP:CG	5:E:49:SER:N	2.66	0.52
5:E:190:LEU:C	5:E:191:LYS:HG2	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:115:MET:O	7:G:164:LYS:HD3	2.09	0.52
11:K:18:LYS:C	11:K:19:LEU:HD23	2.34	0.52
1:A:41:MET:O	1:A:42:ASP:O	2.27	0.52
1:A:108:MET:H	1:A:171:GLN:HE22	1.58	0.52
1:A:385:ILE:HG22	1:A:386:ASP:N	2.24	0.52
1:A:783:THR:HG21	1:A:815:PHE:CZ	2.45	0.52
1:A:914:GLU:C	1:A:916:GLY:H	2.18	0.52
2:B:193:LYS:HZ3	12:L:32:ALA:HB1	1.73	0.52
2:B:222:ILE:H	2:B:240:ILE:HD12	1.74	0.52
2:B:259:TYR:HD1	2:B:259:TYR:H	1.58	0.52
2:B:658:ILE:CG2	2:B:662:MET:HE2	2.36	0.52
2:B:860:MET:HG2	2:B:861:ASP:H	1.74	0.52
2:B:862:GLN:HG2	2:B:963:PHE:CD1	2.34	0.52
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.23	0.52
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.45	0.52
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.28	0.52
2:B:470:LYS:C	2:B:472:ALA:N	2.67	0.52
2:B:560:GLU:O	2:B:561:TRP:CD1	2.62	0.52
2:B:619:ILE:O	2:B:622:LYS:N	2.41	0.52
2:B:1176:ASN:C	2:B:1178:ASN:N	2.66	0.52
3:C:25:VAL:HG12	3:C:26:ASP:H	1.74	0.52
4:D:192:LYS:HD2	4:D:199:ASN:HA	1.91	0.52
12:L:30:ILE:CG2	12:L:31:CYS:N	2.72	0.52
1:A:886:ILE:CG2	1:A:887:GLY:N	2.73	0.52
1:A:889:SER:CB	1:A:1297:GLU:HG3	2.38	0.52
1:A:954:TRP:HB3	1:A:955:PRO:HD2	1.90	0.52
1:A:1015:VAL:O	1:A:1016:THR:C	2.53	0.52
1:A:1195:LEU:HD11	1:A:1267:MET:HE1	1.91	0.52
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.92	0.52
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.74	0.52
2:B:603:LEU:HB3	2:B:609:ILE:HD11	1.91	0.52
2:B:620:ARG:NH2	9:I:68:LEU:HD21	2.25	0.52
4:D:120:GLU:HG2	4:D:120:GLU:O	2.10	0.52
8:H:43:ASN:OD1	8:H:45:GLU:HB3	2.10	0.52
1:A:512:VAL:O	1:A:512:VAL:HG12	2.08	0.52
1:A:677:ARG:HA	1:A:680:THR:OG1	2.10	0.52
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.10	0.52
1:A:1444:MET:HG2	7:G:59:GLY:O	2.10	0.52
2:B:644:GLU:C	2:B:646:LEU:N	2.68	0.52
4:D:219:THR:HG22	4:D:220:LEU:O	2.10	0.52
1:A:434:ARG:NH2	1:A:440:ASP:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:LEU:O	1:A:511:ILE:N	2.43	0.52
1:A:722:LEU:HD23	1:A:799:PHE:CG	2.44	0.52
1:A:751:SER:O	1:A:752:LYS:HG2	2.09	0.52
1:A:1215:ARG:NH1	1:A:1272:THR:O	2.43	0.52
1:A:1308:THR:HG23	1:A:1310:GLY:H	1.74	0.52
2:B:307:ASP:C	2:B:309:GLN:N	2.64	0.52
2:B:990:ILE:HG22	2:B:991:GLY:N	2.25	0.52
5:E:157:SER:C	5:E:159:ASP:N	2.66	0.52
5:E:182:ASP:O	5:E:185:ALA:HB3	2.10	0.52
10:J:3:VAL:HA	10:J:53:HIS:HD1	1.73	0.52
11:K:50:LEU:HD11	11:K:75:ILE:HD13	1.92	0.52
12:L:42:ARG:HG3	12:L:42:ARG:NH1	2.25	0.52
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.93	0.52
1:A:399:HIS:CG	1:A:400:PRO:N	2.77	0.52
1:A:665:GLY:HA2	2:B:1026:LEU:HD21	1.92	0.52
1:A:962:ARG:O	1:A:965:GLN:N	2.43	0.52
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.09	0.52
4:D:53:SER:C	4:D:55:ALA:N	2.64	0.52
5:E:155:ARG:NH1	5:E:194:GLU:OE2	2.43	0.52
9:I:99:LEU:C	9:I:100:PHE:HD1	2.16	0.52
11:K:52:ASN:O	11:K:54:ARG:N	2.42	0.52
12:L:32:ALA:HB3	12:L:55:ILE:HG13	1.88	0.52
1:A:1209:MET:SD	1:A:1236:LEU:HB3	2.50	0.52
2:B:68:THR:CG2	2:B:91:SER:HB3	2.39	0.52
2:B:203:PHE:N	2:B:203:PHE:CD1	2.77	0.52
2:B:357:GLN:HA	2:B:374:LYS:NZ	2.25	0.52
2:B:461:LEU:HD12	2:B:461:LEU:H	1.75	0.52
2:B:831:SER:CB	2:B:994:TYR:HH	2.22	0.52
2:B:842:ASN:ND2	2:B:845:SER:N	2.53	0.52
4:D:20:GLU:CD	4:D:20:GLU:H	2.17	0.52
4:D:73:SER:CB	7:G:21:ARG:HH21	2.23	0.52
5:E:21:GLU:O	5:E:24:LYS:HG2	2.10	0.52
8:H:100:THR:HG23	8:H:138:GLU:HA	1.92	0.52
9:I:34:TYR:CE2	9:I:36:GLU:HB3	2.41	0.52
9:I:93:LYS:H	9:I:93:LYS:CD	2.23	0.52
10:J:14:VAL:O	10:J:14:VAL:HG12	2.08	0.52
1:A:107:CYS:HA	1:A:171:GLN:HE22	1.74	0.51
1:A:868:TYR:HE1	1:A:1064:VAL:CG1	2.23	0.51
1:A:1365:TYR:C	1:A:1365:TYR:CD2	2.88	0.51
2:B:233:PRO:HD2	14:1:11:DA:OP1	2.10	0.51
2:B:847:ASP:OD2	11:K:6:ARG:NH2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:916:THR:CG2	2:B:935:ARG:HD2	2.40	0.51
3:C:221:TYR:CD1	3:C:222:LYS:N	2.78	0.51
4:D:153:ARG:C	4:D:154:PHE:HD2	2.16	0.51
7:G:111:THR:HG23	7:G:114:LEU:HB2	1.91	0.51
8:H:59:ILE:CG2	8:H:60:ALA:N	2.73	0.51
8:H:128:ASN:ND2	8:H:128:ASN:C	2.68	0.51
12:L:38:LEU:HD12	12:L:38:LEU:C	2.35	0.51
13:2:2:DC:H2''	13:2:3:DT:H71	1.91	0.51
1:A:666:ILE:HD12	1:A:667:GLY:H	1.73	0.51
1:A:1095:THR:CG2	1:A:1112:LYS:HB2	2.40	0.51
1:A:1385:THR:O	1:A:1387:HIS:N	2.43	0.51
2:B:134:LYS:HD3	2:B:134:LYS:H	1.74	0.51
2:B:509:ALA:O	2:B:511:PRO:N	2.44	0.51
2:B:552:MET:C	2:B:554:ILE:H	2.19	0.51
3:C:176:ILE:O	3:C:176:ILE:HG22	2.09	0.51
5:E:89:GLY:C	5:E:91:LYS:N	2.66	0.51
5:E:134:THR:C	5:E:135:PHE:HD1	2.17	0.51
5:E:171:LYS:HE2	5:E:174:GLN:CD	2.34	0.51
6:F:111:LEU:N	6:F:111:LEU:CD1	2.73	0.51
1:A:41:MET:H	1:A:41:MET:HE3	1.75	0.51
1:A:53:LEU:O	1:A:54:ASN:C	2.53	0.51
1:A:685:GLU:HG3	1:A:686:ALA:H	1.74	0.51
1:A:695:LYS:C	1:A:697:ALA:N	2.67	0.51
1:A:831:THR:O	1:A:834:THR:HG22	2.09	0.51
1:A:1293:SER:HB3	1:A:1297:GLU:OE1	2.10	0.51
2:B:308:TRP:CH2	9:I:45:ARG:HG2	2.45	0.51
2:B:481:GLN:NE2	15:3:7:G:H4'	2.25	0.51
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.43	0.51
3:C:91:HIS:O	3:C:91:HIS:CD2	2.62	0.51
5:E:177:ARG:O	5:E:212:ARG:HD3	2.10	0.51
6:F:76:LYS:O	6:F:79:ARG:HD3	2.10	0.51
1:A:93:VAL:HG21	1:A:301:ALA:HA	1.90	0.51
1:A:555:ASP:O	1:A:556:TRP:O	2.28	0.51
1:A:670:ILE:HG23	1:A:805:LEU:HD21	1.92	0.51
1:A:806:ARG:HH22	2:B:729:ILE:HD11	1.75	0.51
2:B:327:ARG:HH22	2:B:371:GLU:HG2	1.76	0.51
2:B:552:MET:HA	2:B:552:MET:HE3	1.93	0.51
3:C:66:ARG:O	3:C:69:LEU:HD12	2.10	0.51
4:D:51:ASN:C	4:D:52:LEU:O	2.52	0.51
5:E:172:GLU:C	5:E:174:GLN:H	2.18	0.51
7:G:87:VAL:CG2	7:G:103:VAL:HG21	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:61:ASP:O	9:I:63:GLY:N	2.43	0.51
11:K:55:LYS:HB2	11:K:81:TYR:CE1	2.45	0.51
1:A:11:LEU:HD23	1:A:11:LEU:C	2.35	0.51
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.44	0.51
1:A:503:GLN:NE2	6:F:90:ARG:HH21	2.09	0.51
1:A:1019:CYS:O	1:A:1020:CYS:C	2.54	0.51
2:B:469:GLN:CG	2:B:470:LYS:H	2.21	0.51
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.40	0.51
4:D:124:GLU:CD	4:D:124:GLU:H	2.18	0.51
4:D:130:LEU:C	4:D:132:GLN:N	2.67	0.51
1:A:63:ARG:N	1:A:74:MET:HE2	2.26	0.51
1:A:64:ASN:O	1:A:65:LEU:C	2.52	0.51
1:A:523:ILE:HG13	1:A:622:VAL:CG2	2.38	0.51
1:A:1148:ILE:CG1	1:A:1198:ASP:HB2	2.40	0.51
1:A:1349:TYR:C	1:A:1349:TYR:CD2	2.89	0.51
2:B:31:TRP:CD1	2:B:807:ARG:NH2	2.78	0.51
5:E:192:ARG:HH11	5:E:192:ARG:HG3	1.76	0.51
6:F:138:LEU:O	6:F:140:ASP:N	2.44	0.51
8:H:84:ALA:C	8:H:86:ASP:N	2.68	0.51
1:A:16:GLU:OE1	4:D:13:ARG:NH2	2.42	0.51
1:A:115:LEU:CD1	1:A:142:CYS:HB3	2.40	0.51
1:A:595:THR:C	1:A:596:THR:HG23	2.36	0.51
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.91	0.51
1:A:845:LEU:O	1:A:846:GLU:C	2.52	0.51
2:B:251:ILE:O	2:B:251:ILE:HG22	2.11	0.51
2:B:563:MET:HE1	2:B:580:VAL:HB	1.93	0.51
2:B:638:PHE:O	2:B:740:HIS:HA	2.11	0.51
2:B:885:MET:HA	2:B:936:ASP:CB	2.41	0.51
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.44	0.51
3:C:164:ALA:O	3:C:165:LYS:C	2.53	0.51
7:G:111:THR:O	7:G:114:LEU:N	2.39	0.51
7:G:115:MET:HB3	7:G:116:PRO:CD	2.40	0.51
13:2:4:DA:H2"	13:2:5:DC:C6	2.45	0.51
1:A:139:TRP:O	1:A:140:THR:C	2.54	0.51
1:A:276:LEU:HD13	1:A:293:GLU:HA	1.92	0.51
1:A:537:ARG:NH1	8:H:120:GLY:O	2.44	0.51
1:A:608:ILE:C	1:A:610:GLY:H	2.18	0.51
1:A:665:GLY:HA2	2:B:1026:LEU:HD22	1.93	0.51
1:A:886:ILE:HG23	1:A:887:GLY:N	2.25	0.51
1:A:984:LYS:HG2	1:A:988:LEU:HD12	1.91	0.51
1:A:1116:LEU:C	1:A:1116:LEU:HD12	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:VAL:O	2:B:45:SER:C	2.54	0.51
2:B:90:ILE:CD1	2:B:432:MET:SD	2.98	0.51
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.92	0.51
2:B:850:LEU:HD12	2:B:850:LEU:C	2.33	0.51
3:C:7:GLN:HE21	11:K:104:ASN:ND2	2.09	0.51
5:E:48:ASP:HB3	5:E:54:GLN:CD	2.36	0.51
9:I:55:THR:HG22	9:I:55:THR:O	2.09	0.51
1:A:218:ASP:O	1:A:219:PHE:C	2.53	0.51
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.42	0.51
1:A:470:LEU:N	1:A:470:LEU:CD2	2.74	0.51
1:A:690:VAL:HG13	1:A:691:LEU:N	2.25	0.51
1:A:1385:THR:C	1:A:1387:HIS:N	2.69	0.51
2:B:230:ALA:HB3	2:B:231:PRO:HD3	1.93	0.51
2:B:305:VAL:O	2:B:305:VAL:HG12	2.10	0.51
8:H:106:GLU:C	8:H:108:SER:H	2.16	0.51
9:I:74:GLU:HB3	9:I:81:ARG:HD2	1.92	0.51
1:A:356:ASP:O	1:A:358:ASN:N	2.43	0.51
1:A:1006:ILE:CD1	5:E:163:GLU:HG3	2.41	0.51
2:B:90:ILE:HD12	2:B:432:MET:CE	2.41	0.51
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.41	0.51
2:B:879:ARG:HH22	2:B:885:MET:CE	2.23	0.51
2:B:996:ARG:HH22	3:C:175:ALA:H	1.59	0.51
2:B:1056:SER:HB3	2:B:1066:SER:OG	2.10	0.51
3:C:242:GLN:CA	3:C:245:VAL:HG23	2.37	0.51
7:G:91:VAL:CG1	7:G:92:VAL:N	2.74	0.51
10:J:51:LEU:O	10:J:51:LEU:HD12	2.11	0.51
1:A:401:GLY:C	1:A:435:HIS:HD2	2.18	0.50
2:B:204:ILE:C	2:B:205:ILE:HD12	2.35	0.50
2:B:402:GLY:HA2	2:B:695:ALA:HB3	1.93	0.50
2:B:642:ASP:CA	2:B:649:LYS:HA	2.41	0.50
3:C:69:LEU:HB3	10:J:6:ARG:CD	2.41	0.50
3:C:213:PRO:O	3:C:214:ASN:HB3	2.11	0.50
8:H:26:ILE:HD11	8:H:49:VAL:CG1	2.38	0.50
8:H:40:LEU:HD13	8:H:123:MET:CE	2.33	0.50
10:J:53:HIS:CD2	10:J:55:ASP:N	2.79	0.50
1:A:443:LEU:CD1	2:B:1146:PHE:CE2	2.93	0.50
1:A:533:LYS:CE	1:A:745:GLN:HE22	2.24	0.50
1:A:605:MET:HE2	1:A:607:ILE:HG12	1.93	0.50
1:A:858:ASN:ND2	1:A:860:LEU:N	2.44	0.50
2:B:383:ASN:O	2:B:384:ARG:C	2.54	0.50
4:D:5:THR:O	4:D:5:THR:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:155:ARG:CB	4:D:155:ARG:HH11	2.23	0.50
5:E:22:MET:HE3	5:E:26:ARG:CZ	2.41	0.50
5:E:157:SER:O	5:E:159:ASP:N	2.44	0.50
1:A:687:LYS:C	1:A:690:VAL:HG12	2.36	0.50
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.46	0.50
1:A:1202:MET:HE1	1:A:1212:VAL:CG2	2.41	0.50
1:A:1329:THR:HG22	1:A:1331:SER:N	2.21	0.50
1:A:1343:ALA:HB2	5:E:150:VAL:HG22	1.94	0.50
2:B:196:PRO:HG2	2:B:197:PHE:H	1.76	0.50
2:B:277:LYS:CE	2:B:336:ARG:HD3	2.42	0.50
2:B:408:LEU:HD21	2:B:545:ILE:HD12	1.93	0.50
2:B:575:PRO:HG2	2:B:576:ASP:H	1.77	0.50
7:G:144:ARG:O	7:G:168:LEU:HD23	2.12	0.50
8:H:95:TYR:HE2	8:H:97:MET:CG	2.19	0.50
2:B:37:PHE:C	2:B:37:PHE:HD1	2.19	0.50
2:B:399:ASP:OD2	2:B:510:LYS:HG3	2.12	0.50
2:B:473:MET:HE3	2:B:474:SER:N	2.27	0.50
4:D:179:GLN:O	4:D:183:LEU:HB2	2.11	0.50
5:E:106:GLN:HE22	5:E:129:PRO:HB2	1.76	0.50
6:F:77:ASP:O	6:F:78:GLN:CB	2.50	0.50
9:I:55:THR:HG23	9:I:86:PHE:CZ	2.46	0.50
9:I:61:ASP:C	9:I:63:GLY:N	2.64	0.50
9:I:62:ILE:O	9:I:62:ILE:HG12	2.12	0.50
11:K:12:LEU:H	11:K:12:LEU:HD12	1.77	0.50
12:L:60:ARG:HG2	12:L:61:THR:N	2.23	0.50
1:A:89:PRO:HB2	1:A:204:THR:HG22	1.93	0.50
1:A:298:PHE:O	1:A:302:THR:HB	2.12	0.50
1:A:326:ARG:HG2	1:A:326:ARG:HH11	1.76	0.50
1:A:1104:ILE:C	1:A:1106:ASN:N	2.70	0.50
1:A:1112:LYS:O	1:A:1114:PRO:HD3	2.11	0.50
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.93	0.50
2:B:751:VAL:O	2:B:752:ALA:C	2.54	0.50
2:B:872:GLU:CD	2:B:914:LYS:HE3	2.36	0.50
2:B:957:ASN:HD22	2:B:961:LEU:HB2	1.75	0.50
2:B:1106:ARG:NH2	2:B:1111:MET:HE2	2.27	0.50
2:B:1187:ASN:HD21	2:B:1190:ASP:HB3	1.77	0.50
3:C:100:THR:CG2	3:C:102:GLN:HE21	2.24	0.50
4:D:53:SER:H	4:D:148:LEU:CD2	2.24	0.50
4:D:219:THR:CG2	4:D:220:LEU:O	2.60	0.50
5:E:29:PHE:C	5:E:30:ILE:HG13	2.37	0.50
1:A:478:TYR:O	1:A:479:ASN:CB	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:PHE:O	1:A:650:GLN:HB2	2.12	0.50
1:A:684:ALA:O	1:A:687:LYS:N	2.45	0.50
2:B:25:ILE:HG21	2:B:658:ILE:CD1	2.42	0.50
2:B:27:ALA:O	2:B:29:ASP:N	2.45	0.50
2:B:39:ARG:NE	2:B:665:GLU:HG2	2.27	0.50
2:B:822:ASN:ND2	10:J:52:THR:HG21	2.27	0.50
2:B:1117:GLN:HE21	2:B:1199:ALA:HB2	1.76	0.50
2:B:1197:PRO:HG2	2:B:1200:ALA:CB	2.42	0.50
3:C:18:VAL:O	3:C:20:PHE:HD2	1.94	0.50
7:G:153:GLN:CG	7:G:154:VAL:HG23	2.41	0.50
8:H:30:SER:HB3	8:H:33:GLN:O	2.12	0.50
8:H:41:ASP:C	8:H:42:ILE:HG13	2.37	0.50
10:J:13:VAL:O	10:J:14:VAL:HG23	2.12	0.50
1:A:12:ARG:NH2	2:B:1192:TYR:CE2	2.80	0.50
1:A:828:ALA:C	1:A:831:THR:HG22	2.35	0.50
1:A:983:ILE:HG23	1:A:983:ILE:O	2.11	0.50
2:B:424:LEU:O	2:B:428:ILE:HG13	2.12	0.50
2:B:653:VAL:HG23	2:B:689:LEU:HB3	1.93	0.50
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.33	0.50
8:H:129:TYR:CE1	8:H:130:ARG:HD2	2.46	0.50
10:J:14:VAL:HG13	10:J:50:ILE:HD11	1.94	0.50
12:L:53:HIS:O	12:L:55:ILE:HD13	2.12	0.50
1:A:55:ASP:O	1:A:55:ASP:OD2	2.28	0.50
1:A:463:ILE:HD11	1:A:469:ARG:HG3	1.94	0.50
1:A:555:ASP:O	1:A:556:TRP:C	2.54	0.50
1:A:1030:ARG:NH1	1:A:1035:TYR:OH	2.45	0.50
1:A:1402:PHE:CD1	1:A:1403:GLU:HG2	2.46	0.50
2:B:1102:LYS:O	2:B:1122:ARG:NH1	2.43	0.50
3:C:31:ASN:O	3:C:32:SER:C	2.52	0.50
7:G:111:THR:HG23	7:G:111:THR:O	2.11	0.50
1:A:1142:THR:O	1:A:1145:SER:OG	2.30	0.50
2:B:35:SER:O	2:B:39:ARG:HG3	2.12	0.50
2:B:469:GLN:O	2:B:470:LYS:HB2	2.12	0.50
2:B:507:LYS:C	2:B:508:LEU:HD23	2.37	0.50
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.93	0.50
2:B:1106:ARG:HH21	2:B:1111:MET:HE2	1.75	0.50
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.92	0.50
3:C:83:SER:HG	3:C:160:LYS:HD3	1.77	0.50
4:D:16:LYS:O	4:D:18:VAL:N	2.36	0.50
5:E:122:LYS:O	5:E:123:LEU:HD23	2.11	0.50
6:F:74:ILE:HD12	6:F:144:GLU:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:17:ARG:HG3	9:I:28:GLU:OE1	2.12	0.50
1:A:295:LEU:O	1:A:298:PHE:HB3	2.11	0.49
1:A:1210:GLY:O	1:A:1214:GLU:HG2	2.12	0.49
2:B:284:ILE:HD13	2:B:333:PHE:CD2	2.44	0.49
2:B:710:LEU:CA	2:B:733:HIS:HB3	2.36	0.49
2:B:766:ARG:NH2	15:3:11:U:O2	2.43	0.49
2:B:1068:GLY:O	2:B:1069:PHE:C	2.54	0.49
2:B:1115:THR:CG2	2:B:1117:GLN:HB2	2.42	0.49
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.42	0.49
3:C:242:GLN:O	3:C:244:VAL:N	2.45	0.49
12:L:55:ILE:O	12:L:56:LEU:HB2	2.12	0.49
1:A:219:PHE:CE2	1:A:231:PRO:HD2	2.47	0.49
1:A:336:ILE:HD13	1:A:340:LEU:HD12	1.93	0.49
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.46	0.49
1:A:600:PRO:HA	8:H:25:ARG:NH1	2.27	0.49
1:A:663:SER:OG	1:A:664:THR:N	2.41	0.49
2:B:98:THR:O	2:B:126:SER:HB2	2.12	0.49
2:B:254:LEU:HD12	2:B:272:THR:O	2.13	0.49
2:B:461:LEU:HD12	2:B:461:LEU:N	2.27	0.49
2:B:758:PHE:HE1	2:B:1027:ILE:HG22	1.77	0.49
3:C:114:TYR:OH	10:J:19:GLU:OE1	2.29	0.49
5:E:177:ARG:HD3	5:E:215:MET:SD	2.52	0.49
7:G:1:MET:SD	7:G:79:PHE:CE1	3.05	0.49
7:G:13:LEU:HD13	7:G:22:MET:HE2	1.94	0.49
8:H:92:ASP:C	8:H:93:TYR:CD1	2.89	0.49
8:H:124:ARG:C	8:H:124:ARG:HD3	2.37	0.49
11:K:51:LEU:HD22	11:K:59:ALA:HB3	1.93	0.49
12:L:34:CYS:HB3	12:L:51:CYS:SG	2.52	0.49
1:A:470:LEU:HD13	1:A:487:MET:HE1	1.94	0.49
2:B:570:VAL:HG23	2:B:573:GLN:HB3	1.94	0.49
2:B:794:ASN:C	2:B:795:ILE:HD12	2.37	0.49
11:K:37:LYS:O	11:K:38:GLU:HG2	2.12	0.49
11:K:60:ALA:O	11:K:73:LEU:HD12	2.12	0.49
1:A:418:SER:C	1:A:420:ARG:N	2.71	0.49
1:A:608:ILE:C	1:A:610:GLY:N	2.69	0.49
1:A:718:VAL:O	1:A:722:LEU:HD12	2.12	0.49
1:A:809:THR:H	1:A:812:GLU:HB2	1.77	0.49
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.27	0.49
1:A:1166:ASP:OD2	1:A:1239:ARG:NE	2.44	0.49
1:A:1259:MET:CE	1:A:1263:ILE:HG13	2.43	0.49
1:A:1308:THR:HG23	1:A:1309:ASP:H	1.73	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:SER:HA	2:B:171:PRO:HA	1.94	0.49
2:B:865:LYS:C	2:B:866:TYR:HD1	2.20	0.49
2:B:995:ARG:HH11	3:C:165:LYS:HA	1.77	0.49
2:B:1196:ILE:HB	2:B:1197:PRO:HD2	1.93	0.49
11:K:40:HIS:O	11:K:41:THR:C	2.54	0.49
1:A:69:THR:O	1:A:71:GLN:HG3	2.12	0.49
1:A:171:GLN:HA	1:A:171:GLN:OE1	2.12	0.49
1:A:444:PHE:CE2	1:A:487:MET:HE3	2.47	0.49
1:A:1115:SER:C	1:A:1308:THR:HG22	2.37	0.49
2:B:59:LEU:HD11	2:B:417:PHE:CZ	2.48	0.49
2:B:295:GLY:N	2:B:298:LEU:HD23	2.28	0.49
2:B:830:TYR:O	2:B:832:GLY:N	2.46	0.49
4:D:73:SER:HB3	7:G:21:ARG:HH21	1.77	0.49
5:E:121:MET:C	5:E:123:LEU:H	2.20	0.49
8:H:123:MET:HG2	8:H:124:ARG:N	2.26	0.49
10:J:12:LYS:O	10:J:14:VAL:HG23	2.13	0.49
12:L:30:ILE:CG2	12:L:31:CYS:H	2.25	0.49
1:A:311:GLN:O	1:A:313:GLN:N	2.45	0.49
2:B:311:LEU:O	2:B:312:GLU:C	2.55	0.49
3:C:33:LEU:HG	3:C:37:MET:CE	2.36	0.49
4:D:51:ASN:O	4:D:52:LEU:C	2.53	0.49
5:E:28:TYR:CE1	5:E:78:LEU:HD13	2.47	0.49
7:G:106:MET:HG2	7:G:107:LYS:N	2.28	0.49
9:I:78:CYS:SG	9:I:106:CYS:SG	3.11	0.49
10:J:53:HIS:CD2	10:J:54:VAL:C	2.91	0.49
11:K:24:ASP:OD1	11:K:26:LYS:N	2.46	0.49
12:L:61:THR:HG22	12:L:63:ARG:H	1.77	0.49
1:A:54:ASN:HA	1:A:58:LEU:HD12	1.93	0.49
1:A:289:ILE:C	1:A:291:GLU:H	2.21	0.49
1:A:402:ALA:HB1	1:A:433:GLU:O	2.13	0.49
1:A:464:PRO:HG2	1:A:465:TYR:CD1	2.48	0.49
1:A:590:ARG:NH1	1:A:592:ASP:OD1	2.46	0.49
1:A:739:ASP:OD2	8:H:19:ARG:HD2	2.12	0.49
1:A:1242:VAL:CG1	1:A:1243:VAL:H	2.26	0.49
1:A:1329:THR:HG22	1:A:1330:ASN:N	2.28	0.49
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.43	0.49
2:B:708:GLU:O	2:B:709:ASP:C	2.54	0.49
2:B:842:ASN:ND2	2:B:845:SER:OG	2.45	0.49
4:D:134:THR:CG2	4:D:135:GLY:N	2.75	0.49
6:F:69:LEU:HB3	6:F:71:GLU:OE2	2.13	0.49
10:J:2:ILE:HG22	10:J:3:VAL:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.28	0.49
15:3:11:U:O2	15:3:11:U:H2'	2.12	0.49
1:A:63:ARG:HA	1:A:74:MET:CE	2.41	0.49
1:A:323:LYS:H	1:A:323:LYS:CD	2.21	0.49
1:A:897:TYR:HB3	1:A:936:LEU:CD1	2.43	0.49
1:A:969:GLN:HG3	1:A:969:GLN:O	2.12	0.49
1:A:1067:LEU:HD12	1:A:1067:LEU:O	2.12	0.49
1:A:1205:LYS:O	1:A:1206:ASP:C	2.55	0.49
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.13	0.49
2:B:48:LEU:O	2:B:51:PHE:N	2.43	0.49
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.94	0.49
2:B:615:MET:CB	2:B:626:ILE:HG12	2.43	0.49
3:C:179:GLU:O	3:C:180:TYR:HB3	2.13	0.49
5:E:7:ARG:HD2	5:E:8:ASN:N	2.28	0.49
8:H:99:GLY:HA3	8:H:117:SER:O	2.12	0.49
11:K:53:ASP:C	11:K:55:LYS:H	2.20	0.49
1:A:38:PRO:HG2	1:A:39:GLU:OE2	2.12	0.49
1:A:167:CYS:HB2	1:A:169:ASN:HD21	1.75	0.49
1:A:416:ARG:NH1	1:A:417:TYR:HE2	2.02	0.49
1:A:433:GLU:CD	2:B:1108:ARG:HH22	2.21	0.49
1:A:583:PRO:HG2	1:A:586:ILE:HG13	1.95	0.49
1:A:774:ARG:CZ	1:A:797:LYS:HG3	2.43	0.49
2:B:129:PHE:CE2	2:B:166:PHE:HB2	2.48	0.49
2:B:258:LEU:O	2:B:258:LEU:CG	2.57	0.49
2:B:467:GLY:N	2:B:475:SER:HB3	2.28	0.49
5:E:27:GLY:O	5:E:65:THR:HG23	2.12	0.49
5:E:93:MET:HG2	5:E:123:LEU:HD12	1.95	0.49
6:F:89:GLU:C	6:F:93:ILE:HD12	2.38	0.49
6:F:118:LEU:O	6:F:122:MET:HG3	2.13	0.49
8:H:100:THR:CG2	8:H:138:GLU:HG2	2.43	0.49
1:A:34:LYS:HZ1	1:A:57:ARG:NH2	2.11	0.49
1:A:37:PHE:N	1:A:37:PHE:HD1	2.10	0.49
1:A:77:CYS:C	1:A:78:PRO:O	2.54	0.49
1:A:89:PRO:O	1:A:204:THR:HG21	2.13	0.49
1:A:106:VAL:CG1	1:A:107:CYS:N	2.76	0.49
1:A:525:GLN:O	1:A:526:ASP:C	2.56	0.49
1:A:833:GLU:O	1:A:837:ILE:HG13	2.13	0.49
1:A:904:THR:O	1:A:904:THR:HG22	2.13	0.49
2:B:134:LYS:HD3	2:B:134:LYS:N	2.27	0.49
2:B:912:ILE:O	2:B:938:SER:HB3	2.13	0.49
2:B:1040:ASN:O	2:B:1041:GLU:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:ALA:O	3:C:174:ALA:HB3	2.12	0.49
6:F:136:ARG:O	6:F:143:PHE:HA	2.13	0.49
11:K:48:ALA:O	11:K:51:LEU:N	2.37	0.49
11:K:93:SER:O	11:K:97:LYS:HG3	2.13	0.49
1:A:34:LYS:CB	1:A:36:ARG:NH1	2.75	0.48
1:A:173:THR:HG23	1:A:173:THR:O	2.13	0.48
1:A:500:GLU:OE1	2:B:1145:SER:N	2.46	0.48
1:A:578:LEU:HD23	1:A:612:ILE:CD1	2.43	0.48
1:A:596:THR:C	1:A:598:LEU:N	2.70	0.48
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.46	0.48
1:A:920:LEU:HD23	1:A:920:LEU:C	2.38	0.48
1:A:1053:PHE:O	1:A:1056:SER:N	2.46	0.48
1:A:1422:ARG:HD3	2:B:1224:PHE:CE2	2.47	0.48
2:B:63:ILE:HD12	2:B:421:PHE:CZ	2.47	0.48
2:B:460:ALA:C	2:B:462:ALA:H	2.21	0.48
2:B:654:ARG:HG3	2:B:654:ARG:NH1	2.21	0.48
5:E:16:PHE:O	5:E:17:ARG:C	2.55	0.48
5:E:98:ILE:O	5:E:102:GLU:HG3	2.13	0.48
5:E:164:LEU:HD22	5:E:211:TYR:CD2	2.48	0.48
7:G:26:LEU:O	7:G:29:LYS:N	2.45	0.48
10:J:16:ASP:OD1	10:J:16:ASP:N	2.46	0.48
11:K:24:ASP:OD2	11:K:74:ARG:NH1	2.45	0.48
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.48	0.48
1:A:541:ILE:HD13	1:A:549:MET:CE	2.30	0.48
1:A:720:ARG:O	1:A:720:ARG:HG2	2.13	0.48
1:A:1264:GLU:OE2	9:I:46:HIS:CD2	2.66	0.48
2:B:293:PRO:C	2:B:294:ASP:O	2.55	0.48
2:B:361:LEU:CD2	2:B:377:PHE:CD2	2.96	0.48
2:B:461:LEU:H	2:B:461:LEU:CD1	2.26	0.48
2:B:704:ALA:HB1	2:B:710:LEU:HB2	1.95	0.48
2:B:744:HIS:CD2	2:B:745:PRO:CD	2.86	0.48
2:B:792:MET:H	2:B:857:ARG:HA	1.77	0.48
3:C:8:VAL:HG12	3:C:9:LYS:H	1.78	0.48
4:D:13:ARG:O	4:D:15:LEU:N	2.47	0.48
4:D:155:ARG:HH11	4:D:155:ARG:HB3	1.78	0.48
5:E:157:SER:C	5:E:159:ASP:H	2.20	0.48
11:K:53:ASP:HB3	11:K:56:VAL:CG2	2.43	0.48
1:A:785:PRO:HG2	1:A:786:HIS:CD2	2.48	0.48
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.95	0.48
2:B:505:ASP:O	2:B:506:GLY:C	2.55	0.48
2:B:506:GLY:O	2:B:507:LYS:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:593:PRO:C	2:B:595:ARG:N	2.69	0.48
2:B:709:ASP:OD1	2:B:710:LEU:HD23	2.13	0.48
2:B:827:ILE:HG22	2:B:827:ILE:O	2.13	0.48
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.94	0.48
3:C:239:PRO:O	3:C:241:ASP:N	2.45	0.48
3:C:248:ILE:CD1	11:K:101:LEU:HD22	2.42	0.48
5:E:69:ILE:HA	5:E:72:PHE:O	2.13	0.48
7:G:125:SER:OG	7:G:128:PRO:HA	2.13	0.48
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.95	0.48
1:A:92:HIS:O	1:A:93:VAL:C	2.56	0.48
1:A:356:ASP:HB2	1:A:469:ARG:NH1	2.29	0.48
1:A:658:LEU:HD12	1:A:658:LEU:O	2.13	0.48
1:A:700:ASN:C	1:A:701:LEU:HD23	2.38	0.48
2:B:63:ILE:O	2:B:63:ILE:HG13	2.14	0.48
2:B:771:SER:O	2:B:775:LYS:HE3	2.14	0.48
2:B:1068:GLY:O	2:B:1069:PHE:O	2.31	0.48
3:C:14:SER:OG	3:C:15:LYS:N	2.44	0.48
5:E:192:ARG:HG3	5:E:192:ARG:NH1	2.29	0.48
6:F:90:ARG:HG3	6:F:91:ALA:N	2.27	0.48
1:A:145:LYS:HA	1:A:145:LYS:CE	2.35	0.48
1:A:774:ARG:HB2	1:A:797:LYS:O	2.13	0.48
1:A:852:TYR:O	6:F:81:THR:HG22	2.14	0.48
2:B:639:ILE:CG2	2:B:641:GLU:HG2	2.43	0.48
2:B:860:MET:O	2:B:861:ASP:HB2	2.13	0.48
2:B:956:THR:CG2	2:B:960:GLY:HA2	2.43	0.48
6:F:116:ASP:O	6:F:117:PRO:C	2.54	0.48
9:I:16:PRO:HB3	9:I:27:PHE:CE2	2.48	0.48
9:I:55:THR:OG1	9:I:100:PHE:HD2	1.96	0.48
1:A:381:THR:O	1:A:382:PRO:C	2.55	0.48
1:A:391:LEU:HD23	1:A:401:GLY:N	2.29	0.48
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.94	0.48
1:A:1241:ARG:O	1:A:1242:VAL:CG2	2.61	0.48
1:A:1453:TYR:O	1:A:1454:MET:HB3	2.13	0.48
2:B:120:ARG:NH1	12:L:54:ARG:HD2	2.29	0.48
2:B:313:MET:HE2	2:B:390:LEU:CD2	2.43	0.48
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.79	0.48
4:D:32:GLU:OE1	7:G:41:LYS:HE2	2.14	0.48
7:G:27:LYS:HD3	7:G:51:TYR:CE2	2.48	0.48
9:I:34:TYR:HD2	9:I:34:TYR:C	2.18	0.48
1:A:802:ASN:ND2	1:A:812:GLU:OE1	2.37	0.48
1:A:1244:ARG:HG2	1:A:1244:ARG:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1259:MET:O	1:A:1259:MET:HE3	2.13	0.48
2:B:48:LEU:HD23	2:B:173:MET:SD	2.53	0.48
2:B:364:ILE:O	2:B:365:THR:CB	2.61	0.48
2:B:542:MET:CE	2:B:747:MET:HE2	2.43	0.48
2:B:846:ILE:HG23	2:B:974:PRO:CG	2.41	0.48
2:B:885:MET:HA	2:B:936:ASP:HB2	1.96	0.48
3:C:263:THR:C	3:C:265:MET:N	2.70	0.48
1:A:106:VAL:HG21	1:A:214:ILE:CD1	2.43	0.48
1:A:372:LYS:HA	1:A:435:HIS:CE1	2.48	0.48
2:B:327:ARG:O	2:B:331:LEU:HD13	2.13	0.48
2:B:483:LEU:CD1	2:B:491:THR:HG23	2.38	0.48
2:B:497:ARG:NH2	2:B:775:LYS:HZ2	2.12	0.48
2:B:831:SER:HB2	2:B:833:TYR:HD1	1.79	0.48
2:B:1006:ILE:HG22	10:J:45:CYS:HB3	1.95	0.48
4:D:155:ARG:CG	4:D:155:ARG:HH11	2.27	0.48
5:E:186:LEU:O	5:E:187:TYR:C	2.56	0.48
9:I:80:SER:OG	9:I:105:SER:HB2	2.14	0.48
1:A:147:VAL:HG22	1:A:170:THR:HA	1.95	0.48
1:A:1129:GLU:O	1:A:1130:GLN:C	2.56	0.48
2:B:126:SER:CB	2:B:172:ILE:HD11	2.44	0.48
2:B:210:LYS:HD2	2:B:481:GLN:O	2.13	0.48
2:B:479:VAL:O	2:B:480:SER:HB3	2.13	0.48
2:B:654:ARG:O	2:B:657:HIS:N	2.47	0.48
2:B:1099:VAL:CG1	2:B:1100:ASP:N	2.76	0.48
3:C:125:MET:HE2	3:C:127:ARG:NH2	2.28	0.48
4:D:154:PHE:HE1	4:D:163:VAL:CG1	2.26	0.48
5:E:6:GLU:HA	5:E:9:ILE:HD12	1.95	0.48
5:E:68:SER:HB3	5:E:75:MET:HE1	1.94	0.48
1:A:224:PHE:HE2	1:A:234:MET:HE2	1.79	0.48
1:A:688:LYS:HE3	1:A:691:LEU:HD23	1.96	0.48
2:B:68:THR:HA	2:B:90:ILE:O	2.14	0.48
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.96	0.48
2:B:582:VAL:HG22	2:B:626:ILE:HG22	1.95	0.48
2:B:708:GLU:CG	2:B:709:ASP:H	2.09	0.48
3:C:64:ALA:O	3:C:65:HIS:C	2.57	0.48
3:C:99:LEU:HD22	3:C:99:LEU:N	2.27	0.48
3:C:241:ASP:CG	3:C:242:GLN:N	2.71	0.48
4:D:31:GLN:C	4:D:33:PHE:H	2.22	0.48
4:D:156:ASP:C	4:D:158:GLU:N	2.70	0.48
5:E:13:TRP:O	5:E:16:PHE:HB3	2.14	0.48
9:I:60:GLN:CD	9:I:107:SER:HG	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLN:C	1:A:73:GLY:H	2.22	0.47
1:A:84:ILE:CD1	1:A:270:LEU:HD13	2.44	0.47
1:A:254:GLU:O	1:A:256:GLN:N	2.47	0.47
1:A:302:THR:HA	1:A:305:ASP:O	2.14	0.47
1:A:401:GLY:C	1:A:435:HIS:CD2	2.92	0.47
1:A:709:THR:CG2	1:A:710:LEU:H	2.25	0.47
1:A:1243:VAL:HG12	1:A:1244:ARG:N	2.29	0.47
1:A:1431:GLY:HA3	2:B:1152:MET:HE2	1.96	0.47
2:B:732:SER:HB2	2:B:734:HIS:NE2	2.29	0.47
3:C:147:LEU:N	3:C:147:LEU:CD2	2.73	0.47
4:D:63:LEU:HD22	4:D:133:THR:OG1	2.13	0.47
7:G:90:THR:HG22	7:G:91:VAL:O	2.13	0.47
7:G:127:PRO:HG3	7:G:139:ILE:HG21	1.96	0.47
9:I:55:THR:HG23	9:I:86:PHE:HZ	1.79	0.47
11:K:31:VAL:HG23	11:K:83:PRO:HG3	1.95	0.47
1:A:886:ILE:CG2	1:A:952:ALA:HB2	2.44	0.47
1:A:1036:ARG:HG2	1:A:1036:ARG:NH1	2.29	0.47
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.40	0.47
1:A:1322:ILE:O	1:A:1322:ILE:HG13	2.14	0.47
2:B:773:MET:O	2:B:775:LYS:N	2.46	0.47
2:B:875:GLU:O	2:B:877:PRO:CD	2.60	0.47
2:B:944:THR:CG2	2:B:1122:ARG:NH2	2.72	0.47
2:B:1152:MET:HE1	2:B:1196:ILE:HA	1.96	0.47
6:F:94:LEU:HD22	6:F:122:MET:HG2	1.96	0.47
8:H:58:THR:HG22	8:H:59:ILE:N	2.25	0.47
9:I:86:PHE:CE1	9:I:100:PHE:HB2	2.49	0.47
11:K:108:GLU:O	11:K:112:GLN:HG2	2.14	0.47
1:A:474:VAL:HG22	1:A:474:VAL:O	2.14	0.47
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.49	0.47
1:A:567:LYS:CE	8:H:46:LEU:HB2	2.44	0.47
1:A:1153:TYR:CE1	9:I:42:LEU:HD13	2.49	0.47
1:A:1193:LEU:HD12	1:A:1193:LEU:C	2.39	0.47
2:B:31:TRP:CZ2	2:B:807:ARG:HB2	2.49	0.47
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.96	0.47
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.95	0.47
8:H:96:VAL:HA	8:H:142:LEU:O	2.14	0.47
14:1:15:DG:H2'	14:1:16:DT:H71	1.95	0.47
1:A:69:THR:O	1:A:70:CYS:C	2.57	0.47
1:A:108:MET:HB3	1:A:210:ILE:CD1	2.44	0.47
1:A:1168:GLU:OE2	1:A:1172:LEU:HD11	2.14	0.47
2:B:54:PHE:HE1	2:B:414:ALA:HA	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:VAL:HG23	2:B:109:THR:N	2.29	0.47
2:B:509:ALA:HB1	2:B:513:GLN:CD	2.39	0.47
2:B:654:ARG:H	2:B:657:HIS:HD2	1.60	0.47
2:B:737:THR:O	2:B:738:PHE:C	2.57	0.47
3:C:50:GLU:OE1	12:L:64:LEU:HD12	2.14	0.47
3:C:63:ILE:O	3:C:64:ALA:C	2.57	0.47
3:C:111:THR:O	3:C:147:LEU:HD23	2.14	0.47
11:K:109:TRP:O	11:K:112:GLN:HB2	2.15	0.47
12:L:34:CYS:SG	12:L:51:CYS:SG	3.13	0.47
1:A:55:ASP:H	1:A:56:PRO:HD3	1.76	0.47
1:A:608:ILE:HD12	1:A:613:ILE:HD12	1.97	0.47
1:A:831:THR:HG23	1:A:832:ALA:N	2.29	0.47
1:A:901:LEU:HA	1:A:907:THR:OG1	2.14	0.47
1:A:1048:ASN:HD22	1:A:1048:ASN:N	2.13	0.47
1:A:1450:LEU:HD21	7:G:19:GLY:O	2.15	0.47
2:B:47:GLN:O	2:B:173:MET:HE1	2.14	0.47
2:B:376:PHE:HB2	2:B:566:LEU:HD21	1.96	0.47
2:B:407:ASP:C	2:B:408:LEU:HD12	2.39	0.47
2:B:505:ASP:HA	13:2:1:DA:N7	2.29	0.47
2:B:831:SER:CB	2:B:994:TYR:OH	2.63	0.47
2:B:855:PHE:HZ	2:B:857:ARG:NH1	2.13	0.47
2:B:859:TYR:N	2:B:859:TYR:CD1	2.83	0.47
2:B:1010:LEU:HD12	2:B:1010:LEU:N	2.29	0.47
2:B:1103:ILE:HG23	2:B:1103:ILE:O	2.14	0.47
3:C:39:ALA:HA	3:C:164:ALA:CB	2.44	0.47
3:C:73:GLN:HE21	3:C:75:MET:N	2.10	0.47
3:C:100:THR:HG22	3:C:101:LEU:N	2.29	0.47
4:D:29:LEU:N	4:D:29:LEU:CD2	2.77	0.47
4:D:69:ALA:HA	4:D:72:ARG:HG3	1.96	0.47
4:D:123:LEU:HD13	4:D:123:LEU:C	2.38	0.47
4:D:196:PRO:O	4:D:197:SER:C	2.58	0.47
7:G:127:PRO:HG2	7:G:138:THR:HG21	1.95	0.47
8:H:11:GLN:C	8:H:28:ALA:HB1	2.39	0.47
1:A:293:GLU:O	1:A:296:LEU:N	2.47	0.47
1:A:664:THR:HG22	2:B:1014:PRO:CB	2.44	0.47
1:A:743:VAL:O	1:A:747:VAL:HG23	2.14	0.47
1:A:826:ASP:HB2	1:A:830:LYS:HD3	1.96	0.47
1:A:907:THR:HG23	1:A:908:LEU:N	2.30	0.47
2:B:25:ILE:HD11	2:B:653:VAL:O	2.14	0.47
2:B:225:VAL:HA	2:B:237:VAL:O	2.14	0.47
2:B:792:MET:HA	2:B:856:PHE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:89:GLU:O	3:C:90:ASP:CB	2.58	0.47
3:C:181:ASP:N	3:C:182:PRO:CD	2.76	0.47
4:D:156:ASP:O	4:D:157:GLN:C	2.57	0.47
5:E:10:SER:O	5:E:13:TRP:HB3	2.15	0.47
7:G:87:VAL:HG23	7:G:103:VAL:HG21	1.95	0.47
8:H:33:GLN:C	8:H:35:GLN:H	2.22	0.47
1:A:49:LYS:HD3	1:A:55:ASP:HB3	1.97	0.47
1:A:108:MET:HA	1:A:210:ILE:CD1	2.43	0.47
1:A:244:PRO:CB	1:A:245:PRO:CD	2.84	0.47
1:A:381:THR:CG2	1:A:382:PRO:HD2	2.38	0.47
1:A:382:PRO:HB3	1:A:428:TYR:HE2	1.80	0.47
1:A:567:LYS:HZ1	8:H:46:LEU:HB2	1.75	0.47
1:A:569:LYS:HD3	1:A:571:LEU:HD11	1.96	0.47
1:A:577:ILE:O	1:A:580:VAL:HG23	2.15	0.47
1:A:687:LYS:HE2	1:A:795:GLU:OE2	2.15	0.47
1:A:711:ARG:HH21	9:I:87:GLN:NE2	2.11	0.47
1:A:730:GLY:C	1:A:732:LEU:N	2.71	0.47
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	2.14	0.47
1:A:861:GLY:O	1:A:862:ASN:C	2.58	0.47
1:A:1451:VAL:O	1:A:1454:MET:HG2	2.14	0.47
2:B:466:TRP:O	2:B:468:GLU:N	2.48	0.47
2:B:619:ILE:HG22	2:B:620:ARG:N	2.29	0.47
2:B:620:ARG:CZ	9:I:68:LEU:HD21	2.44	0.47
2:B:745:PRO:O	2:B:748:ILE:HG13	2.14	0.47
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.49	0.47
2:B:969:ARG:HD3	3:C:61:GLU:OE2	2.15	0.47
2:B:996:ARG:HH22	3:C:175:ALA:N	2.12	0.47
2:B:1034:VAL:O	2:B:1037:LEU:N	2.48	0.47
3:C:22:LEU:HD21	11:K:101:LEU:HD11	1.97	0.47
3:C:44:LEU:HD21	3:C:159:ALA:CB	2.44	0.47
3:C:184:ASN:OD1	3:C:187:LYS:CA	2.61	0.47
4:D:63:LEU:HD23	4:D:63:LEU:HA	1.74	0.47
4:D:118:THR:HG21	4:D:121:LYS:HE3	1.95	0.47
5:E:31:THR:HG1	5:E:34:GLU:H	1.62	0.47
5:E:153:HIS:O	5:E:154:ILE:HG13	2.13	0.47
7:G:27:LYS:CE	7:G:54:ILE:HB	2.40	0.47
7:G:106:MET:HE3	7:G:108:VAL:HG22	1.96	0.47
7:G:142:ARG:C	7:G:143:ILE:HG13	2.39	0.47
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.34	0.47
9:I:44:TYR:HD1	9:I:45:ARG:H	1.62	0.47
9:I:51:ASN:O	9:I:54:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:CD2	1:A:54:ASN:N	2.48	0.47
1:A:316:GLN:HB2	1:A:322:VAL:HG23	1.96	0.47
2:B:48:LEU:HA	2:B:173:MET:SD	2.55	0.47
2:B:113:TYR:HE2	2:B:192:LEU:HD21	1.80	0.47
2:B:360:PHE:HD2	2:B:374:LYS:HD3	1.80	0.47
2:B:405:ARG:HA	2:B:631:GLY:O	2.15	0.47
2:B:638:PHE:HB2	2:B:741:CYS:O	2.14	0.47
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.97	0.47
4:D:200:ASN:N	4:D:200:ASN:OD1	2.47	0.47
5:E:164:LEU:HD13	5:E:211:TYR:CE2	2.49	0.47
7:G:114:LEU:HG	7:G:162:SER:HB3	1.97	0.47
8:H:59:ILE:O	8:H:60:ALA:HB3	2.14	0.47
9:I:10:CYS:O	9:I:11:ASN:C	2.55	0.47
11:K:78:THR:HG22	11:K:79:GLU:N	2.30	0.47
12:L:29:TYR:CD2	12:L:29:TYR:N	2.83	0.47
1:A:316:GLN:O	1:A:317:LYS:C	2.57	0.47
1:A:419:LYS:HG3	1:A:420:ARG:HG3	1.96	0.47
1:A:709:THR:CG2	1:A:710:LEU:N	2.75	0.47
1:A:1132:LYS:O	1:A:1135:ARG:HD2	2.15	0.47
2:B:1076:HIS:CD2	11:K:40:HIS:NE2	2.83	0.47
2:B:1107:ALA:O	2:B:1108:ARG:O	2.33	0.47
2:B:1115:THR:HG22	2:B:1117:GLN:HB2	1.96	0.47
4:D:176:GLU:OE2	4:D:197:SER:HB2	2.14	0.47
8:H:7:ASP:O	8:H:8:ASP:HB2	2.15	0.47
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.97	0.47
1:A:167:CYS:HB2	1:A:169:ASN:HD22	1.79	0.47
1:A:870:GLU:HG2	5:E:208:TYR:CD2	2.49	0.47
1:A:1005:GLU:O	1:A:1009:ASN:HB2	2.15	0.47
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	1.96	0.47
1:A:1265:ASN:C	1:A:1267:MET:N	2.72	0.47
2:B:247:GLY:C	2:B:249:ARG:N	2.68	0.47
2:B:460:ALA:C	2:B:462:ALA:N	2.72	0.47
2:B:704:ALA:HB2	2:B:738:PHE:CD2	2.49	0.47
2:B:935:ARG:HG3	2:B:935:ARG:O	2.15	0.47
5:E:136:ASN:OD1	5:E:138:ALA:N	2.48	0.47
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.45	0.47
9:I:50:THR:CG2	9:I:51:ASN:N	2.75	0.47
9:I:62:ILE:HD11	9:I:86:PHE:HE2	1.80	0.47
1:A:34:LYS:HZ1	1:A:57:ARG:HH21	1.62	0.46
1:A:409:SER:O	1:A:410:GLY:C	2.57	0.46
1:A:443:LEU:CD2	1:A:455:MET:HE2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:LYS:H	1:A:773:LYS:HD2	1.80	0.46
1:A:1029:ARG:HH11	1:A:1029:ARG:CG	2.28	0.46
2:B:189:LEU:O	2:B:190:TYR:C	2.58	0.46
2:B:661:LEU:C	2:B:663:ALA:N	2.73	0.46
3:C:120:ILE:HG21	3:C:124:LEU:HD11	1.97	0.46
3:C:177:GLU:HG3	3:C:231:ASN:ND2	2.18	0.46
11:K:83:PRO:O	11:K:84:LYS:C	2.57	0.46
1:A:225:ASN:ND2	1:A:227:VAL:N	2.63	0.46
1:A:228:PHE:CE2	4:D:15:LEU:HD23	2.50	0.46
1:A:278:THR:O	1:A:278:THR:HG22	2.16	0.46
1:A:983:ILE:O	1:A:983:ILE:CG2	2.63	0.46
1:A:1132:LYS:HA	1:A:1135:ARG:HD2	1.97	0.46
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.45	0.46
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.55	0.46
2:B:785:TYR:CD1	2:B:785:TYR:C	2.93	0.46
2:B:1106:ARG:NH1	2:B:1126:GLY:HA2	2.30	0.46
3:C:73:GLN:NE2	3:C:74:SER:H	2.13	0.46
3:C:146:LYS:C	3:C:147:LEU:HD23	2.39	0.46
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.96	0.46
5:E:42:PHE:HZ	5:E:58:MET:HE3	1.78	0.46
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.97	0.46
6:F:111:LEU:HD12	6:F:111:LEU:H	1.81	0.46
7:G:116:PRO:HG2	7:G:119:LEU:HB2	1.97	0.46
11:K:40:HIS:HD1	11:K:61:TYR:HH	1.56	0.46
12:L:61:THR:HG21	12:L:63:ARG:HG3	1.96	0.46
1:A:33:ALA:HA	1:A:57:ARG:HH12	1.80	0.46
1:A:42:ASP:HB3	1:A:45:GLN:H	1.81	0.46
1:A:56:PRO:O	1:A:57:ARG:NH1	2.48	0.46
1:A:93:VAL:HG23	1:A:304:MET:HE3	1.96	0.46
1:A:596:THR:C	1:A:598:LEU:H	2.23	0.46
1:A:785:PRO:HG2	1:A:786:HIS:HD2	1.81	0.46
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.30	0.46
1:A:1198:ASP:OD2	1:A:1200:ALA:HB3	2.15	0.46
2:B:1048:THR:OG1	2:B:1049:ASP:N	2.48	0.46
2:B:1067:ARG:NH2	3:C:194:GLU:OE2	2.49	0.46
4:D:218:GLU:O	4:D:219:THR:C	2.58	0.46
5:E:35:VAL:O	5:E:37:LEU:N	2.47	0.46
5:E:129:PRO:O	5:E:130:ALA:C	2.59	0.46
7:G:22:MET:O	7:G:25:TYR:N	2.48	0.46
8:H:95:TYR:CE2	8:H:97:MET:HE2	2.50	0.46
9:I:110:PHE:CD2	9:I:110:PHE:N	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:111:THR:HG22	9:I:113:ASP:N	2.31	0.46
12:L:38:LEU:HG	12:L:39:SER:H	1.80	0.46
1:A:182:VAL:CG2	1:A:201:VAL:HG22	2.46	0.46
1:A:356:ASP:C	1:A:358:ASN:H	2.22	0.46
1:A:385:ILE:CD1	1:A:426:LEU:HB2	2.46	0.46
1:A:463:ILE:HB	1:A:464:PRO:CD	2.45	0.46
1:A:966:ASN:O	1:A:967:ALA:C	2.59	0.46
1:A:1199:ARG:O	1:A:1200:ALA:C	2.57	0.46
2:B:481:GLN:HE21	15:3:7:G:H4'	1.79	0.46
2:B:843:GLN:N	2:B:994:TYR:O	2.23	0.46
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.96	0.46
5:E:112:TYR:CE1	5:E:136:ASN:HA	2.50	0.46
5:E:128:PRO:HA	5:E:129:PRO:C	2.41	0.46
6:F:72:LYS:H	6:F:72:LYS:HG2	1.49	0.46
7:G:7:LEU:CB	7:G:74:TYR:HE2	2.23	0.46
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.76	0.46
1:A:41:MET:HB2	1:A:49:LYS:HA	1.94	0.46
1:A:533:LYS:HE3	1:A:745:GLN:HE22	1.80	0.46
1:A:1030:ARG:HG3	1:A:1034:GLU:OE2	2.15	0.46
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.31	0.46
1:A:1120:LEU:HD13	1:A:1124:HIS:O	2.14	0.46
1:A:1135:ARG:C	1:A:1137:ALA:H	2.23	0.46
3:C:66:ARG:HH12	10:J:2:ILE:CB	2.29	0.46
3:C:258:ILE:HG23	11:K:19:LEU:HD11	1.98	0.46
4:D:134:THR:HG22	4:D:136:GLY:H	1.80	0.46
6:F:127:GLU:O	6:F:128:LYS:C	2.58	0.46
6:F:128:LYS:HD3	6:F:149:GLU:O	2.15	0.46
9:I:84:VAL:O	9:I:84:VAL:HG22	2.16	0.46
1:A:69:THR:HG22	2:B:1174:LYS:HD3	1.98	0.46
1:A:315:LEU:H	1:A:315:LEU:CD2	2.04	0.46
2:B:221:ASN:OD1	2:B:242:SER:HA	2.16	0.46
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.96	0.46
2:B:875:GLU:OE2	2:B:934:LYS:HE2	2.16	0.46
3:C:22:LEU:HD11	11:K:101:LEU:HD21	1.98	0.46
3:C:66:ARG:C	3:C:68:GLY:N	2.73	0.46
3:C:238:ILE:HG22	3:C:243:VAL:HG23	1.98	0.46
7:G:115:MET:HE1	7:G:130:TYR:CZ	2.51	0.46
8:H:27:GLU:HG3	8:H:39:THR:HA	1.98	0.46
8:H:32:THR:HG22	8:H:33:GLN:OE1	2.16	0.46
9:I:74:GLU:HB3	9:I:81:ARG:CD	2.44	0.46
9:I:93:LYS:HD3	9:I:93:LYS:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:LYS:C	1:A:690:VAL:N	2.70	0.46
1:A:709:THR:HG22	1:A:711:ARG:H	1.79	0.46
1:A:841:LEU:HD23	1:A:841:LEU:HA	1.79	0.46
1:A:858:ASN:ND2	1:A:858:ASN:C	2.52	0.46
1:A:962:ARG:O	1:A:964:ILE:N	2.49	0.46
1:A:1206:ASP:O	1:A:1274:ARG:CZ	2.63	0.46
2:B:172:ILE:CD1	2:B:178:ASN:HD22	2.26	0.46
2:B:644:GLU:OE2	2:B:646:LEU:HB2	2.16	0.46
2:B:1006:ILE:HG23	10:J:43:ARG:HG3	1.98	0.46
3:C:3:GLU:CG	3:C:4:GLU:HG3	2.41	0.46
3:C:52:GLU:OE1	3:C:154:LYS:CE	2.63	0.46
4:D:191:ALA:O	4:D:193:THR:N	2.48	0.46
7:G:158:HIS:CD2	7:G:159:ALA:N	2.83	0.46
8:H:106:GLU:O	8:H:108:SER:N	2.35	0.46
9:I:82:GLU:HB3	9:I:104:LEU:CG	2.46	0.46
10:J:37:SER:OG	10:J:47:ARG:NH2	2.49	0.46
1:A:75:ASN:O	1:A:76:GLU:HB2	2.16	0.46
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.98	0.46
1:A:567:LYS:HB3	8:H:95:TYR:C	2.39	0.46
1:A:1027:ALA:O	1:A:1028:THR:C	2.58	0.46
2:B:38:PHE:HD1	2:B:811:TYR:CD2	2.34	0.46
2:B:432:MET:C	2:B:434:ARG:H	2.24	0.46
2:B:504:ARG:C	2:B:506:GLY:N	2.74	0.46
2:B:908:GLU:O	2:B:909:ASP:C	2.57	0.46
2:B:1003:ALA:HA	3:C:178:PHE:O	2.16	0.46
2:B:1181:GLU:H	2:B:1188:LYS:HA	1.80	0.46
3:C:33:LEU:O	3:C:33:LEU:HD12	2.15	0.46
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.97	0.46
4:D:119:ARG:HD3	4:D:221:TYR:HE2	1.79	0.46
5:E:50:MET:HG2	5:E:52:ARG:HE	1.79	0.46
5:E:90:VAL:HB	5:E:117:THR:HG21	1.97	0.46
9:I:94:ASP:O	9:I:95:THR:O	2.34	0.46
10:J:62:ARG:HG2	10:J:62:ARG:O	2.15	0.46
11:K:91:CYS:O	11:K:94:ILE:N	2.49	0.46
12:L:38:LEU:HG	12:L:39:SER:N	2.31	0.46
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.15	0.46
2:B:1025:HIS:O	2:B:1026:LEU:C	2.57	0.46
3:C:75:MET:HE1	3:C:239:PRO:HG2	1.98	0.46
4:D:52:LEU:HD21	4:D:147:TYR:HE2	1.81	0.46
4:D:196:PRO:C	4:D:198:LEU:N	2.74	0.46
6:F:103:MET:CE	7:G:66:GLY:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:13:LEU:HD22	7:G:17:PHE:HB2	1.96	0.46
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.81	0.46
10:J:56:LEU:O	10:J:59:LYS:N	2.47	0.46
11:K:110:ASN:C	11:K:112:GLN:H	2.23	0.46
1:A:88:LYS:HG3	1:A:276:LEU:CD2	2.45	0.46
1:A:761:MET:O	1:A:803:SER:HB2	2.16	0.46
1:A:1203:ASN:O	1:A:1206:ASP:N	2.49	0.46
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.98	0.46
2:B:263:GLY:O	2:B:264:SER:C	2.59	0.46
2:B:307:ASP:O	2:B:308:TRP:C	2.58	0.46
2:B:377:PHE:O	2:B:379:GLY:N	2.49	0.46
2:B:635:ARG:HH22	2:B:742:GLU:CD	2.23	0.46
2:B:759:PRO:C	2:B:761:HIS:N	2.74	0.46
2:B:914:LYS:HE2	2:B:937:ALA:CB	2.46	0.46
2:B:1138:MET:HE3	2:B:1143:ALA:HB3	1.97	0.46
3:C:243:VAL:O	3:C:243:VAL:CG1	2.64	0.46
4:D:35:LEU:HD11	4:D:173:HIS:CD2	2.50	0.46
4:D:146:GLN:O	4:D:147:TYR:C	2.58	0.46
4:D:187:THR:C	4:D:189:ASP:N	2.72	0.46
5:E:105:PHE:O	5:E:106:GLN:HB2	2.16	0.46
8:H:11:GLN:HE21	8:H:52:GLN:HA	1.80	0.46
8:H:130:ARG:HA	8:H:133:ASN:HB2	1.98	0.46
1:A:12:ARG:HB3	2:B:1218:THR:CG2	2.47	0.45
1:A:61:ILE:CG2	1:A:62:ASP:H	2.14	0.45
1:A:897:TYR:N	1:A:897:TYR:CD1	2.84	0.45
1:A:1293:SER:OG	1:A:1295:THR:CG2	2.65	0.45
2:B:46:GLN:OE1	2:B:47:GLN:HG2	2.15	0.45
2:B:227:LYS:H	2:B:395:GLN:CD	2.23	0.45
2:B:408:LEU:N	2:B:408:LEU:CD1	2.77	0.45
2:B:591:ARG:O	2:B:592:ASN:C	2.57	0.45
2:B:899:ILE:CG2	2:B:900:ALA:N	2.79	0.45
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.97	0.45
5:E:198:ILE:HD11	5:E:212:ARG:HG3	1.97	0.45
6:F:79:ARG:HH22	6:F:150:GLU:CD	2.23	0.45
8:H:108:SER:O	8:H:109:LYS:HB3	2.16	0.45
12:L:48:CYS:HB3	12:L:51:CYS:O	2.17	0.45
1:A:289:ILE:O	1:A:292:ALA:N	2.43	0.45
1:A:343:LYS:NZ	2:B:1151:LEU:O	2.42	0.45
1:A:567:LYS:HZ2	8:H:46:LEU:C	2.24	0.45
1:A:1293:SER:OG	1:A:1295:THR:HG23	2.16	0.45
2:B:637:LEU:HD11	2:B:703:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:778:MET:CE	2:B:1094:ARG:HG2	2.43	0.45
2:B:826:ALA:HB2	2:B:1087:PHE:HE2	1.81	0.45
3:C:166:GLU:C	11:K:6:ARG:NH1	2.74	0.45
4:D:186:ASP:O	4:D:211:LEU:HD13	2.16	0.45
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.98	0.45
6:F:111:LEU:CD1	6:F:111:LEU:H	2.29	0.45
7:G:18:PHE:HA	7:G:22:MET:HE3	1.99	0.45
8:H:38:LEU:HD12	8:H:39:THR:N	2.30	0.45
11:K:6:ARG:O	11:K:9:LEU:HG	2.16	0.45
11:K:17:SER:O	11:K:18:LYS:C	2.60	0.45
1:A:481:ASP:OD1	15:3:11:U:H5''	2.17	0.45
1:A:688:LYS:O	1:A:690:VAL:N	2.48	0.45
2:B:313:MET:CE	2:B:386:LEU:HD22	2.47	0.45
2:B:604:ARG:HB2	2:B:609:ILE:HG13	1.98	0.45
2:B:995:ARG:O	2:B:996:ARG:C	2.59	0.45
2:B:1197:PRO:HG2	2:B:1200:ALA:HB2	1.98	0.45
5:E:75:MET:O	5:E:76:GLY:O	2.35	0.45
6:F:109:VAL:HG13	6:F:127:GLU:OE1	2.16	0.45
8:H:62:SER:OG	8:H:64:ASN:ND2	2.47	0.45
8:H:135:LEU:HD13	8:H:137:GLN:OE1	2.16	0.45
9:I:68:LEU:CB	9:I:84:VAL:HG23	2.46	0.45
1:A:150:THR:HG22	1:A:150:THR:O	2.17	0.45
1:A:369:SER:CB	11:K:2:ASN:OD1	2.64	0.45
1:A:442:VAL:HG21	1:A:489:LEU:HD11	1.99	0.45
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.52	0.45
1:A:869:GLY:C	1:A:871:ASP:H	2.24	0.45
1:A:1353:TYR:HD2	1:A:1353:TYR:O	2.00	0.45
1:A:1387:HIS:CE1	13:2:4:DA:H4'	2.52	0.45
2:B:25:ILE:HG22	2:B:658:ILE:HD12	1.97	0.45
2:B:243:ALA:CB	2:B:250:PHE:O	2.64	0.45
2:B:805:THR:CA	2:B:809:MET:HE3	2.46	0.45
2:B:1032:SER:HB3	2:B:1089:PRO:HG2	1.99	0.45
2:B:1081:LEU:HD12	2:B:1085:ILE:HD11	1.99	0.45
3:C:112:ASN:HD22	3:C:112:ASN:N	2.12	0.45
4:D:52:LEU:H	4:D:182:SER:HB3	1.82	0.45
4:D:138:ASN:HD21	7:G:35:GLU:CB	2.29	0.45
5:E:20:LYS:O	5:E:21:GLU:C	2.59	0.45
7:G:139:ILE:HG23	7:G:140:LYS:N	2.31	0.45
8:H:37:LYS:HD2	8:H:126:GLU:OE1	2.16	0.45
14:1:22:DC:H2''	14:1:23:BRU:OP2	2.16	0.45
1:A:709:THR:HG23	9:I:94:ASP:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1289:ARG:HD2	1:A:1303:GLU:OE2	2.16	0.45
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.31	0.45
2:B:370:PHE:HD2	2:B:373:ARG:HD3	1.82	0.45
2:B:1073:TYR:OH	3:C:179:GLU:HG3	2.15	0.45
3:C:99:LEU:N	3:C:99:LEU:CD2	2.80	0.45
3:C:265:MET:HE3	3:C:265:MET:HB2	1.90	0.45
4:D:206:GLU:O	4:D:210:ILE:HG13	2.16	0.45
12:L:55:ILE:CG1	12:L:56:LEU:H	2.23	0.45
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.45	0.45
1:A:536:LEU:O	1:A:537:ARG:C	2.58	0.45
1:A:985:ASP:O	1:A:986:ILE:C	2.58	0.45
2:B:758:PHE:N	2:B:759:PRO:CD	2.80	0.45
2:B:860:MET:HG2	2:B:861:ASP:N	2.32	0.45
2:B:916:THR:HB	2:B:935:ARG:HG3	1.97	0.45
3:C:20:PHE:HE1	3:C:22:LEU:HD13	1.82	0.45
4:D:35:LEU:N	4:D:35:LEU:CD1	2.80	0.45
4:D:124:GLU:CD	4:D:124:GLU:N	2.74	0.45
8:H:129:TYR:HA	8:H:131:ASN:HD21	1.82	0.45
10:J:22:LEU:HD12	10:J:22:LEU:HA	1.71	0.45
12:L:29:TYR:N	12:L:29:TYR:HD2	2.13	0.45
1:A:53:LEU:O	1:A:56:PRO:HG3	2.17	0.45
1:A:57:ARG:O	1:A:58:LEU:O	2.34	0.45
1:A:80:HIS:O	1:A:243:PRO:HB3	2.15	0.45
1:A:90:VAL:HG13	1:A:297:GLN:OE1	2.16	0.45
1:A:281:HIS:C	1:A:282:ASN:HD22	2.24	0.45
1:A:416:ARG:C	1:A:417:TYR:CD2	2.95	0.45
1:A:693:VAL:HA	1:A:696:GLU:HB3	1.98	0.45
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.16	0.45
1:A:1199:ARG:CG	1:A:1236:LEU:HD11	2.46	0.45
1:A:1212:VAL:O	1:A:1213:GLY:C	2.60	0.45
1:A:1438:THR:O	1:A:1438:THR:HG22	2.17	0.45
2:B:244:LEU:HD13	2:B:247:GLY:O	2.16	0.45
2:B:281:PRO:O	2:B:282:ILE:C	2.59	0.45
2:B:578:THR:O	2:B:589:VAL:HG13	2.15	0.45
2:B:615:MET:CG	2:B:626:ILE:HG12	2.46	0.45
2:B:797:TYR:HE1	2:B:854:LEU:CD2	2.29	0.45
2:B:842:ASN:O	2:B:846:ILE:HG13	2.17	0.45
2:B:1050:ILE:CG2	2:B:1051:THR:N	2.79	0.45
7:G:61:ILE:C	7:G:62:LEU:O	2.57	0.45
7:G:121:PHE:HB2	7:G:130:TYR:CE2	2.52	0.45
9:I:55:THR:OG1	9:I:100:PHE:CD2	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:68:PHE:N	11:K:68:PHE:CD2	2.80	0.45
14:1:12:DG:H2'	14:1:13:DT:H72	1.98	0.45
1:A:260:ASP:O	1:A:261:ASP:C	2.58	0.45
1:A:273:ASN:O	1:A:274:ILE:C	2.59	0.45
1:A:573:SER:O	1:A:576:GLN:HB2	2.16	0.45
1:A:645:LEU:HG	1:A:649:ILE:CD1	2.47	0.45
1:A:685:GLU:HG3	1:A:686:ALA:N	2.32	0.45
1:A:843:LYS:NZ	1:A:1401:SER:OG	2.49	0.45
2:B:68:THR:HG22	2:B:91:SER:HB3	1.97	0.45
2:B:642:ASP:CA	2:B:649:LYS:HG3	2.47	0.45
3:C:24:ASN:CG	3:C:24:ASN:O	2.59	0.45
3:C:70:ILE:HD11	3:C:144:ILE:HD11	1.99	0.45
4:D:195:ILE:HB	4:D:198:LEU:HD12	1.99	0.45
8:H:39:THR:O	8:H:123:MET:HA	2.17	0.45
10:J:48:ARG:HE	10:J:49:MET:CE	2.29	0.45
1:A:384:ASN:O	1:A:385:ILE:C	2.56	0.45
1:A:424:ILE:CG2	1:A:425:GLN:N	2.79	0.45
1:A:731:ARG:O	1:A:735:VAL:HG23	2.17	0.45
1:A:853:ASP:OD1	1:A:855:THR:CG2	2.65	0.45
2:B:113:TYR:CE2	2:B:192:LEU:HD21	2.51	0.45
2:B:205:ILE:C	2:B:207:GLY:N	2.73	0.45
2:B:218:SER:O	2:B:241:ARG:NH1	2.50	0.45
2:B:244:LEU:HD11	2:B:366:GLN:HE21	1.74	0.45
2:B:269:ILE:HG22	2:B:282:ILE:HG23	1.99	0.45
2:B:294:ASP:C	2:B:296:GLU:N	2.72	0.45
2:B:515:HIS:CD2	2:B:517:THR:HG23	2.52	0.45
2:B:520:GLY:C	2:B:521:LEU:HD23	2.42	0.45
2:B:603:LEU:HB3	2:B:609:ILE:CD1	2.47	0.45
2:B:848:ARG:HD3	10:J:11:GLY:HA2	1.97	0.45
3:C:123:ASN:OD1	3:C:124:LEU:N	2.50	0.45
4:D:176:GLU:C	4:D:178:ALA:N	2.72	0.45
10:J:34:THR:O	10:J:35:ALA:C	2.58	0.45
10:J:58:GLU:HA	10:J:61:LEU:HD12	1.99	0.45
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.99	0.45
1:A:476:SER:HB2	1:A:477:PRO:HD3	1.98	0.45
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.81	0.45
1:A:1208:THR:O	1:A:1211:GLN:HB2	2.17	0.45
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.85	0.45
1:A:1410:PHE:HA	2:B:1212:ILE:HD11	1.98	0.45
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.52	0.45
2:B:435:THR:C	2:B:437:GLU:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:659:ALA:HA	2:B:662:MET:HE3	1.99	0.45
2:B:840:ILE:CG2	2:B:994:TYR:HD1	2.31	0.45
2:B:1115:THR:HG22	2:B:1117:GLN:N	2.30	0.45
4:D:53:SER:HA	4:D:56:ARG:CB	2.47	0.45
9:I:7:CYS:HB2	9:I:34:TYR:CD1	2.51	0.45
9:I:98:VAL:HG13	9:I:100:PHE:CE1	2.44	0.45
11:K:24:ASP:OD1	11:K:24:ASP:C	2.60	0.45
1:A:12:ARG:NH2	2:B:1192:TYR:CZ	2.83	0.44
1:A:122:MET:HA	1:A:141:LEU:CD1	2.47	0.44
1:A:174:ILE:HG22	1:A:175:ARG:N	2.30	0.44
1:A:367:PRO:HB3	1:A:465:TYR:O	2.18	0.44
1:A:791:ASP:C	1:A:791:ASP:OD1	2.60	0.44
1:A:946:VAL:HG12	1:A:947:PHE:CE2	2.50	0.44
1:A:960:ILE:O	1:A:961:ARG:C	2.60	0.44
1:A:1291:VAL:HG22	1:A:1292:PRO:CD	2.47	0.44
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.82	0.44
2:B:542:MET:CE	2:B:747:MET:HG3	2.47	0.44
2:B:604:ARG:C	2:B:606:LYS:H	2.24	0.44
2:B:1001:PHE:HD1	2:B:1001:PHE:O	2.00	0.44
2:B:1102:LYS:C	2:B:1122:ARG:NH1	2.75	0.44
2:B:1197:PRO:O	2:B:1198:TYR:C	2.59	0.44
4:D:15:LEU:C	4:D:17:LYS:H	2.25	0.44
5:E:92:THR:O	5:E:95:THR:HB	2.17	0.44
7:G:22:MET:O	7:G:23:LYS:C	2.59	0.44
7:G:51:TYR:C	7:G:51:TYR:HD2	2.23	0.44
1:A:90:VAL:CG1	1:A:297:GLN:CD	2.90	0.44
1:A:254:GLU:HB2	2:B:935:ARG:HH22	1.82	0.44
1:A:351:THR:H	1:A:468:PHE:HE1	1.65	0.44
1:A:806:ARG:HH12	2:B:729:ILE:HD12	1.81	0.44
1:A:988:LEU:O	1:A:992:ASP:HB2	2.17	0.44
1:A:1206:ASP:HB3	1:A:1274:ARG:HH12	1.83	0.44
1:A:1336:MET:HE2	1:A:1381:LEU:HG	1.99	0.44
2:B:273:LEU:HD22	2:B:360:PHE:HD1	1.82	0.44
2:B:377:PHE:C	2:B:379:GLY:H	2.24	0.44
2:B:506:GLY:O	2:B:507:LYS:HB2	2.16	0.44
2:B:506:GLY:O	2:B:507:LYS:HG2	2.17	0.44
2:B:519:TRP:HE1	2:B:635:ARG:NH2	2.16	0.44
2:B:866:TYR:O	2:B:867:GLY:C	2.60	0.44
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.99	0.44
5:E:124:VAL:N	5:E:125:PRO:CD	2.80	0.44
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:207:ARG:NH1	5:E:207:ARG:CB	2.80	0.44
7:G:129:SER:CB	7:G:138:THR:HG1	2.30	0.44
1:A:115:LEU:HD22	1:A:119:ASN:CB	2.48	0.44
1:A:137:ALA:O	1:A:138:ILE:C	2.61	0.44
1:A:196:GLU:HG2	1:A:197:PRO:N	2.32	0.44
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.66	0.44
1:A:244:PRO:O	1:A:246:VAL:N	2.51	0.44
1:A:326:ARG:HG2	1:A:326:ARG:NH1	2.32	0.44
1:A:498:ARG:O	1:A:501:LEU:N	2.51	0.44
1:A:913:LEU:CG	1:A:914:GLU:N	2.80	0.44
1:A:1094:VAL:HG13	1:A:1113:THR:CG2	2.47	0.44
1:A:1150:SER:HB3	1:A:1195:LEU:CD2	2.48	0.44
1:A:1444:MET:HE3	1:A:1444:MET:HB2	1.74	0.44
2:B:171:PRO:HD2	2:B:457:LEU:HD13	2.00	0.44
2:B:186:GLU:HG3	10:J:62:ARG:HH22	1.81	0.44
2:B:522:VAL:CG1	2:B:523:CYS:N	2.79	0.44
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.30	0.44
2:B:620:ARG:NH2	9:I:86:PHE:HB3	2.33	0.44
2:B:916:THR:CB	2:B:935:ARG:HD2	2.44	0.44
2:B:1214:PRO:O	2:B:1214:PRO:HG2	2.18	0.44
3:C:182:PRO:HD2	3:C:210:GLU:OE1	2.17	0.44
4:D:20:GLU:O	4:D:20:GLU:HG2	2.17	0.44
4:D:35:LEU:H	4:D:35:LEU:CD1	2.30	0.44
5:E:63:ASN:HB3	5:E:64:PRO:HD2	1.99	0.44
5:E:144:ILE:HG13	5:E:145:THR:H	1.83	0.44
6:F:85:MET:HE2	6:F:93:ILE:CD1	2.46	0.44
6:F:99:LEU:O	6:F:103:MET:HG3	2.17	0.44
6:F:154:ASP:HB3	6:F:155:LEU:H	1.64	0.44
10:J:7:CYS:O	10:J:8:PHE:C	2.60	0.44
1:A:89:PRO:CG	1:A:205:GLU:HG3	2.47	0.44
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.53	0.44
1:A:233:TRP:C	1:A:235:ILE:N	2.71	0.44
1:A:300:VAL:O	1:A:300:VAL:HG12	2.18	0.44
1:A:774:ARG:H	1:A:774:ARG:HG2	1.59	0.44
1:A:899:VAL:CB	1:A:929:LEU:HD12	2.36	0.44
1:A:1116:LEU:HD12	1:A:1117:THR:N	2.32	0.44
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.83	0.44
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.66	0.44
2:B:309:GLN:HG3	9:I:52:ILE:HD12	2.00	0.44
2:B:426:LYS:HG3	2:B:426:LYS:O	2.17	0.44
2:B:797:TYR:HE1	2:B:854:LEU:HD23	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:864:LYS:HG3	2:B:872:GLU:CD	2.42	0.44
2:B:1072:MET:HB2	2:B:1085:ILE:HD12	2.00	0.44
3:C:214:ASN:O	3:C:217:ASP:OD2	2.33	0.44
3:C:239:PRO:O	3:C:240:VAL:C	2.60	0.44
4:D:153:ARG:CZ	4:D:184:ALA:HA	2.47	0.44
4:D:185:CYS:HB2	4:D:211:LEU:HD21	2.00	0.44
5:E:11:ARG:O	5:E:13:TRP:N	2.50	0.44
5:E:37:LEU:CD1	5:E:41:ASP:HB2	2.47	0.44
7:G:56:ILE:O	7:G:57:GLN:HB2	2.18	0.44
9:I:56:ALA:O	9:I:57:GLY:C	2.60	0.44
11:K:53:ASP:OD2	11:K:81:TYR:OH	2.35	0.44
14:1:11:DA:H2''	14:1:12:DG:H5'	1.99	0.44
1:A:523:ILE:CG1	1:A:622:VAL:HG22	2.44	0.44
1:A:688:LYS:CE	1:A:691:LEU:HD23	2.47	0.44
1:A:742:ASN:O	1:A:743:VAL:C	2.61	0.44
1:A:1423:GLY:O	1:A:1424:VAL:C	2.57	0.44
2:B:801:LYS:N	10:J:52:THR:HG22	2.33	0.44
2:B:912:ILE:HD11	2:B:966:VAL:HG23	2.00	0.44
3:C:22:LEU:HB2	3:C:230:MET:HE3	2.00	0.44
3:C:69:LEU:HD12	3:C:69:LEU:N	2.20	0.44
5:E:78:LEU:HD23	5:E:78:LEU:C	2.43	0.44
5:E:91:LYS:C	5:E:93:MET:N	2.76	0.44
8:H:33:GLN:NE2	8:H:129:TYR:CE2	2.85	0.44
8:H:143:LEU:C	8:H:144:ILE:HG13	2.41	0.44
1:A:38:PRO:CA	1:A:270:LEU:HD23	2.47	0.44
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.53	0.44
1:A:337:ARG:HD3	2:B:1132:GLU:CD	2.42	0.44
1:A:360:GLU:HB2	1:A:363:GLN:HG3	1.99	0.44
1:A:442:VAL:HG23	1:A:489:LEU:HD11	1.99	0.44
1:A:699:ALA:O	1:A:700:ASN:HB3	2.18	0.44
1:A:774:ARG:O	1:A:775:ILE:C	2.58	0.44
1:A:1447:GLU:C	1:A:1447:GLU:OE1	2.60	0.44
2:B:56:ASP:HB3	2:B:57:TYR:CD1	2.53	0.44
2:B:277:LYS:HZ1	2:B:336:ARG:HD3	1.82	0.44
2:B:644:GLU:OE1	2:B:644:GLU:HA	2.15	0.44
2:B:882:THR:O	2:B:883:LEU:HB2	2.17	0.44
2:B:1020:ARG:NH1	2:B:1020:ARG:CG	2.80	0.44
3:C:124:LEU:HD12	3:C:124:LEU:H	1.81	0.44
3:C:133:ILE:HD12	3:C:236:GLY:C	2.43	0.44
3:C:233:GLU:OE1	10:J:12:LYS:HE2	2.18	0.44
4:D:195:ILE:HG22	4:D:198:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:43:ASN:C	8:H:45:GLU:H	2.26	0.44
11:K:90:ALA:O	11:K:94:ILE:HG13	2.18	0.44
1:A:289:ILE:C	1:A:291:GLU:N	2.75	0.44
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.98	0.44
4:D:70:PHE:O	4:D:71:LYS:HG3	2.17	0.44
7:G:145:VAL:HG12	7:G:146:LYS:N	2.33	0.44
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.98	0.44
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.47	0.44
11:K:53:ASP:O	11:K:56:VAL:N	2.49	0.44
11:K:67:PHE:C	11:K:68:PHE:HD2	2.25	0.44
11:K:79:GLU:C	11:K:81:TYR:H	2.26	0.44
1:A:562:THR:HA	1:A:563:PRO:HD3	1.90	0.44
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.99	0.44
1:A:850:VAL:HG12	1:A:1060:PRO:HA	2.00	0.44
1:A:1134:ILE:HG13	1:A:1134:ILE:H	1.52	0.44
1:A:1450:LEU:CD2	7:G:19:GLY:O	2.65	0.44
2:B:212:LEU:HD23	2:B:480:SER:HB2	2.00	0.44
2:B:272:THR:HG23	2:B:279:ASP:OD1	2.18	0.44
2:B:652:LYS:HB3	2:B:689:LEU:HD22	1.99	0.44
2:B:707:PRO:HG2	2:B:708:GLU:N	2.30	0.44
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.53	0.44
2:B:801:LYS:H	10:J:52:THR:HG22	1.82	0.44
2:B:866:TYR:HB2	2:B:870:ILE:HB	2.00	0.44
2:B:948:ILE:O	2:B:968:VAL:HG13	2.18	0.44
2:B:1064:TYR:O	2:B:1065:GLN:C	2.60	0.44
3:C:15:LYS:O	3:C:240:VAL:HG22	2.18	0.44
3:C:66:ARG:O	3:C:68:GLY:N	2.51	0.44
6:F:99:LEU:HD21	7:G:65:ASP:C	2.43	0.44
6:F:140:ASP:C	6:F:140:ASP:OD1	2.60	0.44
7:G:88:ASP:OD2	7:G:88:ASP:N	2.45	0.44
8:H:38:LEU:HD13	8:H:125:LEU:HD12	1.99	0.44
9:I:14:LEU:HA	9:I:28:GLU:O	2.18	0.44
11:K:27:ALA:HB1	11:K:28:PRO:HD2	1.99	0.44
11:K:78:THR:HG22	11:K:79:GLU:H	1.83	0.44
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.53	0.44
1:A:325:ILE:CG2	2:B:1210:MET:HE2	2.48	0.44
1:A:433:GLU:OE2	2:B:1108:ARG:NH2	2.51	0.44
1:A:516:SER:O	1:A:518:LYS:N	2.51	0.44
1:A:789:LYS:CD	2:B:620:ARG:HH12	2.30	0.44
1:A:1171:GLN:H	1:A:1171:GLN:HG3	1.49	0.44
2:B:185:THR:H	2:B:188:ASP:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:MET:O	2:B:311:LEU:C	2.61	0.44
2:B:710:LEU:C	2:B:711:GLU:HG2	2.43	0.44
2:B:953:LEU:HD22	2:B:965:LYS:HB2	2.00	0.44
2:B:1131:GLY:N	2:B:1134:GLU:OE1	2.50	0.44
3:C:16:ASP:O	3:C:17:ASN:CG	2.61	0.44
4:D:64:VAL:O	4:D:66:ARG:N	2.50	0.44
5:E:67:GLU:O	5:E:70:SER:HB2	2.18	0.44
10:J:16:ASP:O	10:J:18:TRP:N	2.51	0.44
1:A:349:ALA:C	2:B:1128:LEU:HD11	2.43	0.43
1:A:596:THR:O	1:A:597:LEU:C	2.59	0.43
1:A:605:MET:HE1	1:A:612:ILE:HG23	2.00	0.43
1:A:1167:GLU:O	1:A:1170:ILE:HD12	2.17	0.43
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.80	0.43
1:A:1259:MET:HA	1:A:1262:LYS:CD	2.41	0.43
2:B:186:GLU:CG	10:J:62:ARG:HH12	2.30	0.43
2:B:186:GLU:HG3	10:J:62:ARG:NH2	2.33	0.43
2:B:414:ALA:O	2:B:415:GLN:C	2.61	0.43
2:B:418:LYS:HE2	2:B:422:LYS:CE	2.48	0.43
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.48	0.43
2:B:966:VAL:HG12	2:B:967:ARG:H	1.82	0.43
2:B:1045:SER:O	2:B:1046:PRO:O	2.35	0.43
5:E:100:ILE:HG23	5:E:105:PHE:HB2	2.00	0.43
5:E:154:ILE:O	5:E:196:VAL:HA	2.17	0.43
6:F:152:ILE:HG22	6:F:153:VAL:N	2.33	0.43
9:I:25:LEU:HB3	9:I:38:ALA:CB	2.48	0.43
9:I:59:VAL:C	9:I:61:ASP:H	2.26	0.43
10:J:19:GLU:O	10:J:20:SER:C	2.60	0.43
11:K:91:CYS:O	11:K:92:ASN:C	2.60	0.43
12:L:38:LEU:CG	12:L:39:SER:N	2.81	0.43
1:A:67:CYS:O	1:A:68:GLN:HG3	2.18	0.43
1:A:122:MET:HA	1:A:141:LEU:HD11	2.00	0.43
1:A:511:ILE:HA	1:A:521:MET:HE3	2.01	0.43
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.48	0.43
1:A:1397:LEU:CB	1:A:1426:GLU:OE1	2.65	0.43
1:A:1404:GLU:O	1:A:1405:THR:C	2.60	0.43
2:B:522:VAL:HG12	2:B:523:CYS:N	2.31	0.43
2:B:535:LEU:HA	2:B:535:LEU:HD23	1.70	0.43
2:B:604:ARG:CA	2:B:609:ILE:HG13	2.47	0.43
2:B:687:GLU:O	2:B:688:GLY:C	2.60	0.43
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.48	0.43
3:C:124:LEU:O	3:C:125:MET:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:136:ASP:OD2	3:C:137:LYS:N	2.52	0.43
5:E:59:SER:O	5:E:60:PHE:HB3	2.17	0.43
5:E:80:VAL:HG12	5:E:82:PHE:HE1	1.83	0.43
6:F:111:LEU:C	6:F:113:GLY:N	2.76	0.43
8:H:11:GLN:O	8:H:28:ALA:HB1	2.18	0.43
9:I:8:ARG:HG2	9:I:34:TYR:CE1	2.52	0.43
10:J:21:TYR:HB2	10:J:39:LEU:CD1	2.48	0.43
1:A:356:ASP:HA	1:A:357:PRO:HD2	1.78	0.43
1:A:433:GLU:CD	2:B:1108:ARG:NH2	2.76	0.43
1:A:498:ARG:O	1:A:499:ALA:C	2.61	0.43
1:A:915:SER:O	1:A:919:ILE:HB	2.18	0.43
2:B:351:TYR:CD1	2:B:355:ILE:HD11	2.53	0.43
2:B:831:SER:HB3	2:B:994:TYR:OH	2.18	0.43
2:B:880:THR:HG22	2:B:880:THR:O	2.17	0.43
3:C:70:ILE:CD1	3:C:144:ILE:HD11	2.49	0.43
5:E:102:GLU:C	5:E:104:ASN:H	2.26	0.43
6:F:79:ARG:CG	6:F:144:GLU:HB3	2.49	0.43
10:J:64:ASN:CB	10:J:65:PRO:CD	2.89	0.43
1:A:34:LYS:HD3	1:A:57:ARG:NH2	2.32	0.43
1:A:1387:HIS:NE2	13:2:4:DA:H5'	2.33	0.43
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.18	0.43
3:C:172:PRO:O	3:C:235:VAL:HG23	2.18	0.43
4:D:177:VAL:O	4:D:177:VAL:HG12	2.19	0.43
7:G:127:PRO:O	7:G:138:THR:HG21	2.17	0.43
10:J:1:MET:H3	10:J:56:LEU:N	2.16	0.43
10:J:24:LEU:HA	10:J:28:ASP:HB2	1.99	0.43
10:J:56:LEU:O	10:J:57:ILE:C	2.60	0.43
11:K:55:LYS:CB	11:K:81:TYR:CD1	3.01	0.43
1:A:108:MET:SD	1:A:210:ILE:HD13	2.58	0.43
1:A:718:VAL:HG12	1:A:722:LEU:HD11	2.00	0.43
1:A:896:ARG:NH2	1:A:1030:ARG:NH2	2.66	0.43
2:B:63:ILE:HG23	2:B:64:CYS:SG	2.58	0.43
2:B:165:VAL:HG11	2:B:448:ILE:CD1	2.48	0.43
2:B:520:GLY:O	2:B:521:LEU:HD23	2.18	0.43
2:B:589:VAL:HG12	2:B:590:HIS:O	2.19	0.43
2:B:805:THR:HA	2:B:809:MET:HE1	2.01	0.43
2:B:840:ILE:HG21	2:B:994:TYR:CD1	2.53	0.43
2:B:980:PHE:HD2	2:B:1094:ARG:HA	1.82	0.43
2:B:1037:LEU:CD2	2:B:1064:TYR:HE1	2.32	0.43
2:B:1045:SER:O	2:B:1048:THR:CG2	2.67	0.43
5:E:11:ARG:C	5:E:13:TRP:N	2.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.66	0.43
8:H:24:CYS:SG	8:H:44:VAL:HG21	2.58	0.43
8:H:130:ARG:HH11	8:H:130:ARG:H	1.65	0.43
1:A:306:ASN:CG	1:A:306:ASN:O	2.60	0.43
1:A:325:ILE:O	1:A:326:ARG:C	2.61	0.43
1:A:849:MET:HB3	1:A:1063:MET:SD	2.58	0.43
1:A:856:THR:O	1:A:856:THR:HG22	2.16	0.43
1:A:942:PHE:HE1	5:E:207:ARG:HD3	1.83	0.43
1:A:1365:TYR:CE2	1:A:1369:ALA:HB2	2.54	0.43
2:B:282:ILE:HG13	2:B:283:VAL:N	2.33	0.43
2:B:468:GLU:HB3	2:B:469:GLN:H	1.32	0.43
2:B:582:VAL:HG22	2:B:626:ILE:HG21	2.01	0.43
2:B:789:MET:HE2	2:B:953:LEU:HD22	2.00	0.43
2:B:830:TYR:C	2:B:832:GLY:N	2.77	0.43
2:B:887:HIS:CD2	2:B:887:HIS:N	2.87	0.43
3:C:101:LEU:HD12	3:C:118:LEU:CD2	2.47	0.43
3:C:185:LYS:HE2	3:C:213:PRO:HA	1.99	0.43
7:G:21:ARG:HD2	7:G:24:GLN:CB	2.49	0.43
8:H:104:PHE:CD2	8:H:114:VAL:HG12	2.54	0.43
9:I:50:THR:HG21	9:I:52:ILE:HG12	1.96	0.43
9:I:98:VAL:CG1	9:I:100:PHE:HE1	2.29	0.43
9:I:104:LEU:N	9:I:104:LEU:HD23	2.33	0.43
13:2:4:DA:H2''	13:2:5:DC:H6	1.83	0.43
1:A:49:LYS:CD	1:A:55:ASP:HB3	2.49	0.43
1:A:255:SER:O	1:A:256:GLN:HG3	2.19	0.43
1:A:341:MET:HE3	1:A:341:MET:HB3	1.89	0.43
1:A:414:ASP:OD1	1:A:416:ARG:HG2	2.19	0.43
1:A:711:ARG:HA	9:I:97:MET:HE2	2.00	0.43
1:A:1053:PHE:O	1:A:1054:LEU:C	2.62	0.43
1:A:1067:LEU:HD12	1:A:1067:LEU:C	2.44	0.43
2:B:729:ILE:O	2:B:729:ILE:HG22	2.18	0.43
2:B:874:PHE:HB3	2:B:896:ASP:O	2.19	0.43
2:B:1148:LYS:HE3	7:G:64:THR:OG1	2.19	0.43
3:C:77:ILE:HG23	3:C:161:LYS:HE3	1.99	0.43
3:C:97:VAL:HG12	3:C:99:LEU:CD2	2.48	0.43
3:C:233:GLU:CG	3:C:234:SER:N	2.82	0.43
4:D:118:THR:HG21	4:D:121:LYS:CE	2.48	0.43
7:G:13:LEU:HD21	7:G:17:PHE:CB	2.49	0.43
9:I:55:THR:HG21	9:I:109:ILE:HD13	2.00	0.43
9:I:95:THR:HG22	9:I:96:SER:N	2.34	0.43
11:K:31:VAL:CG2	11:K:83:PRO:HG3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:19:DT:H2''	14:1:20:DG:O5'	2.18	0.43
1:A:244:PRO:O	1:A:245:PRO:C	2.62	0.43
1:A:598:LEU:CD1	8:H:124:ARG:HB2	2.48	0.43
1:A:794:PRO:C	1:A:796:SER:N	2.76	0.43
1:A:1315:GLU:C	1:A:1317:MET:H	2.27	0.43
1:A:1451:VAL:HG12	1:A:1452:LYS:N	2.34	0.43
2:B:65:GLU:HG3	2:B:66:ASP:H	1.84	0.43
2:B:244:LEU:HD12	2:B:250:PHE:HD1	1.84	0.43
2:B:287:ARG:HB3	2:B:330:ALA:HB2	2.01	0.43
2:B:957:ASN:O	2:B:958:GLN:C	2.61	0.43
3:C:235:VAL:CG1	10:J:13:VAL:HG22	2.48	0.43
4:D:216:ASN:C	4:D:218:GLU:N	2.73	0.43
5:E:91:LYS:O	5:E:93:MET:N	2.51	0.43
5:E:157:SER:OG	5:E:160:GLU:HG3	2.19	0.43
6:F:133:VAL:HG13	6:F:146:TRP:O	2.18	0.43
7:G:127:PRO:O	7:G:128:PRO:C	2.62	0.43
9:I:82:GLU:OE2	9:I:104:LEU:HD12	2.19	0.43
1:A:69:THR:C	1:A:71:GLN:N	2.75	0.43
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.67	0.43
1:A:270:LEU:O	1:A:274:ILE:HG13	2.19	0.43
1:A:457:ALA:HB3	1:A:506:ALA:HA	2.00	0.43
1:A:754:SER:O	1:A:757:ASN:HB2	2.18	0.43
1:A:786:HIS:HE1	2:B:705:MET:HE1	1.80	0.43
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.18	0.43
1:A:1040:GLN:O	1:A:1041:ALA:C	2.61	0.43
2:B:57:TYR:HD1	2:B:57:TYR:H	1.65	0.43
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.52	0.43
2:B:711:GLU:H	2:B:712:PRO:HD2	1.83	0.43
2:B:765:PRO:O	2:B:766:ARG:C	2.62	0.43
2:B:1069:PHE:H	2:B:1069:PHE:HD1	1.66	0.43
3:C:80:LEU:HD12	3:C:94:LYS:O	2.18	0.43
3:C:174:ALA:O	3:C:175:ALA:HB3	2.19	0.43
3:C:213:PRO:HG2	3:C:214:ASN:H	1.83	0.43
4:D:32:GLU:O	4:D:33:PHE:CG	2.72	0.43
4:D:138:ASN:C	4:D:140:ASP:N	2.74	0.43
6:F:84:TYR:N	6:F:84:TYR:CD1	2.87	0.43
7:G:53:ASN:N	7:G:53:ASN:ND2	2.67	0.43
1:A:162:VAL:HG12	1:A:163:SER:N	2.34	0.43
1:A:372:LYS:O	1:A:435:HIS:HE1	2.02	0.43
1:A:482:PHE:C	1:A:484:GLY:N	2.77	0.43
1:A:939:ASP:OD1	1:A:1023:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:ASN:C	1:A:954:TRP:CD1	2.97	0.43
1:A:1120:LEU:H	1:A:1120:LEU:HG	1.37	0.43
3:C:101:LEU:C	3:C:102:GLN:HG3	2.43	0.43
4:D:195:ILE:O	4:D:196:PRO:C	2.62	0.43
5:E:2:ASP:C	5:E:3:GLN:HG2	2.43	0.43
7:G:126:ASN:HD22	7:G:127:PRO:N	2.17	0.43
8:H:106:GLU:C	8:H:108:SER:N	2.77	0.43
11:K:91:CYS:O	11:K:94:ILE:HB	2.19	0.43
1:A:6:TYR:CD1	1:A:7:SER:N	2.87	0.42
1:A:106:VAL:CG1	1:A:107:CYS:H	2.31	0.42
1:A:417:TYR:O	1:A:418:SER:C	2.62	0.42
1:A:478:TYR:O	1:A:479:ASN:HB3	2.19	0.42
1:A:1050:GLU:O	1:A:1053:PHE:HB3	2.19	0.42
1:A:1410:PHE:HD2	2:B:1212:ILE:CD1	2.32	0.42
2:B:39:ARG:HE	2:B:665:GLU:HG2	1.83	0.42
2:B:51:PHE:O	2:B:52:ASN:C	2.62	0.42
2:B:67:SER:O	2:B:68:THR:O	2.36	0.42
2:B:508:LEU:HD23	2:B:508:LEU:N	2.34	0.42
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.90	0.42
2:B:614:SER:C	2:B:615:MET:HG3	2.43	0.42
2:B:654:ARG:H	2:B:657:HIS:CD2	2.36	0.42
2:B:705:MET:HA	2:B:705:MET:CE	2.41	0.42
2:B:1187:ASN:OD1	2:B:1188:LYS:N	2.52	0.42
3:C:181:ASP:CG	3:C:185:LYS:H	2.27	0.42
4:D:14:ARG:O	4:D:16:LYS:N	2.44	0.42
5:E:72:PHE:CD1	5:E:72:PHE:N	2.86	0.42
5:E:161:LYS:C	5:E:163:GLU:N	2.76	0.42
6:F:138:LEU:C	6:F:140:ASP:H	2.28	0.42
7:G:111:THR:O	7:G:112:LYS:C	2.62	0.42
8:H:12:VAL:CG2	8:H:53:ASP:HB2	2.49	0.42
8:H:100:THR:HG22	8:H:101:ALA:N	2.34	0.42
8:H:113:ALA:HB1	8:H:124:ARG:HE	1.83	0.42
12:L:59:ALA:O	12:L:60:ARG:O	2.37	0.42
1:A:102:VAL:HG21	1:A:234:MET:HE1	1.99	0.42
1:A:244:PRO:O	1:A:247:ARG:N	2.51	0.42
1:A:372:LYS:O	1:A:435:HIS:CE1	2.72	0.42
1:A:690:VAL:HG23	1:A:718:VAL:HG13	2.00	0.42
1:A:888:GLY:O	1:A:940:ARG:NH2	2.52	0.42
1:A:940:ARG:O	1:A:941:LYS:C	2.62	0.42
1:A:1035:TYR:O	1:A:1036:ARG:HB2	2.18	0.42
1:A:1283:VAL:O	1:A:1306:LEU:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1334:ASP:C	1:A:1336:MET:N	2.75	0.42
2:B:29:ASP:CB	2:B:658:ILE:HD13	2.49	0.42
2:B:476:ARG:O	2:B:477:ALA:C	2.60	0.42
2:B:770:GLN:OE1	2:B:983:ARG:CA	2.56	0.42
3:C:213:PRO:O	3:C:214:ASN:CB	2.67	0.42
7:G:88:ASP:HA	7:G:143:ILE:O	2.19	0.42
8:H:16:ASP:O	8:H:24:CYS:HA	2.18	0.42
10:J:16:ASP:CG	10:J:17:LYS:HD2	2.44	0.42
11:K:86:ALA:HA	11:K:89:ASN:ND2	2.34	0.42
1:A:107:CYS:CB	1:A:114:LEU:HD21	2.40	0.42
1:A:359:LEU:HA	1:A:359:LEU:HD23	1.80	0.42
1:A:883:LEU:O	1:A:884:ASP:C	2.62	0.42
1:A:935:GLN:O	1:A:938:LYS:N	2.52	0.42
1:A:1259:MET:HE3	1:A:1263:ILE:HG13	2.01	0.42
1:A:1385:THR:O	1:A:1386:ARG:C	2.61	0.42
2:B:103:ASN:ND2	2:B:108:VAL:O	2.52	0.42
2:B:398:ARG:CB	2:B:398:ARG:HH11	2.32	0.42
2:B:466:TRP:CE3	2:B:466:TRP:HA	2.54	0.42
2:B:579:ARG:HG2	2:B:579:ARG:HH11	1.82	0.42
2:B:841:MET:O	2:B:993:THR:HB	2.19	0.42
2:B:866:TYR:HB3	2:B:870:ILE:HD12	2.01	0.42
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.52	0.42
2:B:1082:MET:HA	3:C:189:THR:HA	2.01	0.42
2:B:1099:VAL:HG13	2:B:1100:ASP:H	1.84	0.42
3:C:10:ILE:C	3:C:11:ARG:O	2.60	0.42
3:C:97:VAL:HG21	3:C:129:ILE:HG22	2.00	0.42
4:D:155:ARG:HG3	4:D:219:THR:HG21	1.96	0.42
5:E:56:LYS:HZ3	5:E:84:ASP:N	2.14	0.42
1:A:549:MET:CE	1:A:656:TRP:HD1	2.32	0.42
1:A:774:ARG:HG3	1:A:797:LYS:HB3	2.01	0.42
1:A:1011:GLN:HE22	1:A:1015:VAL:HG21	1.85	0.42
2:B:65:GLU:HG3	2:B:66:ASP:N	2.35	0.42
2:B:398:ARG:NH1	2:B:398:ARG:CB	2.82	0.42
2:B:600:LEU:HA	2:B:603:LEU:HB2	2.00	0.42
2:B:603:LEU:HD13	2:B:608:ASP:CB	2.40	0.42
2:B:936:ASP:CG	2:B:937:ALA:H	2.27	0.42
2:B:1212:ILE:O	2:B:1214:PRO:HD3	2.19	0.42
3:C:62:PHE:C	3:C:62:PHE:CD2	2.97	0.42
4:D:29:LEU:HB3	7:G:82:PHE:HE2	1.82	0.42
5:E:153:HIS:CE1	5:E:184:VAL:HG11	2.54	0.42
10:J:57:ILE:HG23	10:J:58:GLU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:47:ARG:HH11	11:K:47:ARG:CB	2.23	0.42
1:A:49:LYS:HZ1	1:A:61:ILE:H	1.62	0.42
1:A:125:ALA:C	1:A:127:ALA:N	2.75	0.42
1:A:356:ASP:C	1:A:356:ASP:OD1	2.62	0.42
1:A:1232:ASN:O	1:A:1233:ASP:O	2.38	0.42
1:A:1387:HIS:CD2	13:2:4:DA:H5'	2.54	0.42
2:B:498:THR:O	2:B:536:VAL:HA	2.18	0.42
2:B:734:HIS:O	2:B:735:ALA:CB	2.66	0.42
2:B:798:TYR:CE2	3:C:62:PHE:CZ	2.94	0.42
2:B:1104:HIS:HB2	2:B:1122:ARG:HD2	2.01	0.42
2:B:1156:ASP:O	2:B:1157:ALA:C	2.63	0.42
3:C:221:TYR:HD1	3:C:222:LYS:N	2.17	0.42
3:C:258:ILE:N	3:C:258:ILE:CD1	2.83	0.42
4:D:40:HIS:HE1	7:G:7:LEU:O	2.01	0.42
4:D:176:GLU:C	4:D:178:ALA:H	2.26	0.42
7:G:49:LEU:HG	7:G:76:ALA:HA	2.02	0.42
7:G:154:VAL:HB	7:G:155:SER:H	1.41	0.42
1:A:75:ASN:HD22	2:B:1116:ARG:NH1	2.17	0.42
1:A:141:LEU:HD23	1:A:141:LEU:HA	1.84	0.42
1:A:253:ASN:ND2	2:B:884:ARG:HD2	2.35	0.42
1:A:313:GLN:O	1:A:314:ALA:C	2.62	0.42
1:A:369:SER:HB3	11:K:2:ASN:CG	2.44	0.42
1:A:381:THR:HG23	1:A:382:PRO:CD	2.39	0.42
1:A:904:THR:O	1:A:904:THR:CG2	2.68	0.42
1:A:1155:ASP:OD2	1:A:1162:VAL:N	2.47	0.42
2:B:95:ILE:CD1	2:B:130:VAL:HG22	2.50	0.42
2:B:236:HIS:O	2:B:237:VAL:HG23	2.20	0.42
2:B:360:PHE:CE2	2:B:361:LEU:HD13	2.54	0.42
2:B:558:LEU:O	2:B:559:SER:C	2.62	0.42
2:B:703:ILE:HA	2:B:740:HIS:O	2.20	0.42
2:B:758:PHE:CE1	2:B:1027:ILE:CG2	3.02	0.42
2:B:878:GLN:HB3	2:B:879:ARG:HH11	1.85	0.42
5:E:112:TYR:C	5:E:112:TYR:CD1	2.97	0.42
8:H:102:TYR:OH	8:H:122:LEU:HD22	2.20	0.42
11:K:82:ASP:OD1	11:K:84:LYS:N	2.53	0.42
1:A:12:ARG:HB3	2:B:1218:THR:HG22	2.02	0.42
1:A:103:CYS:SG	1:A:108:MET:HE1	2.59	0.42
1:A:377:PRO:O	1:A:377:PRO:HG2	2.20	0.42
1:A:382:PRO:HD3	1:A:428:TYR:HD2	1.81	0.42
1:A:683:ILE:O	1:A:684:ALA:C	2.63	0.42
1:A:710:LEU:O	1:A:714:PHE:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:LEU:HB3	1:A:785:PRO:HD2	2.02	0.42
1:A:842:VAL:HG11	2:B:1136:ASP:CG	2.44	0.42
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.85	0.42
1:A:1287:TYR:CD1	1:A:1305:VAL:HG21	2.54	0.42
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.18	0.42
1:A:1454:MET:O	1:A:1454:MET:HG3	2.20	0.42
2:B:210:LYS:HE2	2:B:461:LEU:O	2.20	0.42
2:B:280:ILE:HG23	2:B:281:PRO:HD2	2.02	0.42
2:B:469:GLN:O	2:B:472:ALA:CB	2.62	0.42
2:B:637:LEU:O	2:B:690:VAL:HG13	2.19	0.42
2:B:736:THR:O	2:B:736:THR:HG22	2.19	0.42
2:B:1202:LEU:O	2:B:1203:LEU:C	2.62	0.42
3:C:79:GLN:HG3	3:C:79:GLN:O	2.18	0.42
3:C:98:VAL:HG13	3:C:157:CYS:O	2.17	0.42
3:C:114:TYR:C	3:C:116:LYS:H	2.28	0.42
3:C:241:ASP:CG	3:C:242:GLN:H	2.27	0.42
4:D:122:GLU:HA	4:D:125:SER:HB3	2.00	0.42
4:D:189:ASP:O	4:D:190:GLU:C	2.62	0.42
7:G:59:GLY:CA	7:G:70:PHE:CD2	3.01	0.42
7:G:90:THR:CG2	7:G:91:VAL:N	2.83	0.42
9:I:8:ARG:HG2	9:I:34:TYR:CD1	2.54	0.42
1:A:153:PRO:HD3	1:A:161:LEU:HD13	2.01	0.42
1:A:277:GLU:O	1:A:277:GLU:HG2	2.20	0.42
1:A:492:PRO:O	1:A:493:GLN:NE2	2.52	0.42
1:A:1305:VAL:CG1	1:A:1306:LEU:N	2.83	0.42
1:A:1334:ASP:O	1:A:1337:GLU:N	2.43	0.42
1:A:1431:GLY:O	2:B:1152:MET:HE2	2.19	0.42
2:B:236:HIS:C	2:B:237:VAL:HG23	2.45	0.42
2:B:487:THR:O	2:B:490:SER:HB3	2.20	0.42
2:B:552:MET:HA	2:B:552:MET:CE	2.49	0.42
2:B:557:PHE:HZ	2:B:603:LEU:HD11	1.85	0.42
2:B:831:SER:HB2	2:B:833:TYR:CD1	2.55	0.42
5:E:11:ARG:O	5:E:12:LEU:C	2.62	0.42
5:E:22:MET:HG3	5:E:187:TYR:CD1	2.55	0.42
5:E:33:GLU:C	5:E:35:VAL:N	2.78	0.42
5:E:35:VAL:C	5:E:37:LEU:N	2.76	0.42
5:E:39:LEU:HG	5:E:43:LYS:HE3	2.00	0.42
5:E:47:CYS:HB3	5:E:51:GLY:HA2	2.02	0.42
5:E:91:LYS:C	5:E:93:MET:H	2.27	0.42
5:E:144:ILE:C	5:E:146:HIS:N	2.77	0.42
7:G:90:THR:O	7:G:102:GLN:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:109:LYS:HG2	8:H:110:ASP:N	2.34	0.42
9:I:111:THR:CG2	9:I:113:ASP:H	2.32	0.42
12:L:58:LYS:O	12:L:58:LYS:HG2	2.19	0.42
14:1:10:DA:C2'	14:1:11:DA:C8	3.02	0.42
1:A:92:HIS:O	1:A:94:GLY:N	2.53	0.42
1:A:233:TRP:C	1:A:235:ILE:H	2.27	0.42
1:A:369:SER:HB3	11:K:2:ASN:OD1	2.19	0.42
1:A:614:PHE:CD1	1:A:614:PHE:C	2.98	0.42
1:A:667:GLY:C	3:C:192:TRP:HZ2	2.28	0.42
1:A:851:HIS:O	1:A:853:ASP:N	2.53	0.42
1:A:925:LEU:C	1:A:927:VAL:N	2.77	0.42
1:A:1111:MET:HE2	1:A:1113:THR:O	2.19	0.42
1:A:1148:ILE:HD11	1:A:1198:ASP:HB2	2.01	0.42
1:A:1277:GLU:O	1:A:1279:ILE:N	2.52	0.42
2:B:98:THR:HG23	2:B:127:GLY:O	2.20	0.42
2:B:247:GLY:O	2:B:248:SER:HB3	2.20	0.42
2:B:294:ASP:HB2	9:I:12:ASN:HA	2.02	0.42
2:B:641:GLU:O	2:B:643:ASP:N	2.51	0.42
2:B:686:ASN:C	2:B:688:GLY:N	2.70	0.42
2:B:1187:ASN:OD1	2:B:1190:ASP:N	2.53	0.42
3:C:50:GLU:OE1	12:L:64:LEU:CD1	2.68	0.42
3:C:59:ALA:O	3:C:62:PHE:HB3	2.19	0.42
4:D:51:ASN:O	4:D:54:GLU:HB3	2.20	0.42
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.54	0.42
7:G:13:LEU:HD12	7:G:26:LEU:HD21	2.01	0.42
7:G:126:ASN:ND2	7:G:127:PRO:HA	2.23	0.42
1:A:241:VAL:HA	1:A:242:PRO:HD2	1.95	0.42
1:A:687:LYS:CE	1:A:795:GLU:OE2	2.68	0.42
1:A:1165:GLU:H	1:A:1165:GLU:HG3	1.61	0.42
1:A:1166:ASP:OD2	1:A:1239:ARG:CD	2.68	0.42
1:A:1332:PHE:CE1	1:A:1381:LEU:HD13	2.55	0.42
2:B:244:LEU:HD21	2:B:366:GLN:HE21	1.84	0.42
2:B:637:LEU:HD22	2:B:741:CYS:C	2.45	0.42
2:B:700:SER:C	2:B:701:ILE:CG2	2.93	0.42
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.35	0.42
3:C:160:LYS:O	3:C:161:LYS:O	2.38	0.42
5:E:49:SER:OG	5:E:50:MET:N	2.48	0.42
5:E:68:SER:O	5:E:72:PHE:O	2.37	0.42
5:E:181:ALA:O	5:E:182:ASP:C	2.62	0.42
7:G:44:TYR:CE2	7:G:105:PRO:HB2	2.55	0.42
7:G:88:ASP:CB	7:G:144:ARG:HA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:101:VAL:CG1	7:G:102:GLN:N	2.80	0.42
7:G:102:GLN:HG3	7:G:106:MET:O	2.20	0.42
8:H:129:TYR:HA	8:H:131:ASN:ND2	2.35	0.42
9:I:101:PHE:N	9:I:101:PHE:HD1	2.16	0.42
11:K:53:ASP:C	11:K:55:LYS:N	2.78	0.42
1:A:351:THR:N	1:A:468:PHE:HE1	2.17	0.41
1:A:565:ILE:HG12	8:H:97:MET:HG2	2.02	0.41
1:A:714:PHE:CG	9:I:97:MET:HE1	2.54	0.41
1:A:1104:ILE:O	1:A:1105:LEU:C	2.63	0.41
1:A:1131:ALA:O	1:A:1132:LYS:C	2.62	0.41
1:A:1225:PHE:CE2	1:A:1227:ILE:HD11	2.55	0.41
1:A:1308:THR:HG21	1:A:1310:GLY:O	2.20	0.41
1:A:1402:PHE:CG	1:A:1403:GLU:HG2	2.55	0.41
2:B:223:VAL:HG21	2:B:380:TYR:HE2	1.85	0.41
2:B:370:PHE:HD2	2:B:373:ARG:CD	2.33	0.41
2:B:778:MET:HE1	2:B:1094:ARG:HH11	1.84	0.41
2:B:978:ASP:OD1	2:B:1098:MET:HB3	2.20	0.41
2:B:1222:ARG:O	2:B:1222:ARG:CG	2.68	0.41
3:C:20:PHE:CE1	3:C:22:LEU:HD13	2.55	0.41
4:D:35:LEU:HD11	4:D:173:HIS:NE2	2.35	0.41
4:D:167:LEU:HB3	4:D:177:VAL:HG13	2.02	0.41
6:F:120:ILE:O	6:F:123:LYS:HB3	2.20	0.41
8:H:118:PHE:O	8:H:119:GLY:C	2.63	0.41
8:H:130:ARG:HH11	8:H:130:ARG:CA	2.32	0.41
8:H:130:ARG:CA	8:H:133:ASN:HB2	2.50	0.41
1:A:21:LEU:HD11	1:A:1414:ALA:CA	2.49	0.41
1:A:120:GLU:C	1:A:122:MET:N	2.79	0.41
1:A:160:GLN:H	1:A:160:GLN:HG3	1.53	0.41
1:A:479:ASN:HD22	1:A:479:ASN:HA	1.70	0.41
1:A:730:GLY:C	1:A:732:LEU:H	2.27	0.41
1:A:1072:ILE:O	1:A:1075:PRO:HG2	2.20	0.41
1:A:1094:VAL:O	1:A:1095:THR:C	2.63	0.41
1:A:1217:LYS:O	1:A:1221:LYS:HA	2.19	0.41
1:A:1239:ARG:HH22	1:A:1241:ARG:HH22	1.67	0.41
2:B:27:ALA:C	2:B:29:ASP:N	2.78	0.41
2:B:123:THR:OG1	2:B:458:LYS:HE2	2.19	0.41
2:B:637:LEU:CD1	2:B:693:ILE:HD11	2.47	0.41
2:B:758:PHE:O	2:B:761:HIS:HB2	2.19	0.41
2:B:1022:THR:HG23	2:B:1022:THR:O	2.20	0.41
3:C:62:PHE:C	3:C:62:PHE:HD2	2.28	0.41
4:D:128:VAL:O	4:D:129:LEU:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:75:PRO:O	6:F:77:ASP:O	2.38	0.41
8:H:41:ASP:O	8:H:42:ILE:HG13	2.20	0.41
9:I:54:GLU:HB3	9:I:100:PHE:CE2	2.54	0.41
11:K:55:LYS:CB	11:K:81:TYR:CE1	3.03	0.41
1:A:425:GLN:O	1:A:426:LEU:O	2.38	0.41
1:A:507:VAL:HB	1:A:508:PRO:HD3	2.01	0.41
1:A:645:LEU:HG	1:A:649:ILE:HD12	2.01	0.41
1:A:1208:THR:HB	1:A:1211:GLN:HG3	2.01	0.41
1:A:1315:GLU:C	1:A:1317:MET:N	2.78	0.41
2:B:38:PHE:CD1	2:B:811:TYR:CD2	3.08	0.41
2:B:500:THR:O	2:B:501:PRO:C	2.63	0.41
2:B:642:ASP:HB3	2:B:649:LYS:HG3	2.02	0.41
2:B:835:GLN:HE21	2:B:835:GLN:HB2	1.58	0.41
2:B:871:THR:O	2:B:917:PRO:HG3	2.20	0.41
2:B:1115:THR:HG22	2:B:1117:GLN:CB	2.49	0.41
3:C:3:GLU:CD	3:C:4:GLU:HG3	2.45	0.41
5:E:124:VAL:HB	5:E:125:PRO:HD3	2.00	0.41
5:E:153:HIS:O	5:E:154:ILE:CG1	2.68	0.41
10:J:14:VAL:CG1	10:J:14:VAL:O	2.69	0.41
1:A:40:THR:CB	1:A:41:MET:HE2	2.48	0.41
1:A:125:ALA:C	1:A:127:ALA:H	2.27	0.41
1:A:130:ASP:O	1:A:131:SER:C	2.61	0.41
1:A:208:LEU:C	1:A:208:LEU:HD23	2.45	0.41
1:A:427:GLN:HB2	1:A:430:TRP:CD1	2.55	0.41
1:A:855:THR:HA	1:A:866:PHE:O	2.20	0.41
2:B:100:PRO:HG3	2:B:172:ILE:HD12	2.03	0.41
2:B:903:VAL:HG12	2:B:904:ARG:N	2.35	0.41
2:B:1152:MET:SD	2:B:1157:ALA:HA	2.61	0.41
3:C:10:ILE:CD1	11:K:108:GLU:HB3	2.51	0.41
3:C:62:PHE:O	3:C:66:ARG:HG3	2.19	0.41
4:D:119:ARG:CD	4:D:221:TYR:HE2	2.34	0.41
4:D:135:GLY:C	4:D:137:ASN:H	2.27	0.41
5:E:69:ILE:O	5:E:69:ILE:HG22	2.21	0.41
8:H:4:THR:CG2	8:H:5:LEU:N	2.83	0.41
10:J:3:VAL:N	10:J:53:HIS:CE1	2.86	0.41
10:J:52:THR:HG22	10:J:52:THR:O	2.20	0.41
1:A:595:THR:O	1:A:596:THR:CG2	2.69	0.41
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.84	0.41
1:A:691:LEU:O	1:A:694:THR:HB	2.21	0.41
1:A:850:VAL:CG2	1:A:868:TYR:HB2	2.50	0.41
2:B:265:SER:O	2:B:266:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:546:SER:O	2:B:546:SER:OG	2.38	0.41
2:B:769:TYR:C	2:B:771:SER:N	2.79	0.41
3:C:167:HIS:CD2	3:C:168:ALA:H	2.37	0.41
5:E:22:MET:O	5:E:26:ARG:HG3	2.20	0.41
6:F:109:VAL:CG1	6:F:110:ASP:N	2.78	0.41
9:I:56:ALA:O	9:I:57:GLY:O	2.38	0.41
1:A:102:VAL:CG1	1:A:211:PHE:CE1	3.03	0.41
1:A:257:ARG:HB3	1:A:258:GLY:H	1.60	0.41
1:A:492:PRO:HB2	1:A:497:THR:HG22	2.01	0.41
1:A:510:GLN:OE1	1:A:510:GLN:HA	2.18	0.41
1:A:699:ALA:HB3	1:A:701:LEU:HG	2.03	0.41
1:A:720:ARG:CZ	1:A:720:ARG:HB3	2.51	0.41
1:A:804:TYR:OH	2:B:763:GLN:HA	2.20	0.41
1:A:857:ARG:CZ	6:F:139:PRO:HG3	2.50	0.41
1:A:961:ARG:HG2	1:A:965:GLN:HE21	1.85	0.41
1:A:1029:ARG:NH1	1:A:1029:ARG:CG	2.83	0.41
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.27	0.41
2:B:314:LEU:O	2:B:315:LYS:C	2.63	0.41
2:B:321:GLY:O	2:B:322:PHE:C	2.63	0.41
2:B:365:THR:HG21	2:B:370:PHE:CG	2.54	0.41
2:B:387:LEU:HD12	2:B:387:LEU:N	2.32	0.41
2:B:566:LEU:O	2:B:567:GLU:C	2.63	0.41
2:B:583:ASN:CG	2:B:628:THR:HG22	2.46	0.41
2:B:603:LEU:HD22	2:B:603:LEU:HA	1.84	0.41
2:B:638:PHE:HD2	2:B:638:PHE:HA	1.79	0.41
3:C:143:LEU:O	3:C:143:LEU:HG	2.21	0.41
4:D:128:VAL:C	4:D:130:LEU:H	2.29	0.41
6:F:117:PRO:O	6:F:118:LEU:C	2.64	0.41
7:G:26:LEU:O	7:G:27:LYS:C	2.63	0.41
8:H:80:ARG:HB3	8:H:81:PRO:HD2	2.03	0.41
9:I:6:PHE:CD2	9:I:6:PHE:N	2.89	0.41
9:I:82:GLU:CD	9:I:104:LEU:HD12	2.46	0.41
1:A:253:ASN:HB3	2:B:935:ARG:NH1	2.36	0.41
1:A:316:GLN:HB2	1:A:322:VAL:CG2	2.51	0.41
1:A:755:PHE:O	1:A:756:ILE:C	2.63	0.41
1:A:853:ASP:OD1	1:A:853:ASP:C	2.63	0.41
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	2.02	0.41
2:B:496:ARG:HB3	2:B:496:ARG:HH11	1.86	0.41
2:B:637:LEU:HD23	2:B:637:LEU:HA	1.81	0.41
2:B:860:MET:CG	2:B:861:ASP:N	2.83	0.41
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:189:THR:CG2	3:C:190:ASP:N	2.78	0.41
3:C:252:GLN:HE21	11:K:95:ILE:CG2	2.21	0.41
4:D:66:ARG:CD	4:D:133:THR:HB	2.39	0.41
4:D:154:PHE:CE1	4:D:163:VAL:CG2	3.03	0.41
4:D:155:ARG:CG	4:D:155:ARG:NH1	2.82	0.41
6:F:98:ALA:HB1	6:F:117:PRO:HB2	2.03	0.41
8:H:44:VAL:O	8:H:44:VAL:CG1	2.67	0.41
9:I:106:CYS:O	9:I:107:SER:HB2	2.21	0.41
1:A:146:MET:C	1:A:171:GLN:HB2	2.46	0.41
1:A:452:LYS:HB2	2:B:1141:HIS:CE1	2.56	0.41
1:A:535:THR:HG21	1:A:617:VAL:N	2.36	0.41
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.86	0.41
1:A:629:LEU:HD22	1:A:633:VAL:CG2	2.50	0.41
1:A:1385:THR:CG2	1:A:1386:ARG:N	2.83	0.41
2:B:95:ILE:HG13	2:B:129:PHE:O	2.21	0.41
2:B:237:VAL:CG1	2:B:238:ALA:N	2.84	0.41
2:B:507:LYS:HD3	2:B:507:LYS:HA	1.96	0.41
2:B:648:HIS:ND1	2:B:648:HIS:N	2.64	0.41
2:B:877:PRO:C	2:B:878:GLN:HG3	2.45	0.41
2:B:1073:TYR:CD1	2:B:1073:TYR:N	2.89	0.41
3:C:66:ARG:HH22	10:J:2:ILE:CG2	2.32	0.41
3:C:82:TYR:O	3:C:85:ASP:N	2.46	0.41
3:C:186:LEU:N	3:C:186:LEU:CD1	2.82	0.41
5:E:9:ILE:O	5:E:10:SER:C	2.64	0.41
7:G:1:MET:O	7:G:2:PHE:C	2.64	0.41
8:H:58:THR:HB	8:H:143:LEU:HD13	2.03	0.41
10:J:13:VAL:C	10:J:14:VAL:HG23	2.45	0.41
10:J:32:GLU:H	10:J:32:GLU:CD	2.28	0.41
14:1:15:DG:C8	14:1:16:DT:C7	3.03	0.41
1:A:407:ARG:O	1:A:408:ASP:C	2.64	0.41
1:A:416:ARG:NH1	1:A:417:TYR:CE2	2.84	0.41
1:A:789:LYS:HD3	2:B:620:ARG:HH12	1.86	0.41
1:A:818:MET:HE2	1:A:818:MET:HB3	1.91	0.41
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.36	0.41
1:A:919:ILE:CD1	1:A:983:ILE:HD12	2.49	0.41
1:A:962:ARG:O	1:A:963:ILE:C	2.64	0.41
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.36	0.41
1:A:1192:LEU:HG	1:A:1193:LEU:N	2.36	0.41
1:A:1259:MET:HE2	1:A:1263:ILE:HD11	2.02	0.41
1:A:1334:ASP:O	1:A:1336:MET:N	2.54	0.41
1:A:1377:THR:O	1:A:1378:GLN:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1385:THR:C	1:A:1387:HIS:H	2.29	0.41
2:B:63:ILE:HD12	2:B:421:PHE:CD2	2.56	0.41
2:B:240:ILE:HG23	2:B:240:ILE:O	2.21	0.41
2:B:332:ASP:OD1	2:B:348:ARG:HD2	2.20	0.41
2:B:466:TRP:O	2:B:467:GLY:C	2.62	0.41
2:B:544:CYS:C	2:B:545:ILE:HG13	2.45	0.41
2:B:563:MET:HE2	2:B:587:HIS:O	2.21	0.41
2:B:654:ARG:O	2:B:657:HIS:HB2	2.20	0.41
2:B:654:ARG:O	2:B:656:GLY:N	2.54	0.41
2:B:700:SER:O	2:B:701:ILE:HG22	2.21	0.41
2:B:882:THR:HG22	2:B:883:LEU:N	2.35	0.41
2:B:912:ILE:O	2:B:938:SER:CB	2.69	0.41
2:B:1137:CYS:O	2:B:1140:ALA:HB3	2.21	0.41
3:C:16:ASP:OD1	3:C:16:ASP:N	2.53	0.41
3:C:100:THR:CG2	3:C:101:LEU:N	2.84	0.41
3:C:164:ALA:O	3:C:167:HIS:O	2.38	0.41
3:C:234:SER:OG	3:C:235:VAL:N	2.54	0.41
3:C:242:GLN:HA	3:C:245:VAL:CG2	2.42	0.41
3:C:251:LEU:O	3:C:255:VAL:HG23	2.20	0.41
4:D:123:LEU:HB3	4:D:124:GLU:OE2	2.20	0.41
4:D:156:ASP:O	4:D:159:THR:N	2.54	0.41
5:E:74:ASP:N	5:E:74:ASP:OD1	2.53	0.41
5:E:108:GLY:O	5:E:132:ILE:HG23	2.21	0.41
5:E:111:VAL:CG1	5:E:137:GLU:HG2	2.51	0.41
7:G:51:TYR:O	7:G:51:TYR:CD2	2.73	0.41
8:H:48:PRO:O	8:H:49:VAL:HG23	2.21	0.41
8:H:61:SER:O	8:H:62:SER:HB2	2.20	0.41
8:H:83:GLN:C	8:H:85:GLY:N	2.79	0.41
9:I:70:ARG:HA	9:I:83:ASN:O	2.21	0.41
9:I:87:GLN:O	9:I:88:SER:C	2.62	0.41
9:I:88:SER:C	9:I:90:GLN:N	2.79	0.41
10:J:2:ILE:HG13	10:J:57:ILE:HD12	2.03	0.41
11:K:57:LEU:CB	11:K:76:GLN:HG2	2.42	0.41
1:A:39:GLU:OE2	1:A:39:GLU:N	2.54	0.41
1:A:41:MET:HE3	1:A:41:MET:N	2.36	0.41
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.51	0.41
1:A:96:ILE:HA	1:A:99:ILE:HD12	2.03	0.41
1:A:569:LYS:HB3	1:A:571:LEU:HD13	2.02	0.41
1:A:846:GLU:OE1	1:A:1425:SER:OG	2.39	0.41
1:A:897:TYR:HB3	1:A:936:LEU:HD12	2.01	0.41
1:A:1104:ILE:C	1:A:1106:ASN:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1148:ILE:HG12	1:A:1198:ASP:HB2	2.03	0.41
1:A:1157:ASP:C	1:A:1159:ARG:H	2.29	0.41
1:A:1387:HIS:O	1:A:1391:ARG:HG3	2.21	0.41
1:A:1425:SER:O	1:A:1426:GLU:C	2.63	0.41
1:A:1436:ILE:O	1:A:1438:THR:N	2.54	0.41
2:B:113:TYR:CE2	2:B:192:LEU:CD2	3.04	0.41
2:B:345:LYS:CA	2:B:348:ARG:HE	2.20	0.41
2:B:558:LEU:O	2:B:561:TRP:N	2.54	0.41
2:B:597:MET:CE	2:B:624:LEU:HD11	2.51	0.41
2:B:679:TYR:CE1	2:B:683:SER:HB3	2.56	0.41
3:C:91:HIS:ND1	3:C:158:VAL:HG11	2.36	0.41
4:D:17:LYS:HD2	4:D:18:VAL:HG13	2.02	0.41
4:D:208:GLU:O	4:D:212:LYS:HE3	2.21	0.41
5:E:65:THR:O	5:E:69:ILE:CD1	2.69	0.41
7:G:137:ILE:CG2	7:G:143:ILE:HD11	2.51	0.41
1:A:464:PRO:O	1:A:465:TYR:HB2	2.21	0.40
1:A:533:LYS:HE3	1:A:745:GLN:NE2	2.36	0.40
1:A:982:THR:HB	1:A:985:ASP:H	1.86	0.40
1:A:1193:LEU:HB2	1:A:1260:LEU:CD2	2.50	0.40
2:B:189:LEU:HA	2:B:192:LEU:HB2	2.02	0.40
2:B:292:ILE:HD11	2:B:327:ARG:H	1.86	0.40
2:B:400:HIS:O	2:B:402:GLY:N	2.54	0.40
2:B:583:ASN:OD1	2:B:628:THR:HG22	2.20	0.40
2:B:661:LEU:C	2:B:663:ALA:H	2.27	0.40
2:B:742:GLU:O	2:B:743:ILE:C	2.65	0.40
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.52	0.40
3:C:10:ILE:H	3:C:10:ILE:HG13	1.70	0.40
4:D:22:GLU:H	4:D:22:GLU:HG3	1.68	0.40
8:H:99:GLY:CA	8:H:117:SER:O	2.70	0.40
1:A:110:CYS:HB3	1:A:167:CYS:SG	2.61	0.40
1:A:532:ARG:O	1:A:535:THR:HB	2.21	0.40
1:A:598:LEU:O	1:A:598:LEU:HD23	2.22	0.40
1:A:603:ASN:HB3	1:A:604:GLY:H	1.74	0.40
1:A:1450:LEU:CD1	6:F:131:PRO:HG3	2.51	0.40
2:B:347:LYS:HG2	2:B:347:LYS:H	1.67	0.40
2:B:1096:ARG:CG	2:B:1097:HIS:N	2.84	0.40
3:C:77:ILE:C	3:C:79:GLN:H	2.29	0.40
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.61	0.40
4:D:142:LYS:O	4:D:146:GLN:HG3	2.22	0.40
5:E:153:HIS:C	5:E:154:ILE:HG13	2.46	0.40
6:F:121:ALA:O	6:F:122:MET:C	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:26:LEU:HD11	7:G:70:PHE:CD1	2.55	0.40
8:H:138:GLU:C	8:H:139:ASN:O	2.62	0.40
9:I:93:LYS:N	9:I:93:LYS:CD	2.83	0.40
9:I:101:PHE:HD1	9:I:101:PHE:H	1.69	0.40
1:A:41:MET:HB2	1:A:42:ASP:H	1.64	0.40
1:A:259:GLU:OE1	1:A:259:GLU:HA	2.22	0.40
1:A:939:ASP:OD2	1:A:1023:ARG:NH1	2.55	0.40
1:A:964:ILE:O	1:A:965:GLN:C	2.64	0.40
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.21	0.40
1:A:1138:ILE:HG13	1:A:1139:GLU:N	2.36	0.40
1:A:1193:LEU:HD12	1:A:1194:ARG:H	1.81	0.40
2:B:118:ARG:HG2	2:B:204:ILE:HD13	2.04	0.40
2:B:203:PHE:N	2:B:203:PHE:HD1	2.18	0.40
2:B:307:ASP:O	2:B:309:GLN:N	2.53	0.40
2:B:345:LYS:C	2:B:347:LYS:H	2.30	0.40
2:B:371:GLU:N	2:B:371:GLU:CD	2.79	0.40
2:B:393:LYS:HA	2:B:393:LYS:HE3	2.02	0.40
2:B:405:ARG:CZ	2:B:632:ARG:HG2	2.51	0.40
2:B:654:ARG:CG	2:B:654:ARG:NH1	2.78	0.40
2:B:708:GLU:O	2:B:710:LEU:N	2.54	0.40
4:D:8:PHE:CD2	7:G:6:ASP:O	2.71	0.40
4:D:15:LEU:HD12	4:D:15:LEU:C	2.46	0.40
5:E:177:ARG:C	5:E:212:ARG:HD3	2.46	0.40
7:G:114:LEU:HD12	7:G:114:LEU:HA	1.94	0.40
8:H:103:LYS:HG2	8:H:104:PHE:N	2.37	0.40
11:K:89:ASN:O	11:K:90:ALA:C	2.65	0.40
1:A:444:PHE:CZ	1:A:487:MET:HE3	2.57	0.40
1:A:711:ARG:HH21	9:I:87:GLN:HE22	1.67	0.40
1:A:920:LEU:HD23	1:A:921:GLY:N	2.37	0.40
1:A:922:ASP:OD1	1:A:924:LYS:HB2	2.20	0.40
1:A:954:TRP:CD1	1:A:954:TRP:N	2.89	0.40
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	2.04	0.40
1:A:1444:MET:O	6:F:133:VAL:N	2.52	0.40
2:B:44:VAL:HG21	2:B:199:MET:O	2.21	0.40
2:B:465:ASN:N	2:B:465:ASN:ND2	2.62	0.40
2:B:966:VAL:CG1	2:B:967:ARG:N	2.85	0.40
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.86	0.40
3:C:44:LEU:C	3:C:44:LEU:HD23	2.47	0.40
3:C:77:ILE:HD13	3:C:77:ILE:HA	1.85	0.40
3:C:184:ASN:HD22	3:C:189:THR:HB	1.83	0.40
3:C:239:PRO:HB2	3:C:241:ASP:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:128:VAL:O	4:D:130:LEU:N	2.54	0.40
5:E:58:MET:O	5:E:59:SER:C	2.64	0.40
5:E:170:LEU:C	5:E:171:LYS:O	2.63	0.40
5:E:175:LEU:HA	5:E:176:PRO:HD3	1.86	0.40
7:G:21:ARG:HD2	7:G:24:GLN:HB3	2.03	0.40
7:G:137:ILE:HG23	7:G:143:ILE:HD11	2.03	0.40
9:I:50:THR:HG22	9:I:52:ILE:N	2.35	0.40
1:A:26:GLU:O	1:A:29:ALA:N	2.54	0.40
1:A:414:ASP:OD1	1:A:416:ARG:CG	2.70	0.40
1:A:741:ASN:ND2	1:A:744:LYS:H	2.18	0.40
1:A:767:GLN:NE2	1:A:774:ARG:CB	2.79	0.40
1:A:786:HIS:N	1:A:786:HIS:HD2	2.18	0.40
1:A:1152:ILE:HA	1:A:1192:LEU:O	2.21	0.40
1:A:1206:ASP:O	1:A:1274:ARG:NH2	2.55	0.40
1:A:1208:THR:HG22	1:A:1210:GLY:N	2.36	0.40
1:A:1283:VAL:CG1	1:A:1284:MET:N	2.83	0.40
1:A:1313:LEU:C	1:A:1315:GLU:N	2.79	0.40
2:B:221:ASN:N	2:B:241:ARG:O	2.53	0.40
2:B:507:LYS:HA	2:B:512:ARG:HE	1.87	0.40
2:B:558:LEU:O	2:B:560:GLU:N	2.54	0.40
2:B:882:THR:HB	2:B:934:LYS:C	2.46	0.40
2:B:889:THR:HG23	2:B:891:ASP:H	1.86	0.40
3:C:7:GLN:HG3	11:K:104:ASN:ND2	2.34	0.40
3:C:66:ARG:O	3:C:67:LEU:C	2.65	0.40
3:C:236:GLY:C	3:C:238:ILE:N	2.79	0.40
5:E:28:TYR:O	5:E:65:THR:HG22	2.21	0.40
5:E:33:GLU:C	5:E:35:VAL:H	2.30	0.40
5:E:56:LYS:HE2	5:E:84:ASP:CB	2.39	0.40
7:G:27:LYS:O	7:G:31:LEU:HD23	2.22	0.40
10:J:36:LEU:HB2	10:J:47:ARG:NH1	2.35	0.40
11:K:67:PHE:C	11:K:68:PHE:CD2	2.99	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1406/1733 (81%)	1004 (71%)	279 (20%)	123 (9%)	0	7
2	B	1094/1224 (89%)	774 (71%)	202 (18%)	118 (11%)	0	5
3	C	264/347 (76%)	181 (69%)	48 (18%)	35 (13%)	0	3
4	D	174/221 (79%)	124 (71%)	33 (19%)	17 (10%)	0	6
5	E	212/215 (99%)	144 (68%)	46 (22%)	22 (10%)	0	5
6	F	85/155 (55%)	72 (85%)	8 (9%)	5 (6%)	1	13
7	G	169/171 (99%)	137 (81%)	24 (14%)	8 (5%)	2	17
8	H	130/146 (89%)	84 (65%)	27 (21%)	19 (15%)	0	3
9	I	112/122 (92%)	77 (69%)	26 (23%)	9 (8%)	1	8
10	J	63/70 (90%)	38 (60%)	14 (22%)	11 (18%)	0	1
11	K	112/120 (93%)	86 (77%)	22 (20%)	4 (4%)	2	22
12	L	42/70 (60%)	20 (48%)	13 (31%)	9 (21%)	0	1
All	All	3863/4594 (84%)	2741 (71%)	742 (19%)	380 (10%)	0	6

All (380) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	48	ALA
1	A	57	ARG
1	A	58	LEU
1	A	67	CYS
1	A	70	CYS
1	A	74	MET
1	A	93	VAL
1	A	96	ILE
1	A	130	ASP
1	A	154	SER
1	A	167	CYS
1	A	219	PHE
1	A	250	ILE
1	A	255	SER
1	A	286	HIS
1	A	331	GLY
1	A	332	LYS
1	A	399	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	410	GLY
1	A	424	ILE
1	A	517	ASN
1	A	556	TRP
1	A	567	LYS
1	A	597	LEU
1	A	598	LEU
1	A	1002	GLY
1	A	1112	LYS
1	A	1114	PRO
1	A	1115	SER
1	A	1223	ASP
1	A	1231	ASP
1	A	1233	ASP
1	A	1242	VAL
1	A	1255	GLU
1	A	1314	SER
1	A	1405	THR
2	B	21	GLU
2	B	67	SER
2	B	68	THR
2	B	100	PRO
2	B	108	VAL
2	B	186	GLU
2	B	294	ASP
2	B	295	GLY
2	B	334	ILE
2	B	365	THR
2	B	367	LEU
2	B	466	TRP
2	B	502	ILE
2	B	507	LYS
2	B	510	LYS
2	B	641	GLU
2	B	643	ASP
2	B	708	GLU
2	B	709	ASP
2	B	731	VAL
2	B	746	SER
2	B	751	VAL
2	B	879	ARG
2	B	907	GLY

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	958	GLN
2	B	1046	PRO
2	B	1069	PHE
2	B	1097	HIS
2	B	1108	ARG
2	B	1157	ALA
2	B	1171	VAL
2	B	1176	ASN
2	B	1188	LYS
2	B	1222	ARG
3	C	90	ASP
3	C	110	THR
3	C	142	VAL
3	C	149	LYS
3	C	161	LYS
3	C	184	ASN
3	C	209	TYR
3	C	215	GLU
3	C	216	GLY
3	C	237	SER
3	C	240	VAL
4	D	5	THR
4	D	8	PHE
4	D	17	LYS
4	D	19	GLU
4	D	52	LEU
4	D	199	ASN
4	D	218	GLU
5	E	36	GLU
5	E	115	ASN
7	G	112	LYS
7	G	139	ILE
8	H	17	PRO
8	H	77	ARG
8	H	92	ASP
8	H	107	VAL
8	H	128	ASN
8	H	134	ASN
8	H	140	ALA
9	I	11	ASN
9	I	57	GLY
9	I	95	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	J	2	ILE
10	J	6	ARG
10	J	17	LYS
10	J	28	ASP
10	J	64	ASN
12	L	50	ASP
12	L	59	ALA
12	L	60	ARG
1	A	5	GLN
1	A	43	GLU
1	A	54	ASN
1	A	59	GLY
1	A	63	ARG
1	A	66	LYS
1	A	76	GLU
1	A	128	ILE
1	A	244	PRO
1	A	318	SER
1	A	322	VAL
1	A	357	PRO
1	A	400	PRO
1	A	426	LEU
1	A	510	GLN
1	A	543	LEU
1	A	583	PRO
1	A	619	LYS
1	A	673	GLY
1	A	731	ARG
1	A	755	PHE
1	A	846	GLU
1	A	852	TYR
1	A	891	ALA
1	A	1105	LEU
1	A	1124	HIS
1	A	1281	ARG
1	A	1438	THR
2	B	27	ALA
2	B	28	GLU
2	B	45	SER
2	B	259	TYR
2	B	282	ILE
2	B	364	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	401	PHE
2	B	435	THR
2	B	449	ASN
2	B	450	ALA
2	B	460	ALA
2	B	461	LEU
2	B	467	GLY
2	B	506	GLY
2	B	509	ALA
2	B	619	ILE
2	B	642	ASP
2	B	655	LYS
2	B	728	ARG
2	B	735	ALA
2	B	792	MET
2	B	848	ARG
2	B	869	SER
2	B	881	ASN
2	B	892	LYS
2	B	1035	ALA
2	B	1103	ILE
3	C	74	SER
3	C	126	GLY
3	C	141	GLY
3	C	224	GLN
3	C	231	ASN
4	D	14	ARG
4	D	32	GLU
4	D	119	ARG
4	D	131	GLU
4	D	136	GLY
4	D	157	GLN
4	D	192	LYS
4	D	197	SER
5	E	45	LYS
5	E	59	SER
5	E	74	ASP
5	E	76	GLY
5	E	104	ASN
5	E	106	GLN
6	F	128	LYS
6	F	139	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	G	154	VAL
8	H	21	ASN
8	H	32	THR
8	H	59	ILE
8	H	82	PRO
8	H	95	TYR
9	I	9	ASP
9	I	62	ILE
9	I	106	CYS
10	J	14	VAL
10	J	24	LEU
10	J	55	ASP
11	K	53	ASP
12	L	28	LYS
12	L	35	SER
12	L	53	HIS
1	A	41	MET
1	A	109	HIS
1	A	138	ILE
1	A	148	CYS
1	A	253	ASN
1	A	259	GLU
1	A	308	ILE
1	A	311	GLN
1	A	423	ASP
1	A	591	PHE
1	A	718	VAL
1	A	738	LYS
1	A	789	LYS
1	A	795	GLU
1	A	963	ILE
1	A	968	GLN
1	A	1016	THR
1	A	1122	PRO
1	A	1206	ASP
1	A	1221	LYS
1	A	1277	GLU
1	A	1278	ASN
1	A	1309	ASP
1	A	1386	ARG
2	B	24	PRO
2	B	56	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	221	ASN
2	B	249	ARG
2	B	258	LEU
2	B	277	LYS
2	B	322	PHE
2	B	323	VAL
2	B	333	PHE
2	B	383	ASN
2	B	433	GLN
2	B	468	GLU
2	B	559	SER
2	B	567	GLU
2	B	575	PRO
2	B	694	ASP
2	B	711	GLU
2	B	810	GLU
2	B	884	ARG
2	B	906	SER
2	B	1065	GLN
2	B	1155	SER
2	B	1175	LEU
2	B	1186	ASP
2	B	1214	PRO
3	C	12	GLU
3	C	78	GLU
3	C	172	PRO
3	C	197	SER
3	C	208	GLU
3	C	214	ASN
3	C	243	VAL
5	E	73	PRO
5	E	92	THR
5	E	167	ARG
5	E	173	SER
5	E	183	PRO
6	F	112	GLU
6	F	154	ASP
12	L	40	LEU
12	L	54	ARG
1	A	42	ASP
1	A	169	ASN
1	A	249	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	256	GLN
1	A	592	ASP
1	A	689	LYS
1	A	821	ARG
1	A	884	ASP
1	A	885	THR
1	A	1054	LEU
1	A	1127	ASP
1	A	1229	SER
2	B	58	THR
2	B	106	ASP
2	B	257	LYS
2	B	267	ARG
2	B	384	ARG
2	B	648	HIS
2	B	752	ALA
2	B	818	PRO
2	B	937	ALA
2	B	1003	ALA
2	B	1017	ILE
2	B	1223	ASP
3	C	173	ALA
3	C	182	PRO
3	C	202	PRO
3	C	213	PRO
4	D	16	LYS
4	D	219	THR
5	E	65	THR
5	E	130	ALA
5	E	158	SER
5	E	192	ARG
7	G	20	PRO
7	G	63	PRO
8	H	62	SER
8	H	91	ASP
8	H	129	TYR
9	I	8	ARG
10	J	27	GLU
11	K	14	GLU
1	A	68	GLN
1	A	69	THR
1	A	284	ALA

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	958	VAL
1	A	1204	ASP
1	A	1365	TYR
2	B	22	SER
2	B	114	PRO
2	B	115	GLN
2	B	250	PHE
2	B	251	ILE
2	B	309	GLN
2	B	480	SER
2	B	636	PRO
2	B	945	GLU
2	B	1181	GLU
3	C	11	ARG
3	C	60	ASP
3	C	107	SER
3	C	132	PRO
3	C	175	ALA
5	E	12	LEU
5	E	83	CYS
6	F	78	GLN
7	G	115	MET
8	H	90	ALA
8	H	109	LYS
9	I	78	CYS
10	J	42	LYS
10	J	62	ARG
11	K	41	THR
11	K	54	ARG
1	A	35	ILE
1	A	599	SER
1	A	986	ILE
1	A	1130	GLN
2	B	483	LEU
2	B	688	GLY
2	B	774	GLY
3	C	223	ALA
5	E	122	LYS
8	H	8	ASP
1	A	51	GLY
1	A	285	PRO
1	A	312	PRO

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Mol	Chain	Res	Type
1	A	683	ILE
1	A	1104	ILE
2	B	758	PHE
2	B	1034	VAL
12	L	55	ILE
1	A	604	GLY
1	A	666	ILE
1	A	1335	ILE
1	A	1454	MET
2	B	283	VAL
2	B	992	ILE
3	C	10	ILE
5	E	51	GLY
5	E	129	PRO
7	G	128	PRO
1	A	245	PRO
7	G	136	VAL
1	A	61	ILE
1	A	336	ILE
2	B	712	PRO
2	B	901	PRO
3	C	176	ILE
9	I	59	VAL
2	B	1018	PRO
8	H	44	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1239/1520 (82%)	1084 (88%)	155 (12%)	4 22
2	B	964/1061 (91%)	832 (86%)	132 (14%)	3 20
3	C	234/299 (78%)	197 (84%)	37 (16%)	2 15
4	D	160/200 (80%)	133 (83%)	27 (17%)	2 13
5	E	196/197 (100%)	177 (90%)	19 (10%)	8 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	77/137 (56%)	66 (86%)	11 (14%)	3	19
7	G	152/152 (100%)	140 (92%)	12 (8%)	11	37
8	H	118/128 (92%)	102 (86%)	16 (14%)	3	20
9	I	108/116 (93%)	96 (89%)	12 (11%)	6	27
10	J	60/65 (92%)	54 (90%)	6 (10%)	7	30
11	K	99/102 (97%)	86 (87%)	13 (13%)	4	21
12	L	39/57 (68%)	35 (90%)	4 (10%)	7	30
All	All	3446/4034 (85%)	3002 (87%)	444 (13%)	4	22

All (444) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	12	ARG
1	A	18	GLN
1	A	34	LYS
1	A	37	PHE
1	A	39	GLU
1	A	41	MET
1	A	57	ARG
1	A	62	ASP
1	A	68	GLN
1	A	69	THR
1	A	93	VAL
1	A	117	GLU
1	A	120	GLU
1	A	121	LEU
1	A	141	LEU
1	A	145	LYS
1	A	152	VAL
1	A	155	GLU
1	A	160	GLN
1	A	161	LEU
1	A	182	VAL
1	A	196	GLU
1	A	200	ARG
1	A	208	LEU
1	A	219	PHE
1	A	244	PRO
1	A	245	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	249	SER
1	A	250	ILE
1	A	265	LYS
1	A	289	ILE
1	A	290	GLU
1	A	302	THR
1	A	315	LEU
1	A	317	LYS
1	A	322	VAL
1	A	324	SER
1	A	344	ARG
1	A	345	VAL
1	A	353	ILE
1	A	369	SER
1	A	373	THR
1	A	375	THR
1	A	379	VAL
1	A	385	ILE
1	A	394	ASN
1	A	408	ASP
1	A	417	TYR
1	A	425	GLN
1	A	443	LEU
1	A	445	ASN
1	A	449	SER
1	A	461	LYS
1	A	462	VAL
1	A	469	ARG
1	A	470	LEU
1	A	475	THR
1	A	481	ASP
1	A	493	GLN
1	A	498	ARG
1	A	504	LEU
1	A	505	CYS
1	A	511	ILE
1	A	512	VAL
1	A	518	LYS
1	A	524	VAL
1	A	535	THR
1	A	544	ASP
1	A	562	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	590	ARG
1	A	593	GLU
1	A	597	LEU
1	A	618	GLU
1	A	629	LEU
1	A	641	VAL
1	A	666	ILE
1	A	680	THR
1	A	685	GLU
1	A	688	LYS
1	A	691	LEU
1	A	701	LEU
1	A	702	LEU
1	A	738	LYS
1	A	762	SER
1	A	768	GLN
1	A	774	ARG
1	A	783	THR
1	A	786	HIS
1	A	805	LEU
1	A	810	PRO
1	A	821	ARG
1	A	827	THR
1	A	834	THR
1	A	838	GLN
1	A	850	VAL
1	A	856	THR
1	A	858	ASN
1	A	871	ASP
1	A	907	THR
1	A	937	VAL
1	A	941	LYS
1	A	955	PRO
1	A	963	ILE
1	A	969	GLN
1	A	983	ILE
1	A	993	LEU
1	A	1004	ASN
1	A	1029	ARG
1	A	1046	LEU
1	A	1067	LEU
1	A	1074	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1078	GLN
1	A	1095	THR
1	A	1110	ASN
1	A	1114	PRO
1	A	1116	LEU
1	A	1120	LEU
1	A	1122	PRO
1	A	1124	HIS
1	A	1129	GLU
1	A	1134	ILE
1	A	1135	ARG
1	A	1146	VAL
1	A	1170	ILE
1	A	1171	GLN
1	A	1187	GLN
1	A	1193	LEU
1	A	1199	ARG
1	A	1217	LYS
1	A	1260	LEU
1	A	1269	GLU
1	A	1276	VAL
1	A	1288	ASP
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1308	THR
1	A	1311	VAL
1	A	1333	ILE
1	A	1345	ARG
1	A	1353	TYR
1	A	1355	VAL
1	A	1365	TYR
1	A	1368	MET
1	A	1370	LEU
1	A	1386	ARG
1	A	1394	THR
1	A	1398	MET
1	A	1436	ILE
1	A	1444	MET
1	A	1445	ILE
1	A	1447	GLU
1	A	1449	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1451	VAL
2	B	20	ASP
2	B	22	SER
2	B	25	ILE
2	B	30	SER
2	B	35	SER
2	B	46	GLN
2	B	57	TYR
2	B	68	THR
2	B	98	THR
2	B	100	PRO
2	B	130	VAL
2	B	134	LYS
2	B	175	ARG
2	B	183	GLU
2	B	194	GLU
2	B	203	PHE
2	B	217	ARG
2	B	218	SER
2	B	222	ILE
2	B	225	VAL
2	B	261	ARG
2	B	262	GLU
2	B	272	THR
2	B	287	ARG
2	B	298	LEU
2	B	323	VAL
2	B	324	ILE
2	B	361	LEU
2	B	364	ILE
2	B	371	GLU
2	B	393	LYS
2	B	401	PHE
2	B	416	LEU
2	B	425	THR
2	B	430	ARG
2	B	446	LEU
2	B	452	THR
2	B	465	ASN
2	B	466	TRP
2	B	479	VAL
2	B	482	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	485	ARG
2	B	487	THR
2	B	493	SER
2	B	496	ARG
2	B	498	THR
2	B	505	ASP
2	B	508	LEU
2	B	516	ASN
2	B	518	HIS
2	B	555	ILE
2	B	572	HIS
2	B	580	VAL
2	B	582	VAL
2	B	597	MET
2	B	603	LEU
2	B	609	ILE
2	B	616	ILE
2	B	618	ASP
2	B	626	ILE
2	B	636	PRO
2	B	644	GLU
2	B	678	GLU
2	B	693	ILE
2	B	705	MET
2	B	714	GLU
2	B	730	ARG
2	B	737	THR
2	B	743	ILE
2	B	748	ILE
2	B	754	SER
2	B	786	ASN
2	B	790	ASP
2	B	805	THR
2	B	811	TYR
2	B	815	ARG
2	B	825	VAL
2	B	830	TYR
2	B	831	SER
2	B	835	GLN
2	B	837	ASP
2	B	839	MET
2	B	857	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	859	TYR
2	B	865	LYS
2	B	878	GLN
2	B	879	ARG
2	B	887	HIS
2	B	889	THR
2	B	915	THR
2	B	945	GLU
2	B	946	ASN
2	B	953	LEU
2	B	954	VAL
2	B	957	ASN
2	B	959	ASP
2	B	987	LYS
2	B	989	THR
2	B	997	GLU
2	B	999	MET
2	B	1001	PHE
2	B	1007	VAL
2	B	1022	THR
2	B	1034	VAL
2	B	1048	THR
2	B	1049	ASP
2	B	1053	GLU
2	B	1060	ARG
2	B	1073	TYR
2	B	1084	GLN
2	B	1087	PHE
2	B	1095	LEU
2	B	1098	MET
2	B	1103	ILE
2	B	1113	VAL
2	B	1119	VAL
2	B	1122	ARG
2	B	1124	ARG
2	B	1150	ARG
2	B	1151	LEU
2	B	1152	MET
2	B	1159	ARG
2	B	1160	VAL
2	B	1165	ILE
2	B	1172	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	1175	LEU
2	B	1183	LYS
2	B	1185	CYS
2	B	1193	GLN
2	B	1202	LEU
2	B	1214	PRO
2	B	1218	THR
3	C	22	LEU
3	C	23	SER
3	C	25	VAL
3	C	26	ASP
3	C	33	LEU
3	C	54	ASN
3	C	55	THR
3	C	56	THR
3	C	67	LEU
3	C	69	LEU
3	C	74	SER
3	C	77	ILE
3	C	78	GLU
3	C	83	SER
3	C	89	GLU
3	C	91	HIS
3	C	99	LEU
3	C	117	ASP
3	C	119	VAL
3	C	129	ILE
3	C	133	ILE
3	C	145	CYS
3	C	147	LEU
3	C	166	GLU
3	C	176	ILE
3	C	192	TRP
3	C	197	SER
3	C	202	PRO
3	C	217	ASP
3	C	226	ASP
3	C	235	VAL
3	C	238	ILE
3	C	240	VAL
3	C	245	VAL
3	C	259	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	262	LEU
3	C	266	ASP
4	D	11	ARG
4	D	14	ARG
4	D	15	LEU
4	D	16	LYS
4	D	17	LYS
4	D	21	GLU
4	D	22	GLU
4	D	23	ASN
4	D	29	LEU
4	D	34	GLN
4	D	40	HIS
4	D	70	PHE
4	D	74	GLN
4	D	123	LEU
4	D	124	GLU
4	D	149	THR
4	D	155	ARG
4	D	159	THR
4	D	183	LEU
4	D	187	THR
4	D	200	ASN
4	D	207	LEU
4	D	213	GLU
4	D	214	LEU
4	D	219	THR
4	D	220	LEU
4	D	221	TYR
5	E	2	ASP
5	E	10	SER
5	E	31	THR
5	E	33	GLU
5	E	37	LEU
5	E	65	THR
5	E	66	GLU
5	E	72	PHE
5	E	74	ASP
5	E	78	LEU
5	E	92	THR
5	E	99	HIS
5	E	115	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	E	134	THR
5	E	171	LYS
5	E	183	PRO
5	E	191	LYS
5	E	212	ARG
5	E	215	MET
6	F	72	LYS
6	F	79	ARG
6	F	84	TYR
6	F	90	ARG
6	F	111	LEU
6	F	112	GLU
6	F	119	ARG
6	F	122	MET
6	F	131	PRO
6	F	147	SER
6	F	153	VAL
7	G	1	MET
7	G	8	SER
7	G	12	THR
7	G	13	LEU
7	G	31	LEU
7	G	51	TYR
7	G	61	ILE
7	G	74	TYR
7	G	101	VAL
7	G	118	ASP
7	G	154	VAL
7	G	168	LEU
8	H	11	GLN
8	H	23	VAL
8	H	26	ILE
8	H	27	GLU
8	H	36	CYS
8	H	46	LEU
8	H	53	ASP
8	H	61	SER
8	H	88	SER
8	H	89	LEU
8	H	91	ASP
8	H	102	TYR
8	H	111	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	H	130	ARG
8	H	138	GLU
8	H	143	LEU
9	I	6	PHE
9	I	12	ASN
9	I	21	GLU
9	I	34	TYR
9	I	59	VAL
9	I	84	VAL
9	I	85	PHE
9	I	86	PHE
9	I	93	LYS
9	I	101	PHE
9	I	110	PHE
9	I	114	GLN
10	J	2	ILE
10	J	3	VAL
10	J	13	VAL
10	J	25	LEU
10	J	43	ARG
10	J	53	HIS
11	K	25	THR
11	K	31	VAL
11	K	34	THR
11	K	47	ARG
11	K	50	LEU
11	K	51	LEU
11	K	61	TYR
11	K	89	ASN
11	K	103	THR
11	K	107	THR
11	K	111	LEU
11	K	113	THR
11	K	114	LEU
12	L	27	LEU
12	L	38	LEU
12	L	55	ILE
12	L	65	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	18	GLN
1	A	54	ASN
1	A	68	GLN
1	A	71	GLN
1	A	75	ASN
1	A	169	ASN
1	A	171	GLN
1	A	213	HIS
1	A	225	ASN
1	A	253	ASN
1	A	282	ASN
1	A	299	HIS
1	A	339	ASN
1	A	394	ASN
1	A	435	HIS
1	A	445	ASN
1	A	447	GLN
1	A	479	ASN
1	A	493	GLN
1	A	503	GLN
1	A	515	GLN
1	A	517	ASN
1	A	611	GLN
1	A	631	HIS
1	A	698	GLN
1	A	723	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	786	HIS
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	994	GLN
1	A	1048	ASN
1	A	1128	GLN
1	A	1140	HIS
1	A	1187	GLN
1	A	1203	ASN
1	A	1258	HIS
1	A	1265	ASN
1	A	1312	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1390	ASN
1	A	1432	GLN
2	B	103	ASN
2	B	121	ASN
2	B	178	ASN
2	B	236	HIS
2	B	366	GLN
2	B	383	ASN
2	B	395	GLN
2	B	433	GLN
2	B	465	ASN
2	B	481	GLN
2	B	515	HIS
2	B	518	HIS
2	B	538	ASN
2	B	587	HIS
2	B	610	ASN
2	B	667	GLN
2	B	786	ASN
2	B	794	ASN
2	B	821	GLN
2	B	842	ASN
2	B	862	GLN
2	B	878	GLN
2	B	887	HIS
2	B	957	ASN
2	B	975	GLN
2	B	984	HIS
2	B	1062	HIS
2	B	1065	GLN
2	B	1076	HIS
2	B	1084	GLN
2	B	1112	GLN
2	B	1117	GLN
2	B	1161	HIS
2	B	1179	GLN
2	B	1193	GLN
2	B	1195	HIS
3	C	7	GLN
3	C	65	HIS
3	C	73	GLN
3	C	79	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	91	HIS
3	C	102	GLN
3	C	112	ASN
3	C	140	ASN
3	C	151	GLN
3	C	167	HIS
3	C	231	ASN
3	C	252	GLN
4	D	9	GLN
4	D	40	HIS
4	D	132	GLN
4	D	138	ASN
4	D	143	ASN
4	D	216	ASN
5	E	3	GLN
5	E	54	GLN
5	E	101	GLN
5	E	104	ASN
5	E	106	GLN
5	E	113	GLN
5	E	115	ASN
5	E	143	ASN
5	E	147	HIS
5	E	174	GLN
6	F	104	ASN
7	G	14	HIS
7	G	53	ASN
7	G	122	ASN
7	G	126	ASN
7	G	131	GLN
7	G	158	HIS
8	H	11	GLN
8	H	64	ASN
8	H	83	GLN
8	H	128	ASN
8	H	131	ASN
8	H	133	ASN
8	H	134	ASN
9	I	12	ASN
9	I	23	ASN
9	I	46	HIS
9	I	79	HIS

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Mol	Chain	Res	Type
9	I	87	GLN
9	I	90	GLN
9	I	108	HIS
10	J	53	HIS
10	J	64	ASN
11	K	29	ASN
11	K	65	HIS
11	K	76	GLN
11	K	89	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	3	10/18 (55%)	2 (20%)	1 (10%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	3	3	A
15	3	11	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	3	2	A

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	BRU	1	23	15,14	18,21,22	3.92	1 (5%)	25,30,33	1.03	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BRU	1	23	15,14	-	0/7/21/22	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	23	BRU	BR-C5	-16.54	1.50	1.88

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	23	BRU	C6-C5-C4	-2.86	117.77	120.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	1	23	BRU	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	1416/1733 (81%)	0.01	36 (2%) 58 34	15, 63, 100, 128	0
2	B	1112/1224 (90%)	0.32	55 (4%) 35 20	15, 74, 111, 122	0
3	C	266/347 (76%)	-0.05	1 (0%) 88 70	31, 63, 93, 111	0
4	D	178/221 (80%)	0.42	9 (5%) 33 19	40, 75, 106, 115	0
5	E	214/215 (99%)	0.37	2 (0%) 81 56	41, 87, 115, 124	0
6	F	87/155 (56%)	-0.37	0 100 100	17, 44, 73, 84	0
7	G	171/171 (100%)	0.07	0 100 100	44, 64, 92, 100	0
8	H	134/146 (91%)	0.73	8 (5%) 27 17	67, 95, 112, 117	0
9	I	114/122 (93%)	0.52	3 (2%) 57 33	62, 93, 109, 114	0
10	J	65/70 (92%)	-0.08	0 100 100	41, 60, 85, 92	0
11	K	114/120 (95%)	-0.21	1 (0%) 81 56	28, 66, 82, 92	0
12	L	44/70 (62%)	0.95	6 (13%) 7 6	42, 100, 111, 114	0
13	2	7/12 (58%)	1.27	1 (14%) 6 6	112, 116, 123, 124	0
14	1	18/26 (69%)	1.15	3 (16%) 4 5	68, 109, 126, 131	0
15	3	11/18 (61%)	1.07	1 (9%) 15 11	92, 97, 123, 126	0
All	All	3951/4650 (84%)	0.18	126 (3%) 50 29	15, 70, 109, 131	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	GLY	6.9
2	B	883	LEU	5.8
2	B	709	ASP	5.7
1	A	253	ASN	4.9
15	3	1	C	4.9
12	L	27	LEU	4.8
4	D	24	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	69	THR	4.7
2	B	882	THR	4.6
2	B	70	ILE	4.6
2	B	251	ILE	4.2
2	B	733	HIS	4.1
1	A	1254	ALA	4.1
2	B	446	LEU	3.7
2	B	250	PHE	3.6
1	A	252	PHE	3.6
2	B	241	ARG	3.6
11	K	114	LEU	3.6
2	B	734	HIS	3.6
2	B	710	LEU	3.5
14	1	10	DA	3.5
2	B	108	VAL	3.5
8	H	132	LEU	3.5
1	A	2	VAL	3.4
1	A	251	SER	3.3
1	A	1081	LEU	3.3
1	A	56	PRO	3.2
2	B	134	LYS	3.1
1	A	256	GLN	3.1
14	1	28	DA	3.1
1	A	71	GLN	3.1
2	B	472	ALA	3.1
2	B	880	THR	3.0
1	A	51	GLY	3.0
8	H	136	LYS	2.9
2	B	934	LYS	2.9
1	A	255	SER	2.9
1	A	66	LYS	2.9
1	A	1080	THR	2.9
2	B	436	VAL	2.8
8	H	127	GLY	2.8
2	B	933	SER	2.8
4	D	18	VAL	2.8
2	B	506	GLY	2.8
2	B	918	ILE	2.7
8	H	83	GLN	2.7
2	B	431	TYR	2.7
1	A	159	THR	2.7
2	B	507	LYS	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	154	SER	2.7
2	B	870	ILE	2.7
1	A	157	ASP	2.6
12	L	37	LYS	2.6
1	A	1455	PRO	2.6
2	B	712	PRO	2.6
4	D	12	ARG	2.5
3	C	3	GLU	2.5
5	E	125	PRO	2.5
2	B	69	LEU	2.5
2	B	473	MET	2.5
4	D	3	VAL	2.5
2	B	868	MET	2.5
2	B	295	GLY	2.5
2	B	643	ASP	2.5
8	H	90	ALA	2.4
2	B	66	ASP	2.4
1	A	1256	GLU	2.4
1	A	257	ARG	2.4
4	D	13	ARG	2.4
9	I	4	PHE	2.4
1	A	1257	ASP	2.4
2	B	715	ALA	2.4
2	B	252	SER	2.4
2	B	101	MET	2.4
1	A	1187	GLN	2.3
1	A	59	GLY	2.3
2	B	723	VAL	2.3
2	B	962	LYS	2.3
2	B	335	GLY	2.3
4	D	23	ASN	2.3
1	A	1454	MET	2.3
1	A	50	ILE	2.3
2	B	884	ARG	2.3
2	B	714	GLU	2.3
2	B	505	ASP	2.3
4	D	25	ALA	2.2
2	B	468	GLU	2.2
4	D	11	ARG	2.2
1	A	65	LEU	2.2
12	L	49	LYS	2.2
2	B	879	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	266	ALA	2.2
12	L	53	HIS	2.2
2	B	115	GLN	2.2
2	B	265	SER	2.2
8	H	108	SER	2.2
2	B	584	GLY	2.2
9	I	76	PRO	2.2
1	A	44	THR	2.2
2	B	508	LEU	2.2
1	A	109	HIS	2.1
2	B	106	ASP	2.1
2	B	731	VAL	2.1
13	2	7	DT	2.1
8	H	84	ALA	2.1
2	B	866	TYR	2.1
1	A	155	GLU	2.1
1	A	161	LEU	2.1
8	H	64	ASN	2.1
2	B	244	LEU	2.1
2	B	881	ASN	2.1
2	B	246	LYS	2.1
1	A	158	PRO	2.1
2	B	725	PRO	2.1
12	L	28	LYS	2.1
1	A	254	GLU	2.1
4	D	119	ARG	2.1
12	L	54	ARG	2.1
14	1	11	DA	2.0
1	A	153	PRO	2.0
1	A	1092	LYS	2.0
5	E	131	THR	2.0
9	I	21	GLU	2.0
2	B	370	PHE	2.0
1	A	1110	ASN	2.0
2	B	708	GLU	2.0

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

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( $\text{\AA}^2$ )	Q<0.9
14	BRU	1	23	20/21	0.84	0.16	81,90,95,98	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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( $\text{\AA}^2$ )	Q<0.9
16	ZN	I	1122	1/1	0.95	0.07	124,124,124,124	0
17	MG	A	2458	1/1	0.95	0.07	52,52,52,52	0
16	ZN	L	1071	1/1	0.99	0.05	86,86,86,86	0
16	ZN	A	2456	1/1	0.99	0.03	70,70,70,70	0
16	ZN	I	1121	1/1	1.00	0.02	74,74,74,74	0
16	ZN	A	2457	1/1	1.00	0.01	35,35,35,35	0
16	ZN	J	1066	1/1	1.00	0.01	39,39,39,39	0
16	ZN	B	2225	1/1	1.00	0.01	32,32,32,32	0
16	ZN	C	1269	1/1	1.00	0.02	27,27,27,27	0

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

There are no such residues in this entry.