



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:48 am BST

PDB ID : 3HOV  
Title : Complete RNA polymerase II elongation complex II  
Authors : Sydow, J.F.; Brueckner, F.; Cheung, A.C.M.; Damsma, G.E.; Dengl, S.;  
Lehmann, E.; Vassilyev, D.; Cramer, P.  
Deposited on : 2009-06-03  
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

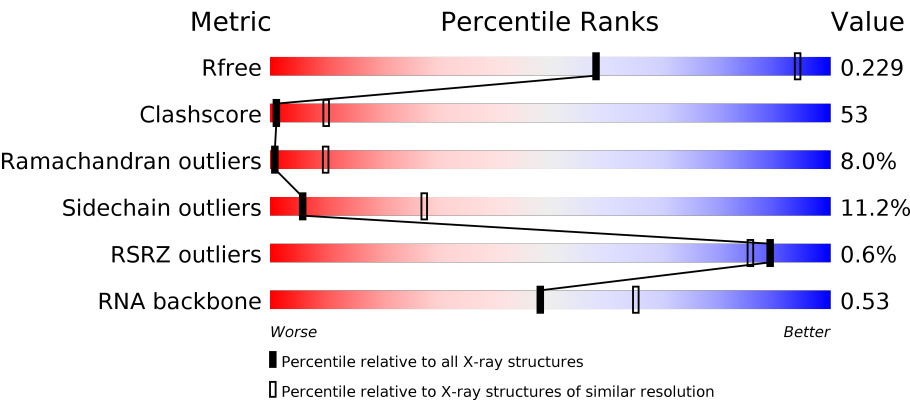
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

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





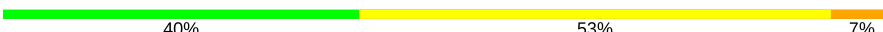
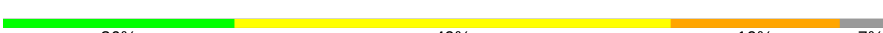


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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><div>%</div><div><div></div><div>27%</div><div>44%</div><div>9%</div><div>•</div><div>18%</div></div></div>
2	B	1224	<div><div>%</div><div><div></div><div>25%</div><div>52%</div><div>12%</div><div>10%</div></div></div>
3	C	318	<div><div></div><div><div></div><div>26%</div><div>46%</div><div>11%</div><div>16%</div></div></div>
4	D	221	<div><div></div><div><div></div><div>25%</div><div>44%</div><div>10%</div><div>•</div><div>19%</div></div></div>

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	T	26	
14	N	13	
15	P	17	

## 2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 31777 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
1	A	1416	Total	C	N	O	S	0	0	0
			11143	7021	1949	2111	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1104	Total	C	N	O	S	0	0	0
			8779	5560	1537	1627	55			

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a DNA chain called 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*A\*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
13	T	17	Total	Br	C	N	O	P	0	0	0
			347	1	166	61	103	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	5	Total	C	N	O	P	0	0	0
			97	48	18	27	4			

- Molecule 15 is a RNA chain called 5'-R(\*UP\*GP\*CP\*AP\*UP\*UP\*UP\*CP\*GP\*AP\*CP\*CP\*AP\*GP\*GP\*CP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	10	Total	C	N	O	P	0	0	0
			215	96	42	67	10			

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

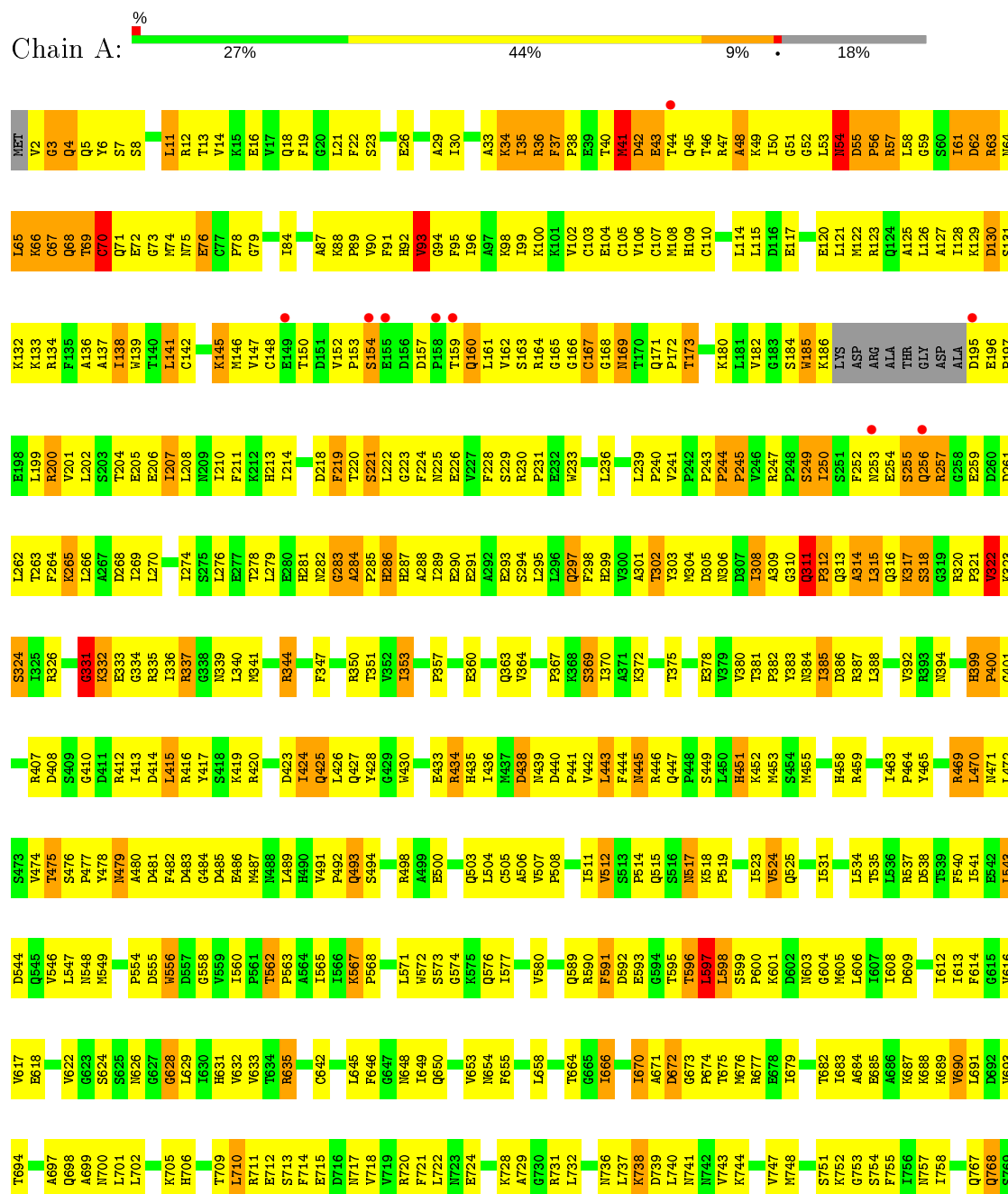
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

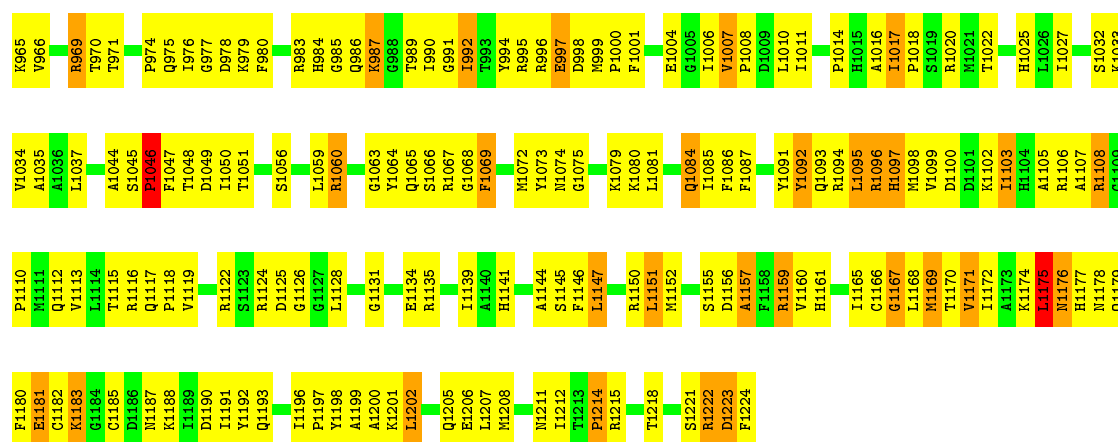
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



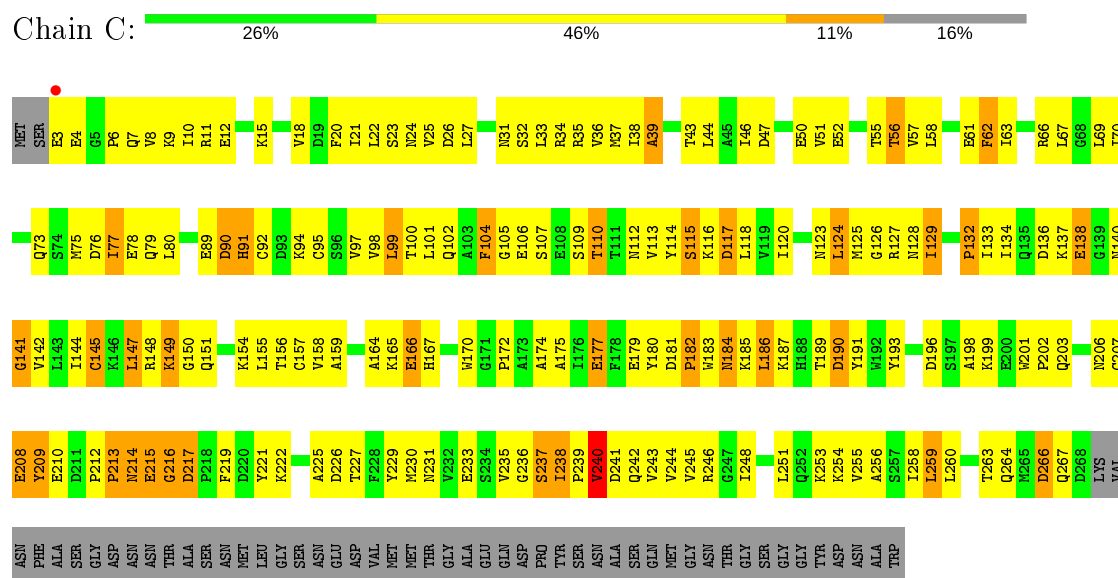




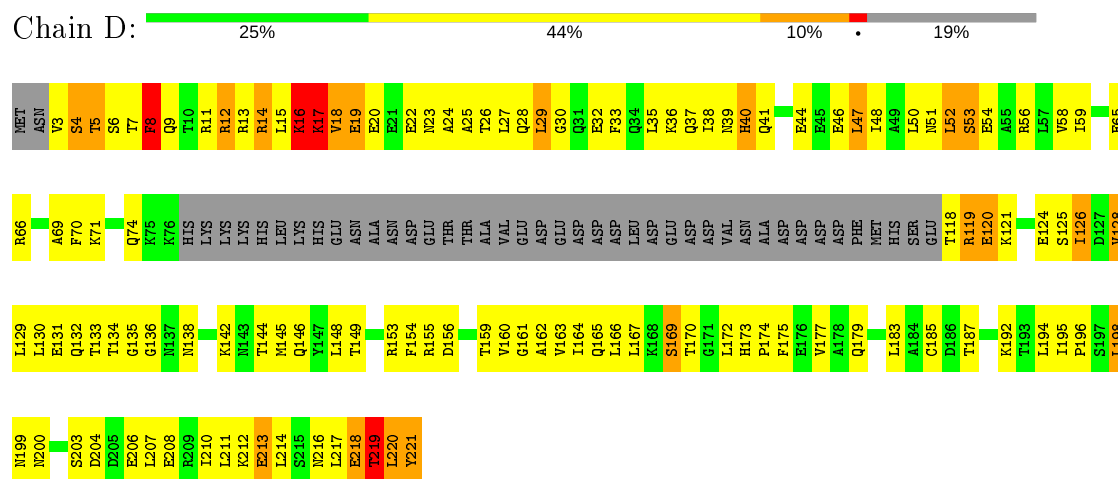
E336	S771	A704	D642	V580	R512	A447	F377	P316	Q255	T185	T123	D61
D837	A705	B706	D643	F581	Q513	I448	L378	C317	V256	E186	Y124	I62
S338	M773	B707	E644	N583	H515	M449	G379	V318	K257	S187	S125	I63
M839	G774	F707	S645	N583	H515	A450	Y380	E319	L258	D188	S126	O54
I840	K775	E708	L646	N586	T517	K451	M381	D320	Y259	L189	G127	B65
M841	Q776	D709	G647	N586	H518	T452	I382	V823	G260	Y190	L128	D66
N842	A777	L710	H648	V589	H519	T453	I383	I324	K261	K191	F129	S67
S845	M778	E711	K649	H590	G520	T454	N384	Q325	E262	L192	V130	I68
I846	Q779	F712	E650	H590	G520	S455	L385	D326	S264	K193	L69	I69
D847	V780	A713	L651	N592	L521	G456	L386	R327	G265	E194	I70	TYR
D847	E714	K652	K652	N592	L521	L457	L387	E328	S265			LEU
R848	Y785	A715	V653	P593	E526	K458	T329	E328	A266	M199	ARG	GLU
G849	N786	ASN	R654	A594	T527	Y459	D391	T329	R267		THR	GLN
L850	V787	E716	K655	R595	P528	A460	D391	A330	Y202	F203	T77	LEU
F851	V788	GLU	G656	L596	E529	L461	R392	L331	I269		ALA	ASP
	M789	ASN	H657	M597	G530	K470	K393	L331	I204	I204	ALA	GLN
	D790	ASP	I658	N598	Q531	LVS	G402	F333	I205	I205	ILE	HIS
L854	T791	LEU	A659	T599	A532	A472	R405	I334	D272	D272	ASP	GLY
F855	M792	D722	K660	L600	A532	M465	R405	I334	I280	R217	LYS	SER
F856	A793	F723	R601	L601	L535	M466	L406	ILE	I282	S218	GLY	T26
S958	N794	H734	M662	R601	L535	G467	D399	ARG	V283	N221	LEU	T28
G859	S958	R728	A663	L603	K537	Q469	H400	GLY	I284	M221	ILE	GLU
M860	L796	T729	T664	R604	M538	K470	F401	THR	I285	I222	ALA	I90
D861	R730	E730	E665	R605	L539	LVS	G402	ALA	I285	V223	ALA	S91
Q862	V731		Y666	K606	L542	A472	K418	LEU	F286	Q224	GLU	S91
R863	Q732		Q667	G607	M542	M473	D407	LYS	I286	I222	ILE	I90
K864	H733		D668	D608	L545	S474	L403	K345	I286	I222	ILE	I90
S865	A801	H734	ILE	I609	S546	S475	L403	K345	I286	I222	ILE	I90
K866	R802	T736	GLU	N610	S546	R476	L403	K345	I286	I222	ILE	I90
G867	L803		GLY	P611	V547	A477	L403	K345	I286	I222	ILE	I90
M868	G804		GLY	P612	G548	G478	L403	K345	I286	I222	ILE	I90
S869	R934	F738	PHE	P613	T549	V479	L403	K345	I286	I222	ILE	I90
I870	T806	T739	GLU	P614	D550	S480	L403	K345	I286	I222	ILE	I90
T871	R807	H740	ASP	M615	P551	A472	L403	K345	I286	I222	ILE	I90
E872	A808	C741	VAL	I616	M552	L483	L403	K345	I286	I222	ILE	I90
T873	M809	E742	GLU	R617	P553	M484	L403	K345	I286	I222	ILE	I90
F874	E810	I743	D678	D618	L554	R485	L403	K345	I286	I222	ILE	I90
K875	Y811	H744	Y679	I619	L555	Y486	L403	K345	I286	I222	ILE	I90
T876	L812	F745		R620	T556	T487	L403	K345	I286	I222	ILE	I90
P877	K813	S746	S682	E621	F557	K426	L403	K345	I286	I222	ILE	I90
Q878	F814	M747		K622	F557	K426	L403	K345	I286	I222	ILE	I90
R879	R815	I748	L685	E523	S559	T491	L403	K345	I286	I222	ILE	I90
S880	E816	L749	M686	L624	E560	L492	L403	K345	I286	I222	ILE	I90
ASN	L817	G750	E687	K625	M561	S493	L403	K345	I286	I222	ILE	I90
THR	P818	V751	G688	I626	G562	L492	L403	K345	I286	I222	ILE	I90
LEU	A819	A752	L689	F627	M563	R496	L403	K345	I286	I222	ILE	I90
R884	G820		P690	T628	Q432	R497	L403	K345	I286	I222	ILE	I90
M885	Q821	I756	E691	D629	L566	T498	L403	K345	I286	I222	ILE	I90
K886	F757	F757	F692	A630	L566	T498	L403	K345	I286	I222	ILE	I90
H887	I824	F758	D693	G631	Y569	P501	L403	K345	I286	I222	ILE	I90
G888	V825	F759	L694	R632	V570	I502	L403	K345	I286	I222	ILE	I90
T889	A826	D760	A695	V633	P571	GLY	L403	K345	I286	I222	ILE	I90
Y890	I827		E696	Y634	H572	ARG	L403	K345	I286	I222	ILE	I90
D891			E697	R635	Q573	ASP	L403	K345	I286	I222	ILE	I90
R992	Y830	Q763	E698	P636	S574	GLY	L403	K345	I286	I222	ILE	I90
L893	S831	F765	E699	L637	P575	LVS	L403	K345	I286	I222	ILE	I90
D894	G832	R766	F699	F638	D576	ASN	L403	K345	I286	I222	ILE	I90
R895	H833	S700	I701	I639	A577	A509	L403	K345	I286	I222	ILE	I90
T896	K834	Y769	L702	V640	T578	LVS	L403	K345	I286	I222	ILE	I90
C897	R935	D770	I703	R641	B570	D511	L403	K345	I286	I222	ILE	I90



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

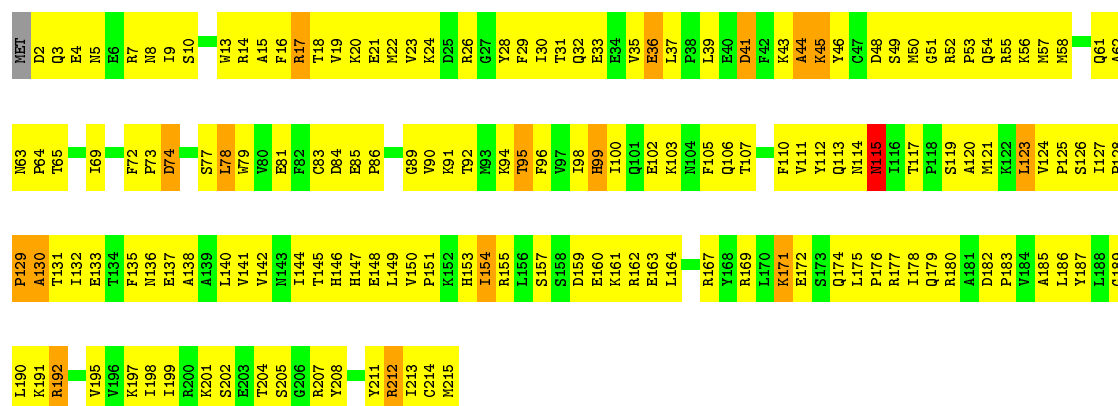


- Molecule 4: DNA-directed RNA polymerase II subunit RPB4

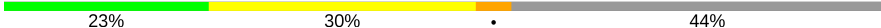


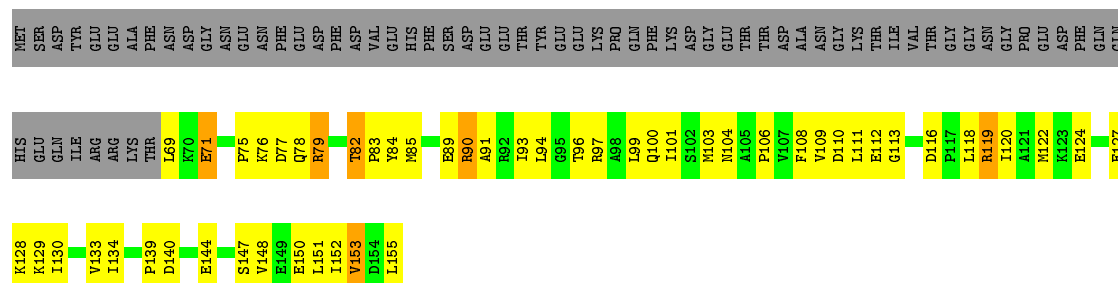
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 



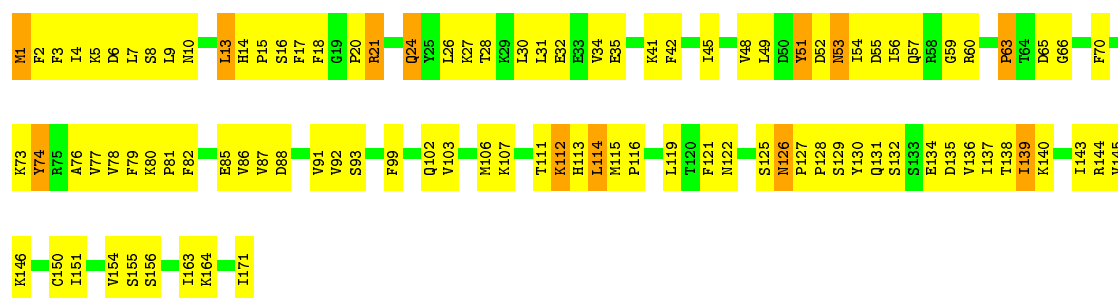
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 



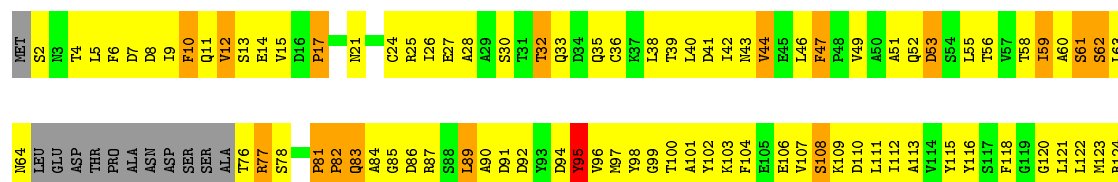
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G: 



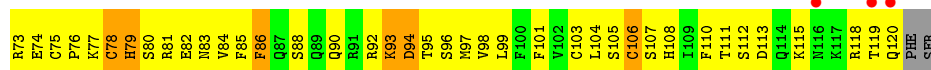
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 

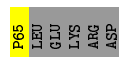




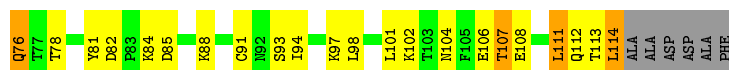
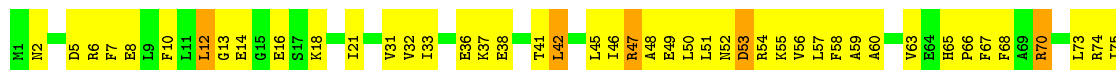
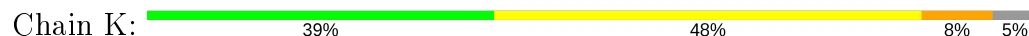
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



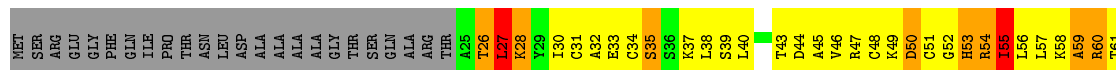
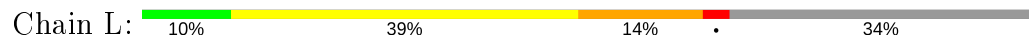
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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

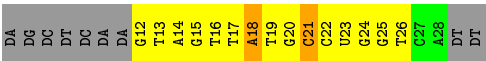


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

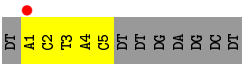


- Molecule 13: 5'-D(\*AP\*GP\*CP\*TP\*CP\*AP\*A\*GP\*TP\*AP\*GP\*TP\*TP\*AP\*TP\*GP\*CP\*C  
P\*(BRU)P\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3'





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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	222.25Å 393.38Å 283.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50 49.17 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.50) 99.9 (49.17-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.76 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.210 , 0.226 0.214 , 0.229	Depositor DCC
$R_{free}$ test set	4056 reflections (2.61%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.9	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 99.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.024 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	31777	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.49	0/11342	0.77	12/15337 (0.1%)
2	B	0.48	0/8948	0.74	1/12062 (0.0%)
3	C	0.47	0/2133	0.75	1/2891 (0.0%)
4	D	0.45	0/1444	0.72	1/1935 (0.1%)
5	E	0.45	0/1788	0.68	1/2406 (0.0%)
6	F	0.56	0/717	0.80	1/967 (0.1%)
7	G	0.48	0/1368	0.76	1/1844 (0.1%)
8	H	0.43	0/1094	0.72	0/1481
9	I	0.44	0/989	0.71	0/1331
10	J	0.50	0/541	0.83	0/727
11	K	0.48	0/937	0.67	0/1265
12	L	0.57	0/365	0.84	0/485
13	T	0.54	0/365	0.85	0/560
14	N	0.57	0/108	0.78	0/164
15	P	0.45	0/240	0.82	1/372 (0.3%)
All	All	0.48	0/32379	0.75	19/43827 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
8	H	0	1
13	T	0	3
All	All	0	5

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	PRO	N-CA-C	-6.45	95.34	112.10
3	C	39	ALA	N-CA-C	6.38	128.24	111.00
1	A	55	ASP	N-CA-CB	6.13	121.63	110.60
1	A	3	GLY	N-CA-C	-6.04	97.99	113.10
15	P	1	C	N1-C1'-C2'	5.90	121.67	114.00
1	A	311	GLN	N-CA-C	5.87	126.84	111.00
5	E	171	LYS	N-CA-C	-5.69	95.65	111.00
1	A	1116	LEU	CA-CB-CG	5.65	128.29	115.30
1	A	331	GLY	N-CA-C	5.63	127.17	113.10
1	A	4	GLN	N-CA-C	5.53	125.93	111.00
4	D	8	PHE	N-CA-C	5.44	125.69	111.00
6	F	71	GLU	N-CA-C	-5.38	96.48	111.00
7	G	65	ASP	N-CA-C	-5.36	96.52	111.00
1	A	1403	GLU	N-CA-C	5.32	125.37	111.00
1	A	54	ASN	C-N-CA	5.28	134.90	121.70
1	A	78	PRO	N-CA-C	-5.16	98.68	112.10
1	A	998	LEU	CA-CB-CG	-5.16	103.43	115.30
1	A	459	ARG	NE-CZ-NH1	-5.12	117.74	120.30
2	B	363	HIS	N-CA-C	-5.04	97.40	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1192	TYR	Sidechain
8	H	102	TYR	Sidechain
13	T	18	DA	Sidechain
13	T	19	DT	Sidechain
13	T	21	DC	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	1194	0
2	B	8779	0	8808	1069	0
3	C	2095	0	2051	259	0
4	D	1434	0	1460	156	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1752	0	1776	193	0
6	F	705	0	731	75	0
7	G	1340	0	1357	133	0
8	H	1076	0	1046	159	0
9	I	971	0	929	118	0
10	J	532	0	542	77	0
11	K	919	0	929	82	0
12	L	363	0	388	85	0
13	T	347	0	192	20	0
14	N	97	0	58	6	0
15	P	215	0	111	7	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
All	All	31777	0	31595	3348	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 53.

All (3348) 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:559:SER:HA	2:B:563:MET:HB3	1.20	1.18
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.08	1.17
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.28	1.14
2:B:261:ARG:HH11	2:B:261:ARG:HB3	1.12	1.13
1:A:53:LEU:HD23	1:A:54:ASN:N	1.65	1.12
1:A:567:LYS:HB3	8:H:96:VAL:H	1.06	1.11
1:A:53:LEU:HD23	1:A:54:ASN:H	0.97	1.10
1:A:901:LEU:H	1:A:926:GLN:NE2	1.47	1.10
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.21	1.10
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.30	1.07
8:H:4:THR:HA	8:H:60:ALA:HB2	1.30	1.07
1:A:34:LYS:HE3	1:A:57:ARG:HH12	1.13	1.06
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.36	1.06
2:B:278:GLN:HG2	2:B:279:ASP:H	1.14	1.06
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.31	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.37	1.05
9:I:93:LYS:H	9:I:93:LYS:HD3	1.22	1.04
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.35	1.04
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.21	1.03
1:A:41:MET:HB3	1:A:49:LYS:HA	1.40	1.03
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.58	1.01
2:B:430:ARG:HB3	2:B:430:ARG:HH11	1.25	1.01
2:B:510:LYS:CG	2:B:511:PRO:HD3	1.91	1.01
12:L:26:THR:HG22	12:L:27:LEU:H	1.22	1.01
1:A:1385:THR:HG23	1:A:1387:HIS:H	1.24	1.00
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.25	1.00
3:C:177:GLU:HG3	3:C:231:ASN:HB3	1.42	1.00
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.43	0.99
5:E:56:LYS:HE2	5:E:84:ASP:HB2	1.45	0.99
2:B:120:ARG:HH12	12:L:54:ARG:HH11	1.08	0.98
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.46	0.98
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.46	0.98
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.26	0.98
8:H:95:TYR:HE2	8:H:97:MET:HG3	1.25	0.98
2:B:510:LYS:HG3	2:B:511:PRO:HD3	0.99	0.98
1:A:308:ILE:HG22	1:A:309:ALA:H	1.26	0.98
12:L:55:ILE:HG12	12:L:56:LEU:H	1.27	0.97
1:A:108:MET:HA	1:A:210:ILE:HD13	1.40	0.97
1:A:34:LYS:CE	1:A:57:ARG:HH12	1.76	0.97
12:L:38:LEU:HD11	12:L:49:LYS:HE2	1.47	0.97
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.42	0.97
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.45	0.97
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.00	0.96
4:D:118:THR:HB	4:D:121:LYS:HB2	1.44	0.96
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.30	0.96
2:B:508:LEU:N	14:N:1:DA:HO5'	1.61	0.96
1:A:90:VAL:HB	1:A:297:GLN:NE2	1.80	0.96
10:J:64:ASN:HB3	10:J:65:PRO:CD	1.95	0.96
10:J:16:ASP:OD1	10:J:17:LYS:HD2	1.66	0.96
1:A:567:LYS:HB3	8:H:96:VAL:N	1.80	0.95
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.31	0.95
9:I:111:THR:HG22	9:I:112:SER:H	1.30	0.95
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.48	0.95
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.49	0.95
1:A:688:LYS:HD2	1:A:691:LEU:HD23	1.46	0.95
2:B:510:LYS:HG3	2:B:511:PRO:CD	1.95	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.48	0.94
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.65	0.94
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.47	0.94
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.03	0.94
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.50	0.94
2:B:751:VAL:HG13	2:B:812:LEU:HD22	1.49	0.93
5:E:114:ASN:O	5:E:115:ASN:HB3	1.66	0.93
9:I:50:THR:HG22	9:I:51:ASN:H	1.33	0.93
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.51	0.93
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.48	0.93
1:A:754:SER:H	1:A:757:ASN:HD22	1.10	0.93
1:A:41:MET:CB	1:A:49:LYS:HA	1.99	0.92
1:A:858:ASN:ND2	1:A:860:LEU:H	1.66	0.92
2:B:261:ARG:NH1	2:B:261:ARG:HB3	1.83	0.92
1:A:567:LYS:HZ1	8:H:43:ASN:HB3	1.35	0.92
1:A:903:ASN:HD22	1:A:904:THR:N	1.67	0.92
1:A:830:LYS:O	1:A:834:THR:HB	1.70	0.92
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.50	0.92
3:C:56:THR:HG21	3:C:145:CYS:SG	2.10	0.92
1:A:34:LYS:HZ2	1:A:57:ARG:HH22	1.13	0.92
1:A:741:ASN:HD22	1:A:744:LYS:H	1.18	0.92
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.49	0.92
4:D:155:ARG:HD3	4:D:221:TYR:HE1	1.34	0.91
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.68	0.91
13:T:24:DG:H2''	13:T:25:DG:H5'	1.52	0.91
2:B:579:ARG:HB2	2:B:586:TRP:NE1	1.85	0.91
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.53	0.91
2:B:603:LEU:HD13	2:B:608:ASP:HB2	1.50	0.91
1:A:855:THR:HG21	1:A:857:ARG:HE	1.33	0.91
9:I:111:THR:HG22	9:I:113:ASP:H	1.32	0.91
1:A:517:ASN:HD22	1:A:1364:ASN:HD22	1.04	0.90
8:H:59:ILE:HG22	8:H:60:ALA:H	1.36	0.90
1:A:1116:LEU:N	1:A:1308:THR:HG22	1.86	0.90
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.51	0.90
1:A:315:LEU:H	1:A:315:LEU:HD23	1.36	0.90
2:B:996:ARG:HH12	3:C:174:ALA:HA	1.36	0.90
6:F:103:MET:CE	7:G:66:GLY:H	1.82	0.90
2:B:879:ARG:CZ	2:B:879:ARG:H	1.83	0.90
2:B:806:THR:HG22	2:B:808:ALA:H	1.34	0.90
1:A:1387:HIS:O	1:A:1391:ARG:HG3	1.72	0.90
7:G:34:VAL:HG11	7:G:74:TYR:HE1	1.37	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:82:PRO:C	8:H:84:ALA:H	1.73	0.90
1:A:344:ARG:HH11	1:A:344:ARG:HB3	1.36	0.89
1:A:913:LEU:HD12	1:A:914:GLU:H	1.38	0.89
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.55	0.89
1:A:1385:THR:HG22	1:A:1388:GLY:H	1.35	0.89
1:A:66:LYS:NZ	1:A:68:GLN:H	1.71	0.89
2:B:120:ARG:NH1	12:L:54:ARG:HH11	1.70	0.89
2:B:766:ARG:NH2	2:B:1020:ARG:HH11	1.70	0.89
2:B:36:ALA:HA	2:B:39:ARG:HD2	1.54	0.89
2:B:744:HIS:HD2	2:B:745:PRO:HD2	1.37	0.89
4:D:154:PHE:CD1	4:D:163:VAL:HG21	2.08	0.88
1:A:381:THR:HG22	1:A:383:TYR:H	1.36	0.88
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.53	0.88
2:B:516:ASN:N	2:B:516:ASN:HD22	1.70	0.88
8:H:130:ARG:HH11	8:H:130:ARG:HB2	1.38	0.88
2:B:766:ARG:HH22	2:B:1020:ARG:HH11	1.18	0.88
2:B:642:ASP:HA	2:B:649:LYS:HA	1.54	0.88
5:E:78:LEU:HB2	5:E:107:THR:HB	1.53	0.88
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.56	0.88
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.54	0.88
1:A:901:LEU:H	1:A:926:GLN:HE21	1.20	0.88
2:B:168:GLY:H	2:B:450:ALA:HB1	1.38	0.88
2:B:706:GLN:HE22	2:B:730:ARG:HD3	1.38	0.88
7:G:1:MET:HE1	7:G:79:PHE:HA	1.56	0.87
1:A:61:ILE:HG22	1:A:62:ASP:H	1.40	0.87
1:A:534:LEU:O	1:A:574:GLY:HA3	1.73	0.87
1:A:66:LYS:HZ3	1:A:68:GLN:H	1.22	0.87
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.57	0.87
9:I:111:THR:HG22	9:I:112:SER:N	1.86	0.86
1:A:107:CYS:HA	1:A:171:GLN:NE2	1.90	0.86
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.58	0.86
2:B:469:GLN:O	2:B:472:ALA:HB3	1.74	0.86
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.05	0.86
12:L:28:LYS:HE3	12:L:39:SER:OG	1.75	0.86
2:B:1065:GLN:HE21	2:B:1067:ARG:H	0.87	0.85
2:B:1187:ASN:HD21	2:B:1190:ASP:HB3	1.41	0.85
4:D:130:LEU:HD13	4:D:142:LYS:HG2	1.58	0.85
1:A:40:THR:HG22	1:A:41:MET:HG3	1.59	0.85
13:T:16:DT:H5'	13:T:16:DT:H6	1.41	0.85
1:A:853:ASP:OD1	1:A:855:THR:HB	1.74	0.85
2:B:243:ALA:HA	2:B:250:PHE:O	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:12:ARG:HH11	4:D:12:ARG:HG2	1.42	0.85
5:E:153:HIS:O	5:E:154:ILE:HG13	1.76	0.85
1:A:1364:ASN:OD1	1:A:1366:ARG:HG2	1.77	0.84
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.57	0.84
13:T:13:DT:H2"	13:T:14:DA:OP2	1.77	0.84
7:G:128:PRO:O	7:G:138:THR:HG23	1.77	0.84
2:B:616:ILE:HG13	2:B:697:GLU:HG3	1.59	0.84
3:C:50:GLU:OE1	12:L:64:LEU:HD22	1.76	0.84
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.07	0.84
5:E:198:ILE:HD11	5:E:212:ARG:HG3	1.60	0.84
1:A:315:LEU:N	1:A:315:LEU:HD23	1.92	0.84
1:A:265:LYS:HE3	1:A:265:LYS:N	1.92	0.84
1:A:316:GLN:HG2	1:A:317:LYS:HG2	1.60	0.84
3:C:115:SER:HB3	3:C:141:GLY:O	1.78	0.84
3:C:123:ASN:ND2	3:C:125:MET:HG3	1.92	0.84
1:A:822:GLU:HG3	2:B:513:GLN:HE21	1.43	0.84
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.58	0.84
8:H:42:ILE:HG23	8:H:95:TYR:HE1	1.42	0.84
10:J:1:MET:N	10:J:57:ILE:H	1.76	0.84
2:B:879:ARG:NH1	2:B:879:ARG:H	1.76	0.83
3:C:73:GLN:NE2	3:C:75:MET:HB2	1.93	0.83
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.13	0.83
5:E:197:LYS:HE2	5:E:199:ILE:HD11	1.60	0.83
8:H:89:LEU:C	8:H:91:ASP:H	1.81	0.83
2:B:705:MET:H	2:B:710:LEU:HD12	1.43	0.83
8:H:59:ILE:HG22	8:H:60:ALA:N	1.93	0.83
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.59	0.83
2:B:531:GLN:HG2	2:B:532:ALA:H	1.44	0.83
1:A:596:THR:O	1:A:598:LEU:N	2.12	0.83
1:A:629:LEU:O	1:A:633:VAL:HG23	1.79	0.83
2:B:583:ASN:ND2	2:B:628:THR:HG22	1.91	0.83
1:A:567:LYS:CB	8:H:95:TYR:HA	2.09	0.83
9:I:6:PHE:HB3	9:I:12:ASN:O	1.78	0.83
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.09	0.82
12:L:40:LEU:HD13	12:L:44:ASP:HB3	1.60	0.82
1:A:43:GLU:HG3	1:A:46:THR:HB	1.59	0.82
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.59	0.82
2:B:56:ASP:HB3	2:B:57:TYR:CD1	2.14	0.82
12:L:32:ALA:CB	12:L:55:ILE:HG13	2.09	0.82
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.15	0.82
1:A:1127:ASP:OD2	1:A:1130:GLN:HB2	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:744:HIS:CD2	2:B:745:PRO:HD2	2.14	0.82
15:P:3:A:H2'	15:P:4:C:C6	2.14	0.82
1:A:256:GLN:O	1:A:257:ARG:HB2	1.79	0.82
1:A:567:LYS:HD3	8:H:95:TYR:CD2	2.14	0.82
10:J:48:ARG:HE	10:J:49:MET:HE2	1.44	0.82
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.44	0.82
2:B:278:GLN:HG2	2:B:279:ASP:N	1.93	0.82
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.59	0.82
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.60	0.82
7:G:122:ASN:ND2	7:G:125:SER:HB3	1.95	0.82
12:L:55:ILE:H	12:L:55:ILE:HD13	1.44	0.82
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.60	0.81
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.10	0.81
1:A:288:ALA:HA	1:A:291:GLU:CD	2.01	0.81
1:A:503:GLN:HE21	6:F:90:ARG:NH2	1.78	0.81
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.61	0.81
3:C:112:ASN:HB3	3:C:114:TYR:CE1	2.15	0.81
1:A:353:ILE:HG21	1:A:487:MET:CG	2.10	0.81
2:B:172:ILE:HD13	2:B:178:ASN:HD22	1.44	0.81
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.61	0.81
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.10	0.81
4:D:154:PHE:CE1	4:D:163:VAL:HG21	2.15	0.81
1:A:710:LEU:H	1:A:710:LEU:HD12	1.44	0.81
1:A:63:ARG:HA	1:A:74:MET:HE2	1.62	0.81
7:G:34:VAL:HG11	7:G:74:TYR:CE1	2.15	0.81
1:A:1110:ASN:N	1:A:1110:ASN:HD22	1.78	0.81
1:A:866:PHE:O	1:A:867:ILE:HD12	1.78	0.81
2:B:622:LYS:HE2	9:I:59:VAL:CG2	2.09	0.81
2:B:995:ARG:HH12	3:C:165:LYS:HG2	1.45	0.81
1:A:34:LYS:HE3	1:A:57:ARG:NH1	1.96	0.81
1:A:55:ASP:N	1:A:56:PRO:HD3	1.96	0.81
2:B:465:ASN:HD22	2:B:465:ASN:N	1.78	0.81
2:B:56:ASP:HB3	2:B:57:TYR:HD1	1.45	0.81
7:G:26:LEU:HD12	7:G:56:ILE:HD11	1.63	0.80
12:L:30:ILE:O	12:L:56:LEU:HA	1.80	0.80
1:A:754:SER:N	1:A:757:ASN:HD22	1.78	0.80
1:A:767:GLN:NE2	1:A:774:ARG:HB3	1.96	0.80
2:B:579:ARG:HG2	2:B:579:ARG:HH11	1.46	0.80
12:L:47:ARG:HH11	12:L:47:ARG:HB2	1.46	0.80
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.60	0.80
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:THR:HG22	1:A:710:LEU:H	1.44	0.80
1:A:901:LEU:HA	1:A:907:THR:OG1	1.81	0.80
3:C:238:ILE:HG22	3:C:243:VAL:HG23	1.64	0.80
3:C:7:GLN:HE21	11:K:104:ASN:ND2	1.77	0.80
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.63	0.80
2:B:916:THR:HB	2:B:935:ARG:HD2	1.64	0.80
1:A:1409:LEU:HD13	2:B:1207:LEU:HD11	1.63	0.80
3:C:148:ARG:H	3:C:151:GLN:HG3	1.45	0.80
1:A:595:THR:O	1:A:596:THR:HG23	1.80	0.80
11:K:57:LEU:HB2	11:K:76:GLN:HG2	1.61	0.80
1:A:34:LYS:HZ2	1:A:57:ARG:NH2	1.80	0.80
1:A:66:LYS:HD3	1:A:67:CYS:N	1.97	0.80
1:A:738:LYS:HG3	1:A:740:LEU:HG	1.61	0.80
2:B:744:HIS:HD2	2:B:745:PRO:CD	1.93	0.80
8:H:58:THR:HG22	8:H:59:ILE:H	1.48	0.80
10:J:63:TYR:O	10:J:64:ASN:HB2	1.79	0.79
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.65	0.79
3:C:66:ARG:NH1	10:J:2:ILE:HG21	1.98	0.79
6:F:111:LEU:H	6:F:111:LEU:HD12	1.45	0.79
8:H:130:ARG:HB2	8:H:130:ARG:NH1	1.96	0.79
1:A:1081:LEU:HD11	1:A:1098:VAL:H	1.47	0.79
1:A:858:ASN:HD22	1:A:858:ASN:C	1.84	0.79
4:D:159:THR:O	4:D:163:VAL:HG23	1.82	0.79
1:A:416:ARG:HH11	1:A:417:TYR:HE1	1.29	0.79
5:E:19:VAL:O	5:E:23:VAL:HG23	1.82	0.79
5:E:9:ILE:HD11	5:E:53:PRO:HD3	1.65	0.79
9:I:111:THR:CG2	9:I:112:SER:H	1.95	0.79
3:C:8:VAL:O	3:C:9:LYS:HG3	1.83	0.79
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.65	0.79
2:B:294:ASP:O	2:B:296:GLU:N	2.14	0.79
1:A:372:LYS:HA	1:A:435:HIS:ND1	1.98	0.79
1:A:53:LEU:CD2	1:A:54:ASN:H	1.88	0.79
1:A:567:LYS:NZ	8:H:43:ASN:HB3	1.98	0.79
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.65	0.78
2:B:542:MET:HG2	2:B:747:MET:HE3	1.66	0.78
8:H:130:ARG:HD3	8:H:130:ARG:N	1.97	0.78
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.48	0.78
2:B:583:ASN:HD21	2:B:628:THR:CG2	1.94	0.78
2:B:917:PRO:O	2:B:918:ILE:HG13	1.83	0.78
1:A:503:GLN:NE2	6:F:90:ARG:NH2	2.32	0.78
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.22	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:VAL:HG21	2:B:508:LEU:HD13	1.64	0.78
2:B:766:ARG:HH21	2:B:1020:ARG:CD	1.96	0.78
2:B:1004:GLU:HG3	10:J:42:LYS:HZ1	1.49	0.78
9:I:50:THR:HG22	9:I:51:ASN:N	1.99	0.78
2:B:25:ILE:CG2	2:B:658:ILE:HD12	2.13	0.78
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.19	0.78
12:L:47:ARG:HG2	12:L:48:CYS:H	1.47	0.78
1:A:225:ASN:HD22	1:A:228:PHE:H	1.32	0.78
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	1.84	0.78
7:G:138:THR:HG22	7:G:139:ILE:N	1.99	0.78
8:H:95:TYR:HE2	8:H:97:MET:CG	1.97	0.78
2:B:25:ILE:HG21	2:B:658:ILE:HD12	1.65	0.78
2:B:65:GLU:OE1	2:B:418:LYS:HE3	1.84	0.78
2:B:289:LEU:HD13	2:B:375:ALA:HB2	1.64	0.78
2:B:241:ARG:HG2	2:B:253:THR:CG2	2.13	0.77
5:E:84:ASP:O	5:E:86:PRO:HD3	1.84	0.77
4:D:71:LYS:HA	4:D:74:GLN:HB2	1.66	0.77
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.64	0.77
1:A:687:LYS:O	1:A:690:VAL:HG12	1.83	0.77
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.66	0.77
2:B:815:ARG:HH11	2:B:815:ARG:HB2	1.50	0.77
4:D:14:ARG:HB3	4:D:14:ARG:HH11	1.48	0.77
1:A:1161:THR:HG22	1:A:1163:ILE:N	1.99	0.77
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.65	0.77
2:B:613:VAL:HG22	2:B:628:THR:HA	1.67	0.77
2:B:796:LEU:HD21	2:B:821:GLN:HE21	1.50	0.77
3:C:11:ARG:HD3	3:C:209:TYR:CE2	2.20	0.77
1:A:783:THR:HG21	1:A:796:SER:O	1.85	0.77
1:A:961:ARG:HG2	1:A:965:GLN:HE21	1.49	0.77
9:I:105:SER:O	9:I:106:CYS:HB3	1.83	0.77
1:A:55:ASP:C	1:A:57:ARG:H	1.87	0.77
1:A:770:VAL:HG12	1:A:771:GLU:HG3	1.66	0.77
2:B:221:ASN:OD1	2:B:242:SER:HA	1.84	0.77
1:A:1329:THR:HG22	1:A:1331:SER:N	2.00	0.77
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.13	0.77
8:H:127:GLY:O	8:H:128:ASN:HB2	1.83	0.77
6:F:69:LEU:HB3	6:F:71:GLU:OE1	1.84	0.77
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.25	0.76
11:K:65:HIS:CD2	11:K:67:PHE:H	2.02	0.76
12:L:32:ALA:HB2	12:L:55:ILE:HG13	1.67	0.76
1:A:934:LYS:O	1:A:937:VAL:HG12	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.66	0.76
4:D:14:ARG:HH22	4:D:16:LYS:HZ3	1.32	0.76
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.83	0.76
7:G:126:ASN:HD22	7:G:127:PRO:HA	1.51	0.76
1:A:250:ILE:O	1:A:250:ILE:HG22	1.84	0.76
1:A:122:MET:HA	1:A:141:LEU:HD11	1.66	0.76
1:A:1112:LYS:O	1:A:1114:PRO:HD3	1.85	0.76
2:B:995:ARG:NH1	3:C:165:LYS:HG2	2.00	0.76
3:C:167:HIS:CD2	12:L:70:ARG:HB3	2.21	0.76
1:A:157:ASP:OD2	1:A:159:THR:HB	1.85	0.76
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.15	0.76
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.68	0.76
2:B:745:PRO:O	2:B:748:ILE:HG12	1.86	0.75
1:A:297:GLN:HE21	1:A:297:GLN:HA	1.49	0.75
1:A:567:LYS:HB2	8:H:95:TYR:HA	1.64	0.75
4:D:162:ALA:HA	4:D:165:GLN:HE21	1.49	0.75
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.65	0.75
1:A:1329:THR:HG22	1:A:1331:SER:H	1.51	0.75
1:A:697:ALA:HB2	1:A:702:LEU:HD11	1.69	0.75
7:G:14:HIS:CD2	7:G:16:SER:H	2.04	0.75
9:I:111:THR:HG22	9:I:113:ASP:N	2.01	0.75
2:B:707:PRO:HG2	2:B:708:GLU:H	1.51	0.75
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.21	0.75
5:E:112:TYR:O	5:E:137:GLU:HG3	1.86	0.75
8:H:55:LEU:HD22	8:H:144:ILE:HG22	1.68	0.75
12:L:53:HIS:HB3	12:L:55:ILE:CD1	2.16	0.75
2:B:644:GLU:OE2	2:B:646:LEU:HB3	1.86	0.75
4:D:155:ARG:HD3	4:D:221:TYR:CE1	2.21	0.75
9:I:80:SER:OG	9:I:105:SER:HB2	1.87	0.75
1:A:1308:THR:HG23	1:A:1309:ASP:N	2.01	0.75
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.66	0.74
1:A:69:THR:O	1:A:71:GLN:N	2.20	0.74
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.69	0.74
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.22	0.74
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.21	0.74
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.86	0.74
5:E:23:VAL:O	5:E:28:TYR:HB2	1.87	0.74
2:B:880:THR:HB	2:B:934:LYS:HD2	1.68	0.74
3:C:120:ILE:HG21	3:C:124:LEU:HD11	1.69	0.74
12:L:47:ARG:NH1	12:L:47:ARG:HB2	2.02	0.74
1:A:416:ARG:NH1	1:A:417:TYR:HE1	1.84	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:ILE:HD13	1:A:1037:LEU:HA	1.69	0.74
4:D:12:ARG:HG2	4:D:12:ARG:NH1	1.99	0.74
1:A:288:ALA:HA	1:A:291:GLU:OE1	1.87	0.74
2:B:824:ILE:HG12	10:J:48:ARG:HH12	1.52	0.74
10:J:44:TYR:HD2	10:J:44:TYR:H	1.35	0.74
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.69	0.74
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.69	0.74
2:B:890:TYR:O	2:B:893:LEU:HB2	1.88	0.74
3:C:165:LYS:O	11:K:6:ARG:NH1	2.21	0.74
5:E:15:ALA:O	5:E:19:VAL:HG23	1.87	0.74
1:A:672:ASP:HB3	1:A:736:ASN:OD1	1.87	0.73
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.16	0.73
2:B:427:ASP:HA	2:B:430:ARG:HD2	1.70	0.73
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.69	0.73
1:A:901:LEU:N	1:A:926:GLN:NE2	2.31	0.73
2:B:39:ARG:HH21	2:B:665:GLU:HG2	1.53	0.73
2:B:732:SER:HB2	2:B:734:HIS:CE1	2.23	0.73
6:F:82:THR:HG23	6:F:84:TYR:H	1.52	0.73
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.70	0.73
1:A:1444:MET:CG	7:G:60:ARG:HA	2.18	0.73
2:B:37:PHE:HE1	2:B:41:LYS:HD3	1.53	0.73
2:B:969:ARG:HD2	3:C:61:GLU:OE2	1.87	0.73
7:G:126:ASN:HD22	7:G:127:PRO:CA	1.99	0.73
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.70	0.73
1:A:446:ARG:HB2	1:A:487:MET:SD	2.28	0.73
2:B:39:ARG:HH21	2:B:665:GLU:CG	2.01	0.73
1:A:122:MET:HA	1:A:141:LEU:CD1	2.18	0.73
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.70	0.73
1:A:1006:ILE:HD11	5:E:163:GLU:HG3	1.69	0.73
7:G:139:ILE:HG23	7:G:140:LYS:N	2.01	0.73
1:A:2:VAL:HG22	1:A:3:GLY:H	1.53	0.73
1:A:369:SER:HB3	11:K:2:ASN:OD1	1.88	0.73
2:B:292:ILE:HD11	2:B:327:ARG:H	1.53	0.73
7:G:139:ILE:HG23	7:G:140:LYS:H	1.53	0.73
1:A:571:LEU:HD22	8:H:46:LEU:HD11	1.70	0.73
1:A:913:LEU:HD12	1:A:914:GLU:N	2.04	0.73
2:B:547:VAL:HG12	2:B:612:GLU:OE2	1.88	0.73
1:A:567:LYS:CB	8:H:96:VAL:H	1.96	0.73
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.22	0.73
2:B:805:THR:HG22	2:B:806:THR:H	1.51	0.73
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:66:ARG:NH2	10:J:3:VAL:O	2.22	0.73
13:T:15:DG:C2'	13:T:16:DT:H71	2.19	0.73
1:A:518:LYS:HE2	1:A:624:SER:O	1.89	0.73
4:D:66:ARG:HD2	4:D:133:THR:HB	1.70	0.73
1:A:12:ARG:HD2	2:B:1218:THR:HB	1.70	0.72
1:A:675:THR:O	1:A:679:ILE:HG13	1.88	0.72
1:A:879:GLU:O	1:A:955:PRO:HA	1.89	0.72
1:A:1141:THR:CG2	1:A:1205:LYS:HD3	2.19	0.72
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.69	0.72
2:B:652:LYS:HB3	2:B:689:LEU:HD23	1.68	0.72
2:B:800:GLN:HB3	10:J:52:THR:HG22	1.69	0.72
6:F:77:ASP:O	6:F:78:GLN:HB2	1.90	0.72
5:E:22:MET:HE3	5:E:26:ARG:HE	1.53	0.72
10:J:30:LEU:HD11	10:J:38:ARG:HH11	1.55	0.72
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.72	0.72
5:E:22:MET:HE3	5:E:26:ARG:NE	2.04	0.72
5:E:44:ALA:O	5:E:45:LYS:HB2	1.89	0.72
7:G:112:LYS:HA	7:G:115:MET:CE	2.19	0.72
7:G:13:LEU:HD22	7:G:17:PHE:HB2	1.72	0.72
1:A:265:LYS:HE3	1:A:265:LYS:CA	2.19	0.72
1:A:709:THR:HG22	1:A:710:LEU:N	2.04	0.72
2:B:364:ILE:O	2:B:365:THR:HB	1.89	0.72
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.71	0.72
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.24	0.72
1:A:40:THR:HG23	1:A:54:ASN:HD21	1.54	0.72
2:B:309:GLN:CD	9:I:52:ILE:HD11	2.08	0.72
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.19	0.72
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.69	0.72
1:A:249:SER:O	1:A:250:ILE:HG13	1.90	0.72
4:D:156:ASP:HB2	4:D:159:THR:HG23	1.70	0.72
2:B:193:LYS:NZ	12:L:32:ALA:HB1	2.05	0.72
1:A:1158:PRO:O	1:A:1159:ARG:HG3	1.89	0.72
1:A:855:THR:HG21	1:A:857:ARG:NE	2.03	0.72
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.24	0.72
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.20	0.72
1:A:56:PRO:O	1:A:57:ARG:NE	2.23	0.72
1:A:903:ASN:ND2	1:A:905:ASP:H	1.87	0.72
2:B:35:SER:HA	2:B:811:TYR:HE2	1.55	0.72
1:A:1223:ASP:HA	1:A:1243:VAL:HG22	1.72	0.72
2:B:549:THR:HG22	2:B:550:ASP:H	1.55	0.72
2:B:953:LEU:O	2:B:953:LEU:HD23	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:CYS:HA	1:A:171:GLN:HE22	1.53	0.71
1:A:534:LEU:HG	1:A:534:LEU:O	1.90	0.71
1:A:61:ILE:HG22	1:A:62:ASP:N	2.04	0.71
1:A:535:THR:CG2	1:A:616:VAL:HA	2.19	0.71
1:A:646:PHE:O	1:A:650:GLN:HG3	1.90	0.71
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.54	0.71
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.73	0.71
2:B:638:PHE:HD2	2:B:690:VAL:HG12	1.54	0.71
2:B:654:ARG:HH11	2:B:654:ARG:HG3	1.55	0.71
2:B:798:TYR:HE2	3:C:62:PHE:CZ	2.08	0.71
12:L:26:THR:HG22	12:L:27:LEU:N	2.00	0.71
1:A:49:LYS:HZ1	1:A:61:ILE:N	1.89	0.71
3:C:128:ASN:O	3:C:129:ILE:HG13	1.89	0.71
1:A:1210:GLY:O	1:A:1214:GLU:HG2	1.91	0.71
1:A:332:LYS:C	1:A:334:GLY:H	1.93	0.71
2:B:1016:ALA:O	2:B:1020:ARG:HG3	1.90	0.71
3:C:183:TRP:O	3:C:185:LYS:N	2.24	0.71
3:C:57:VAL:HG11	10:J:60:PHE:CB	2.12	0.71
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.25	0.71
6:F:96:THR:O	6:F:100:GLN:HG3	1.89	0.71
12:L:55:ILE:HG12	12:L:56:LEU:N	2.02	0.71
7:G:88:ASP:HB3	7:G:144:ARG:HA	1.73	0.71
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.56	0.71
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.26	0.71
1:A:858:ASN:HD22	1:A:860:LEU:H	1.39	0.71
12:L:38:LEU:CD1	12:L:49:LYS:HE2	2.20	0.71
1:A:590:ARG:O	1:A:591:PHE:HB2	1.91	0.71
4:D:14:ARG:HB3	4:D:14:ARG:NH1	2.05	0.71
11:K:36:GLU:OE2	11:K:70:ARG:HD3	1.91	0.71
1:A:438:ASP:O	1:A:439:ASN:HB2	1.91	0.70
2:B:244:LEU:HD21	2:B:366:GLN:HE21	1.55	0.70
2:B:165:VAL:HG11	2:B:448:ILE:HD13	1.71	0.70
2:B:706:GLN:NE2	2:B:730:ARG:HD3	2.05	0.70
5:E:14:ARG:HH21	5:E:141:VAL:HG12	1.54	0.70
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.55	0.70
1:A:1258:HIS:O	1:A:1262:LYS:HE3	1.90	0.70
1:A:367:PRO:HG2	1:A:370:ILE:HD12	1.71	0.70
1:A:399:HIS:O	1:A:401:GLY:N	2.24	0.70
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.20	0.70
2:B:1063:GLY:O	3:C:202:PRO:HG2	1.91	0.70
2:B:345:LYS:HE3	2:B:349:ILE:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:589:VAL:HG12	2:B:590:HIS:H	1.55	0.70
2:B:603:LEU:HD12	2:B:609:ILE:HG12	1.74	0.70
2:B:615:MET:HB3	2:B:626:ILE:HG12	1.74	0.70
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.21	0.70
1:A:517:ASN:ND2	1:A:1364:ASN:HD22	1.86	0.70
1:A:42:ASP:O	1:A:44:THR:N	2.24	0.70
1:A:722:LEU:H	1:A:722:LEU:HD12	1.56	0.70
2:B:766:ARG:HH21	2:B:1020:ARG:HD3	1.56	0.70
2:B:553:PRO:O	2:B:557:PHE:HB2	1.92	0.70
3:C:32:SER:O	3:C:36:VAL:HG23	1.91	0.70
9:I:93:LYS:H	9:I:93:LYS:CD	1.99	0.70
1:A:512:VAL:HA	1:A:519:PRO:HA	1.73	0.70
5:E:117:THR:HG22	5:E:119:SER:H	1.56	0.70
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.26	0.70
1:A:284:ALA:O	1:A:286:HIS:N	2.23	0.70
1:A:310:GLY:O	1:A:312:PRO:HD2	1.91	0.70
2:B:363:HIS:O	2:B:364:ILE:HB	1.92	0.70
5:E:204:THR:HG23	5:E:205:SER:N	2.06	0.70
8:H:42:ILE:HG23	8:H:95:TYR:CE1	2.26	0.70
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.27	0.70
7:G:26:LEU:HD12	7:G:56:ILE:CD1	2.22	0.70
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.73	0.70
1:A:1223:ASP:HA	1:A:1243:VAL:CG2	2.22	0.70
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.73	0.70
2:B:737:THR:HG21	9:I:66:PRO:HA	1.72	0.70
2:B:863:GLU:OE2	2:B:873:THR:HA	1.91	0.70
5:E:176:PRO:O	5:E:212:ARG:HA	1.92	0.70
2:B:944:THR:HG21	2:B:1122:ARG:NH2	2.06	0.69
2:B:393:LYS:HE3	2:B:393:LYS:HA	1.74	0.69
1:A:1433:MET:HE1	7:G:63:PRO:HB2	1.74	0.69
1:A:1385:THR:HG23	1:A:1387:HIS:N	2.04	0.69
3:C:147:LEU:N	3:C:147:LEU:HD23	2.08	0.69
7:G:112:LYS:HA	7:G:115:MET:HE2	1.72	0.69
7:G:116:PRO:HG2	7:G:119:LEU:HB2	1.74	0.69
2:B:807:ARG:NH1	2:B:807:ARG:HB3	2.07	0.69
3:C:244:VAL:O	3:C:248:ILE:HG13	1.91	0.69
2:B:378:LEU:O	2:B:382:ILE:HG13	1.92	0.69
2:B:168:GLY:HA2	2:B:454:THR:OG1	1.93	0.69
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.74	0.69
2:B:653:VAL:HG23	2:B:689:LEU:HB3	1.72	0.69
3:C:203:GLN:HG2	3:C:207:CYS:SG	2.33	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:180:ARG:HB2	5:E:215:MET:OXT	1.92	0.69
5:E:79:TRP:HE1	5:E:81:GLU:HB2	1.58	0.69
12:L:34:CYS:HB3	12:L:51:CYS:SG	2.32	0.69
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.33	0.69
3:C:208:GLU:O	3:C:210:GLU:N	2.25	0.69
2:B:295:GLY:N	2:B:298:LEU:HD23	2.08	0.69
2:B:405:ARG:NE	2:B:629:ASP:OD2	2.22	0.69
4:D:134:THR:HG22	4:D:135:GLY:N	2.08	0.69
6:F:111:LEU:HD12	6:F:111:LEU:N	2.07	0.69
12:L:61:THR:HG22	12:L:63:ARG:HG3	1.75	0.69
12:L:61:THR:CG2	12:L:63:ARG:HG3	2.23	0.69
1:A:709:THR:HG21	1:A:711:ARG:HG3	1.75	0.69
2:B:562:GLY:HA3	2:B:590:HIS:ND1	2.08	0.69
2:B:873:THR:O	2:B:914:LYS:HA	1.93	0.69
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.74	0.69
13:T:15:DG:H2''	13:T:16:DT:H71	1.75	0.69
1:A:11:LEU:O	1:A:11:LEU:HD23	1.93	0.69
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.27	0.69
2:B:710:LEU:CA	2:B:733:HIS:HB3	2.22	0.69
6:F:103:MET:HE1	7:G:66:GLY:H	1.57	0.69
7:G:1:MET:SD	7:G:79:PHE:CD1	2.86	0.69
11:K:113:THR:O	11:K:114:LEU:HB2	1.93	0.69
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.28	0.69
2:B:1004:GLU:HG3	10:J:42:LYS:NZ	2.07	0.69
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.75	0.69
2:B:345:LYS:O	2:B:347:LYS:HG2	1.91	0.69
2:B:365:THR:HG21	2:B:370:PHE:CG	2.28	0.69
2:B:579:ARG:HA	2:B:589:VAL:HG13	1.74	0.69
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.22	0.69
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.75	0.69
10:J:12:LYS:O	10:J:14:VAL:HG23	1.92	0.69
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.74	0.69
12:L:47:ARG:CG	12:L:48:CYS:H	2.06	0.69
15:P:1:C:H2'	15:P:1:C:O2	1.92	0.68
1:A:883:LEU:HD11	1:A:1017:LEU:HD11	1.75	0.68
1:A:1150:SER:HB3	1:A:1195:LEU:HD23	1.73	0.68
1:A:186:LYS:NZ	1:A:197:PRO:HD3	2.07	0.68
8:H:82:PRO:C	8:H:84:ALA:N	2.46	0.68
2:B:294:ASP:C	2:B:296:GLU:H	1.96	0.68
2:B:244:LEU:HD21	2:B:366:GLN:NE2	2.08	0.68
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1214:GLU:O	1:A:1218:GLN:HG2	1.93	0.68
1:A:503:GLN:HE21	6:F:90:ARG:HH21	1.41	0.68
1:A:822:GLU:HG3	2:B:513:GLN:NE2	2.08	0.68
5:E:117:THR:HB	5:E:120:ALA:HB2	1.74	0.68
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.59	0.68
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.57	0.68
1:A:860:LEU:HD11	1:A:1393:ASN:HB2	1.76	0.68
1:A:381:THR:HG22	1:A:383:TYR:N	2.08	0.68
2:B:295:GLY:H	2:B:298:LEU:HD23	1.58	0.68
2:B:642:ASP:CA	2:B:649:LYS:HG3	2.23	0.68
7:G:139:ILE:HD13	7:G:140:LYS:HE3	1.74	0.68
1:A:308:ILE:HG22	1:A:309:ALA:N	2.06	0.68
5:E:78:LEU:HB2	5:E:107:THR:CB	2.24	0.68
1:A:567:LYS:CB	1:A:568:PRO:CD	2.72	0.68
11:K:47:ARG:HB3	11:K:47:ARG:NH1	2.06	0.68
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.24	0.68
2:B:558:LEU:HD21	2:B:600:LEU:HD11	1.76	0.68
10:J:1:MET:H2	10:J:57:ILE:H	1.38	0.68
1:A:37:PHE:CD1	1:A:37:PHE:N	2.59	0.68
2:B:875:GLU:O	2:B:877:PRO:HD3	1.93	0.68
4:D:208:GLU:O	4:D:212:LYS:HG3	1.92	0.68
6:F:69:LEU:O	6:F:71:GLU:HG3	1.94	0.68
2:B:345:LYS:HG2	2:B:346:GLU:H	1.58	0.67
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.76	0.67
2:B:259:TYR:H	2:B:259:TYR:HD1	1.43	0.67
2:B:705:MET:N	2:B:710:LEU:HD12	2.09	0.67
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.59	0.67
4:D:7:THR:O	4:D:9:GLN:N	2.27	0.67
5:E:117:THR:HB	5:E:120:ALA:CB	2.24	0.67
5:E:29:PHE:O	5:E:30:ILE:HG13	1.94	0.67
8:H:135:LEU:HB2	8:H:137:GLN:HE21	1.58	0.67
1:A:34:LYS:HG2	1:A:57:ARG:HH22	1.59	0.67
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.93	0.67
1:A:11:LEU:HB2	2:B:1193:GLN:HG3	1.75	0.67
2:B:293:PRO:HD2	2:B:296:GLU:OE1	1.94	0.67
9:I:50:THR:HG22	9:I:52:ILE:H	1.59	0.67
1:A:672:ASP:OD1	1:A:674:PRO:HD2	1.95	0.67
2:B:241:ARG:HG2	2:B:253:THR:HG22	1.77	0.67
2:B:559:SER:CA	2:B:563:MET:HB3	2.12	0.67
1:A:1144:LYS:HB2	1:A:1268:LEU:O	1.93	0.67
2:B:613:VAL:HG13	2:B:627:PHE:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:62:ILE:HD11	9:I:86:PHE:HE2	1.57	0.67
1:A:500:GLU:OE2	1:A:1438:THR:HG21	1.95	0.67
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.76	0.67
1:A:684:ALA:O	1:A:687:LYS:HB2	1.94	0.67
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.77	0.67
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.30	0.67
3:C:133:ILE:CD1	3:C:237:SER:HA	2.25	0.67
1:A:75:ASN:HD22	2:B:1116:ARG:NH1	1.92	0.67
6:F:147:SER:OG	6:F:150:GLU:HG3	1.94	0.67
1:A:1095:THR:CG2	1:A:1112:LYS:HD2	2.24	0.67
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.09	0.67
1:A:167:CYS:HB2	1:A:169:ASN:ND2	2.10	0.67
2:B:288:ALA:HB1	2:B:331:LEU:HD12	1.75	0.67
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.77	0.67
2:B:577:ALA:CB	2:B:589:VAL:HG11	2.20	0.67
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.77	0.67
1:A:145:LYS:HA	1:A:145:LYS:HE3	1.77	0.67
2:B:649:LYS:HD3	2:B:736:THR:O	1.95	0.67
8:H:25:ARG:HH22	8:H:122:LEU:HD12	1.60	0.67
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	1.76	0.66
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.59	0.66
6:F:82:THR:HG23	6:F:84:TYR:N	2.10	0.66
8:H:11:GLN:HA	8:H:53:ASP:O	1.95	0.66
8:H:14:GLU:HG2	8:H:15:VAL:N	2.09	0.66
10:J:64:ASN:HB3	10:J:65:PRO:HD2	1.78	0.66
11:K:63:VAL:HG23	11:K:63:VAL:O	1.96	0.66
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.24	0.66
1:A:266:LEU:HD21	1:A:303:TYR:CE1	2.30	0.66
2:B:430:ARG:CB	2:B:430:ARG:HH11	2.04	0.66
2:B:644:GLU:HB3	2:B:648:HIS:O	1.94	0.66
2:B:807:ARG:HB3	2:B:807:ARG:HH11	1.61	0.66
8:H:100:THR:HG23	8:H:138:GLU:HA	1.77	0.66
10:J:64:ASN:HD22	10:J:65:PRO:HD3	1.60	0.66
1:A:184:SER:CB	1:A:199:LEU:HD23	2.26	0.66
2:B:345:LYS:CG	2:B:346:GLU:H	2.07	0.66
3:C:10:ILE:HG22	3:C:11:ARG:O	1.96	0.66
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.76	0.66
2:B:308:TRP:CH2	9:I:45:ARG:HG2	2.29	0.66
12:L:26:THR:CG2	12:L:27:LEU:H	2.03	0.66
1:A:1094:VAL:HG13	1:A:1113:THR:CG2	2.26	0.66
1:A:1148:ILE:HD11	1:A:1198:ASP:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ASP:O	1:A:63:ARG:C	2.33	0.66
2:B:865:LYS:HG2	2:B:961:LEU:HD21	1.78	0.66
6:F:109:VAL:HG12	6:F:110:ASP:N	2.10	0.66
2:B:273:LEU:HD21	2:B:360:PHE:CD1	2.31	0.66
10:J:48:ARG:HE	10:J:49:MET:CE	2.08	0.66
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.24	0.66
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.78	0.66
1:A:1445:ILE:H	1:A:1445:ILE:HD12	1.60	0.66
1:A:72:GLU:HB3	1:A:76:GLU:HG2	1.78	0.66
4:D:4:SER:O	4:D:5:THR:HB	1.95	0.66
1:A:335:ARG:HH12	2:B:1206:GLU:CD	1.99	0.66
2:B:172:ILE:CD1	2:B:178:ASN:HD22	2.09	0.66
2:B:57:TYR:HD1	2:B:57:TYR:N	1.93	0.66
4:D:18:VAL:O	4:D:19:GLU:HB2	1.94	0.66
10:J:1:MET:N	10:J:56:LEU:N	2.43	0.66
1:A:316:GLN:HG2	1:A:317:LYS:N	2.10	0.66
2:B:1181:GLU:HA	2:B:1187:ASN:O	1.96	0.66
2:B:313:MET:SD	2:B:390:LEU:HD21	2.35	0.66
2:B:842:ASN:ND2	2:B:845:SER:OG	2.29	0.66
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.77	0.66
4:D:134:THR:HG22	4:D:135:GLY:H	1.61	0.66
1:A:110:CYS:HB3	1:A:167:CYS:SG	2.36	0.65
1:A:388:LEU:O	1:A:392:VAL:HG23	1.96	0.65
1:A:741:ASN:ND2	1:A:744:LYS:H	1.93	0.65
2:B:357:GLN:O	2:B:366:GLN:HA	1.96	0.65
2:B:570:VAL:HG21	2:B:573:GLN:CD	2.16	0.65
3:C:148:ARG:N	3:C:151:GLN:HG3	2.11	0.65
3:C:189:THR:HG22	3:C:190:ASP:N	2.11	0.65
6:F:99:LEU:O	6:F:103:MET:HG2	1.97	0.65
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.29	0.65
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.17	0.65
2:B:422:LYS:O	2:B:426:LYS:HG2	1.96	0.65
2:B:402:GLY:HA2	2:B:695:ALA:HB3	1.75	0.65
3:C:189:THR:HG22	3:C:190:ASP:H	1.62	0.65
7:G:53:ASN:HD22	7:G:53:ASN:N	1.94	0.65
8:H:143:LEU:N	8:H:143:LEU:HD12	2.11	0.65
1:A:425:GLN:N	1:A:425:GLN:OE1	2.30	0.65
1:A:49:LYS:NZ	1:A:61:ILE:HG13	2.10	0.65
1:A:828:ALA:HB1	2:B:530:GLY:HA2	1.78	0.65
2:B:483:LEU:HD11	2:B:491:THR:CG2	2.27	0.65
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:PRO:HB2	3:C:25:VAL:HG22	1.77	0.65
2:B:798:TYR:HE2	3:C:62:PHE:CE2	2.14	0.65
4:D:220:LEU:HG	4:D:221:TYR:H	1.60	0.65
5:E:111:VAL:HG12	5:E:137:GLU:HG2	1.77	0.65
6:F:69:LEU:HB3	6:F:71:GLU:CD	2.16	0.65
12:L:49:LYS:O	12:L:50:ASP:HB2	1.95	0.65
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.77	0.65
1:A:184:SER:HB3	1:A:199:LEU:HD23	1.79	0.65
8:H:130:ARG:HH11	8:H:130:ARG:CB	2.07	0.65
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.78	0.65
2:B:1147:LEU:HD22	2:B:1151:LEU:HD22	1.78	0.65
2:B:1202:LEU:O	2:B:1206:GLU:HG3	1.97	0.65
1:A:102:VAL:CG1	1:A:211:PHE:HE1	2.10	0.65
1:A:1386:ARG:HB2	1:A:1403:GLU:HG3	1.77	0.65
1:A:353:ILE:HD12	1:A:470:LEU:HD21	1.78	0.65
3:C:104:PHE:HE2	3:C:150:GLY:HA2	1.62	0.65
3:C:73:GLN:HE21	3:C:75:MET:HB2	1.62	0.65
1:A:562:THR:HB	8:H:98:TYR:HD2	1.62	0.65
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	1.97	0.65
1:A:1259:MET:HE2	1:A:1263:ILE:HD11	1.78	0.65
1:A:869:GLY:O	5:E:204:THR:HG21	1.97	0.65
2:B:60:GLN:O	2:B:63:ILE:HG22	1.97	0.65
2:B:847:ASP:C	2:B:849:GLY:H	2.00	0.65
1:A:1041:ALA:O	1:A:1045:VAL:HG23	1.97	0.65
1:A:134:ARG:HD2	1:A:221:SER:O	1.97	0.65
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.32	0.65
2:B:418:LYS:HE2	2:B:422:LYS:NZ	2.12	0.65
2:B:1147:LEU:CD2	2:B:1151:LEU:HD22	2.27	0.65
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.27	0.65
2:B:792:MET:HG2	2:B:855:PHE:HE1	1.62	0.65
4:D:71:LYS:HG2	4:D:74:GLN:HG3	1.78	0.65
11:K:12:LEU:HD23	11:K:16:GLU:O	1.97	0.65
1:A:207:ILE:HG22	1:A:211:PHE:CE2	2.32	0.64
1:A:886:ILE:HG23	1:A:887:GLY:N	2.12	0.64
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.32	0.64
2:B:1084:GLN:NE2	2:B:1084:GLN:N	2.44	0.64
1:A:341:MET:HE1	2:B:1135:ARG:NH1	2.12	0.64
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.79	0.64
2:B:859:TYR:OH	2:B:941:LEU:HD12	1.96	0.64
3:C:124:LEU:O	3:C:127:ARG:HG2	1.97	0.64
7:G:139:ILE:HG23	7:G:140:LYS:HG3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.78	0.64
2:B:189:LEU:O	2:B:192:LEU:N	2.29	0.64
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.78	0.64
3:C:73:GLN:HE21	3:C:75:MET:H	1.44	0.64
6:F:89:GLU:OE2	6:F:134:ILE:HG21	1.97	0.64
1:A:960:ILE:O	1:A:963:ILE:HG22	1.97	0.64
1:A:977:LYS:HB3	1:A:978:PRO:HD2	1.79	0.64
4:D:220:LEU:CG	4:D:221:TYR:H	2.10	0.64
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.33	0.64
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.33	0.64
2:B:120:ARG:NH1	12:L:54:ARG:HD2	2.12	0.64
2:B:705:MET:H	2:B:710:LEU:CD1	2.11	0.64
3:C:177:GLU:CG	3:C:231:ASN:HB3	2.25	0.64
3:C:69:LEU:N	3:C:69:LEU:HD12	2.12	0.64
1:A:34:LYS:HG3	1:A:36:ARG:HH22	1.62	0.64
1:A:535:THR:HG21	1:A:617:VAL:H	1.62	0.64
1:A:1150:SER:HB3	1:A:1195:LEU:CD2	2.28	0.64
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.78	0.64
1:A:67:CYS:C	1:A:68:GLN:HG3	2.17	0.64
1:A:854:ASN:HD22	1:A:1000:LEU:HD23	1.63	0.64
2:B:638:PHE:CD2	2:B:690:VAL:HG12	2.32	0.64
1:A:1215:ARG:NH1	1:A:1272:THR:O	2.31	0.64
2:B:1183:LYS:HE3	2:B:1183:LYS:O	1.97	0.64
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.33	0.64
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.78	0.64
2:B:185:THR:H	2:B:188:ASP:HB2	1.63	0.64
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.80	0.64
2:B:313:MET:HE2	2:B:390:LEU:HD11	1.78	0.64
2:B:359:GLU:O	2:B:362:PRO:HD3	1.98	0.64
4:D:29:LEU:N	4:D:29:LEU:HD22	2.12	0.64
5:E:79:TRP:HB2	5:E:105:PHE:CE1	2.32	0.64
12:L:32:ALA:HB3	12:L:55:ILE:HG13	1.79	0.64
2:B:954:VAL:O	12:L:55:ILE:O	2.15	0.64
1:A:129:LYS:O	1:A:130:ASP:CB	2.46	0.64
1:A:68:GLN:O	1:A:68:GLN:OE1	2.15	0.64
2:B:549:THR:HB	2:B:628:THR:OG1	1.96	0.64
2:B:737:THR:CG2	9:I:66:PRO:HA	2.28	0.64
8:H:84:ALA:HA	8:H:87:ARG:HD2	1.80	0.64
8:H:8:ASP:OD2	8:H:9:ILE:N	2.30	0.64
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.87	0.64
1:A:321:PRO:O	1:A:322:VAL:HB	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:470:LYS:C	2:B:472:ALA:N	2.52	0.64
2:B:955:THR:CG2	2:B:956:THR:N	2.59	0.64
5:E:179:GLN:O	5:E:182:ASP:HB2	1.98	0.64
1:A:351:THR:CG2	2:B:1103:ILE:HA	2.27	0.63
3:C:138:GLU:OE1	3:C:138:GLU:N	2.31	0.63
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.33	0.63
2:B:620:ARG:NH1	9:I:68:LEU:HD21	2.13	0.63
1:A:265:LYS:HE3	1:A:265:LYS:HA	1.79	0.63
1:A:287:HIS:HA	1:A:290:GLU:HG2	1.80	0.63
2:B:273:LEU:HD21	2:B:360:PHE:HD1	1.63	0.63
2:B:811:TYR:N	2:B:811:TYR:CD1	2.65	0.63
10:J:14:VAL:HG12	10:J:14:VAL:O	1.97	0.63
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.32	0.63
12:L:34:CYS:HB3	12:L:51:CYS:HG	1.63	0.63
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.80	0.63
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.81	0.63
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	1.97	0.63
2:B:244:LEU:HD11	2:B:366:GLN:HE22	1.63	0.63
2:B:425:THR:HA	2:B:428:ILE:HD12	1.81	0.63
2:B:879:ARG:CZ	2:B:879:ARG:N	2.59	0.63
3:C:18:VAL:O	3:C:18:VAL:HG12	1.97	0.63
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.80	0.63
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.33	0.63
12:L:34:CYS:CB	12:L:51:CYS:HG	2.10	0.63
5:E:120:ALA:O	5:E:123:LEU:HG	1.98	0.63
9:I:7:CYS:SG	9:I:8:ARG:O	2.56	0.63
1:A:1420:ASP:O	1:A:1421:CYS:HB2	1.98	0.63
1:A:601:LYS:HD3	1:A:603:ASN:HD21	1.63	0.63
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.79	0.63
15:P:5:C:O2'	15:P:6:A:H5'	1.99	0.63
1:A:108:MET:HA	1:A:210:ILE:CD1	2.23	0.63
2:B:307:ASP:OD2	2:B:310:MET:HB2	1.99	0.63
2:B:284:ILE:HD13	2:B:333:PHE:CD2	2.34	0.63
5:E:111:VAL:CG1	5:E:137:GLU:HG2	2.29	0.63
5:E:37:LEU:CD1	5:E:41:ASP:HB2	2.29	0.63
7:G:13:LEU:CD2	7:G:17:PHE:HB2	2.29	0.63
1:A:1235:LYS:HG2	1:A:1237:ILE:HD11	1.79	0.63
1:A:1241:ARG:O	1:A:1242:VAL:HB	1.98	0.63
1:A:903:ASN:C	1:A:903:ASN:HD22	2.00	0.63
4:D:207:LEU:HD12	4:D:207:LEU:O	1.99	0.63
8:H:130:ARG:H	8:H:130:ARG:HD3	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.28	0.63
1:A:106:VAL:HG12	1:A:107:CYS:N	2.13	0.63
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.81	0.63
1:A:973:ILE:HD11	1:A:1041:ALA:CB	2.29	0.63
2:B:589:VAL:HG12	2:B:590:HIS:N	2.14	0.63
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.80	0.63
6:F:103:MET:HE2	7:G:66:GLY:H	1.60	0.63
1:A:1107:VAL:HG12	1:A:1107:VAL:O	1.99	0.63
1:A:1450:LEU:HG	1:A:1450:LEU:O	1.98	0.63
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.33	0.63
2:B:108:VAL:HG23	2:B:109:THR:N	2.14	0.63
6:F:119:ARG:HG3	6:F:119:ARG:HH11	1.64	0.63
1:A:1187:GLN:HG3	1:A:1188:GLN:H	1.64	0.62
1:A:416:ARG:HG3	1:A:417:TYR:CE1	2.34	0.62
2:B:345:LYS:CE	2:B:349:ILE:HD11	2.29	0.62
3:C:123:ASN:HD21	3:C:125:MET:HG3	1.61	0.62
4:D:39:ASN:ND2	4:D:41:GLN:HB2	2.14	0.62
4:D:71:LYS:HA	4:D:74:GLN:CB	2.29	0.62
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.64	0.62
8:H:82:PRO:O	8:H:84:ALA:N	2.31	0.62
1:A:98:LYS:O	1:A:102:VAL:HG23	1.99	0.62
1:A:1241:ARG:O	1:A:1242:VAL:CB	2.48	0.62
2:B:429:PHE:HA	2:B:432:MET:HE2	1.81	0.62
2:B:70:ILE:H	2:B:429:PHE:HE1	1.46	0.62
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.29	0.62
1:A:698:GLN:HA	9:I:97:MET:O	1.99	0.62
12:L:30:ILE:HG22	12:L:31:CYS:N	2.14	0.62
2:B:955:THR:OG1	12:L:55:ILE:HA	1.99	0.62
2:B:1174:LYS:O	2:B:1176:ASN:N	2.31	0.62
2:B:334:ILE:O	2:B:334:ILE:HG22	1.99	0.62
2:B:498:THR:HG22	2:B:537:LYS:H	1.63	0.62
2:B:579:ARG:HG2	2:B:579:ARG:NH1	2.10	0.62
2:B:766:ARG:HH21	2:B:1020:ARG:HD2	1.64	0.62
5:E:171:LYS:HG2	5:E:174:GLN:CD	2.19	0.62
8:H:139:ASN:O	8:H:140:ALA:CB	2.46	0.62
9:I:61:ASP:C	9:I:63:GLY:H	2.02	0.62
1:A:472:LEU:O	1:A:475:THR:HB	1.99	0.62
2:B:465:ASN:ND2	2:B:465:ASN:N	2.47	0.62
2:B:515:HIS:CD2	2:B:517:THR:HG23	2.35	0.62
2:B:846:ILE:CG2	2:B:974:PRO:HG2	2.27	0.62
2:B:955:THR:HG22	2:B:956:THR:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1224:PHE:CE1	5:E:171:LYS:HG3	2.34	0.62
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.80	0.62
4:D:33:PHE:CE1	7:G:80:LYS:HD3	2.35	0.62
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.29	0.62
1:A:70:CYS:O	1:A:72:GLU:HG2	1.99	0.62
2:B:916:THR:HB	2:B:935:ARG:CD	2.30	0.62
8:H:38:LEU:HD13	8:H:125:LEU:CD1	2.30	0.62
2:B:351:TYR:O	2:B:355:ILE:HG13	1.99	0.62
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.31	0.62
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.29	0.62
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.30	0.62
1:A:153:PRO:HB3	1:A:161:LEU:HD22	1.81	0.62
1:A:185:TRP:CH2	1:A:200:ARG:HG2	2.34	0.62
1:A:503:GLN:NE2	6:F:90:ARG:HH21	1.93	0.62
2:B:240:ILE:HG23	2:B:254:LEU:HB3	1.82	0.62
2:B:516:ASN:H	2:B:516:ASN:HD22	1.48	0.62
3:C:133:ILE:HD11	3:C:237:SER:HA	1.82	0.62
7:G:138:THR:HG22	7:G:139:ILE:H	1.64	0.62
1:A:794:PRO:HG2	1:A:795:GLU:OE2	1.99	0.62
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.80	0.62
2:B:769:TYR:CD1	2:B:987:LYS:NZ	2.67	0.62
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.82	0.62
9:I:50:THR:HG21	9:I:52:ILE:HG12	1.81	0.62
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.80	0.62
1:A:1130:GLN:O	1:A:1134:ILE:HG13	2.00	0.62
1:A:148:CYS:HB3	1:A:167:CYS:O	2.00	0.62
1:A:62:ASP:O	1:A:64:ASN:HB2	2.00	0.62
2:B:305:VAL:HG12	2:B:305:VAL:O	2.00	0.62
5:E:22:MET:HE1	5:E:26:ARG:NH2	2.14	0.62
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.81	0.62
11:K:108:GLU:O	11:K:112:GLN:HG2	2.00	0.62
12:L:39:SER:O	12:L:40:LEU:HG	2.00	0.62
12:L:58:LYS:O	12:L:59:ALA:O	2.18	0.62
1:A:35:ILE:HA	1:A:52:GLY:O	1.99	0.62
2:B:1177:HIS:CB	2:B:1179:GLN:HE21	2.12	0.62
2:B:957:ASN:ND2	2:B:961:LEU:HB2	2.14	0.62
5:E:153:HIS:O	5:E:154:ILE:CG1	2.47	0.62
9:I:50:THR:CG2	9:I:51:ASN:H	2.09	0.62
1:A:1120:LEU:HD22	1:A:1125:ALA:HA	1.81	0.61
1:A:129:LYS:O	1:A:130:ASP:HB2	2.00	0.61
1:A:34:LYS:NZ	1:A:57:ARG:HH12	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.65	0.61
2:B:98:THR:O	2:B:126:SER:HB2	2.00	0.61
2:B:234:ILE:HG12	2:B:257:LYS:HG2	1.82	0.61
2:B:806:THR:HG21	2:B:808:ALA:HB3	1.80	0.61
4:D:146:GLN:HA	4:D:149:THR:HG22	1.82	0.61
8:H:55:LEU:HD22	8:H:144:ILE:CG2	2.30	0.61
1:A:1191:TRP:HZ3	9:I:43:VAL:HG21	1.64	0.61
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.35	0.61
2:B:277:LYS:CG	2:B:336:ARG:HG2	2.31	0.61
2:B:57:TYR:CD1	2:B:57:TYR:N	2.64	0.61
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.83	0.61
2:B:865:LYS:HB2	2:B:961:LEU:HD11	1.81	0.61
3:C:43:THR:CG2	3:C:44:LEU:N	2.63	0.61
1:A:1312:ASN:HD21	1:A:1315:GLU:HG3	1.65	0.61
1:A:382:PRO:HB3	1:A:428:TYR:HE2	1.66	0.61
1:A:469:ARG:NH2	2:B:991:GLY:O	2.34	0.61
1:A:907:THR:HG23	1:A:908:LEU:N	2.16	0.61
2:B:1095:LEU:H	2:B:1095:LEU:HD12	1.65	0.61
2:B:277:LYS:HE2	2:B:336:ARG:C	2.21	0.61
2:B:35:SER:O	2:B:39:ARG:HG3	2.01	0.61
8:H:127:GLY:O	8:H:128:ASN:CB	2.47	0.61
1:A:1242:VAL:CG1	1:A:1243:VAL:N	2.63	0.61
1:A:252:PHE:O	1:A:256:GLN:NE2	2.33	0.61
1:A:317:LYS:O	1:A:318:SER:CB	2.47	0.61
2:B:508:LEU:HB3	14:N:1:DA:O3'	2.01	0.61
2:B:996:ARG:NH1	3:C:174:ALA:HA	2.13	0.61
8:H:32:THR:HG22	8:H:33:GLN:OE1	2.01	0.61
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.14	0.61
1:A:535:THR:HG21	1:A:617:VAL:N	2.16	0.61
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.35	0.61
1:A:590:ARG:HG2	1:A:590:ARG:HH11	1.65	0.61
1:A:698:GLN:NE2	9:I:99:LEU:HD11	2.16	0.61
2:B:642:ASP:HA	2:B:649:LYS:HG3	1.81	0.61
5:E:124:VAL:CG1	5:E:132:ILE:HB	2.20	0.61
8:H:4:THR:HG22	8:H:5:LEU:N	2.15	0.61
10:J:30:LEU:HD22	10:J:34:THR:HG21	1.83	0.61
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.83	0.61
11:K:82:ASP:OD1	11:K:84:LYS:N	2.34	0.61
1:A:1225:PHE:CE2	1:A:1227:ILE:HD11	2.36	0.61
1:A:1353:TYR:CD2	1:A:1353:TYR:C	2.73	0.61
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:146:GLN:O	4:D:149:THR:HG22	1.99	0.61
5:E:39:LEU:HG	5:E:43:LYS:HE3	1.82	0.61
9:I:74:GLU:HB3	9:I:81:ARG:CD	2.30	0.61
1:A:1387:HIS:HA	1:A:1391:ARG:HE	1.66	0.61
1:A:150:THR:HG23	1:A:166:GLY:HA2	1.83	0.61
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.81	0.61
2:B:114:PRO:HG2	2:B:115:GLN:H	1.65	0.61
2:B:192:LEU:O	2:B:193:LYS:HB2	2.01	0.61
3:C:251:LEU:O	3:C:255:VAL:HG23	2.00	0.61
8:H:63:LEU:HD11	8:H:141:TYR:CE2	2.36	0.61
9:I:73:ARG:HH12	9:I:112:SER:HB3	1.64	0.61
1:A:331:GLY:O	1:A:332:LYS:O	2.18	0.61
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.28	0.61
1:A:591:PHE:HA	1:A:595:THR:HG21	1.82	0.61
1:A:75:ASN:HD22	2:B:1116:ARG:HH12	1.47	0.61
3:C:181:ASP:OD1	3:C:186:LEU:HD13	2.01	0.61
3:C:221:TYR:CE1	3:C:222:LYS:HG3	2.35	0.61
1:A:84:ILE:CD1	1:A:270:LEU:HD13	2.31	0.61
4:D:35:LEU:H	4:D:35:LEU:HD12	1.64	0.61
5:E:32:GLN:HG3	5:E:36:GLU:OE2	2.00	0.61
6:F:93:ILE:CD1	6:F:134:ILE:HD11	2.30	0.61
6:F:83:PRO:HD2	6:F:84:TYR:HD1	1.65	0.61
10:J:24:LEU:O	10:J:30:LEU:HB2	2.01	0.61
2:B:1096:ARG:HG3	2:B:1097:HIS:H	1.66	0.61
2:B:50:SER:OG	2:B:411:PRO:HD3	2.01	0.61
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.83	0.61
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.15	0.61
7:G:115:MET:HB3	7:G:116:PRO:HD2	1.81	0.61
10:J:1:MET:H1	10:J:56:LEU:N	1.99	0.61
13:T:23:BRU:H6	13:T:23:BRU:H5"	1.83	0.61
1:A:244:PRO:HB2	1:A:245:PRO:CD	2.27	0.60
1:A:710:LEU:N	1:A:710:LEU:HD12	2.15	0.60
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.36	0.60
2:B:277:LYS:HG3	2:B:336:ARG:HG2	1.83	0.60
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.15	0.60
2:B:957:ASN:O	2:B:959:ASP:N	2.33	0.60
5:E:78:LEU:CB	5:E:107:THR:HB	2.28	0.60
5:E:128:PRO:HA	5:E:129:PRO:C	2.21	0.60
6:F:109:VAL:HG13	6:F:127:GLU:OE1	2.01	0.60
10:J:30:LEU:HD11	10:J:38:ARG:NH1	2.15	0.60
1:A:108:MET:O	1:A:109:HIS:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:PRO:HD3	1:A:185:TRP:NE1	2.16	0.60
1:A:420:ARG:O	1:A:424:ILE:HG13	2.01	0.60
1:A:853:ASP:O	1:A:854:ASN:HB2	2.00	0.60
2:B:842:ASN:O	2:B:846:ILE:HG13	2.01	0.60
5:E:99:HIS:CE1	5:E:103:LYS:HG3	2.36	0.60
7:G:126:ASN:HD22	7:G:127:PRO:N	1.99	0.60
1:A:384:ASN:OD1	1:A:388:LEU:HD12	2.00	0.60
2:B:1182:CYS:SG	2:B:1182:CYS:O	2.59	0.60
2:B:172:ILE:HD13	2:B:178:ASN:ND2	2.15	0.60
2:B:756:ILE:O	2:B:759:PRO:HD3	2.01	0.60
3:C:104:PHE:HD2	3:C:105:GLY:N	1.99	0.60
7:G:35:GLU:HG2	7:G:48:VAL:HG23	1.81	0.60
1:A:873:MET:C	1:A:1058:VAL:HG23	2.21	0.60
4:D:8:PHE:CE1	4:D:37:GLN:HB2	2.37	0.60
6:F:118:LEU:O	6:F:122:MET:HG3	2.01	0.60
2:B:120:ARG:HH12	12:L:54:ARG:NH1	1.90	0.60
2:B:217:ARG:C	2:B:217:ARG:HD2	2.22	0.60
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.31	0.60
3:C:183:TRP:O	3:C:185:LYS:HG3	2.01	0.60
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.15	0.60
1:A:185:TRP:HE3	1:A:185:TRP:H	1.50	0.60
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.29	0.60
2:B:1085:ILE:HD12	2:B:1085:ILE:N	2.16	0.60
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.81	0.60
7:G:21:ARG:HD2	7:G:24:GLN:HB3	1.83	0.60
10:J:48:ARG:NE	10:J:49:MET:HE2	2.16	0.60
1:A:107:CYS:HB2	1:A:114:LEU:HD21	1.82	0.60
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.82	0.60
1:A:323:LYS:H	1:A:323:LYS:HD2	1.67	0.60
1:A:96:ILE:HA	1:A:99:ILE:HD12	1.84	0.60
2:B:345:LYS:HG2	2:B:346:GLU:N	2.16	0.60
3:C:226:ASP:O	3:C:227:THR:HB	2.02	0.60
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.37	0.60
1:A:335:ARG:NH1	2:B:1202:LEU:HD13	2.17	0.60
2:B:464:GLY:O	2:B:477:ALA:HA	2.02	0.60
2:B:542:MET:HG2	2:B:747:MET:CE	2.31	0.60
4:D:14:ARG:O	4:D:16:LYS:N	2.32	0.60
1:A:1118:VAL:O	1:A:1305:VAL:HG13	2.02	0.60
2:B:69:LEU:HB3	2:B:429:PHE:CE1	2.36	0.60
3:C:243:VAL:HG12	3:C:243:VAL:O	2.00	0.60
1:A:1167:GLU:O	1:A:1170:ILE:HD12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LYS:O	1:A:269:ILE:HG13	2.02	0.60
1:A:42:ASP:HA	1:A:46:THR:O	2.02	0.60
2:B:292:ILE:HD11	2:B:327:ARG:N	2.16	0.60
2:B:327:ARG:NH2	2:B:371:GLU:HG2	2.17	0.60
2:B:787:VAL:O	2:B:787:VAL:HG12	2.01	0.60
1:A:711:ARG:HH21	9:I:97:MET:HG2	1.66	0.60
11:K:21:ILE:CG2	11:K:31:VAL:HG11	2.31	0.60
1:A:535:THR:HG21	1:A:616:VAL:HA	1.82	0.59
2:B:637:LEU:CD2	2:B:742:GLU:HA	2.32	0.59
2:B:64:CYS:HA	2:B:67:SER:OG	2.02	0.59
2:B:806:THR:CG2	2:B:808:ALA:HB3	2.31	0.59
3:C:263:THR:O	3:C:266:ASP:HB2	2.02	0.59
4:D:52:LEU:O	4:D:54:GLU:N	2.34	0.59
2:B:797:TYR:O	10:J:1:MET:HG2	2.01	0.59
1:A:1114:PRO:O	1:A:1311:VAL:HG23	2.02	0.59
1:A:596:THR:C	1:A:598:LEU:H	2.04	0.59
1:A:998:LEU:HD12	1:A:998:LEU:N	2.17	0.59
2:B:418:LYS:HG2	2:B:422:LYS:HE3	1.83	0.59
3:C:177:GLU:HG3	3:C:231:ASN:HD22	1.64	0.59
5:E:212:ARG:HH11	5:E:212:ARG:HG3	1.66	0.59
7:G:27:LYS:O	7:G:31:LEU:HG	2.02	0.59
11:K:31:VAL:HG12	11:K:32:VAL:N	2.15	0.59
1:A:626:ASN:O	1:A:631:HIS:CD2	2.55	0.59
1:A:7:SER:HB3	2:B:1193:GLN:HE22	1.67	0.59
2:B:778:MET:HE1	2:B:1094:ARG:HD3	1.82	0.59
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.17	0.59
2:B:616:ILE:HD12	2:B:616:ILE:N	2.17	0.59
2:B:708:GLU:HG3	2:B:709:ASP:H	1.65	0.59
4:D:7:THR:HG23	4:D:7:THR:O	2.02	0.59
7:G:119:LEU:HD13	7:G:132:SER:HB2	1.83	0.59
12:L:53:HIS:O	12:L:55:ILE:HD13	2.02	0.59
1:A:66:LYS:NZ	1:A:68:GLN:N	2.48	0.59
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.02	0.59
2:B:254:LEU:HD23	2:B:381:MET:HE3	1.83	0.59
2:B:303:TYR:CD2	2:B:303:TYR:N	2.70	0.59
2:B:531:GLN:HG2	2:B:532:ALA:N	2.15	0.59
2:B:916:THR:HB	2:B:935:ARG:CG	2.33	0.59
3:C:124:LEU:HD21	3:C:129:ILE:O	2.03	0.59
4:D:154:PHE:HE1	4:D:163:VAL:HG11	1.66	0.59
8:H:84:ALA:HB1	8:H:87:ARG:HB2	1.84	0.59
12:L:27:LEU:HD13	12:L:37:LYS:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1177:HIS:HB3	2:B:1179:GLN:HE21	1.66	0.59
5:E:48:ASP:CG	5:E:49:SER:H	2.06	0.59
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.34	0.59
1:A:100:LYS:HE2	1:A:104:GLU:OE2	2.02	0.59
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.83	0.59
1:A:1342:GLU:CG	5:E:198:ILE:HD13	2.32	0.59
1:A:381:THR:HG23	1:A:382:PRO:CD	2.32	0.59
1:A:728:LYS:HA	1:A:731:ARG:NH1	2.18	0.59
1:A:858:ASN:ND2	1:A:858:ASN:C	2.55	0.59
2:B:815:ARG:HB2	2:B:815:ARG:NH1	2.16	0.59
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.84	0.59
1:A:1293:SER:HB2	1:A:1299:VAL:HG21	1.85	0.59
1:A:1063:MET:SD	1:A:1436:ILE:HB	2.42	0.59
1:A:850:VAL:HG21	1:A:1058:VAL:HG11	1.84	0.59
1:A:986:ILE:O	1:A:990:VAL:HG23	2.03	0.59
2:B:168:GLY:HA2	2:B:454:THR:HG1	1.65	0.59
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.17	0.59
2:B:467:GLY:CA	2:B:475:SER:HB3	2.33	0.59
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.03	0.59
3:C:35:ARG:NH1	11:K:41:THR:H	2.01	0.59
1:A:857:ARG:NH1	6:F:139:PRO:HB2	2.17	0.59
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.03	0.59
1:A:67:CYS:O	1:A:68:GLN:HG3	2.03	0.59
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.85	0.59
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.37	0.59
2:B:642:ASP:O	2:B:644:GLU:N	2.28	0.59
2:B:860:MET:HG2	2:B:861:ASP:H	1.67	0.59
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.29	0.59
8:H:25:ARG:NH2	8:H:122:LEU:HD12	2.16	0.59
8:H:139:ASN:O	8:H:140:ALA:HB2	2.02	0.59
1:A:311:GLN:O	1:A:313:GLN:N	2.36	0.59
1:A:41:MET:HB2	1:A:48:ALA:O	2.03	0.59
1:A:694:THR:O	1:A:698:GLN:HG3	2.03	0.59
1:A:728:LYS:O	1:A:732:LEU:HG	2.02	0.59
1:A:768:GLN:CG	1:A:816:HIS:HA	2.30	0.59
2:B:129:PHE:HD2	2:B:166:PHE:HA	1.67	0.59
1:A:1444:MET:HG2	7:G:60:ARG:HA	1.84	0.59
1:A:1206:ASP:HB3	1:A:1274:ARG:HH22	1.67	0.59
1:A:1208:THR:HG22	1:A:1210:GLY:N	2.18	0.59
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.38	0.59
1:A:486:GLU:OE1	2:B:1102:LYS:HD3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:LEU:HD23	2:B:173:MET:SD	2.43	0.59
2:B:806:THR:HG22	2:B:808:ALA:N	2.12	0.59
2:B:868:MET:O	2:B:870:ILE:HG13	2.03	0.59
3:C:114:TYR:CD2	3:C:140:ASN:CB	2.86	0.59
1:A:1110:ASN:ND2	1:A:1110:ASN:N	2.50	0.58
1:A:555:ASP:O	1:A:556:TRP:C	2.40	0.58
1:A:565:ILE:HD13	1:A:567:LYS:HE2	1.84	0.58
1:A:774:ARG:NH2	1:A:797:LYS:HB2	2.18	0.58
2:B:811:TYR:HD1	2:B:811:TYR:H	1.51	0.58
4:D:138:ASN:HD21	7:G:35:GLU:HB3	1.67	0.58
11:K:93:SER:O	11:K:97:LYS:HG3	2.03	0.58
1:A:344:ARG:NH1	1:A:344:ARG:HB3	2.11	0.58
1:A:915:SER:O	1:A:919:ILE:HB	2.02	0.58
2:B:1065:GLN:NE2	2:B:1067:ARG:HG2	2.18	0.58
1:A:1029:ARG:HG3	1:A:1029:ARG:HH11	1.68	0.58
1:A:1081:LEU:HD11	1:A:1098:VAL:N	2.18	0.58
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.32	0.58
2:B:766:ARG:HH22	2:B:1020:ARG:NH1	1.96	0.58
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.33	0.58
4:D:12:ARG:NH1	4:D:14:ARG:HA	2.18	0.58
5:E:136:ASN:OD1	5:E:138:ALA:N	2.37	0.58
1:A:854:ASN:ND2	1:A:1000:LEU:HD23	2.18	0.58
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.04	0.58
1:A:182:VAL:CG2	1:A:201:VAL:HG22	2.33	0.58
2:B:531:GLN:CG	2:B:532:ALA:H	2.11	0.58
2:B:708:GLU:O	2:B:710:LEU:N	2.36	0.58
3:C:167:HIS:NE2	12:L:70:ARG:HB3	2.18	0.58
3:C:209:TYR:HD1	3:C:209:TYR:H	1.49	0.58
5:E:94:LYS:CE	5:E:98:ILE:HD11	2.23	0.58
7:G:138:THR:CG2	7:G:139:ILE:N	2.66	0.58
8:H:128:ASN:ND2	8:H:131:ASN:OD1	2.36	0.58
8:H:4:THR:HA	8:H:60:ALA:CB	2.20	0.58
10:J:53:HIS:CD2	10:J:54:VAL:N	2.72	0.58
1:A:697:ALA:CB	1:A:702:LEU:HD11	2.34	0.58
1:A:718:VAL:O	1:A:721:PHE:HB2	2.03	0.58
2:B:978:ASP:OD2	2:B:1098:MET:HG2	2.04	0.58
2:B:792:MET:HA	2:B:856:PHE:O	2.02	0.58
11:K:21:ILE:HG23	11:K:31:VAL:HG11	1.84	0.58
1:A:1094:VAL:HG13	1:A:1113:THR:HG21	1.86	0.58
1:A:1152:ILE:HD13	1:A:1260:LEU:HD23	1.86	0.58
1:A:132:LYS:HE3	1:A:1411:GLU:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:THR:HG22	1:A:616:VAL:HA	1.85	0.58
1:A:600:PRO:HA	8:H:25:ARG:NH1	2.19	0.58
1:A:606:LEU:HG	1:A:613:ILE:HD12	1.86	0.58
1:A:718:VAL:O	1:A:722:LEU:HD12	2.02	0.58
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.84	0.58
2:B:468:GLU:OE1	2:B:470:LYS:HE3	2.03	0.58
2:B:603:LEU:HB3	2:B:609:ILE:HD11	1.85	0.58
2:B:863:GLU:O	2:B:961:LEU:HD13	2.02	0.58
3:C:73:GLN:HE21	3:C:75:MET:CB	2.16	0.58
4:D:5:THR:O	4:D:5:THR:HG23	2.04	0.58
5:E:177:ARG:HD3	5:E:215:MET:SD	2.43	0.58
6:F:109:VAL:HG12	6:F:110:ASP:H	1.66	0.58
8:H:84:ALA:CA	8:H:87:ARG:HD2	2.32	0.58
11:K:45:LEU:HG	11:K:94:ILE:CD1	2.34	0.58
1:A:573:SER:O	1:A:576:GLN:HB2	2.03	0.58
1:A:12:ARG:HD2	2:B:1218:THR:CB	2.34	0.58
2:B:558:LEU:HD22	2:B:596:LEU:HD21	1.85	0.58
3:C:76:ASP:OD2	3:C:128:ASN:N	2.36	0.58
1:A:35:ILE:CD1	1:A:241:VAL:HG11	2.34	0.58
1:A:698:GLN:O	9:I:98:VAL:HG13	2.03	0.58
2:B:1152:MET:CE	2:B:1157:ALA:HA	2.34	0.58
8:H:145:ARG:O	8:H:146:ARG:HB2	2.03	0.58
1:A:1315:GLU:C	1:A:1317:MET:H	2.08	0.58
2:B:251:ILE:HG22	2:B:251:ILE:O	2.02	0.58
2:B:508:LEU:O	2:B:509:ALA:HB3	2.04	0.58
3:C:166:GLU:HG3	11:K:10:PHE:HZ	1.68	0.58
1:A:41:MET:O	1:A:42:ASP:O	2.22	0.58
2:B:278:GLN:CG	2:B:279:ASP:H	2.00	0.58
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.84	0.58
10:J:44:TYR:N	10:J:44:TYR:CD2	2.72	0.58
1:A:1135:ARG:HG2	1:A:1136:SER:N	2.19	0.57
2:B:1177:HIS:HB2	2:B:1179:GLN:NE2	2.19	0.57
2:B:205:ILE:N	2:B:205:ILE:HD12	2.19	0.57
1:A:1237:ILE:HG22	1:A:1238:ILE:N	2.19	0.57
1:A:66:LYS:O	1:A:67:CYS:HB2	2.04	0.57
1:A:699:ALA:HB3	1:A:701:LEU:HG	1.86	0.57
1:A:922:ASP:OD1	1:A:924:LYS:HB2	2.04	0.57
2:B:637:LEU:HD21	2:B:742:GLU:HA	1.86	0.57
2:B:842:ASN:ND2	2:B:845:SER:H	2.01	0.57
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.36	0.57
4:D:14:ARG:HH22	4:D:16:LYS:NZ	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:97:ARG:HH21	6:F:108:PHE:HE1	1.52	0.57
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.85	0.57
1:A:1293:SER:HB2	1:A:1299:VAL:CG2	2.34	0.57
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.04	0.57
6:F:97:ARG:O	6:F:101:ILE:HG13	2.05	0.57
1:A:1259:MET:HA	1:A:1262:LYS:CD	2.31	0.57
1:A:666:ILE:N	1:A:666:ILE:HD12	2.19	0.57
2:B:292:ILE:HD13	2:B:326:ASP:HA	1.87	0.57
2:B:168:GLY:N	2:B:450:ALA:HB1	2.16	0.57
3:C:89:GLU:O	3:C:90:ASP:HB3	2.05	0.57
1:A:16:GLU:OE1	4:D:13:ARG:NH2	2.38	0.57
11:K:88:LYS:O	11:K:91:CYS:HB2	2.03	0.57
1:A:117:GLU:HA	1:A:123:ARG:HG3	1.85	0.57
1:A:19:PHE:O	1:A:1416:ALA:HA	2.04	0.57
1:A:182:VAL:HG22	1:A:201:VAL:HG22	1.87	0.57
1:A:285:PRO:O	1:A:287:HIS:N	2.37	0.57
1:A:316:GLN:NE2	1:A:317:LYS:HE2	2.19	0.57
1:A:332:LYS:C	1:A:334:GLY:N	2.57	0.57
1:A:35:ILE:O	1:A:35:ILE:HG22	2.02	0.57
1:A:979:SER:OG	1:A:980:ASP:N	2.37	0.57
2:B:582:VAL:HG23	2:B:626:ILE:HB	1.85	0.57
6:F:77:ASP:O	6:F:78:GLN:CB	2.51	0.57
7:G:106:MET:HG2	7:G:107:LYS:N	2.19	0.57
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.85	0.57
1:A:360:GLU:HB2	1:A:363:GLN:HG3	1.85	0.57
1:A:444:PHE:CE2	1:A:487:MET:CE	2.87	0.57
2:B:1166:CYS:O	2:B:1168:LEU:N	2.36	0.57
3:C:113:VAL:HG23	3:C:147:LEU:HD21	1.85	0.57
4:D:128:VAL:HG12	4:D:129:LEU:N	2.20	0.57
4:D:71:LYS:HA	4:D:74:GLN:CG	2.34	0.57
12:L:49:LYS:O	12:L:50:ASP:CB	2.52	0.57
1:A:164:ARG:HG3	1:A:165:GLY:H	1.68	0.57
1:A:907:THR:CG2	1:A:908:LEU:N	2.68	0.57
5:E:178:ILE:HG22	5:E:213:ILE:O	2.05	0.57
12:L:60:ARG:HG2	12:L:61:THR:H	1.69	0.57
1:A:106:VAL:HG21	1:A:214:ILE:CD1	2.33	0.57
1:A:897:TYR:HB3	1:A:936:LEU:HD12	1.85	0.57
1:A:961:ARG:HG2	1:A:965:GLN:NE2	2.17	0.57
2:B:1099:VAL:HG13	2:B:1100:ASP:N	2.20	0.57
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.87	0.57
2:B:351:TYR:CZ	2:B:355:ILE:HD11	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:794:ASN:O	2:B:795:ILE:HD12	2.05	0.57
3:C:241:ASP:O	3:C:245:VAL:HG23	2.05	0.57
3:C:39:ALA:O	3:C:164:ALA:HB3	2.05	0.57
4:D:210:ILE:O	4:D:214:LEU:HD23	2.05	0.57
8:H:106:GLU:C	8:H:108:SER:H	2.08	0.57
8:H:24:CYS:HB2	8:H:44:VAL:CG2	2.31	0.57
9:I:61:ASP:O	9:I:63:GLY:N	2.38	0.57
14:N:2:DC:H1'	14:N:3:DT:H5'	1.86	0.57
1:A:973:ILE:HD11	1:A:1041:ALA:HB2	1.87	0.57
2:B:211:VAL:O	2:B:480:SER:HA	2.05	0.57
2:B:664:THR:HG1	2:B:678:GLU:N	2.03	0.57
1:A:896:ARG:NH2	1:A:1030:ARG:NH2	2.53	0.57
1:A:268:ASP:HB3	1:A:299:HIS:ND1	2.20	0.57
1:A:416:ARG:NH1	1:A:417:TYR:CE1	2.71	0.57
2:B:276:ILE:HA	2:B:336:ARG:O	2.05	0.57
2:B:778:MET:HE3	2:B:1094:ARG:HD3	1.86	0.57
3:C:148:ARG:HD3	3:C:149:LYS:HG3	1.85	0.57
3:C:33:LEU:O	3:C:37:MET:HG3	2.05	0.57
1:A:1139:GLU:O	1:A:1139:GLU:HG2	2.05	0.56
1:A:949:ASP:OD1	1:A:951:GLU:HB2	2.05	0.56
2:B:25:ILE:HD13	2:B:653:VAL:HG12	1.87	0.56
5:E:28:TYR:CE1	5:E:78:LEU:HD13	2.40	0.56
8:H:56:THR:HB	8:H:145:ARG:HG2	1.86	0.56
1:A:311:GLN:O	1:A:312:PRO:C	2.41	0.56
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.40	0.56
2:B:731:VAL:HG12	2:B:734:HIS:NE2	2.20	0.56
3:C:36:VAL:HG21	3:C:251:LEU:HD13	1.87	0.56
4:D:185:CYS:O	4:D:211:LEU:HD22	2.04	0.56
1:A:1200:ALA:HA	1:A:1203:ASN:HD22	1.70	0.56
1:A:332:LYS:O	1:A:334:GLY:N	2.38	0.56
1:A:50:ILE:C	1:A:52:GLY:H	2.09	0.56
1:A:7:SER:HB3	2:B:1193:GLN:NE2	2.20	0.56
2:B:597:MET:HA	2:B:597:MET:CE	2.35	0.56
4:D:155:ARG:CD	4:D:221:TYR:HE1	2.11	0.56
9:I:74:GLU:HB3	9:I:81:ARG:HD2	1.88	0.56
1:A:37:PHE:HD1	1:A:37:PHE:N	2.02	0.56
2:B:97:VAL:HG13	2:B:97:VAL:O	2.06	0.56
4:D:25:ALA:HB1	4:D:196:PRO:HG2	1.86	0.56
8:H:58:THR:HG22	8:H:59:ILE:N	2.18	0.56
12:L:34:CYS:SG	12:L:34:CYS:O	2.64	0.56
1:A:57:ARG:O	1:A:68:GLN:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:ARG:HG2	1:A:720:ARG:O	2.04	0.56
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.70	0.56
4:D:32:GLU:OE1	7:G:41:LYS:HE2	2.05	0.56
8:H:40:LEU:HD13	8:H:123:MET:CE	2.36	0.56
10:J:23:ASN:C	10:J:25:LEU:H	2.09	0.56
1:A:1445:ILE:N	1:A:1445:ILE:HD12	2.21	0.56
1:A:351:THR:HG22	2:B:1103:ILE:CA	2.27	0.56
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.69	0.56
1:A:824:LEU:O	1:A:827:THR:HG22	2.06	0.56
1:A:964:ILE:O	1:A:967:ALA:HB3	2.04	0.56
2:B:303:TYR:HD2	2:B:303:TYR:N	2.03	0.56
2:B:53:GLN:HG2	2:B:547:VAL:CG2	2.36	0.56
1:A:315:LEU:N	1:A:315:LEU:CD2	2.64	0.56
1:A:321:PRO:O	1:A:322:VAL:CB	2.53	0.56
1:A:34:LYS:HG3	1:A:36:ARG:NH2	2.19	0.56
2:B:758:PHE:HE1	2:B:1027:ILE:HG22	1.67	0.56
2:B:1084:GLN:NE2	2:B:1084:GLN:H	2.03	0.56
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.88	0.56
2:B:68:THR:HG22	2:B:91:SER:HA	1.87	0.56
3:C:253:LYS:O	3:C:256:ALA:HB3	2.06	0.56
4:D:13:ARG:C	4:D:15:LEU:H	2.08	0.56
4:D:51:ASN:O	4:D:52:LEU:O	2.24	0.56
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.34	0.56
11:K:65:HIS:HD2	11:K:67:PHE:H	1.51	0.56
1:A:370:ILE:HG12	2:B:1105:ALA:HB2	1.88	0.56
2:B:1096:ARG:CG	2:B:1097:HIS:N	2.69	0.56
2:B:245:GLU:O	2:B:246:LYS:HG3	2.05	0.56
2:B:274:PRO:CG	2:B:359:GLU:HB3	2.36	0.56
2:B:429:PHE:CD1	2:B:432:MET:HE3	2.41	0.56
2:B:557:PHE:CZ	2:B:603:LEU:HD11	2.41	0.56
2:B:601:ARG:O	2:B:605:ARG:HG3	2.06	0.56
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.36	0.56
5:E:157:SER:OG	5:E:160:GLU:HG3	2.06	0.56
5:E:69:ILE:HD12	5:E:69:ILE:H	1.71	0.56
5:E:69:ILE:N	5:E:69:ILE:HD12	2.21	0.56
5:E:94:LYS:O	5:E:98:ILE:HG13	2.05	0.56
1:A:1011:GLN:HE22	1:A:1015:VAL:HG21	1.71	0.56
1:A:929:LEU:HD21	1:A:983:ILE:HG23	1.88	0.56
2:B:1116:ARG:HG3	2:B:1198:TYR:CG	2.41	0.56
2:B:20:ASP:O	2:B:22:SER:N	2.29	0.56
2:B:360:PHE:CZ	2:B:361:LEU:HD13	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.38	0.56
3:C:112:ASN:HB3	3:C:114:TYR:HE1	1.66	0.56
3:C:177:GLU:HG3	3:C:231:ASN:CB	2.26	0.56
11:K:47:ARG:HD3	11:K:59:ALA:O	2.06	0.56
13:T:18:DA:H3'	13:T:18:DA:OP1	2.06	0.56
1:A:1205:LYS:O	1:A:1207:LEU:HG	2.06	0.56
1:A:470:LEU:HD23	1:A:470:LEU:N	2.20	0.56
1:A:741:ASN:HD22	1:A:744:LYS:N	1.96	0.56
1:A:825:ILE:O	1:A:829:VAL:HG23	2.06	0.56
1:A:11:LEU:HB2	2:B:1193:GLN:CG	2.36	0.56
2:B:167:ILE:N	2:B:167:ILE:HD12	2.21	0.56
2:B:345:LYS:CG	2:B:346:GLU:N	2.69	0.56
2:B:575:PRO:HG2	2:B:576:ASP:H	1.69	0.56
2:B:640:VAL:HG23	2:B:740:HIS:HA	1.87	0.56
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.87	0.56
1:A:1170:ILE:HD12	1:A:1170:ILE:H	1.71	0.56
1:A:186:LYS:HZ3	1:A:197:PRO:HD3	1.69	0.56
1:A:230:ARG:HG3	1:A:233:TRP:CZ3	2.41	0.56
1:A:53:LEU:CD2	1:A:54:ASN:N	2.55	0.56
2:B:102:VAL:HG21	2:B:112:LEU:HD13	1.88	0.56
2:B:1177:HIS:CB	2:B:1179:GLN:NE2	2.69	0.56
2:B:637:LEU:HD12	2:B:693:ILE:CD1	2.32	0.56
2:B:731:VAL:HG12	2:B:732:SER:N	2.21	0.56
2:B:935:ARG:HG3	2:B:935:ARG:O	2.05	0.56
3:C:99:LEU:CD2	3:C:99:LEU:N	2.68	0.56
4:D:59:ILE:HG21	4:D:145:MET:SD	2.46	0.56
1:A:401:GLY:C	1:A:435:HIS:HD2	2.09	0.55
1:A:41:MET:HB2	1:A:49:LYS:HA	1.84	0.55
1:A:62:ASP:O	1:A:64:ASN:N	2.39	0.55
1:A:909:ASP:OD1	1:A:911:SER:N	2.37	0.55
2:B:1224:PHE:CZ	5:E:171:LYS:HG3	2.39	0.55
2:B:654:ARG:H	2:B:657:HIS:HD2	1.53	0.55
4:D:4:SER:O	4:D:5:THR:CB	2.54	0.55
6:F:89:GLU:O	6:F:93:ILE:HD12	2.05	0.55
12:L:38:LEU:O	12:L:39:SER:HB3	2.06	0.55
1:A:1006:ILE:CD1	5:E:163:GLU:HG3	2.36	0.55
1:A:117:GLU:H	1:A:117:GLU:CD	2.09	0.55
1:A:90:VAL:HB	1:A:297:GLN:HE21	1.68	0.55
2:B:273:LEU:CD2	2:B:360:PHE:HD1	2.19	0.55
4:D:173:HIS:O	4:D:177:VAL:HG23	2.06	0.55
10:J:23:ASN:O	10:J:25:LEU:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:1:MET:H1	10:J:57:ILE:H	1.54	0.55
1:A:427:GLN:HG3	1:A:430:TRP:CE2	2.40	0.55
2:B:209:GLU:OE2	2:B:485:ARG:NE	2.34	0.55
2:B:309:GLN:HG3	9:I:52:ILE:CD1	2.37	0.55
2:B:383:ASN:O	2:B:387:LEU:HD13	2.06	0.55
2:B:560:GLU:O	2:B:561:TRP:CD1	2.59	0.55
2:B:68:THR:HA	2:B:90:ILE:O	2.07	0.55
5:E:98:ILE:HG22	5:E:102:GLU:HG3	1.88	0.55
9:I:34:TYR:CD2	9:I:35:VAL:N	2.74	0.55
1:A:1109:LYS:C	1:A:1110:ASN:HD22	2.10	0.55
2:B:1152:MET:HE3	2:B:1157:ALA:CB	2.37	0.55
2:B:427:ASP:HA	2:B:430:ARG:CD	2.36	0.55
2:B:916:THR:O	2:B:935:ARG:HG2	2.07	0.55
5:E:2:ASP:O	5:E:3:GLN:HG2	2.06	0.55
6:F:111:LEU:H	6:F:111:LEU:CD1	2.16	0.55
1:A:562:THR:HB	8:H:98:TYR:CD2	2.42	0.55
1:A:709:THR:CG2	1:A:711:ARG:HG3	2.35	0.55
4:D:12:ARG:HH12	4:D:14:ARG:HA	1.71	0.55
5:E:46:TYR:CD2	5:E:58:MET:HG2	2.41	0.55
2:B:1113:VAL:HG23	15:P:1:C:H4'	1.88	0.55
1:A:66:LYS:HZ3	1:A:68:GLN:N	1.98	0.55
2:B:101:MET:HB3	2:B:109:THR:HG22	1.87	0.55
2:B:1096:ARG:HG3	2:B:1097:HIS:N	2.21	0.55
2:B:459:TYR:CZ	2:B:469:GLN:HG3	2.42	0.55
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.87	0.55
8:H:89:LEU:C	8:H:91:ASP:N	2.52	0.55
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.41	0.55
1:A:446:ARG:HH11	1:A:446:ARG:HG2	1.71	0.55
1:A:65:LEU:O	1:A:66:LYS:C	2.44	0.55
1:A:7:SER:OG	2:B:1161:HIS:CE1	2.59	0.55
1:A:886:ILE:HG23	1:A:887:GLY:H	1.72	0.55
1:A:982:THR:HB	1:A:985:ASP:H	1.72	0.55
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.40	0.55
2:B:1115:THR:O	2:B:1116:ARG:HB2	2.06	0.55
2:B:654:ARG:H	2:B:657:HIS:CD2	2.25	0.55
3:C:99:LEU:HD22	3:C:99:LEU:N	2.21	0.55
4:D:118:THR:HG22	4:D:118:THR:O	2.07	0.55
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.42	0.55
8:H:106:GLU:HG2	8:H:112:ILE:CD1	2.37	0.55
8:H:61:SER:O	8:H:62:SER:HB2	2.07	0.55
8:H:84:ALA:CB	8:H:87:ARG:HD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.21	0.55
1:A:120:GLU:HG3	1:A:123:ARG:NH2	2.22	0.55
1:A:1433:MET:CE	7:G:63:PRO:HB2	2.36	0.55
1:A:714:PHE:O	1:A:718:VAL:HG23	2.07	0.55
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.89	0.55
2:B:361:LEU:O	2:B:363:HIS:O	2.25	0.55
2:B:652:LYS:HD2	2:B:688:GLY:O	2.07	0.55
4:D:219:THR:HG22	4:D:220:LEU:O	2.07	0.55
9:I:74:GLU:HB3	9:I:81:ARG:NE	2.22	0.55
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.70	0.55
2:B:1004:GLU:CG	10:J:42:LYS:NZ	2.70	0.55
2:B:47:GLN:O	2:B:173:MET:HE1	2.06	0.55
2:B:333:PHE:O	2:B:334:ILE:HG13	2.07	0.55
2:B:370:PHE:HD2	2:B:373:ARG:HD3	1.72	0.55
3:C:80:LEU:HD11	3:C:95:CYS:CA	2.37	0.55
4:D:12:ARG:CG	4:D:12:ARG:HH11	2.15	0.55
4:D:213:GLU:HA	4:D:213:GLU:OE1	2.07	0.55
2:B:473:MET:HE1	2:B:474:SER:HA	1.89	0.55
3:C:112:ASN:CB	3:C:114:TYR:HE1	2.19	0.55
8:H:130:ARG:HB3	8:H:134:ASN:H	1.72	0.55
12:L:38:LEU:HG	12:L:39:SER:H	1.72	0.55
1:A:1161:THR:CG2	1:A:1163:ILE:H	2.08	0.54
1:A:381:THR:HG21	1:A:383:TYR:CD1	2.42	0.54
1:A:512:VAL:CG1	1:A:512:VAL:O	2.56	0.54
2:B:185:THR:O	2:B:188:ASP:N	2.40	0.54
2:B:434:ARG:O	2:B:436:VAL:HG23	2.07	0.54
2:B:590:HIS:NE2	2:B:592:ASN:O	2.39	0.54
2:B:792:MET:HG2	2:B:855:PHE:CE1	2.41	0.54
2:B:855:PHE:HZ	2:B:857:ARG:HH12	1.54	0.54
4:D:120:GLU:OE1	4:D:120:GLU:O	2.25	0.54
7:G:21:ARG:HD2	7:G:24:GLN:CB	2.37	0.54
7:G:49:LEU:HG	7:G:76:ALA:HA	1.88	0.54
8:H:26:ILE:HG22	8:H:40:LEU:O	2.07	0.54
9:I:82:GLU:HB3	9:I:104:LEU:CG	2.37	0.54
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.89	0.54
1:A:1445:ILE:H	1:A:1445:ILE:CD1	2.18	0.54
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.88	0.54
1:A:645:LEU:HD11	1:A:649:ILE:HD11	1.89	0.54
2:B:108:VAL:HG23	2:B:109:THR:H	1.70	0.54
2:B:427:ASP:HA	2:B:430:ARG:HG3	1.89	0.54
2:B:637:LEU:HD22	2:B:741:CYS:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:GLY:O	2:B:130:VAL:HG13	2.07	0.54
8:H:59:ILE:O	8:H:60:ALA:HB3	2.07	0.54
11:K:47:ARG:O	11:K:47:ARG:HD2	2.08	0.54
1:A:1437:GLY:O	1:A:1439:GLY:N	2.40	0.54
1:A:711:ARG:HA	9:I:97:MET:HE1	1.89	0.54
2:B:313:MET:CE	2:B:386:LEU:HD22	2.37	0.54
5:E:3:GLN:NE2	5:E:52:ARG:HH12	2.05	0.54
8:H:12:VAL:CG1	8:H:26:ILE:HD11	2.37	0.54
1:A:1118:VAL:HG12	1:A:1327:ILE:HG13	1.88	0.54
1:A:598:LEU:O	1:A:599:SER:C	2.46	0.54
1:A:710:LEU:H	1:A:710:LEU:CD1	2.17	0.54
1:A:903:ASN:HD22	1:A:904:THR:H	1.51	0.54
2:B:999:MET:HE3	2:B:999:MET:HA	1.89	0.54
6:F:69:LEU:HD13	6:F:71:GLU:OE1	2.06	0.54
7:G:87:VAL:CG2	7:G:103:VAL:HG21	2.36	0.54
1:A:107:CYS:HB2	1:A:114:LEU:CD2	2.37	0.54
1:A:1312:ASN:ND2	1:A:1315:GLU:HB2	2.22	0.54
1:A:102:VAL:HG13	1:A:222:LEU:HD13	1.89	0.54
1:A:219:PHE:HE1	1:A:230:ARG:HE	1.54	0.54
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.90	0.54
1:A:382:PRO:HD3	1:A:428:TYR:HD2	1.71	0.54
1:A:524:VAL:HG12	1:A:525:GLN:H	1.73	0.54
1:A:89:PRO:C	1:A:204:THR:HG21	2.28	0.54
1:A:984:LYS:HG2	1:A:988:LEU:HD12	1.89	0.54
1:A:443:LEU:HD12	2:B:1146:PHE:CE2	2.43	0.54
2:B:315:LYS:N	2:B:316:PRO:HD2	2.22	0.54
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.90	0.54
4:D:71:LYS:CA	4:D:74:GLN:HB2	2.36	0.54
5:E:207:ARG:HH11	5:E:207:ARG:HB3	1.73	0.54
12:L:58:LYS:O	12:L:58:LYS:HG2	2.08	0.54
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.42	0.54
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.89	0.54
1:A:332:LYS:HG2	1:A:333:GLU:HG2	1.90	0.54
2:B:423:LYS:O	2:B:427:ASP:HB2	2.08	0.54
2:B:794:ASN:C	2:B:795:ILE:HD12	2.27	0.54
3:C:229:TYR:CD1	3:C:229:TYR:N	2.75	0.54
5:E:78:LEU:HA	5:E:107:THR:HB	1.88	0.54
8:H:109:LYS:HG2	8:H:110:ASP:OD1	2.07	0.54
2:B:620:ARG:HH12	9:I:68:LEU:HD21	1.71	0.54
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.89	0.54
1:A:709:THR:HB	1:A:712:GLU:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:639:ILE:CG2	2:B:641:GLU:HG2	2.38	0.54
2:B:875:GLU:O	2:B:877:PRO:CD	2.55	0.54
3:C:31:ASN:O	3:C:34:ARG:HB3	2.07	0.54
3:C:73:GLN:NE2	3:C:75:MET:H	2.06	0.54
5:E:144:ILE:HD13	5:E:183:PRO:HB3	1.90	0.54
10:J:36:LEU:HD11	10:J:51:LEU:HB2	1.89	0.54
12:L:68:GLU:CD	12:L:68:GLU:H	2.11	0.54
1:A:1397:LEU:HB2	1:A:1426:GLU:OE1	2.08	0.54
1:A:500:GLU:O	1:A:504:LEU:HB2	2.08	0.54
1:A:673:GLY:O	1:A:676:MET:HB2	2.08	0.54
2:B:390:LEU:O	2:B:392:ARG:HG3	2.08	0.54
2:B:862:GLN:HG2	2:B:963:PHE:HD1	1.72	0.54
2:B:871:THR:HG22	2:B:872:GLU:O	2.08	0.54
5:E:144:ILE:HG13	5:E:145:THR:H	1.72	0.54
7:G:9:LEU:HD12	7:G:10:ASN:N	2.22	0.54
9:I:73:ARG:HD2	9:I:101:PHE:CE2	2.43	0.54
1:A:1161:THR:HG22	1:A:1162:VAL:N	2.22	0.54
1:A:597:LEU:N	1:A:597:LEU:HD12	2.23	0.54
2:B:247:GLY:C	2:B:249:ARG:H	2.10	0.54
2:B:258:LEU:O	2:B:258:LEU:HG	2.07	0.54
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.73	0.54
2:B:282:ILE:CD1	2:B:382:ILE:HD13	2.38	0.54
2:B:707:PRO:HG2	2:B:708:GLU:N	2.22	0.54
3:C:80:LEU:HD11	3:C:95:CYS:HA	1.90	0.54
4:D:216:ASN:C	4:D:218:GLU:N	2.59	0.54
6:F:90:ARG:HD3	6:F:155:LEU:HD13	1.89	0.54
1:A:600:PRO:HG2	1:A:601:LYS:H	1.72	0.54
1:A:919:ILE:HD13	1:A:983:ILE:HD12	1.88	0.54
2:B:241:ARG:HG2	2:B:253:THR:HG21	1.90	0.54
4:D:14:ARG:NH2	4:D:16:LYS:HD2	2.23	0.54
8:H:84:ALA:HB2	8:H:87:ARG:HD2	1.90	0.54
9:I:62:ILE:HD11	9:I:86:PHE:CE2	2.41	0.54
1:A:1171:GLN:HA	1:A:1174:PHE:CD1	2.43	0.53
1:A:1241:ARG:O	1:A:1242:VAL:HG23	2.08	0.53
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.89	0.53
1:A:879:GLU:OE1	1:A:962:ARG:NH2	2.41	0.53
2:B:244:LEU:HD11	2:B:366:GLN:NE2	2.23	0.53
2:B:289:LEU:CD1	2:B:375:ALA:HB2	2.36	0.53
2:B:449:ASN:C	2:B:451:LYS:H	2.11	0.53
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.90	0.53
2:B:705:MET:CE	2:B:705:MET:HA	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.91	0.53
11:K:65:HIS:HD2	11:K:67:PHE:N	2.05	0.53
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.23	0.53
1:A:1199:ARG:HG3	1:A:1236:LEU:HD11	1.89	0.53
1:A:264:PHE:HB3	1:A:265:LYS:NZ	2.23	0.53
1:A:34:LYS:NZ	1:A:57:ARG:NH1	2.57	0.53
2:B:110:HIS:HB2	12:L:54:ARG:NH2	2.23	0.53
2:B:1124:ARG:O	2:B:1125:ASP:HB3	2.07	0.53
2:B:1181:GLU:OE2	2:B:1188:LYS:HE3	2.07	0.53
2:B:171:PRO:HD2	2:B:457:LEU:HD13	1.91	0.53
2:B:399:ASP:OD2	2:B:510:LYS:HB2	2.07	0.53
2:B:797:TYR:HE1	2:B:854:LEU:HD23	1.73	0.53
2:B:889:THR:HG23	2:B:891:ASP:H	1.72	0.53
3:C:35:ARG:HH12	11:K:41:THR:H	1.54	0.53
3:C:63:ILE:HA	3:C:66:ARG:HG3	1.90	0.53
3:C:80:LEU:CD1	3:C:95:CYS:HA	2.39	0.53
5:E:64:PRO:HB2	5:E:69:ILE:HD11	1.89	0.53
6:F:111:LEU:C	6:F:113:GLY:H	2.10	0.53
7:G:111:THR:CG2	7:G:114:LEU:HD13	2.37	0.53
12:L:47:ARG:HG3	12:L:52:GLY:O	2.09	0.53
1:A:444:PHE:CE2	1:A:487:MET:HE3	2.43	0.53
1:A:508:PRO:O	1:A:511:ILE:HG13	2.09	0.53
1:A:898:ARG:HD2	1:A:899:VAL:H	1.73	0.53
1:A:967:ALA:HA	1:A:1044:TRP:CZ3	2.43	0.53
2:B:129:PHE:HA	2:B:165:VAL:O	2.08	0.53
2:B:360:PHE:HE2	2:B:374:LYS:HB3	1.73	0.53
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.43	0.53
2:B:25:ILE:HG22	2:B:658:ILE:HD12	1.90	0.53
2:B:847:ASP:C	2:B:849:GLY:N	2.62	0.53
2:B:855:PHE:HZ	2:B:857:ARG:NH1	2.05	0.53
3:C:44:LEU:HD21	3:C:159:ALA:CB	2.38	0.53
4:D:35:LEU:N	4:D:35:LEU:HD12	2.23	0.53
7:G:1:MET:SD	7:G:2:PHE:N	2.82	0.53
7:G:52:ASP:C	7:G:53:ASN:HD22	2.12	0.53
1:A:102:VAL:HB	1:A:211:PHE:CE1	2.43	0.53
1:A:115:LEU:HD12	1:A:142:CYS:HB3	1.91	0.53
1:A:22:PHE:HE2	1:A:30:ILE:HD11	1.74	0.53
1:A:903:ASN:ND2	1:A:904:THR:N	2.49	0.53
2:B:237:VAL:HG22	2:B:257:LYS:HA	1.90	0.53
2:B:90:ILE:HD12	2:B:432:MET:SD	2.49	0.53
2:B:622:LYS:NZ	9:I:59:VAL:HG13	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:770:GLN:HG2	2:B:983:ARG:O	2.07	0.53
2:B:801:LYS:O	10:J:52:THR:HG23	2.08	0.53
3:C:8:VAL:HG12	3:C:9:LYS:N	2.22	0.53
4:D:144:THR:HG22	4:D:148:LEU:HD12	1.89	0.53
6:F:94:LEU:HD22	6:F:122:MET:HG2	1.90	0.53
11:K:47:ARG:HH11	11:K:47:ARG:CB	2.13	0.53
1:A:1236:LEU:C	1:A:1237:ILE:HD12	2.29	0.53
1:A:75:ASN:ND2	2:B:1116:ARG:HH12	2.06	0.53
2:B:582:VAL:CG2	2:B:626:ILE:HB	2.38	0.53
5:E:144:ILE:HG13	5:E:145:THR:N	2.23	0.53
5:E:204:THR:CG2	5:E:205:SER:N	2.71	0.53
7:G:87:VAL:HG23	7:G:103:VAL:HG21	1.88	0.53
1:A:1147:THR:HB	9:I:48:LEU:HD12	1.91	0.53
1:A:1173:HIS:O	1:A:1174:PHE:CD2	2.61	0.53
1:A:1206:ASP:O	1:A:1274:ARG:CZ	2.56	0.53
1:A:55:ASP:CG	1:A:55:ASP:O	2.45	0.53
2:B:126:SER:OG	2:B:172:ILE:HD11	2.08	0.53
2:B:661:LEU:HD23	2:B:679:TYR:O	2.08	0.53
3:C:179:GLU:HG2	3:C:180:TYR:N	2.24	0.53
3:C:23:SER:O	3:C:24:ASN:HB3	2.08	0.53
5:E:124:VAL:HB	5:E:125:PRO:HD3	1.90	0.53
5:E:164:LEU:HD21	5:E:211:TYR:CG	2.44	0.53
9:I:111:THR:HG21	9:I:113:ASP:HB2	1.91	0.53
9:I:17:ARG:HG2	9:I:28:GLU:HG2	1.90	0.53
12:L:33:GLU:H	12:L:33:GLU:CD	2.11	0.53
1:A:1148:ILE:HG12	1:A:1198:ASP:HB2	1.90	0.53
1:A:195:ASP:O	1:A:196:GLU:HB3	2.09	0.53
1:A:332:LYS:O	1:A:333:GLU:HB2	2.08	0.53
1:A:399:HIS:CB	1:A:400:PRO:CD	2.86	0.53
1:A:866:PHE:C	1:A:867:ILE:HD12	2.28	0.53
1:A:500:GLU:OE2	2:B:1145:SER:HB2	2.09	0.53
2:B:26:THR:O	2:B:29:ASP:HB2	2.07	0.53
2:B:579:ARG:CA	2:B:589:VAL:HG13	2.38	0.53
2:B:996:ARG:NH2	3:C:175:ALA:H	2.05	0.53
3:C:238:ILE:HD11	3:C:246:ARG:NH1	2.23	0.53
7:G:14:HIS:HD2	7:G:16:SER:H	1.50	0.53
8:H:12:VAL:HA	8:H:28:ALA:HB2	1.91	0.53
11:K:107:THR:HG22	11:K:108:GLU:N	2.23	0.53
1:A:1116:LEU:N	1:A:1308:THR:CG2	2.68	0.53
1:A:1143:LEU:HD12	1:A:1143:LEU:O	2.08	0.53
1:A:1158:PRO:C	1:A:1159:ARG:HG3	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:GLU:CD	1:A:205:GLU:H	2.12	0.53
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.39	0.53
1:A:297:GLN:CA	1:A:297:GLN:HE21	2.20	0.53
1:A:689:LYS:O	1:A:693:VAL:HG23	2.08	0.53
2:B:758:PHE:CE1	2:B:1027:ILE:CG2	2.91	0.53
2:B:785:TYR:CD1	2:B:786:ASN:N	2.77	0.53
7:G:9:LEU:HD12	7:G:10:ASN:H	1.74	0.53
8:H:4:THR:HG22	8:H:6:PHE:H	1.74	0.53
9:I:73:ARG:HH12	9:I:112:SER:CB	2.21	0.53
1:A:317:LYS:O	1:A:318:SER:HB3	2.09	0.53
1:A:709:THR:HB	1:A:712:GLU:HG3	1.91	0.53
1:A:898:ARG:HD2	1:A:899:VAL:N	2.23	0.53
1:A:905:ASP:O	1:A:906:HIS:ND1	2.42	0.53
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.89	0.53
2:B:1116:ARG:HG3	2:B:1198:TYR:CD2	2.43	0.53
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.89	0.53
2:B:779:GLY:O	2:B:795:ILE:HA	2.08	0.53
2:B:955:THR:HG23	2:B:956:THR:H	1.74	0.53
4:D:47:LEU:HD13	4:D:48:ILE:N	2.24	0.53
8:H:106:GLU:HA	8:H:112:ILE:HD12	1.91	0.53
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.39	0.53
12:L:59:ALA:O	12:L:60:ARG:O	2.27	0.53
2:B:405:ARG:NE	2:B:632:ARG:HG2	2.23	0.53
3:C:144:ILE:HG22	3:C:145:CYS:HB3	1.91	0.53
5:E:56:LYS:NZ	5:E:84:ASP:H	2.07	0.53
9:I:92:ARG:HD2	9:I:94:ASP:OD2	2.08	0.53
12:L:52:GLY:O	12:L:53:HIS:C	2.48	0.53
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.38	0.52
1:A:1170:ILE:HG22	1:A:1174:PHE:CZ	2.44	0.52
1:A:1280:GLU:O	1:A:1281:ARG:C	2.48	0.52
1:A:1293:SER:OG	1:A:1295:THR:HG23	2.08	0.52
1:A:278:THR:HG22	1:A:278:THR:O	2.09	0.52
2:B:245:GLU:C	2:B:246:LYS:HG3	2.29	0.52
2:B:431:TYR:CG	2:B:447:ALA:HB2	2.45	0.52
2:B:866:TYR:CG	2:B:870:ILE:HB	2.44	0.52
2:B:936:ASP:OD1	2:B:937:ALA:N	2.41	0.52
4:D:130:LEU:C	4:D:132:GLN:H	2.13	0.52
1:A:1333:ILE:O	1:A:1337:GLU:HG3	2.09	0.52
1:A:1454:MET:HG3	1:A:1454:MET:O	2.09	0.52
1:A:167:CYS:HB2	1:A:169:ASN:HD21	1.72	0.52
1:A:250:ILE:CG2	1:A:250:ILE:O	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLN:O	1:A:314:ALA:C	2.46	0.52
2:B:508:LEU:N	2:B:512:ARG:HE	2.07	0.52
2:B:848:ARG:HH22	2:B:996:ARG:HD3	1.74	0.52
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.08	0.52
4:D:220:LEU:HD23	4:D:221:TYR:N	2.25	0.52
7:G:121:PHE:HB2	7:G:130:TYR:CE2	2.44	0.52
8:H:89:LEU:O	8:H:91:ASP:N	2.42	0.52
1:A:1187:GLN:NE2	1:A:1188:GLN:HE21	2.07	0.52
1:A:335:ARG:NH1	2:B:1206:GLU:OE1	2.42	0.52
2:B:185:THR:O	2:B:186:GLU:C	2.47	0.52
2:B:526:GLU:OE1	2:B:752:ALA:HB3	2.09	0.52
2:B:816:GLU:O	2:B:817:LEU:HD23	2.09	0.52
3:C:213:PRO:O	3:C:214:ASN:HB3	2.10	0.52
3:C:8:VAL:C	3:C:9:LYS:HG3	2.29	0.52
5:E:185:ALA:O	5:E:190:LEU:HG	2.08	0.52
5:E:17:ARG:O	5:E:21:GLU:HG3	2.09	0.52
5:E:61:GLN:HG2	5:E:62:ALA:N	2.25	0.52
8:H:123:MET:HE3	8:H:142:LEU:CD2	2.40	0.52
8:H:11:GLN:C	8:H:28:ALA:HB1	2.29	0.52
11:K:18:LYS:NZ	11:K:38:GLU:HG2	2.23	0.52
2:B:657:HIS:CE1	2:B:689:LEU:HD11	2.44	0.52
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.44	0.52
7:G:139:ILE:CG2	7:G:140:LYS:H	2.21	0.52
1:A:434:ARG:NH2	1:A:440:ASP:OD1	2.43	0.52
1:A:853:ASP:OD1	1:A:855:THR:CB	2.52	0.52
2:B:429:PHE:HD1	2:B:432:MET:HE3	1.73	0.52
2:B:991:GLY:O	2:B:992:ILE:HB	2.09	0.52
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.40	0.52
4:D:203:SER:OG	4:D:206:GLU:HB2	2.09	0.52
5:E:121:MET:C	5:E:123:LEU:H	2.12	0.52
7:G:51:TYR:O	7:G:54:ILE:HG13	2.09	0.52
11:K:57:LEU:HB2	11:K:76:GLN:CG	2.36	0.52
1:A:1365:TYR:CE2	1:A:1369:ALA:HB2	2.44	0.52
1:A:84:ILE:HD11	1:A:270:LEU:HD13	1.92	0.52
1:A:901:LEU:N	1:A:926:GLN:HE21	1.99	0.52
2:B:1033:LYS:HD3	2:B:1059:LEU:HD11	1.92	0.52
2:B:176:SER:O	2:B:182:SER:HB3	2.09	0.52
2:B:906:SER:HA	2:B:946:ASN:HB2	1.92	0.52
4:D:40:HIS:CE1	7:G:7:LEU:O	2.63	0.52
13:T:24:DG:H2''	13:T:25:DG:C5'	2.34	0.52
1:A:1353:TYR:HD2	1:A:1353:TYR:C	2.11	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:NH1	2:B:1206:GLU:CD	2.63	0.52
1:A:720:ARG:O	1:A:724:GLU:HB3	2.09	0.52
1:A:821:ARG:HB2	1:A:821:ARG:NH1	2.25	0.52
1:A:829:VAL:HG21	2:B:508:LEU:CD1	2.37	0.52
2:B:288:ALA:CB	2:B:331:LEU:HD12	2.40	0.52
2:B:336:ARG:HG3	2:B:336:ARG:HH11	1.75	0.52
2:B:639:ILE:HG22	2:B:641:GLU:HG2	1.92	0.52
3:C:6:PRO:CG	11:K:101:LEU:HD12	2.40	0.52
5:E:55:ARG:HH11	5:E:55:ARG:HG3	1.74	0.52
6:F:94:LEU:HD21	6:F:122:MET:HA	1.92	0.52
1:A:598:LEU:CD1	8:H:124:ARG:HB2	2.40	0.52
2:B:619:ILE:HD12	9:I:65:ASP:HB2	1.91	0.52
1:A:1030:ARG:HG2	1:A:1034:GLU:OE2	2.10	0.52
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.91	0.52
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.57	0.52
2:B:1115:THR:HG22	2:B:1117:GLN:HG3	1.92	0.52
2:B:20:ASP:C	2:B:22:SER:H	2.13	0.52
2:B:254:LEU:HD12	2:B:272:THR:O	2.10	0.52
2:B:300:HIS:O	2:B:303:TYR:HE2	1.93	0.52
2:B:712:PRO:O	2:B:733:HIS:NE2	2.43	0.52
2:B:911:ILE:HG21	2:B:966:VAL:HG11	1.90	0.52
2:B:997:GLU:HG2	3:C:39:ALA:HB2	1.91	0.52
3:C:215:GLU:O	3:C:216:GLY:C	2.47	0.52
3:C:254:LYS:HE2	11:K:42:LEU:HD13	1.92	0.52
6:F:76:LYS:O	6:F:79:ARG:HD3	2.09	0.52
9:I:44:TYR:CD1	9:I:45:ARG:N	2.78	0.52
1:A:1100:ARG:O	1:A:1103:GLU:HB3	2.09	0.52
1:A:182:VAL:HG22	1:A:201:VAL:HA	1.91	0.52
1:A:22:PHE:CE2	1:A:30:ILE:HD11	2.45	0.52
1:A:412:ARG:CZ	2:B:1108:ARG:NH1	2.73	0.52
1:A:711:ARG:O	1:A:714:PHE:HB3	2.10	0.52
2:B:301:ILE:HG21	2:B:314:LEU:HD11	1.92	0.52
2:B:614:SER:HB2	2:B:697:GLU:OE1	2.10	0.52
3:C:22:LEU:HD11	11:K:101:LEU:HD21	1.92	0.52
2:B:620:ARG:CZ	9:I:68:LEU:HD21	2.40	0.52
1:A:999:VAL:HG12	1:A:1000:LEU:HG	1.90	0.52
1:A:1100:ARG:NH2	1:A:1351:GLU:CG	2.73	0.52
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.75	0.52
1:A:1291:VAL:HG22	1:A:1292:PRO:CD	2.40	0.52
1:A:442:VAL:CG2	1:A:489:LEU:HD11	2.40	0.52
1:A:628:GLY:O	1:A:632:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:LYS:HE2	1:A:795:GLU:OE2	2.10	0.52
1:A:903:ASN:C	1:A:903:ASN:ND2	2.63	0.52
2:B:1115:THR:HG22	2:B:1117:GLN:CG	2.40	0.52
2:B:234:ILE:HG21	2:B:237:VAL:HG23	1.90	0.52
2:B:878:GLN:O	2:B:879:ARG:C	2.48	0.52
5:E:182:ASP:HB3	5:E:185:ALA:HB2	1.92	0.52
6:F:90:ARG:HG3	6:F:91:ALA:N	2.25	0.52
7:G:138:THR:O	7:G:140:LYS:N	2.43	0.52
1:A:1124:HIS:HB2	1:A:1130:GLN:HG2	1.92	0.51
1:A:44:THR:O	1:A:45:GLN:HB2	2.09	0.51
1:A:512:VAL:HG12	1:A:512:VAL:O	2.09	0.51
1:A:786:HIS:CD2	1:A:786:HIS:N	2.76	0.51
2:B:101:MET:HB3	2:B:109:THR:CG2	2.40	0.51
2:B:1033:LYS:O	2:B:1037:LEU:HG	2.10	0.51
3:C:113:VAL:CG2	3:C:147:LEU:HD21	2.39	0.51
3:C:3:GLU:HG2	3:C:4:GLU:HG3	1.92	0.51
7:G:115:MET:O	7:G:164:LYS:HD3	2.10	0.51
10:J:23:ASN:C	10:J:25:LEU:N	2.62	0.51
12:L:38:LEU:HG	12:L:39:SER:N	2.25	0.51
1:A:367:PRO:HB3	1:A:465:TYR:O	2.10	0.51
1:A:55:ASP:C	1:A:57:ARG:N	2.59	0.51
1:A:609:ASP:HB2	1:A:969:GLN:HE22	1.75	0.51
2:B:1084:GLN:H	2:B:1084:GLN:HE21	1.58	0.51
2:B:331:LEU:O	2:B:334:ILE:HB	2.10	0.51
2:B:847:ASP:O	2:B:849:GLY:N	2.42	0.51
2:B:860:MET:HG2	2:B:861:ASP:N	2.25	0.51
2:B:975:GLN:HG2	2:B:976:ILE:H	1.74	0.51
3:C:18:VAL:CG2	3:C:240:VAL:HB	2.39	0.51
3:C:258:ILE:N	3:C:258:ILE:HD12	2.25	0.51
7:G:1:MET:SD	7:G:79:PHE:CE1	3.03	0.51
4:D:29:LEU:HD12	7:G:82:PHE:CE2	2.44	0.51
3:C:35:ARG:NH1	11:K:41:THR:N	2.58	0.51
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.92	0.51
1:A:1166:ASP:HA	1:A:1169:ILE:HD12	1.92	0.51
1:A:1229:SER:HB2	1:A:1233:ASP:OD2	2.11	0.51
1:A:899:VAL:CG2	1:A:908:LEU:HD21	2.40	0.51
2:B:203:PHE:N	2:B:203:PHE:CD1	2.78	0.51
2:B:604:ARG:C	2:B:606:LYS:H	2.11	0.51
2:B:796:LEU:HD21	2:B:821:GLN:NE2	2.21	0.51
8:H:104:PHE:CZ	8:H:136:LYS:HG3	2.45	0.51
8:H:76:THR:O	8:H:77:ARG:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:7:ASP:O	8:H:8:ASP:HB2	2.11	0.51
13:T:16:DT:H5'	13:T:16:DT:C6	2.32	0.51
1:A:883:LEU:CD2	1:A:1021:LEU:HB2	2.40	0.51
1:A:925:LEU:HD13	1:A:983:ILE:CG2	2.41	0.51
2:B:259:TYR:N	2:B:259:TYR:CD1	2.79	0.51
2:B:654:ARG:NH1	2:B:654:ARG:HG3	2.24	0.51
3:C:133:ILE:HD12	3:C:237:SER:HA	1.92	0.51
4:D:192:LYS:HD2	4:D:199:ASN:HA	1.91	0.51
5:E:65:THR:O	5:E:69:ILE:HD12	2.11	0.51
7:G:139:ILE:CG2	7:G:140:LYS:N	2.71	0.51
8:H:40:LEU:HD13	8:H:123:MET:HE3	1.92	0.51
3:C:235:VAL:HG21	10:J:6:ARG:NH2	2.25	0.51
1:A:446:ARG:HD3	1:A:480:ALA:HB2	1.92	0.51
1:A:554:PRO:HD2	1:A:648:ASN:OD1	2.10	0.51
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.92	0.51
2:B:96:TYR:N	2:B:129:PHE:O	2.33	0.51
2:B:324:ILE:O	2:B:324:ILE:HG22	2.10	0.51
2:B:579:ARG:HD2	2:B:586:TRP:CZ2	2.45	0.51
3:C:133:ILE:HD12	3:C:237:SER:N	2.26	0.51
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.50	0.51
4:D:134:THR:CG2	4:D:135:GLY:N	2.74	0.51
7:G:1:MET:O	7:G:2:PHE:C	2.48	0.51
8:H:123:MET:HG2	8:H:124:ARG:N	2.24	0.51
1:A:1112:LYS:O	1:A:1114:PRO:CD	2.57	0.51
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.91	0.51
2:B:1208:MET:O	2:B:1211:ASN:N	2.43	0.51
2:B:336:ARG:NH1	2:B:336:ARG:HG3	2.26	0.51
2:B:226:PHE:HA	2:B:395:GLN:CG	2.41	0.51
2:B:430:ARG:HB3	2:B:430:ARG:NH1	2.10	0.51
2:B:557:PHE:CE1	2:B:603:LEU:HD11	2.46	0.51
2:B:614:SER:C	2:B:615:MET:HG3	2.31	0.51
2:B:659:ALA:HA	2:B:662:MET:HE2	1.91	0.51
4:D:16:LYS:O	4:D:18:VAL:N	2.42	0.51
4:D:23:ASN:HA	4:D:28:GLN:O	2.11	0.51
7:G:26:LEU:CD1	7:G:56:ILE:HD11	2.37	0.51
9:I:105:SER:O	9:I:106:CYS:CB	2.53	0.51
11:K:8:GLU:O	11:K:37:LYS:HD2	2.11	0.51
1:A:55:ASP:OD2	1:A:55:ASP:O	2.28	0.51
2:B:766:ARG:NH2	2:B:1020:ARG:HD2	2.25	0.51
2:B:168:GLY:HA2	2:B:450:ALA:O	2.10	0.51
2:B:217:ARG:NE	2:B:405:ARG:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:644:GLU:C	2:B:646:LEU:H	2.13	0.51
2:B:850:LEU:HD12	2:B:851:PHE:N	2.26	0.51
2:B:789:MET:CE	2:B:953:LEU:HD22	2.41	0.51
2:B:955:THR:CG2	2:B:956:THR:O	2.59	0.51
5:E:180:ARG:O	5:E:186:LEU:HD21	2.10	0.51
5:E:89:GLY:C	5:E:91:LYS:H	2.13	0.51
8:H:38:LEU:HD12	8:H:124:ARG:O	2.10	0.51
9:I:19:ASP:HB3	9:I:24:ARG:HG2	1.93	0.51
2:B:309:GLN:CG	9:I:52:ILE:HD11	2.39	0.51
11:K:107:THR:O	11:K:111:LEU:HG	2.09	0.51
1:A:1116:LEU:HD12	1:A:1116:LEU:C	2.31	0.51
1:A:164:ARG:HG3	1:A:165:GLY:N	2.26	0.51
1:A:43:GLU:HG2	1:A:48:ALA:HB3	1.92	0.51
1:A:744:LYS:HD3	1:A:748:MET:HE1	1.91	0.51
1:A:8:SER:O	4:D:3:VAL:HG21	2.10	0.51
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.46	0.51
1:A:946:VAL:HG22	5:E:201:LYS:HB3	1.93	0.51
2:B:225:VAL:HG11	2:B:385:LEU:HA	1.92	0.51
2:B:604:ARG:HB2	2:B:609:ILE:HG13	1.92	0.51
2:B:687:GLU:O	2:B:689:LEU:HG	2.11	0.51
3:C:18:VAL:O	3:C:20:PHE:HD2	1.94	0.51
4:D:118:THR:O	4:D:120:GLU:N	2.44	0.51
4:D:35:LEU:HD11	4:D:173:HIS:CD2	2.45	0.51
4:D:69:ALA:C	4:D:71:LYS:H	2.12	0.51
6:F:75:PRO:O	6:F:77:ASP:O	2.29	0.51
12:L:55:ILE:O	12:L:56:LEU:HB2	2.10	0.51
1:A:93:VAL:HG21	1:A:301:ALA:O	2.11	0.51
1:A:482:PHE:C	1:A:484:GLY:H	2.15	0.51
2:B:230:ALA:HB3	2:B:231:PRO:HD3	1.92	0.51
2:B:408:LEU:N	2:B:408:LEU:HD12	2.26	0.51
2:B:69:LEU:HB3	2:B:429:PHE:HE1	1.76	0.51
2:B:999:MET:CE	2:B:999:MET:HA	2.41	0.51
4:D:134:THR:CG2	4:D:135:GLY:H	2.24	0.51
7:G:127:PRO:HG3	7:G:139:ILE:HG21	1.92	0.51
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.46	0.51
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.11	0.51
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.74	0.51
1:A:1095:THR:HG21	1:A:1112:LYS:HD2	1.91	0.51
1:A:184:SER:HB2	1:A:199:LEU:HD23	1.93	0.51
1:A:98:LYS:HE2	1:A:224:PHE:CZ	2.46	0.51
1:A:264:PHE:C	1:A:265:LYS:HE3	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:ILE:HG23	1:A:805:LEU:HD21	1.93	0.51
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.46	0.51
1:A:829:VAL:CG2	2:B:508:LEU:HD13	2.40	0.51
2:B:508:LEU:N	14:N:1:DA:O5'	2.38	0.51
2:B:91:SER:OG	2:B:133:LYS:HB2	2.11	0.51
3:C:196:ASP:CG	3:C:199:LYS:HD3	2.32	0.51
3:C:7:GLN:HE21	11:K:104:ASN:HD21	1.56	0.51
4:D:153:ARG:C	4:D:154:PHE:CD2	2.85	0.51
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.76	0.50
2:B:118:ARG:HG2	2:B:204:ILE:HD13	1.93	0.50
2:B:515:HIS:H	2:B:518:HIS:CD2	2.29	0.50
2:B:622:LYS:HZ3	9:I:59:VAL:HG13	1.76	0.50
2:B:66:ASP:OD2	2:B:422:LYS:HG2	2.11	0.50
4:D:13:ARG:O	4:D:15:LEU:N	2.41	0.50
5:E:129:PRO:O	5:E:130:ALA:C	2.48	0.50
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.93	0.50
8:H:84:ALA:CA	8:H:87:ARG:HB2	2.41	0.50
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.92	0.50
1:A:306:ASN:ND2	1:A:322:VAL:HG12	2.26	0.50
1:A:382:PRO:CB	1:A:428:TYR:HE2	2.23	0.50
1:A:556:TRP:CH2	1:A:558:GLY:HA2	2.46	0.50
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.46	0.50
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.93	0.50
2:B:601:ARG:HD3	2:B:605:ARG:NH2	2.26	0.50
3:C:120:ILE:HG21	3:C:124:LEU:CD1	2.40	0.50
1:A:1277:GLU:C	1:A:1279:ILE:H	2.15	0.50
1:A:1316:VAL:O	1:A:1316:VAL:HG12	2.11	0.50
1:A:306:ASN:HD22	1:A:322:VAL:HG12	1.77	0.50
1:A:709:THR:CB	1:A:712:GLU:HG3	2.41	0.50
2:B:580:VAL:HG22	2:B:624:LEU:HB3	1.93	0.50
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.77	0.50
4:D:194:LEU:HD22	7:G:86:VAL:HG11	1.93	0.50
7:G:1:MET:CE	7:G:80:LYS:H	2.24	0.50
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.92	0.50
1:A:146:MET:O	1:A:147:VAL:HG23	2.12	0.50
1:A:43:GLU:OE2	1:A:48:ALA:CB	2.58	0.50
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.46	0.50
2:B:640:VAL:O	2:B:641:GLU:C	2.50	0.50
2:B:650:GLU:OE2	2:B:651:LEU:HB2	2.10	0.50
2:B:654:ARG:O	2:B:657:HIS:N	2.44	0.50
8:H:113:ALA:HA	8:H:125:LEU:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:52:THR:O	10:J:52:THR:HG22	2.11	0.50
1:A:1280:GLU:O	1:A:1281:ARG:O	2.29	0.50
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.12	0.50
1:A:914:GLU:HB2	1:A:979:SER:O	2.11	0.50
2:B:1056:SER:HB3	2:B:1066:SER:OG	2.11	0.50
2:B:227:LYS:HG3	2:B:395:GLN:OE1	2.11	0.50
2:B:515:HIS:HD2	2:B:517:THR:HG23	1.75	0.50
3:C:7:GLN:HE21	11:K:104:ASN:HD22	1.57	0.50
4:D:56:ARG:HD3	4:D:149:THR:HA	1.93	0.50
5:E:48:ASP:OD1	5:E:52:ARG:HB2	2.11	0.50
8:H:15:VAL:HG21	8:H:49:VAL:O	2.11	0.50
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	2.98	0.50
1:A:1168:GLU:OE2	1:A:1172:LEU:HD11	2.11	0.50
1:A:105:CYS:SG	1:A:139:TRP:HA	2.52	0.50
1:A:47:ARG:NH1	1:A:254:GLU:HG2	2.27	0.50
1:A:655:PHE:O	1:A:658:LEU:HB3	2.11	0.50
1:A:75:ASN:O	1:A:76:GLU:CB	2.59	0.50
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.12	0.50
2:B:118:ARG:CG	2:B:204:ILE:HD13	2.41	0.50
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.94	0.50
2:B:582:VAL:O	2:B:582:VAL:HG12	2.11	0.50
2:B:686:ASN:C	2:B:688:GLY:H	2.15	0.50
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.93	0.50
4:D:29:LEU:HB3	7:G:82:PHE:CE2	2.46	0.50
4:D:39:ASN:ND2	4:D:41:GLN:H	2.09	0.50
5:E:204:THR:HG23	5:E:205:SER:H	1.73	0.50
7:G:138:THR:CG2	7:G:139:ILE:H	2.23	0.50
7:G:55:ASP:OD1	7:G:57:GLN:HG3	2.12	0.50
1:A:1395:GLY:HA3	1:A:1419:ASP:OD2	2.11	0.50
1:A:180:LYS:HZ2	1:A:294:SER:HB3	1.77	0.50
2:B:599:THR:O	2:B:603:LEU:HB2	2.11	0.50
3:C:8:VAL:HG12	3:C:9:LYS:H	1.76	0.50
5:E:154:ILE:HG22	5:E:155:ARG:O	2.11	0.50
7:G:111:THR:HG23	7:G:114:LEU:HB2	1.92	0.50
7:G:1:MET:HE2	7:G:1:MET:C	2.31	0.50
1:A:1207:LEU:HD13	1:A:1273:LEU:HD23	1.94	0.50
1:A:1436:ILE:O	1:A:1437:GLY:C	2.50	0.50
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.77	0.50
2:B:105:SER:O	2:B:106:ASP:HB2	2.12	0.50
2:B:172:ILE:CD1	2:B:178:ASN:ND2	2.73	0.50
2:B:244:LEU:HD11	2:B:250:PHE:HD1	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:605:ARG:HH12	2:B:641:GLU:CG	2.25	0.50
4:D:50:LEU:HD11	7:G:4:ILE:HD11	1.93	0.50
8:H:77:ARG:HG2	8:H:78:SER:H	1.77	0.50
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.41	0.50
9:I:111:THR:CG2	9:I:113:ASP:H	2.14	0.50
2:B:953:LEU:CB	12:L:57:LEU:HD23	2.42	0.50
13:T:16:DT:H2''	13:T:17:DT:C5'	2.41	0.50
1:A:1081:LEU:CD1	1:A:1098:VAL:HG23	2.42	0.50
1:A:1313:LEU:O	1:A:1315:GLU:N	2.44	0.50
1:A:547:LEU:HD21	1:A:560:ILE:HD13	1.94	0.50
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.26	0.50
2:B:37:PHE:HD2	2:B:542:MET:SD	2.35	0.50
2:B:570:VAL:HB	2:B:573:GLN:HB3	1.94	0.50
3:C:123:ASN:CG	3:C:125:MET:H	2.16	0.50
3:C:91:HIS:CD2	3:C:91:HIS:C	2.85	0.50
6:F:76:LYS:HA	6:F:79:ARG:CD	2.42	0.50
8:H:89:LEU:HB2	8:H:91:ASP:CG	2.32	0.50
9:I:58:VAL:HG13	9:I:62:ILE:HD13	1.93	0.50
12:L:47:ARG:CG	12:L:48:CYS:N	2.74	0.50
1:A:1171:GLN:OE1	1:A:1172:LEU:N	2.45	0.49
1:A:1349:TYR:CD2	1:A:1349:TYR:C	2.85	0.49
1:A:1402:PHE:CD2	1:A:1403:GLU:HG2	2.47	0.49
1:A:831:THR:HG23	1:A:832:ALA:N	2.27	0.49
2:B:115:GLN:HG2	2:B:193:LYS:CB	2.41	0.49
2:B:418:LYS:HE2	2:B:422:LYS:HZ1	1.76	0.49
2:B:56:ASP:HB3	2:B:57:TYR:CE1	2.48	0.49
2:B:579:ARG:N	2:B:589:VAL:HG13	2.26	0.49
2:B:957:ASN:HD22	2:B:961:LEU:HB2	1.76	0.49
2:B:96:TYR:HB2	2:B:129:PHE:HB2	1.94	0.49
3:C:101:LEU:HD21	3:C:113:VAL:HG11	1.94	0.49
1:A:447:GLN:NE2	13:T:20:DG:H4'	2.27	0.49
1:A:1050:GLU:O	1:A:1054:LEU:HD12	2.13	0.49
1:A:860:LEU:CD1	1:A:1393:ASN:HD22	2.24	0.49
1:A:1402:PHE:CE2	1:A:1403:GLU:HG2	2.47	0.49
1:A:145:LYS:HE3	1:A:145:LYS:CA	2.43	0.49
1:A:266:LEU:HD21	1:A:303:TYR:CZ	2.47	0.49
1:A:385:ILE:HG22	1:A:386:ASP:N	2.26	0.49
1:A:626:ASN:O	1:A:631:HIS:HD2	1.94	0.49
2:B:1095:LEU:H	2:B:1095:LEU:CD1	2.22	0.49
2:B:519:TRP:C	2:B:519:TRP:CD1	2.85	0.49
2:B:707:PRO:CG	2:B:708:GLU:H	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:906:SER:O	2:B:907:GLY:C	2.50	0.49
4:D:156:ASP:HB2	4:D:159:THR:CG2	2.41	0.49
4:D:161:GLY:O	4:D:165:GLN:HG3	2.11	0.49
7:G:132:SER:HB3	7:G:135:ASP:H	1.77	0.49
1:A:1076:ALA:HA	1:A:1079:MET:HG3	1.93	0.49
1:A:1150:SER:CB	1:A:1195:LEU:HD23	2.42	0.49
1:A:1399:ARG:HB3	1:A:1408:ILE:HD13	1.95	0.49
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.42	0.49
1:A:21:LEU:HD12	1:A:229:SER:HB2	1.94	0.49
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.12	0.49
2:B:558:LEU:CD2	2:B:596:LEU:HD11	2.43	0.49
8:H:106:GLU:O	8:H:108:SER:N	2.36	0.49
1:A:997:LEU:HD13	1:A:1018:PHE:CE2	2.47	0.49
1:A:1081:LEU:HD11	1:A:1098:VAL:HG23	1.94	0.49
1:A:47:ARG:CZ	1:A:254:GLU:HG2	2.43	0.49
1:A:54:ASN:HB3	1:A:247:ARG:HH22	1.77	0.49
1:A:67:CYS:O	1:A:70:CYS:HB3	2.12	0.49
1:A:807:GLY:HA2	2:B:760:ASP:O	2.12	0.49
2:B:508:LEU:O	2:B:509:ALA:CB	2.60	0.49
2:B:580:VAL:HG22	2:B:624:LEU:HD23	1.95	0.49
2:B:638:PHE:HB3	2:B:651:LEU:CD2	2.42	0.49
2:B:796:LEU:CD2	2:B:821:GLN:HE21	2.23	0.49
2:B:887:HIS:N	2:B:887:HIS:CD2	2.81	0.49
5:E:127:ILE:O	5:E:127:ILE:HG13	2.13	0.49
9:I:101:PHE:N	9:I:101:PHE:CD1	2.81	0.49
9:I:6:PHE:CB	9:I:12:ASN:O	2.56	0.49
1:A:378:GLU:OE2	1:A:387:ARG:NH2	2.46	0.49
1:A:41:MET:O	1:A:42:ASP:C	2.50	0.49
1:A:427:GLN:O	1:A:428:TYR:C	2.50	0.49
2:B:1095:LEU:HD12	2:B:1095:LEU:N	2.26	0.49
2:B:953:LEU:CD2	2:B:965:LYS:HB2	2.42	0.49
4:D:220:LEU:CG	4:D:221:TYR:N	2.75	0.49
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.48	0.49
4:D:8:PHE:HZ	7:G:5:LYS:HZ2	1.58	0.49
8:H:12:VAL:HG11	8:H:15:VAL:HG23	1.94	0.49
10:J:64:ASN:CB	10:J:65:PRO:CD	2.78	0.49
1:A:1021:LEU:O	1:A:1024:SER:HB3	2.12	0.49
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.75	0.49
1:A:1315:GLU:O	1:A:1317:MET:N	2.46	0.49
1:A:1138:ILE:HG21	1:A:1316:VAL:HG13	1.95	0.49
1:A:1349:TYR:O	1:A:1350:LYS:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASN:O	1:A:76:GLU:HB2	2.12	0.49
2:B:102:VAL:CG2	2:B:112:LEU:HD13	2.42	0.49
2:B:294:ASP:C	2:B:296:GLU:N	2.64	0.49
3:C:69:LEU:H	3:C:69:LEU:HD12	1.77	0.49
1:A:1207:LEU:CD1	1:A:1273:LEU:HD23	2.42	0.49
1:A:304:MET:O	1:A:324:SER:HB2	2.12	0.49
1:A:598:LEU:HD23	1:A:598:LEU:O	2.12	0.49
2:B:203:PHE:HD1	2:B:203:PHE:N	2.11	0.49
2:B:280:ILE:CG2	2:B:285:ILE:HG13	2.43	0.49
2:B:390:LEU:O	2:B:392:ARG:N	2.45	0.49
2:B:90:ILE:CD1	2:B:432:MET:SD	3.00	0.49
2:B:417:PHE:CE1	2:B:453:ILE:HD13	2.47	0.49
2:B:557:PHE:HZ	2:B:603:LEU:HD21	1.77	0.49
2:B:605:ARG:HH12	2:B:641:GLU:HG3	1.78	0.49
2:B:642:ASP:N	2:B:649:LYS:HG3	2.27	0.49
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.94	0.49
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.95	0.49
4:D:33:PHE:HE1	7:G:80:LYS:HD3	1.74	0.49
5:E:61:GLN:NE2	5:E:105:PHE:CZ	2.80	0.49
7:G:112:LYS:HA	7:G:115:MET:HE3	1.95	0.49
7:G:51:TYR:C	7:G:51:TYR:CD2	2.86	0.49
9:I:118:ARG:HH22	9:I:120:GLN:HB2	1.78	0.49
10:J:27:GLU:C	10:J:29:GLU:H	2.15	0.49
1:A:265:LYS:CE	1:A:265:LYS:HA	2.42	0.49
1:A:671:ALA:HB3	1:A:676:MET:CE	2.43	0.49
1:A:855:THR:CG2	1:A:857:ARG:HE	2.16	0.49
1:A:857:ARG:HD3	1:A:861:GLY:O	2.13	0.49
1:A:883:LEU:HD23	1:A:1021:LEU:HD13	1.94	0.49
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.48	0.49
2:B:468:GLU:HB3	2:B:469:GLN:H	1.39	0.49
2:B:910:VAL:CG1	2:B:938:SER:HB3	2.43	0.49
3:C:105:GLY:O	3:C:149:LYS:O	2.31	0.49
8:H:81:PRO:HB3	8:H:82:PRO:HD2	1.93	0.49
1:A:1155:ASP:CG	1:A:1162:VAL:HG23	2.33	0.49
1:A:145:LYS:HA	1:A:145:LYS:CE	2.43	0.49
1:A:95:PHE:O	1:A:96:ILE:C	2.51	0.49
2:B:797:TYR:HE1	2:B:854:LEU:CD2	2.25	0.49
2:B:857:ARG:HD2	2:B:945:GLU:OE1	2.12	0.49
3:C:44:LEU:HD13	3:C:129:ILE:HG23	1.95	0.49
4:D:50:LEU:HD21	7:G:4:ILE:HD12	1.94	0.49
7:G:14:HIS:HD2	7:G:16:SER:CB	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLY:O	1:A:169:ASN:C	2.51	0.49
3:C:11:ARG:NH2	3:C:206:ASN:OD1	2.46	0.49
1:A:1325:THR:O	5:E:148:GLU:HB2	2.12	0.49
5:E:50:MET:HG2	5:E:52:ARG:NH2	2.28	0.49
9:I:119:THR:HG22	9:I:119:THR:O	2.12	0.49
9:I:73:ARG:O	9:I:83:ASN:ND2	2.44	0.49
11:K:55:LYS:CB	11:K:81:TYR:CD1	2.96	0.49
1:A:1141:THR:HA	1:A:1205:LYS:HZ3	1.78	0.48
1:A:1155:ASP:OD2	1:A:1162:VAL:N	2.38	0.48
1:A:162:VAL:HG12	1:A:163:SER:N	2.28	0.48
1:A:470:LEU:HD23	1:A:470:LEU:H	1.78	0.48
2:B:1197:PRO:HG2	2:B:1200:ALA:CB	2.43	0.48
2:B:326:ASP:OD2	2:B:328:GLU:HB3	2.12	0.48
2:B:43:LEU:HD13	2:B:492:LEU:HD13	1.94	0.48
2:B:449:ASN:O	2:B:451:LYS:N	2.46	0.48
2:B:467:GLY:N	2:B:475:SER:HB3	2.28	0.48
2:B:729:ILE:O	2:B:729:ILE:HG22	2.11	0.48
3:C:104:PHE:HD2	3:C:105:GLY:H	1.60	0.48
5:E:48:ASP:HB3	5:E:54:GLN:NE2	2.28	0.48
7:G:145:VAL:HG12	7:G:146:LYS:N	2.27	0.48
8:H:100:THR:HG22	8:H:101:ALA:N	2.28	0.48
8:H:38:LEU:HD13	8:H:125:LEU:HD12	1.94	0.48
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.94	0.48
1:A:122:MET:CA	1:A:141:LEU:HD11	2.41	0.48
1:A:288:ALA:HA	1:A:291:GLU:CG	2.43	0.48
2:B:284:ILE:HD13	2:B:333:PHE:HD2	1.77	0.48
2:B:831:SER:CB	2:B:994:TYR:OH	2.61	0.48
1:A:1140:HIS:NE2	1:A:1142:THR:HG23	2.28	0.48
1:A:35:ILE:HD12	1:A:241:VAL:HG21	1.95	0.48
1:A:41:MET:O	1:A:50:ILE:HG13	2.12	0.48
2:B:812:LEU:O	2:B:813:LYS:HB2	2.13	0.48
2:B:95:ILE:HG13	2:B:130:VAL:CG2	2.43	0.48
8:H:15:VAL:HG22	8:H:26:ILE:CD1	2.43	0.48
1:A:475:THR:CG2	1:A:476:SER:N	2.75	0.48
2:B:237:VAL:HG22	2:B:257:LYS:HG3	1.94	0.48
2:B:273:LEU:HD12	2:B:280:ILE:HD12	1.95	0.48
2:B:309:GLN:HG3	9:I:52:ILE:HD12	1.95	0.48
2:B:516:ASN:ND2	2:B:516:ASN:N	2.44	0.48
2:B:597:MET:SD	2:B:624:LEU:HD11	2.53	0.48
2:B:654:ARG:N	2:B:657:HIS:HD2	2.11	0.48
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:773:MET:CE	2:B:987:LYS:HD2	2.44	0.48
5:E:177:ARG:O	5:E:212:ARG:HD3	2.13	0.48
6:F:101:ILE:HD13	6:F:120:ILE:CG2	2.43	0.48
7:G:126:ASN:ND2	7:G:127:PRO:HA	2.24	0.48
7:G:129:SER:HB3	7:G:138:THR:OG1	2.13	0.48
1:A:1035:TYR:O	1:A:1036:ARG:HB2	2.13	0.48
1:A:773:LYS:HD2	1:A:773:LYS:H	1.79	0.48
2:B:976:ILE:O	2:B:990:ILE:HB	2.13	0.48
8:H:51:ALA:O	8:H:52:GLN:HB2	2.13	0.48
8:H:82:PRO:HG2	8:H:83:GLN:H	1.78	0.48
9:I:82:GLU:HB3	9:I:104:LEU:CD1	2.43	0.48
11:K:59:ALA:HA	11:K:74:ARG:O	2.14	0.48
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.43	0.48
1:A:1336:MET:HE2	1:A:1381:LEU:HG	1.96	0.48
1:A:196:GLU:CG	1:A:197:PRO:HD2	2.44	0.48
1:A:23:SER:HA	1:A:233:TRP:CD1	2.48	0.48
2:B:1116:ARG:HG3	2:B:1198:TYR:CD1	2.48	0.48
2:B:24:PRO:O	2:B:25:ILE:HG23	2.13	0.48
2:B:552:MET:HA	2:B:552:MET:HE3	1.93	0.48
2:B:638:PHE:HB2	2:B:741:CYS:O	2.13	0.48
2:B:529:GLU:OE1	2:B:769:TYR:CE2	2.66	0.48
5:E:10:SER:O	5:E:14:ARG:HG3	2.13	0.48
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.43	0.48
8:H:94:ASP:O	8:H:95:TYR:HB2	2.14	0.48
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.95	0.48
1:A:1152:ILE:CD1	1:A:1260:LEU:HD23	2.43	0.48
1:A:1453:TYR:O	1:A:1454:MET:HB3	2.13	0.48
1:A:344:ARG:HB2	2:B:1118:PRO:HB2	1.96	0.48
1:A:364:VAL:O	1:A:364:VAL:HG13	2.13	0.48
1:A:41:MET:HA	1:A:50:ILE:H	1.78	0.48
1:A:850:VAL:HG12	1:A:1060:PRO:HA	1.94	0.48
2:B:34:ILE:HG12	2:B:542:MET:HE1	1.96	0.48
3:C:208:GLU:C	3:C:210:GLU:H	2.15	0.48
4:D:119:ARG:HD3	4:D:221:TYR:CE2	2.49	0.48
5:E:78:LEU:CA	5:E:107:THR:HB	2.43	0.48
6:F:103:MET:O	6:F:104:ASN:HB2	2.14	0.48
7:G:21:ARG:HA	7:G:21:ARG:HD3	1.75	0.48
7:G:91:VAL:HG12	7:G:92:VAL:N	2.29	0.48
9:I:84:VAL:O	9:I:84:VAL:HG13	2.12	0.48
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.48	0.48
3:C:166:GLU:C	11:K:6:ARG:NH1	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:61:THR:HG21	12:L:63:ARG:HG3	1.96	0.48
1:A:1107:VAL:CG1	1:A:1333:ILE:HD11	2.44	0.48
1:A:49:LYS:CD	1:A:55:ASP:HB3	2.44	0.48
1:A:629:LEU:CD1	1:A:645:LEU:HD21	2.44	0.48
1:A:341:MET:CE	2:B:1135:ARG:NH1	2.75	0.48
2:B:1197:PRO:HG2	2:B:1200:ALA:HB2	1.95	0.48
2:B:641:GLU:C	2:B:643:ASP:H	2.17	0.48
2:B:710:LEU:HA	2:B:733:HIS:CB	2.34	0.48
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.95	0.48
3:C:186:LEU:HD21	3:C:225:ALA:HB2	1.95	0.48
3:C:233:GLU:OE1	10:J:12:LYS:HE2	2.13	0.48
3:C:91:HIS:HD2	3:C:91:HIS:O	1.97	0.48
7:G:137:ILE:CG2	7:G:143:ILE:HD11	2.44	0.48
1:A:986:ILE:HG21	1:A:1028:THR:HA	1.96	0.48
1:A:1293:SER:HB3	1:A:1297:GLU:OE1	2.14	0.48
1:A:690:VAL:CG1	1:A:691:LEU:N	2.77	0.48
2:B:324:ILE:HD13	2:B:330:ALA:HA	1.96	0.48
2:B:244:LEU:CD2	2:B:366:GLN:HE21	2.25	0.48
5:E:172:GLU:HG2	5:E:213:ILE:CD1	2.44	0.48
1:A:106:VAL:CG1	1:A:107:CYS:N	2.77	0.48
1:A:1168:GLU:O	1:A:1171:GLN:OE1	2.30	0.48
1:A:1317:MET:O	1:A:1322:ILE:HD11	2.14	0.48
1:A:1430:LEU:O	2:B:1196:ILE:HG22	2.13	0.48
1:A:305:ASP:OD2	1:A:326:ARG:HD3	2.12	0.48
1:A:973:ILE:O	1:A:973:ILE:HG22	2.14	0.48
2:B:258:LEU:CG	2:B:258:LEU:O	2.61	0.48
2:B:871:THR:HG22	2:B:872:GLU:N	2.29	0.48
9:I:88:SER:C	9:I:90:GLN:H	2.17	0.48
1:A:1081:LEU:HD11	1:A:1097:GLY:HA3	1.96	0.47
1:A:281:HIS:C	1:A:282:ASN:HD22	2.16	0.47
1:A:593:GLU:C	1:A:595:THR:H	2.16	0.47
1:A:738:LYS:CG	1:A:740:LEU:HG	2.38	0.47
2:B:123:THR:O	2:B:125:SER:N	2.44	0.47
2:B:470:LYS:O	2:B:472:ALA:N	2.46	0.47
3:C:107:SER:C	3:C:109:SER:H	2.17	0.47
3:C:22:LEU:HG	3:C:25:VAL:HG21	1.96	0.47
7:G:125:SER:OG	7:G:128:PRO:HA	2.13	0.47
8:H:145:ARG:O	8:H:146:ARG:CB	2.61	0.47
8:H:89:LEU:HD13	8:H:91:ASP:OD1	2.13	0.47
1:A:1121:GLU:HB3	1:A:1124:HIS:NE2	2.29	0.47
1:A:1239:ARG:HH12	1:A:1241:ARG:HH12	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:ILE:HG13	1:A:613:ILE:HD12	1.95	0.47
2:B:108:VAL:CG2	2:B:109:THR:H	2.25	0.47
2:B:123:THR:HG23	2:B:205:ILE:HA	1.96	0.47
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.95	0.47
2:B:314:LEU:O	2:B:318:VAL:HG23	2.13	0.47
2:B:642:ASP:CA	2:B:649:LYS:HA	2.38	0.47
2:B:696:GLU:O	2:B:699:GLU:HB2	2.15	0.47
2:B:862:GLN:O	2:B:914:LYS:HE3	2.13	0.47
3:C:191:TYR:HD2	3:C:201:TRP:CD1	2.32	0.47
4:D:160:VAL:O	4:D:164:ILE:HG13	2.15	0.47
4:D:220:LEU:CD2	4:D:221:TYR:H	2.27	0.47
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	1.96	0.47
5:E:65:THR:O	5:E:69:ILE:CD1	2.62	0.47
7:G:88:ASP:OD2	7:G:88:ASP:N	2.47	0.47
1:A:1111:MET:HG3	1:A:1114:PRO:HB3	1.95	0.47
1:A:1255:GLU:OE1	1:A:1258:HIS:HB2	2.15	0.47
1:A:1294:PRO:HG2	1:A:1295:THR:HG22	1.97	0.47
1:A:289:ILE:HG22	1:A:290:GLU:N	2.29	0.47
1:A:92:HIS:O	1:A:94:GLY:N	2.47	0.47
2:B:766:ARG:NH2	2:B:1020:ARG:CD	2.73	0.47
2:B:244:LEU:O	2:B:246:LYS:N	2.47	0.47
2:B:287:ARG:NH1	2:B:324:ILE:O	2.47	0.47
2:B:955:THR:HG23	2:B:956:THR:N	2.28	0.47
2:B:996:ARG:HH22	3:C:175:ALA:H	1.61	0.47
3:C:221:TYR:CD1	3:C:222:LYS:N	2.83	0.47
3:C:89:GLU:O	3:C:90:ASP:CB	2.63	0.47
5:E:10:SER:O	5:E:13:TRP:HB3	2.14	0.47
7:G:21:ARG:CZ	7:G:24:GLN:HB2	2.45	0.47
8:H:103:LYS:HG2	8:H:104:PHE:N	2.29	0.47
8:H:104:PHE:CE2	8:H:136:LYS:HG3	2.49	0.47
13:T:16:DT:H2''	13:T:17:DT:O5'	2.14	0.47
1:A:832:ALA:O	13:T:18:DA:H5'	2.15	0.47
1:A:1402:PHE:CE2	1:A:1403:GLU:CG	2.98	0.47
1:A:323:LYS:N	1:A:323:LYS:HD2	2.28	0.47
2:B:222:ILE:N	2:B:240:ILE:HD12	2.28	0.47
2:B:435:THR:C	2:B:437:GLU:H	2.16	0.47
2:B:44:VAL:O	2:B:45:SER:C	2.53	0.47
4:D:216:ASN:C	4:D:218:GLU:H	2.17	0.47
4:D:7:THR:HG21	4:D:32:GLU:CD	2.35	0.47
5:E:155:ARG:HH11	5:E:155:ARG:HG2	1.80	0.47
5:E:192:ARG:HH11	5:E:192:ARG:HG3	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:56:LYS:CE	5:E:84:ASP:H	2.27	0.47
6:F:111:LEU:C	6:F:113:GLY:N	2.68	0.47
8:H:27:GLU:CG	8:H:39:THR:HG23	2.45	0.47
2:B:620:ARG:NH2	9:I:68:LEU:HD21	2.28	0.47
12:L:30:ILE:CG2	12:L:31:CYS:N	2.77	0.47
1:A:1011:GLN:NE2	1:A:1015:VAL:CG2	2.78	0.47
1:A:1029:ARG:CG	1:A:1029:ARG:HH11	2.26	0.47
1:A:36:ARG:HB2	1:A:37:PHE:CE1	2.49	0.47
1:A:698:GLN:HE22	9:I:99:LEU:HD11	1.78	0.47
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.49	0.47
2:B:1045:SER:O	2:B:1048:THR:HG23	2.14	0.47
2:B:605:ARG:CZ	2:B:639:ILE:HD13	2.45	0.47
3:C:22:LEU:CD2	3:C:25:VAL:HG21	2.45	0.47
3:C:43:THR:HG22	3:C:44:LEU:N	2.30	0.47
5:E:112:TYR:CD1	5:E:112:TYR:C	2.88	0.47
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.79	0.47
8:H:44:VAL:O	8:H:44:VAL:HG12	2.15	0.47
1:A:1015:VAL:O	1:A:1015:VAL:HG12	2.14	0.47
1:A:1141:THR:HG23	1:A:1205:LYS:CD	2.42	0.47
1:A:1141:THR:HA	1:A:1205:LYS:NZ	2.29	0.47
1:A:336:ILE:HD13	1:A:340:LEU:HD12	1.97	0.47
1:A:347:PHE:HE2	1:A:375:THR:CG2	2.27	0.47
1:A:565:ILE:O	1:A:565:ILE:HG22	2.13	0.47
2:B:819:ALA:O	2:B:1093:GLN:HG2	2.14	0.47
2:B:466:TRP:CE3	2:B:466:TRP:HA	2.49	0.47
2:B:483:LEU:CD1	2:B:491:THR:HG23	2.42	0.47
2:B:792:MET:H	2:B:857:ARG:HA	1.78	0.47
4:D:155:ARG:HB3	4:D:155:ARG:HH11	1.80	0.47
5:E:22:MET:HE1	5:E:26:ARG:HH21	1.78	0.47
7:G:55:ASP:HB3	7:G:73:LYS:HB2	1.96	0.47
1:A:1081:LEU:CD1	1:A:1097:GLY:HA3	2.45	0.47
1:A:71:GLN:O	1:A:73:GLY:N	2.41	0.47
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.80	0.47
2:B:1068:GLY:O	2:B:1069:PHE:O	2.32	0.47
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.95	0.47
2:B:363:HIS:O	2:B:364:ILE:CB	2.60	0.47
2:B:448:ILE:O	2:B:450:ALA:N	2.47	0.47
2:B:516:ASN:ND2	2:B:516:ASN:H	2.11	0.47
4:D:12:ARG:NH1	4:D:14:ARG:HG2	2.30	0.47
5:E:37:LEU:HD11	5:E:41:ASP:HB2	1.94	0.47
7:G:59:GLY:HA3	7:G:70:PHE:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:9:ILE:HA	8:H:55:LEU:O	2.15	0.47
9:I:61:ASP:C	9:I:63:GLY:N	2.67	0.47
11:K:65:HIS:CD2	11:K:67:PHE:N	2.76	0.47
1:A:1345:ARG:CG	1:A:1372:VAL:HG12	2.45	0.47
1:A:281:HIS:O	1:A:282:ASN:ND2	2.41	0.47
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.50	0.47
1:A:316:GLN:HG2	1:A:317:LYS:H	1.78	0.47
1:A:322:VAL:CG1	1:A:322:VAL:O	2.61	0.47
1:A:598:LEU:HD11	8:H:124:ARG:HB2	1.97	0.47
2:B:1048:THR:OG1	2:B:1050:ILE:HD12	2.14	0.47
2:B:708:GLU:O	2:B:709:ASP:C	2.53	0.47
4:D:15:LEU:O	4:D:17:LYS:HG3	2.14	0.47
5:E:56:LYS:NZ	5:E:84:ASP:N	2.63	0.47
11:K:18:LYS:HZ2	11:K:38:GLU:HG2	1.80	0.47
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.83	0.47
1:A:252:PHE:HB2	1:A:256:GLN:CD	2.35	0.47
1:A:298:PHE:CD2	1:A:299:HIS:HD2	2.33	0.47
1:A:590:ARG:HG2	1:A:590:ARG:NH1	2.27	0.47
1:A:672:ASP:OD2	1:A:674:PRO:HG2	2.15	0.47
2:B:129:PHE:CE2	2:B:166:PHE:HB2	2.50	0.47
2:B:638:PHE:HB3	2:B:651:LEU:HD22	1.97	0.47
3:C:73:GLN:HE21	3:C:75:MET:N	2.11	0.47
7:G:106:MET:CG	7:G:107:LYS:N	2.77	0.47
1:A:1027:ALA:O	1:A:1031:VAL:HG23	2.15	0.47
1:A:1120:LEU:H	1:A:1120:LEU:HG	1.48	0.47
1:A:1366:ARG:HG2	1:A:1366:ARG:HH11	1.80	0.47
1:A:226:GLU:O	1:A:226:GLU:HG2	2.13	0.47
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.96	0.47
1:A:55:ASP:N	1:A:56:PRO:CD	2.73	0.47
1:A:682:THR:HG23	1:A:728:LYS:HE3	1.96	0.47
1:A:916:GLY:O	1:A:919:ILE:HG22	2.14	0.47
2:B:1222:ARG:O	2:B:1222:ARG:HG2	2.15	0.47
2:B:235:SER:OG	2:B:236:HIS:CD2	2.68	0.47
2:B:317:CYS:O	2:B:320:ASP:HB3	2.15	0.47
2:B:335:GLY:O	2:B:336:ARG:HB2	2.15	0.47
2:B:37:PHE:HE1	2:B:41:LYS:CD	2.25	0.47
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.15	0.47
2:B:776:GLN:OE1	2:B:1097:HIS:NE2	2.47	0.47
3:C:11:ARG:HE	3:C:21:ILE:HD11	1.80	0.47
3:C:196:ASP:OD1	3:C:198:ALA:HB3	2.15	0.47
3:C:254:LYS:O	3:C:258:ILE:CD1	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:29:PHE:HA	5:E:65:THR:HG22	1.97	0.47
6:F:111:LEU:O	6:F:113:GLY:N	2.39	0.47
8:H:59:ILE:CG2	8:H:60:ALA:N	2.66	0.47
9:I:4:PHE:CE1	9:I:13:MET:HG3	2.50	0.47
9:I:50:THR:HG22	9:I:52:ILE:N	2.27	0.47
3:C:10:ILE:HG13	11:K:108:GLU:HB3	1.95	0.47
1:A:416:ARG:HG3	1:A:417:TYR:CD1	2.49	0.47
1:A:478:TYR:O	1:A:479:ASN:CB	2.62	0.47
1:A:482:PHE:CE1	2:B:836:GLU:HB2	2.50	0.47
1:A:589:GLN:HA	1:A:605:MET:O	2.15	0.47
1:A:821:ARG:O	1:A:821:ARG:HG3	2.14	0.47
2:B:806:THR:HA	2:B:1045:SER:OG	2.15	0.47
2:B:810:GLU:CB	2:B:815:ARG:HH22	2.28	0.47
3:C:213:PRO:HG2	3:C:214:ASN:H	1.80	0.47
3:C:44:LEU:CD2	3:C:159:ALA:HB1	2.44	0.47
4:D:220:LEU:HD23	4:D:221:TYR:C	2.36	0.47
6:F:106:PRO:HG2	7:G:18:PHE:O	2.15	0.47
8:H:129:TYR:HA	8:H:131:ASN:HD21	1.80	0.47
9:I:59:VAL:C	9:I:61:ASP:H	2.18	0.47
1:A:444:PHE:CE2	1:A:487:MET:HE2	2.48	0.46
1:A:567:LYS:HB3	8:H:95:TYR:CA	2.44	0.46
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.49	0.46
2:B:1169:MET:HE3	2:B:1201:LYS:HG2	1.97	0.46
2:B:129:PHE:HE2	2:B:166:PHE:HB2	1.81	0.46
2:B:345:LYS:HA	2:B:348:ARG:HE	1.80	0.46
3:C:34:ARG:O	3:C:38:ILE:HG13	2.15	0.46
5:E:26:ARG:NH1	5:E:133:GLU:OE2	2.37	0.46
8:H:26:ILE:CD1	8:H:49:VAL:HG11	2.45	0.46
9:I:80:SER:HB2	9:I:103:CYS:SG	2.54	0.46
1:A:1107:VAL:HG13	1:A:1333:ILE:HD11	1.97	0.46
1:A:252:PHE:HB2	1:A:256:GLN:NE2	2.30	0.46
1:A:494:SER:O	1:A:498:ARG:HG2	2.15	0.46
1:A:568:PRO:HG3	8:H:46:LEU:O	2.15	0.46
1:A:549:MET:SD	1:A:577:ILE:CD1	3.03	0.46
1:A:697:ALA:HA	1:A:702:LEU:HG	1.96	0.46
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.79	0.46
2:B:618:ASP:O	2:B:622:LYS:N	2.48	0.46
2:B:745:PRO:O	2:B:747:MET:N	2.47	0.46
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.96	0.46
9:I:88:SER:HB3	9:I:95:THR:HG21	1.98	0.46
12:L:61:THR:HG22	12:L:62:LYS:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:993:LEU:CD2	1:A:1022:LEU:HD21	2.46	0.46
1:A:1241:ARG:O	1:A:1242:VAL:CG2	2.62	0.46
1:A:1365:TYR:CD2	1:A:1365:TYR:C	2.89	0.46
1:A:270:LEU:O	1:A:274:ILE:HG13	2.15	0.46
1:A:886:ILE:CG2	1:A:887:GLY:N	2.79	0.46
2:B:652:LYS:HB3	2:B:689:LEU:CD2	2.43	0.46
2:B:885:MET:HA	2:B:936:ASP:HB2	1.96	0.46
8:H:138:GLU:OE1	8:H:138:GLU:C	2.54	0.46
1:A:601:LYS:HB2	1:A:603:ASN:ND2	2.30	0.46
1:A:65:LEU:HA	1:A:73:GLY:HA2	1.97	0.46
2:B:124:TYR:HE2	2:B:179:CYS:HG	1.63	0.46
2:B:496:ARG:NH1	2:B:539:LEU:HB2	2.29	0.46
2:B:801:LYS:O	10:J:52:THR:CG2	2.64	0.46
2:B:839:MET:HE2	2:B:980:PHE:HB2	1.97	0.46
3:C:189:THR:CG2	3:C:190:ASP:H	2.27	0.46
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.97	0.46
3:C:15:LYS:O	3:C:240:VAL:HG22	2.14	0.46
4:D:47:LEU:HD11	7:G:3:PHE:CD2	2.51	0.46
5:E:175:LEU:HA	5:E:176:PRO:HD3	1.81	0.46
5:E:78:LEU:C	5:E:78:LEU:HD23	2.36	0.46
7:G:111:THR:HG23	7:G:114:LEU:HD13	1.96	0.46
7:G:126:ASN:HA	7:G:127:PRO:C	2.35	0.46
12:L:47:ARG:CD	12:L:52:GLY:HA2	2.45	0.46
13:T:12:DG:H2''	13:T:13:DT:O5'	2.16	0.46
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.51	0.46
2:B:243:ALA:HB2	2:B:251:ILE:HG12	1.97	0.46
2:B:38:PHE:HD1	2:B:811:TYR:CD2	2.34	0.46
2:B:600:LEU:O	2:B:609:ILE:HD11	2.16	0.46
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.97	0.46
3:C:98:VAL:C	3:C:99:LEU:HD22	2.36	0.46
5:E:145:THR:HG21	5:E:187:TYR:CD2	2.51	0.46
8:H:84:ALA:O	8:H:85:GLY:C	2.53	0.46
11:K:31:VAL:CG1	11:K:32:VAL:N	2.77	0.46
11:K:65:HIS:NE2	11:K:67:PHE:CG	2.81	0.46
1:A:218:ASP:O	1:A:219:PHE:C	2.53	0.46
1:A:247:ARG:NH1	1:A:263:THR:HG23	2.30	0.46
1:A:464:PRO:HG2	1:A:465:TYR:CD1	2.51	0.46
1:A:540:PHE:CE2	1:A:565:ILE:HD12	2.51	0.46
1:A:540:PHE:HE2	1:A:565:ILE:HD12	1.80	0.46
1:A:72:GLU:HB3	1:A:76:GLU:CG	2.44	0.46
1:A:71:GLN:C	1:A:73:GLY:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASN:ND2	2:B:1116:ARG:NH1	2.59	0.46
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.98	0.46
2:B:31:TRP:CZ2	2:B:807:ARG:HB2	2.50	0.46
4:D:128:VAL:CG1	4:D:129:LEU:N	2.79	0.46
4:D:7:THR:HB	7:G:42:PHE:CE2	2.51	0.46
8:H:12:VAL:HG13	8:H:26:ILE:HD11	1.96	0.46
8:H:133:ASN:O	8:H:135:LEU:N	2.48	0.46
1:A:1191:TRP:CZ3	9:I:43:VAL:HG21	2.48	0.46
9:I:58:VAL:O	9:I:58:VAL:HG12	2.16	0.46
1:A:1042:PHE:CE2	1:A:1046:LEU:HD11	2.51	0.46
1:A:399:HIS:CG	1:A:400:PRO:N	2.81	0.46
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.50	0.46
1:A:709:THR:CG2	1:A:710:LEU:H	2.21	0.46
1:A:774:ARG:NH1	1:A:797:LYS:HG3	2.30	0.46
2:B:1072:MET:HB2	2:B:1085:ILE:HD13	1.98	0.46
2:B:733:HIS:O	2:B:735:ALA:N	2.44	0.46
3:C:11:ARG:HD3	3:C:209:TYR:CZ	2.49	0.46
3:C:91:HIS:ND1	3:C:158:VAL:HG11	2.30	0.46
3:C:177:GLU:HG3	3:C:231:ASN:ND2	2.31	0.46
2:B:798:TYR:CE2	3:C:62:PHE:CZ	2.97	0.46
3:C:66:ARG:NH1	10:J:2:ILE:CG2	2.75	0.46
5:E:79:TRP:HB2	5:E:105:PHE:HE1	1.77	0.46
5:E:124:VAL:HB	5:E:125:PRO:CD	2.46	0.46
5:E:135:PHE:HD2	5:E:140:LEU:CD2	2.27	0.46
1:A:1450:LEU:HD11	6:F:108:PHE:CZ	2.51	0.46
7:G:126:ASN:C	7:G:126:ASN:HD22	2.15	0.46
7:G:14:HIS:CD2	7:G:16:SER:HB3	2.51	0.46
9:I:82:GLU:OE2	9:I:104:LEU:HB2	2.15	0.46
1:A:133:LYS:O	1:A:136:ALA:HB3	2.16	0.46
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.51	0.46
1:A:555:ASP:O	1:A:556:TRP:O	2.33	0.46
1:A:709:THR:CG2	1:A:710:LEU:N	2.75	0.46
1:A:982:THR:C	1:A:984:LYS:N	2.69	0.46
2:B:486:TYR:CE1	2:B:1096:ARG:NH2	2.84	0.46
2:B:1165:ILE:CD1	2:B:1187:ASN:HD22	2.28	0.46
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.46	0.46
2:B:249:ARG:O	2:B:251:ILE:HG13	2.15	0.46
2:B:277:LYS:HG2	2:B:336:ARG:CB	2.46	0.46
2:B:640:VAL:HG23	2:B:740:HIS:CA	2.46	0.46
3:C:79:GLN:HE21	3:C:127:ARG:HD3	1.81	0.46
5:E:178:ILE:HB	5:E:212:ARG:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:150:CYS:C	7:G:151:ILE:HG13	2.34	0.46
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.45	0.46
12:L:26:THR:C	12:L:27:LEU:HD23	2.36	0.46
12:L:55:ILE:CG1	12:L:56:LEU:H	2.10	0.46
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.16	0.46
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	2.31	0.46
1:A:752:LYS:HD3	1:A:752:LYS:HA	1.72	0.46
2:B:100:PRO:HB2	2:B:180:TYR:HE1	1.79	0.46
2:B:889:THR:HG23	2:B:891:ASP:N	2.31	0.46
3:C:189:THR:CG2	3:C:190:ASP:N	2.78	0.46
3:C:80:LEU:HD11	3:C:95:CYS:C	2.36	0.46
4:D:51:ASN:C	4:D:52:LEU:O	2.53	0.46
5:E:26:ARG:HH22	5:E:133:GLU:CD	2.19	0.46
5:E:89:GLY:C	5:E:91:LYS:N	2.69	0.46
7:G:74:TYR:HD2	7:G:74:TYR:H	1.62	0.46
10:J:21:TYR:HB2	10:J:39:LEU:CD1	2.46	0.46
1:A:1066:VAL:O	1:A:1070:GLN:HG3	2.16	0.46
1:A:1115:SER:OG	1:A:1116:LEU:N	2.49	0.46
1:A:1206:ASP:O	1:A:1274:ARG:NH1	2.48	0.46
1:A:605:MET:HE2	1:A:612:ILE:HG12	1.97	0.46
1:A:69:THR:C	1:A:71:GLN:N	2.68	0.46
2:B:469:GLN:HB3	2:B:470:LYS:H	1.50	0.46
2:B:651:LEU:HD21	2:B:741:CYS:HB3	1.98	0.46
2:B:770:GLN:HB2	2:B:985:GLY:H	1.81	0.46
2:B:790:ASP:OD2	2:B:790:ASP:N	2.46	0.46
3:C:118:LEU:HB2	3:C:132:PRO:HG2	1.98	0.46
3:C:183:TRP:O	3:C:184:ASN:C	2.55	0.46
3:C:243:VAL:CG1	3:C:243:VAL:O	2.64	0.46
5:E:169:ARG:HD3	6:F:140:ASP:OD2	2.15	0.46
5:E:45:LYS:HD3	5:E:46:TYR:CE1	2.51	0.46
8:H:30:SER:HB2	8:H:36:CYS:HB3	1.98	0.46
1:A:1268:LEU:HD11	9:I:48:LEU:HD11	1.98	0.46
12:L:46:VAL:O	12:L:46:VAL:HG12	2.16	0.46
1:A:1386:ARG:HB2	1:A:1403:GLU:CG	2.45	0.45
1:A:541:ILE:HG22	1:A:546:VAL:CG2	2.39	0.45
1:A:905:ASP:C	1:A:906:HIS:ND1	2.70	0.45
2:B:1115:THR:CG2	2:B:1117:GLN:HB2	2.46	0.45
2:B:436:VAL:O	2:B:436:VAL:HG12	2.17	0.45
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.81	0.45
2:B:886:LYS:HB2	2:B:890:TYR:OH	2.16	0.45
2:B:916:THR:CB	2:B:935:ARG:HD2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:LEU:HD11	10:J:2:ILE:HG13	1.98	0.45
4:D:119:ARG:HD3	4:D:221:TYR:CD2	2.51	0.45
5:E:63:ASN:HB3	5:E:64:PRO:HD2	1.97	0.45
6:F:111:LEU:N	6:F:111:LEU:CD1	2.78	0.45
7:G:14:HIS:HD2	7:G:16:SER:HB3	1.80	0.45
7:G:77:VAL:O	7:G:77:VAL:HG12	2.15	0.45
8:H:62:SER:OG	8:H:63:LEU:N	2.49	0.45
11:K:113:THR:O	11:K:114:LEU:CB	2.63	0.45
1:A:335:ARG:O	1:A:339:ASN:HB2	2.15	0.45
1:A:401:GLY:CA	1:A:435:HIS:HD2	2.29	0.45
1:A:567:LYS:CG	1:A:568:PRO:CD	2.89	0.45
2:B:1079:LYS:HA	3:C:27:LEU:HD21	1.98	0.45
2:B:1212:ILE:O	2:B:1214:PRO:HD3	2.14	0.45
2:B:893:LEU:HD22	2:B:897:GLY:C	2.35	0.45
2:B:769:TYR:HD1	2:B:987:LYS:NZ	2.14	0.45
3:C:264:GLN:HG3	3:C:264:GLN:H	1.60	0.45
3:C:34:ARG:NH1	3:C:35:ARG:HG2	2.32	0.45
5:E:147:HIS:HB3	5:E:150:VAL:CG2	2.41	0.45
5:E:56:LYS:NZ	5:E:85:GLU:HG3	2.30	0.45
4:D:8:PHE:CD2	7:G:6:ASP:HB2	2.51	0.45
1:A:789:LYS:HE3	9:I:67:THR:CB	2.46	0.45
1:A:100:LYS:O	1:A:103:CYS:HB2	2.17	0.45
1:A:1205:LYS:O	1:A:1206:ASP:C	2.55	0.45
1:A:173:THR:CG2	1:A:173:THR:O	2.64	0.45
1:A:196:GLU:HG2	1:A:197:PRO:HD2	1.99	0.45
1:A:590:ARG:O	1:A:591:PHE:CB	2.60	0.45
1:A:838:GLN:O	1:A:842:VAL:HG23	2.17	0.45
1:A:843:LYS:HD3	1:A:843:LYS:HA	1.71	0.45
2:B:230:ALA:N	2:B:231:PRO:HD2	2.32	0.45
2:B:308:TRP:HB2	9:I:2:THR:HG22	1.97	0.45
2:B:364:ILE:O	2:B:365:THR:CB	2.60	0.45
2:B:552:MET:HA	2:B:552:MET:CE	2.46	0.45
2:B:664:THR:CG2	2:B:678:GLU:N	2.79	0.45
2:B:878:GLN:HB2	2:B:879:ARG:NH1	2.31	0.45
3:C:137:LYS:HB3	3:C:138:GLU:OE1	2.16	0.45
3:C:97:VAL:HG12	3:C:99:LEU:CD2	2.46	0.45
3:C:97:VAL:HG12	3:C:99:LEU:HD22	1.97	0.45
4:D:8:PHE:CZ	4:D:37:GLN:HB2	2.51	0.45
7:G:129:SER:CB	7:G:138:THR:OG1	2.65	0.45
9:I:82:GLU:HB3	9:I:104:LEU:HG	1.97	0.45
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLY:O	1:A:285:PRO:HD2	2.16	0.45
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.50	0.45
1:A:675:THR:HG21	1:A:736:ASN:CB	2.47	0.45
2:B:461:LEU:HD12	2:B:461:LEU:N	2.31	0.45
3:C:117:ASP:N	3:C:117:ASP:OD1	2.48	0.45
3:C:22:LEU:HD22	3:C:230:MET:CE	2.45	0.45
3:C:242:GLN:C	3:C:244:VAL:H	2.17	0.45
4:D:217:LEU:O	4:D:219:THR:N	2.48	0.45
6:F:85:MET:HB2	6:F:151:LEU:HB3	1.98	0.45
9:I:78:CYS:SG	9:I:106:CYS:SG	3.14	0.45
12:L:38:LEU:CG	12:L:39:SER:N	2.79	0.45
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.99	0.45
1:A:1376:THR:O	1:A:1377:THR:C	2.55	0.45
1:A:305:ASP:OD1	1:A:306:ASN:N	2.48	0.45
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.82	0.45
1:A:49:LYS:HD3	1:A:55:ASP:HB3	1.99	0.45
1:A:341:MET:CE	1:A:843:LYS:HZ3	2.29	0.45
1:A:919:ILE:CD1	1:A:983:ILE:HD12	2.47	0.45
2:B:247:GLY:C	2:B:249:ARG:N	2.70	0.45
2:B:334:ILE:O	2:B:334:ILE:CG2	2.64	0.45
2:B:33:VAL:O	2:B:36:ALA:HB3	2.16	0.45
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.97	0.45
2:B:825:VAL:HG21	2:B:1092:TYR:HE1	1.82	0.45
2:B:842:ASN:HD22	2:B:845:SER:H	1.61	0.45
2:B:859:TYR:CD1	2:B:859:TYR:N	2.85	0.45
2:B:866:TYR:HD2	2:B:870:ILE:HD12	1.82	0.45
4:D:20:GLU:O	4:D:20:GLU:HG2	2.16	0.45
4:D:71:LYS:HA	4:D:74:GLN:HG3	1.97	0.45
4:D:7:THR:HG21	4:D:32:GLU:OE1	2.17	0.45
8:H:98:TYR:C	8:H:118:PHE:HD2	2.20	0.45
1:A:1120:LEU:HD12	1:A:1120:LEU:C	2.36	0.45
1:A:1339:LEU:HD23	5:E:144:ILE:HG22	1.98	0.45
1:A:443:LEU:O	1:A:489:LEU:HD12	2.16	0.45
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.99	0.45
2:B:230:ALA:N	2:B:231:PRO:CD	2.79	0.45
2:B:377:PHE:O	2:B:380:TYR:N	2.50	0.45
2:B:662:MET:HA	2:B:665:GLU:HG3	1.99	0.45
3:C:186:LEU:CD2	3:C:225:ALA:HB2	2.47	0.45
8:H:103:LYS:HB3	8:H:115:TYR:HD1	1.82	0.45
8:H:30:SER:CB	8:H:36:CYS:HB3	2.47	0.45
1:A:265:LYS:CE	1:A:265:LYS:CA	2.92	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:THR:CG2	1:A:383:TYR:H	2.18	0.45
1:A:401:GLY:C	1:A:435:HIS:CD2	2.90	0.45
1:A:523:ILE:HG13	1:A:622:VAL:HG22	1.99	0.45
1:A:577:ILE:O	1:A:580:VAL:HG23	2.16	0.45
1:A:831:THR:O	1:A:834:THR:HG22	2.16	0.45
2:B:277:LYS:HG2	2:B:336:ARG:HB3	1.98	0.45
2:B:425:THR:HG22	2:B:426:LYS:N	2.32	0.45
2:B:429:PHE:HA	2:B:432:MET:CE	2.46	0.45
2:B:51:PHE:O	2:B:54:PHE:HB3	2.17	0.45
2:B:550:ASP:OD1	2:B:552:MET:HB2	2.17	0.45
2:B:552:MET:C	2:B:554:ILE:H	2.20	0.45
2:B:838:SER:HA	2:B:989:THR:O	2.16	0.45
2:B:942:ARG:HB2	2:B:945:GLU:HB2	1.99	0.45
2:B:952:VAL:HG12	2:B:953:LEU:N	2.32	0.45
1:A:483:ASP:O	2:B:979:LYS:HE3	2.16	0.45
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.97	0.45
5:E:61:GLN:NE2	5:E:105:PHE:CE2	2.84	0.45
7:G:155:SER:O	7:G:156:SER:HB3	2.16	0.45
2:B:193:LYS:HZ3	12:L:32:ALA:HB1	1.81	0.45
1:A:849:MET:HB3	1:A:1063:MET:SD	2.57	0.45
1:A:1095:THR:CG2	1:A:1112:LYS:HB2	2.47	0.45
1:A:332:LYS:H	1:A:337:ARG:CB	2.30	0.45
2:B:1166:CYS:SG	2:B:1166:CYS:O	2.75	0.45
2:B:205:ILE:CD1	2:B:205:ILE:N	2.80	0.45
2:B:34:ILE:HD13	2:B:542:MET:HE2	1.98	0.45
4:D:50:LEU:HD21	7:G:4:ILE:CD1	2.47	0.45
6:F:82:THR:CG2	6:F:84:TYR:O	2.64	0.45
8:H:100:THR:OG1	8:H:138:GLU:HG2	2.16	0.45
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.97	0.45
1:A:963:ILE:HD11	1:A:1048:ASN:HB2	1.98	0.45
1:A:1242:VAL:CG1	1:A:1243:VAL:H	2.29	0.45
1:A:1389:PHE:C	1:A:1391:ARG:H	2.20	0.45
1:A:162:VAL:HG12	1:A:163:SER:H	1.82	0.45
1:A:106:VAL:HG21	1:A:214:ILE:HD13	1.96	0.45
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.52	0.45
1:A:743:VAL:O	1:A:747:VAL:HG23	2.17	0.45
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.16	0.45
1:A:962:ARG:O	1:A:964:ILE:N	2.49	0.45
2:B:1167:GLY:N	2:B:1215:ARG:HG2	2.32	0.45
2:B:487:THR:O	2:B:490:SER:HB3	2.17	0.45
2:B:408:LEU:HD21	2:B:545:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:705:MET:HB3	2:B:706:GLN:H	1.61	0.45
2:B:906:SER:O	2:B:941:LEU:HD23	2.17	0.45
5:E:182:ASP:HB3	5:E:185:ALA:CB	2.47	0.45
8:H:4:THR:CG2	8:H:5:LEU:N	2.80	0.45
1:A:1217:LYS:O	1:A:1221:LYS:HA	2.17	0.45
1:A:1189:SER:HB2	1:A:1256:GLU:OE1	2.17	0.45
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.52	0.45
1:A:236:LEU:HD11	1:A:304:MET:HE1	1.99	0.45
1:A:33:ALA:HB1	1:A:56:PRO:HB2	1.99	0.45
1:A:794:PRO:C	1:A:796:SER:H	2.20	0.45
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.50	0.45
1:A:982:THR:C	1:A:984:LYS:H	2.19	0.45
2:B:257:LYS:HB3	2:B:258:LEU:H	1.53	0.45
2:B:62:ILE:HG23	2:B:418:LYS:HG3	1.99	0.45
3:C:101:LEU:O	3:C:102:GLN:HG2	2.17	0.45
1:A:125:ALA:C	1:A:127:ALA:H	2.21	0.44
1:A:1297:GLU:OE1	1:A:1297:GLU:N	2.50	0.44
1:A:23:SER:HA	1:A:233:TRP:NE1	2.32	0.44
1:A:53:LEU:O	1:A:54:ASN:C	2.56	0.44
1:A:690:VAL:CG2	1:A:718:VAL:HG13	2.47	0.44
1:A:789:LYS:HE3	9:I:67:THR:HB	1.99	0.44
1:A:904:THR:HG22	1:A:904:THR:O	2.17	0.44
1:A:929:LEU:N	1:A:929:LEU:CD2	2.80	0.44
1:A:888:GLY:O	1:A:940:ARG:NH2	2.51	0.44
2:B:286:PHE:CG	2:B:297:ILE:HG23	2.52	0.44
2:B:29:ASP:CB	2:B:658:ILE:HD13	2.46	0.44
2:B:785:TYR:CD1	2:B:785:TYR:C	2.91	0.44
2:B:996:ARG:NH2	3:C:38:ILE:HG23	2.32	0.44
5:E:157:SER:C	5:E:159:ASP:N	2.71	0.44
5:E:192:ARG:HG3	5:E:192:ARG:NH1	2.31	0.44
1:A:105:CYS:O	1:A:114:LEU:HG	2.17	0.44
1:A:1148:ILE:O	1:A:1149:ALA:HB2	2.17	0.44
1:A:1315:GLU:C	1:A:1317:MET:N	2.69	0.44
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.98	0.44
1:A:146:MET:CA	1:A:171:GLN:HB2	2.47	0.44
1:A:220:THR:O	1:A:223:GLY:N	2.44	0.44
2:B:110:HIS:CB	12:L:54:ARG:HH22	2.30	0.44
2:B:254:LEU:HD22	2:B:361:LEU:CD1	2.47	0.44
2:B:31:TRP:HA	2:B:31:TRP:CE3	2.52	0.44
2:B:434:ARG:O	2:B:436:VAL:N	2.50	0.44
2:B:473:MET:CE	2:B:474:SER:HA	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:604:ARG:C	2:B:606:LYS:N	2.69	0.44
5:E:169:ARG:HD3	6:F:140:ASP:CG	2.38	0.44
9:I:15:TYR:N	9:I:15:TYR:CD1	2.85	0.44
3:C:235:VAL:HG21	10:J:6:ARG:HH21	1.81	0.44
11:K:46:ILE:O	11:K:50:LEU:HB2	2.17	0.44
1:A:289:ILE:CG2	1:A:290:GLU:N	2.80	0.44
1:A:676:MET:O	1:A:679:ILE:N	2.48	0.44
2:B:274:PRO:O	2:B:275:TYR:HB2	2.17	0.44
2:B:293:PRO:O	2:B:294:ASP:O	2.36	0.44
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.83	0.44
2:B:479:VAL:O	2:B:480:SER:HB3	2.17	0.44
3:C:239:PRO:O	3:C:240:VAL:C	2.54	0.44
4:D:12:ARG:NH1	4:D:14:ARG:CA	2.79	0.44
4:D:29:LEU:HD12	7:G:82:PHE:CZ	2.52	0.44
7:G:116:PRO:HG2	7:G:119:LEU:CB	2.44	0.44
8:H:129:TYR:C	8:H:131:ASN:H	2.21	0.44
1:A:1050:GLU:HG3	1:A:1054:LEU:HD11	1.99	0.44
1:A:1165:GLU:HG2	1:A:1165:GLU:H	1.44	0.44
1:A:1385:THR:HG22	1:A:1388:GLY:N	2.17	0.44
1:A:34:LYS:HG2	1:A:57:ARG:NH2	2.31	0.44
1:A:34:LYS:NZ	1:A:57:ARG:HH22	1.99	0.44
1:A:34:LYS:NZ	1:A:57:ARG:NH2	2.57	0.44
1:A:691:LEU:O	1:A:694:THR:HB	2.17	0.44
2:B:1096:ARG:HB2	2:B:1096:ARG:HH11	1.83	0.44
2:B:204:ILE:HG22	2:B:204:ILE:O	2.16	0.44
2:B:431:TYR:CD1	2:B:447:ALA:HB2	2.52	0.44
2:B:807:ARG:CB	2:B:807:ARG:HH11	2.29	0.44
3:C:124:LEU:O	3:C:125:MET:C	2.55	0.44
3:C:181:ASP:N	3:C:182:PRO:CD	2.80	0.44
3:C:73:GLN:NE2	3:C:75:MET:N	2.65	0.44
4:D:146:GLN:CA	4:D:149:THR:HG22	2.47	0.44
12:L:47:ARG:HG2	12:L:48:CYS:N	2.23	0.44
1:A:1385:THR:CG2	1:A:1388:GLY:H	2.18	0.44
1:A:1446:ASP:O	1:A:1448:GLU:N	2.51	0.44
1:A:700:ASN:O	9:I:115:LYS:HD2	2.18	0.44
1:A:781:ASP:HB3	1:A:790:ASP:H	1.82	0.44
2:B:370:PHE:HD2	2:B:373:ARG:CD	2.29	0.44
2:B:744:HIS:CD2	2:B:745:PRO:CD	2.83	0.44
2:B:860:MET:HG3	2:B:965:LYS:HG2	1.98	0.44
3:C:236:GLY:O	3:C:238:ILE:N	2.51	0.44
4:D:142:LYS:O	4:D:146:GLN:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:LEU:O	5:E:78:LEU:HD23	2.18	0.44
8:H:130:ARG:H	8:H:130:ARG:HH11	1.64	0.44
8:H:11:GLN:O	8:H:28:ALA:HB1	2.17	0.44
9:I:106:CYS:O	9:I:107:SER:HB2	2.17	0.44
2:B:622:LYS:CE	9:I:59:VAL:HG13	2.47	0.44
11:K:50:LEU:HD13	11:K:75:ILE:HG12	2.00	0.44
12:L:34:CYS:O	12:L:35:SER:C	2.56	0.44
12:L:43:THR:O	12:L:43:THR:HG22	2.17	0.44
1:A:1123:GLY:O	1:A:1125:ALA:N	2.51	0.44
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.99	0.44
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.48	0.44
1:A:26:GLU:O	1:A:29:ALA:HB3	2.17	0.44
1:A:40:THR:HG21	1:A:259:GLU:OE2	2.18	0.44
1:A:590:ARG:NH1	1:A:592:ASP:OD2	2.44	0.44
1:A:806:ARG:HH12	2:B:729:ILE:HD11	1.81	0.44
1:A:93:VAL:HG22	1:A:301:ALA:CA	2.41	0.44
2:B:110:HIS:CB	12:L:54:ARG:NH2	2.80	0.44
1:A:69:THR:HG22	2:B:1174:LYS:HD3	2.00	0.44
2:B:240:ILE:HG23	2:B:240:ILE:O	2.17	0.44
2:B:263:GLY:O	2:B:264:SER:C	2.56	0.44
2:B:384:ARG:HE	2:B:384:ARG:HB3	1.59	0.44
2:B:629:ASP:HB3	2:B:632:ARG:HD3	2.00	0.44
2:B:637:LEU:HB2	2:B:693:ILE:CD1	2.48	0.44
2:B:886:LYS:HB2	2:B:890:TYR:CE1	2.53	0.44
2:B:918:ILE:HG21	2:B:935:ARG:NH2	2.32	0.44
4:D:136:GLY:HA2	4:D:142:LYS:NZ	2.32	0.44
4:D:54:GLU:O	4:D:58:VAL:HG23	2.18	0.44
5:E:128:PRO:HA	5:E:129:PRO:O	2.18	0.44
8:H:81:PRO:CB	8:H:82:PRO:CD	2.95	0.44
11:K:53:ASP:OD1	11:K:55:LYS:HB2	2.18	0.44
11:K:53:ASP:HB3	11:K:56:VAL:HG23	2.00	0.44
1:A:1350:LYS:O	1:A:1354:ASN:ND2	2.51	0.44
1:A:298:PHE:O	1:A:302:THR:HB	2.17	0.44
1:A:341:MET:HE1	2:B:1135:ARG:HH12	1.82	0.44
1:A:458:HIS:NE2	1:A:478:TYR:OH	2.35	0.44
1:A:492:PRO:O	1:A:493:GLN:NE2	2.50	0.44
1:A:596:THR:C	1:A:598:LEU:N	2.62	0.44
1:A:934:LYS:NZ	1:A:934:LYS:HB2	2.33	0.44
2:B:260:GLY:O	2:B:267:ARG:HD3	2.17	0.44
2:B:879:ARG:HH22	2:B:885:MET:CE	2.30	0.44
2:B:941:LEU:O	2:B:942:ARG:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:113:VAL:HG23	3:C:147:LEU:CD2	2.48	0.44
3:C:6:PRO:CB	3:C:25:VAL:HG22	2.45	0.44
4:D:218:GLU:O	4:D:219:THR:C	2.55	0.44
4:D:29:LEU:N	4:D:29:LEU:CD2	2.78	0.44
5:E:180:ARG:NH2	5:E:192:ARG:HB2	2.32	0.44
6:F:97:ARG:HH11	6:F:97:ARG:HG3	1.82	0.44
12:L:44:ASP:O	12:L:45:ALA:HB3	2.17	0.44
13:T:23:BRU:H2''	13:T:24:DG:O5'	2.18	0.44
1:A:1313:LEU:C	1:A:1315:GLU:N	2.71	0.44
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.83	0.44
1:A:115:LEU:CD1	1:A:142:CYS:HB3	2.48	0.44
1:A:211:PHE:HD1	1:A:214:ILE:HD12	1.83	0.44
1:A:666:ILE:O	1:A:670:ILE:HD13	2.18	0.44
2:B:244:LEU:CD1	2:B:250:PHE:HD1	2.31	0.44
2:B:280:ILE:HG22	2:B:285:ILE:HG13	2.00	0.44
2:B:287:ARG:CG	2:B:292:ILE:HA	2.46	0.44
2:B:291:ILE:CD1	2:B:300:HIS:NE2	2.81	0.44
2:B:616:ILE:CG2	2:B:700:SER:OG	2.66	0.44
2:B:750:GLY:O	2:B:751:VAL:C	2.55	0.44
2:B:831:SER:HG	2:B:994:TYR:HE1	1.65	0.44
3:C:52:GLU:OE2	3:C:154:LYS:HD2	2.17	0.44
2:B:1124:ARG:HH22	15:P:2:G:P	2.40	0.44
13:T:21:DC:C2	13:T:22:DC:C5	3.06	0.44
1:A:883:LEU:CD1	1:A:1017:LEU:HD11	2.46	0.44
1:A:1268:LEU:O	1:A:1269:GLU:HG3	2.17	0.44
1:A:1354:ASN:O	1:A:1358:SER:HB3	2.17	0.44
1:A:899:VAL:CB	1:A:929:LEU:HD12	2.45	0.44
2:B:1119:VAL:O	2:B:1126:GLY:HA3	2.17	0.44
2:B:467:GLY:HA3	2:B:475:SER:HB3	1.99	0.44
2:B:708:GLU:HG3	2:B:709:ASP:N	2.32	0.44
2:B:707:PRO:O	2:B:708:GLU:O	2.36	0.44
3:C:69:LEU:N	3:C:69:LEU:CD1	2.81	0.44
4:D:39:ASN:HD22	4:D:41:GLN:HB2	1.83	0.44
5:E:28:TYR:CE1	5:E:78:LEU:HB3	2.53	0.44
6:F:97:ARG:NH2	6:F:108:PHE:HE1	2.15	0.44
12:L:48:CYS:HB3	12:L:51:CYS:O	2.17	0.44
13:T:22:DC:H2''	13:T:23:BRU:OP2	2.18	0.44
1:A:613:ILE:O	1:A:614:PHE:HB3	2.18	0.43
2:B:984:HIS:CD2	2:B:1025:HIS:HB2	2.53	0.43
2:B:664:THR:HG23	2:B:678:GLU:N	2.32	0.43
2:B:866:TYR:CD2	2:B:870:ILE:HB	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:984:HIS:NE2	2:B:1025:HIS:HA	2.33	0.43
3:C:112:ASN:CB	3:C:114:TYR:CE1	2.91	0.43
4:D:166:LEU:O	4:D:169:SER:OG	2.36	0.43
4:D:29:LEU:H	4:D:29:LEU:HD22	1.81	0.43
5:E:180:ARG:HG2	5:E:180:ARG:O	2.18	0.43
5:E:79:TRP:NE1	5:E:81:GLU:HB2	2.30	0.43
7:G:126:ASN:C	7:G:126:ASN:ND2	2.71	0.43
7:G:127:PRO:HG2	7:G:138:THR:HG21	2.00	0.43
9:I:73:ARG:NH1	9:I:112:SER:HB3	2.32	0.43
9:I:4:PHE:HE1	9:I:13:MET:HG3	1.83	0.43
10:J:16:ASP:OD1	10:J:17:LYS:N	2.48	0.43
11:K:91:CYS:O	11:K:94:ILE:HB	2.18	0.43
1:A:1072:ILE:O	1:A:1075:PRO:HG2	2.18	0.43
1:A:1155:ASP:OD2	1:A:1161:THR:CG2	2.64	0.43
1:A:1444:MET:HG2	7:G:60:ARG:CA	2.47	0.43
1:A:36:ARG:HB2	1:A:37:PHE:CD1	2.53	0.43
1:A:61:ILE:CG2	1:A:62:ASP:N	2.74	0.43
1:A:61:ILE:O	1:A:62:ASP:C	2.56	0.43
1:A:664:THR:HG22	2:B:1014:PRO:HB3	2.00	0.43
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.53	0.43
1:A:987:VAL:HG12	1:A:988:LEU:N	2.33	0.43
2:B:427:ASP:HA	2:B:430:ARG:CG	2.49	0.43
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.48	0.43
2:B:611:PRO:O	2:B:692:TYR:HB2	2.18	0.43
2:B:616:ILE:HD12	2:B:616:ILE:H	1.79	0.43
2:B:758:PHE:N	2:B:759:PRO:CD	2.81	0.43
2:B:785:TYR:CD2	2:B:795:ILE:HG12	2.53	0.43
3:C:242:GLN:C	3:C:244:VAL:N	2.71	0.43
8:H:128:ASN:C	8:H:128:ASN:ND2	2.71	0.43
11:K:53:ASP:HB3	11:K:56:VAL:CG2	2.48	0.43
1:A:1308:THR:HG23	1:A:1310:GLY:H	1.82	0.43
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.46	0.43
1:A:63:ARG:HA	1:A:74:MET:CE	2.39	0.43
2:B:1181:GLU:HB2	2:B:1188:LYS:HG2	2.00	0.43
2:B:35:SER:HA	2:B:811:TYR:CE2	2.44	0.43
2:B:558:LEU:HD23	2:B:596:LEU:HD11	2.00	0.43
2:B:619:ILE:O	2:B:622:LYS:N	2.46	0.43
2:B:640:VAL:O	2:B:640:VAL:HG12	2.18	0.43
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.51	0.43
2:B:955:THR:HG22	2:B:956:THR:N	2.33	0.43
3:C:254:LYS:O	3:C:258:ILE:HD13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:PRO:HB2	11:K:101:LEU:HD12	1.99	0.43
4:D:14:ARG:C	4:D:16:LYS:H	2.18	0.43
4:D:46:GLU:HG2	4:D:47:LEU:N	2.33	0.43
8:H:41:ASP:HB3	8:H:121:LEU:HD22	1.98	0.43
9:I:8:ARG:O	9:I:10:CYS:N	2.52	0.43
1:A:186:LYS:HZ1	1:A:197:PRO:HD3	1.81	0.43
1:A:88:LYS:HD3	1:A:293:GLU:CD	2.38	0.43
1:A:37:PHE:H	1:A:37:PHE:HD1	1.66	0.43
1:A:66:LYS:HD3	1:A:67:CYS:H	1.81	0.43
1:A:722:LEU:HD23	1:A:799:PHE:CG	2.52	0.43
2:B:125:SER:O	2:B:126:SER:HB3	2.17	0.43
2:B:803:LEU:CD1	2:B:1032:SER:HB3	2.47	0.43
2:B:948:ILE:HG22	2:B:949:VAL:O	2.18	0.43
5:E:29:PHE:C	5:E:30:ILE:HG13	2.38	0.43
5:E:21:GLU:HG2	5:E:35:VAL:HG11	1.99	0.43
6:F:101:ILE:HD13	6:F:120:ILE:HG22	1.99	0.43
7:G:1:MET:O	7:G:1:MET:HE2	2.18	0.43
1:A:1063:MET:SD	1:A:1436:ILE:CG2	3.06	0.43
1:A:1171:GLN:O	1:A:1174:PHE:HB2	2.19	0.43
1:A:1444:MET:HG2	7:G:59:GLY:O	2.19	0.43
1:A:1451:VAL:O	1:A:1454:MET:HG2	2.19	0.43
1:A:780:VAL:O	1:A:782:ARG:HG2	2.18	0.43
1:A:90:VAL:HB	1:A:297:GLN:HE22	1.74	0.43
2:B:1034:VAL:O	2:B:1037:LEU:N	2.51	0.43
2:B:1102:LYS:O	2:B:1103:ILE:C	2.57	0.43
1:A:350:ARG:HB2	2:B:1128:LEU:HD13	2.00	0.43
2:B:293:PRO:O	2:B:296:GLU:HB3	2.18	0.43
6:F:119:ARG:CG	6:F:119:ARG:HH11	2.30	0.43
6:F:76:LYS:HA	6:F:79:ARG:HD2	1.99	0.43
9:I:77:LYS:O	9:I:79:HIS:N	2.51	0.43
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.33	0.43
1:A:1001:ARG:O	1:A:1002:GLY:O	2.36	0.43
1:A:137:ALA:O	1:A:139:TRP:N	2.51	0.43
1:A:134:ARG:HH11	1:A:221:SER:HA	1.83	0.43
1:A:219:PHE:CE2	1:A:231:PRO:HD2	2.54	0.43
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.54	0.43
1:A:392:VAL:HG13	1:A:415:LEU:CD1	2.44	0.43
1:A:65:LEU:O	1:A:66:LYS:O	2.36	0.43
1:A:713:SER:O	1:A:717:ASN:ND2	2.52	0.43
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.52	0.43
1:A:846:GLU:OE1	1:A:1425:SER:OG	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	3.01	0.43
2:B:1065:GLN:HE22	2:B:1067:ARG:HG2	1.81	0.43
2:B:292:ILE:CG2	2:B:325:GLN:O	2.66	0.43
2:B:641:GLU:O	2:B:643:ASP:N	2.51	0.43
2:B:810:GLU:HB2	2:B:815:ARG:NH2	2.33	0.43
2:B:840:ILE:CG2	2:B:994:TYR:HD1	2.31	0.43
2:B:880:THR:HG21	2:B:934:LYS:HE3	2.00	0.43
2:B:890:TYR:OH	2:B:936:ASP:OD2	2.30	0.43
3:C:213:PRO:O	3:C:214:ASN:CB	2.66	0.43
3:C:239:PRO:O	3:C:242:GLN:N	2.51	0.43
5:E:62:ALA:HB3	5:E:78:LEU:CD2	2.48	0.43
7:G:28:THR:HG22	7:G:32:GLU:OE1	2.18	0.43
8:H:4:THR:HG22	8:H:5:LEU:H	1.80	0.43
1:A:709:THR:HG23	9:I:94:ASP:HA	2.01	0.43
3:C:235:VAL:HG13	10:J:13:VAL:HG22	2.01	0.43
11:K:37:LYS:HD3	11:K:37:LYS:HA	1.92	0.43
11:K:55:LYS:HB2	11:K:81:TYR:CE1	2.54	0.43
11:K:85:ASP:O	11:K:88:LYS:HB2	2.17	0.43
1:A:1278:ASN:O	1:A:1310:GLY:HA3	2.17	0.43
1:A:476:SER:HB2	1:A:477:PRO:HD3	2.00	0.43
1:A:485:ASP:OD1	15:P:10:A:O2'	2.36	0.43
1:A:767:GLN:HA	1:A:799:PHE:HA	2.00	0.43
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.66	0.43
1:A:814:PHE:CD2	1:A:814:PHE:O	2.71	0.43
2:B:1096:ARG:CB	2:B:1096:ARG:HH11	2.32	0.43
2:B:365:THR:HG21	2:B:370:PHE:CD1	2.54	0.43
2:B:487:THR:H	2:B:490:SER:HB3	1.84	0.43
2:B:508:LEU:HD23	14:N:2:DC:OP1	2.19	0.43
3:C:109:SER:O	3:C:110:THR:C	2.56	0.43
5:E:17:ARG:CG	5:E:18:THR:N	2.82	0.43
5:E:55:ARG:C	5:E:57:MET:N	2.71	0.43
6:F:84:TYR:CD1	6:F:84:TYR:N	2.87	0.43
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.75	0.43
8:H:123:MET:HE3	8:H:142:LEU:HD22	2.00	0.43
11:K:13:GLY:O	11:K:16:GLU:HG3	2.18	0.43
1:A:1100:ARG:O	1:A:1100:ARG:HD2	2.19	0.43
1:A:1147:THR:HB	9:I:48:LEU:CD1	2.47	0.43
1:A:1154:TYR:CD2	1:A:1156:PRO:HD3	2.54	0.43
1:A:1386:ARG:HB2	1:A:1403:GLU:CB	2.49	0.43
1:A:504:LEU:HD13	6:F:91:ALA:HB2	1.99	0.43
1:A:870:GLU:HG2	5:E:208:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LYS:HG3	1:A:276:LEU:HD21	2.01	0.43
2:B:1131:GLY:N	2:B:1134:GLU:OE1	2.51	0.43
2:B:282:ILE:HG21	2:B:382:ILE:CD1	2.48	0.43
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.54	0.43
2:B:705:MET:HA	2:B:705:MET:HE2	1.99	0.43
2:B:810:GLU:HB2	2:B:815:ARG:HH22	1.83	0.43
2:B:842:ASN:HD22	2:B:845:SER:CB	2.30	0.43
3:C:11:ARG:H	3:C:20:PHE:HA	1.83	0.43
3:C:214:ASN:O	3:C:217:ASP:OD2	2.37	0.43
3:C:264:GLN:O	3:C:267:GLN:HG2	2.19	0.43
3:C:39:ALA:HA	3:C:164:ALA:CB	2.49	0.43
2:B:798:TYR:CE2	3:C:62:PHE:CE2	3.03	0.43
5:E:212:ARG:NH1	5:E:212:ARG:HG3	2.33	0.43
5:E:55:ARG:N	5:E:84:ASP:OD1	2.51	0.43
6:F:69:LEU:C	6:F:71:GLU:HG3	2.39	0.43
10:J:1:MET:H1	10:J:57:ILE:N	2.16	0.43
11:K:60:ALA:O	11:K:73:LEU:HD12	2.18	0.43
1:A:1208:THR:O	1:A:1211:GLN:HB2	2.18	0.43
1:A:13:THR:HB	1:A:1432:GLN:NE2	2.34	0.43
1:A:1450:LEU:HD11	6:F:108:PHE:HZ	1.83	0.43
1:A:690:VAL:HG21	1:A:718:VAL:HG13	1.99	0.43
1:A:897:TYR:CD1	1:A:897:TYR:N	2.87	0.43
1:A:93:VAL:HG23	1:A:304:MET:HE3	2.01	0.43
2:B:290:GLY:O	2:B:292:ILE:HG13	2.19	0.43
2:B:486:TYR:HD1	2:B:775:LYS:O	2.01	0.43
2:B:376:PHE:CB	2:B:566:LEU:HD21	2.49	0.43
3:C:193:TYR:CD1	3:C:193:TYR:C	2.92	0.43
4:D:216:ASN:O	4:D:218:GLU:N	2.52	0.43
5:E:117:THR:HB	5:E:120:ALA:H	1.84	0.43
9:I:17:ARG:HG3	9:I:28:GLU:OE1	2.19	0.43
12:L:53:HIS:HB3	12:L:55:ILE:HD11	1.95	0.43
1:A:1154:TYR:CE2	1:A:1156:PRO:HD3	2.54	0.43
1:A:1215:ARG:O	1:A:1219:THR:N	2.50	0.43
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.32	0.43
1:A:153:PRO:CB	1:A:161:LEU:HD22	2.47	0.43
1:A:471:ASN:O	1:A:474:VAL:HG12	2.19	0.43
1:A:751:SER:O	1:A:752:LYS:HG2	2.19	0.43
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.39	0.43
2:B:299:GLU:OE2	2:B:571:PRO:CG	2.66	0.43
2:B:555:ILE:HG22	2:B:556:THR:N	2.34	0.43
2:B:591:ARG:O	2:B:592:ASN:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:187:LYS:HG2	3:C:219:PHE:CE1	2.54	0.43
3:C:226:ASP:O	3:C:227:THR:CB	2.66	0.43
3:C:69:LEU:O	10:J:6:ARG:HD2	2.19	0.43
4:D:173:HIS:ND1	4:D:174:PRO:HD2	2.34	0.43
8:H:13:SER:HB3	8:H:27:GLU:O	2.19	0.43
1:A:1148:ILE:HG12	9:I:49:ILE:HD12	2.01	0.43
2:B:186:GLU:HG2	10:J:62:ARG:NH2	2.34	0.43
1:A:1203:ASN:O	1:A:1204:ASP:C	2.57	0.42
1:A:1308:THR:HG23	1:A:1309:ASP:H	1.81	0.42
1:A:414:ASP:OD1	1:A:416:ARG:CG	2.66	0.42
1:A:845:LEU:O	1:A:846:GLU:C	2.58	0.42
1:A:963:ILE:HD13	1:A:1049:ILE:CG1	2.49	0.42
2:B:129:PHE:CE2	2:B:166:PHE:CD1	3.07	0.42
3:C:181:ASP:OD2	3:C:185:LYS:N	2.49	0.42
3:C:196:ASP:CB	3:C:199:LYS:HD3	2.49	0.42
4:D:35:LEU:HA	4:D:47:LEU:HB2	2.00	0.42
4:D:69:ALA:C	4:D:71:LYS:N	2.72	0.42
7:G:99:PHE:HZ	7:G:163:ILE:HD13	1.85	0.42
8:H:47:PHE:CD2	8:H:95:TYR:HD1	2.37	0.42
9:I:95:THR:HG22	9:I:96:SER:O	2.18	0.42
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.33	0.42
1:A:1280:GLU:HB3	1:A:1281:ARG:H	1.64	0.42
1:A:565:ILE:HG23	1:A:567:LYS:HG2	2.00	0.42
1:A:834:THR:CG2	1:A:835:GLY:N	2.81	0.42
1:A:2:VAL:CG1	2:B:1157:ALA:O	2.67	0.42
2:B:126:SER:CB	2:B:172:ILE:HD11	2.49	0.42
2:B:269:ILE:HG21	2:B:282:ILE:HD13	2.01	0.42
2:B:317:CYS:O	2:B:320:ASP:N	2.52	0.42
2:B:953:LEU:HB2	12:L:57:LEU:HD23	2.00	0.42
3:C:177:GLU:CG	3:C:231:ASN:HD22	2.32	0.42
5:E:135:PHE:CD2	5:E:140:LEU:HD21	2.50	0.42
1:A:1342:GLU:HG3	5:E:198:ILE:HD13	2.00	0.42
5:E:55:ARG:NH1	5:E:55:ARG:HG3	2.34	0.42
9:I:69:PRO:HB2	9:I:85:PHE:CZ	2.54	0.42
1:A:1166:ASP:OD2	1:A:1239:ARG:HD2	2.19	0.42
1:A:1289:ARG:HH12	1:A:1326:ARG:NH1	2.18	0.42
1:A:1325:THR:OG1	5:E:146:HIS:O	2.37	0.42
1:A:207:ILE:HG22	1:A:211:PHE:CD2	2.53	0.42
1:A:264:PHE:HB3	1:A:265:LYS:HZ1	1.84	0.42
1:A:419:LYS:HG3	1:A:420:ARG:HG3	2.01	0.42
1:A:901:LEU:HB2	1:A:926:GLN:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1190:ASP:C	2:B:1191:ILE:HG13	2.40	0.42
2:B:235:SER:C	2:B:236:HIS:HD2	2.21	0.42
2:B:34:ILE:HG12	2:B:542:MET:CE	2.48	0.42
2:B:558:LEU:O	2:B:560:GLU:N	2.52	0.42
2:B:570:VAL:HG21	2:B:573:GLN:NE2	2.34	0.42
2:B:629:ASP:HB3	2:B:632:ARG:CD	2.49	0.42
2:B:766:ARG:HD3	2:B:766:ARG:HA	1.78	0.42
3:C:147:LEU:N	3:C:147:LEU:CD2	2.79	0.42
3:C:174:ALA:O	3:C:175:ALA:HB3	2.18	0.42
3:C:47:ASP:O	3:C:47:ASP:CG	2.58	0.42
4:D:6:SER:OG	4:D:7:THR:N	2.52	0.42
5:E:13:TRP:O	5:E:16:PHE:HB3	2.19	0.42
5:E:78:LEU:HB2	5:E:107:THR:CG2	2.49	0.42
6:F:97:ARG:NH2	6:F:108:PHE:CE1	2.87	0.42
6:F:127:GLU:O	6:F:129:LYS:HG3	2.18	0.42
1:A:537:ARG:NH1	8:H:120:GLY:O	2.50	0.42
1:A:1268:LEU:CD1	9:I:48:LEU:HD11	2.49	0.42
3:C:7:GLN:NE2	11:K:104:ASN:ND2	2.55	0.42
2:B:992:ILE:HD11	11:K:66:PRO:HB2	2.00	0.42
1:A:1001:ARG:O	1:A:1002:GLY:C	2.57	0.42
1:A:153:PRO:HB3	1:A:161:LEU:CD2	2.47	0.42
1:A:305:ASP:C	1:A:305:ASP:OD1	2.57	0.42
1:A:322:VAL:HG12	1:A:322:VAL:O	2.19	0.42
1:A:567:LYS:HD3	8:H:95:TYR:CE2	2.54	0.42
1:A:642:CYS:O	1:A:645:LEU:HB3	2.19	0.42
1:A:65:LEU:HB2	1:A:71:GLN:NE2	2.34	0.42
1:A:878:ILE:HG22	1:A:879:GLU:N	2.34	0.42
2:B:1068:GLY:O	2:B:1069:PHE:C	2.58	0.42
2:B:1161:HIS:NE2	2:B:1175:LEU:HD21	2.34	0.42
2:B:174:LEU:HD22	2:B:202:TYR:CE1	2.54	0.42
2:B:216:GLU:OE2	2:B:401:PHE:HE1	2.03	0.42
2:B:431:TYR:CG	2:B:447:ALA:CB	3.02	0.42
2:B:44:VAL:HG21	2:B:199:MET:O	2.20	0.42
2:B:704:ALA:HB2	2:B:738:PHE:CE2	2.54	0.42
2:B:863:GLU:OE1	2:B:962:LYS:HB2	2.19	0.42
4:D:170:THR:HB	4:D:172:LEU:HG	2.01	0.42
4:D:35:LEU:H	4:D:35:LEU:CD1	2.31	0.42
5:E:157:SER:O	5:E:159:ASP:N	2.52	0.42
5:E:62:ALA:HB3	5:E:78:LEU:HD22	2.01	0.42
8:H:15:VAL:HG22	8:H:26:ILE:HD12	2.01	0.42
8:H:82:PRO:O	8:H:83:GLN:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:52:ASN:O	11:K:54:ARG:N	2.53	0.42
2:B:900:ALA:HB3	12:L:61:THR:OG1	2.19	0.42
1:A:1030:ARG:NH1	1:A:1035:TYR:OH	2.52	0.42
1:A:38:PRO:HA	1:A:270:LEU:HD23	2.00	0.42
1:A:350:ARG:HB2	2:B:1128:LEU:CD1	2.49	0.42
1:A:865:GLN:OE1	1:A:1370:LEU:HD23	2.20	0.42
2:B:110:HIS:HB3	12:L:54:ARG:HH22	1.84	0.42
2:B:447:ALA:O	2:B:449:ASN:N	2.52	0.42
2:B:545:ILE:HG12	2:B:633:VAL:HG22	2.01	0.42
2:B:658:ILE:HG22	2:B:662:MET:HE2	2.01	0.42
2:B:956:THR:HA	2:B:961:LEU:O	2.20	0.42
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.34	0.42
3:C:175:ALA:HB2	10:J:10:CYS:HB2	2.00	0.42
3:C:31:ASN:O	3:C:35:ARG:HG3	2.19	0.42
5:E:64:PRO:O	5:E:69:ILE:HD11	2.20	0.42
9:I:70:ARG:HA	9:I:83:ASN:O	2.20	0.42
10:J:43:ARG:HD3	10:J:43:ARG:H	1.83	0.42
11:K:48:ALA:O	11:K:51:LEU:N	2.45	0.42
1:A:1029:ARG:CG	1:A:1029:ARG:NH1	2.81	0.42
1:A:838:GLN:HG2	1:A:1073:GLY:HA3	2.01	0.42
1:A:506:ALA:O	1:A:507:VAL:C	2.58	0.42
1:A:614:PHE:HB3	8:H:122:LEU:HD21	2.01	0.42
1:A:953:ASN:C	1:A:954:TRP:CD1	2.93	0.42
2:B:281:PRO:O	2:B:283:VAL:N	2.52	0.42
2:B:601:ARG:HD3	2:B:605:ARG:CZ	2.49	0.42
2:B:847:ASP:OD2	11:K:6:ARG:NH2	2.52	0.42
2:B:912:ILE:O	2:B:938:SER:HA	2.20	0.42
2:B:996:ARG:NH1	3:C:175:ALA:H	2.18	0.42
3:C:260:LEU:O	3:C:264:GLN:HG3	2.20	0.42
4:D:13:ARG:C	4:D:15:LEU:N	2.73	0.42
4:D:162:ALA:HA	4:D:165:GLN:NE2	2.26	0.42
4:D:179:GLN:O	4:D:183:LEU:HB2	2.20	0.42
4:D:8:PHE:HD2	7:G:6:ASP:O	2.02	0.42
5:E:191:LYS:O	5:E:192:ARG:C	2.57	0.42
8:H:24:CYS:CB	8:H:44:VAL:HG21	2.41	0.42
9:I:76:PRO:HD3	9:I:110:PHE:CG	2.55	0.42
1:A:108:MET:O	1:A:109:HIS:CB	2.62	0.42
1:A:125:ALA:O	1:A:127:ALA:N	2.53	0.42
1:A:1444:MET:O	6:F:133:VAL:N	2.50	0.42
1:A:820:GLY:O	1:A:823:GLY:N	2.53	0.42
2:B:839:MET:HE3	2:B:1010:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:PHE:HB2	2:B:566:LEU:HD21	2.02	0.42
2:B:377:PHE:CD2	2:B:381:MET:HE2	2.55	0.42
4:D:12:ARG:NH1	4:D:14:ARG:N	2.68	0.42
5:E:112:TYR:OH	5:E:136:ASN:HB2	2.19	0.42
7:G:81:PRO:HG3	7:G:106:MET:SD	2.59	0.42
8:H:84:ALA:C	8:H:86:ASP:N	2.70	0.42
12:L:47:ARG:NH2	12:L:54:ARG:HG2	2.34	0.42
1:A:1166:ASP:OD2	1:A:1239:ARG:CD	2.68	0.42
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.35	0.42
1:A:798:GLY:HA2	1:A:815:PHE:CD1	2.55	0.42
1:A:912:LEU:HB2	1:A:913:LEU:H	1.72	0.42
2:B:1065:GLN:NE2	2:B:1067:ARG:N	2.45	0.42
2:B:1183:LYS:HE3	2:B:1183:LYS:N	2.35	0.42
2:B:1221:SER:O	2:B:1223:ASP:N	2.53	0.42
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.38	0.42
2:B:191:LYS:HB3	2:B:191:LYS:HE2	1.85	0.42
2:B:228:LYS:HA	2:B:228:LYS:HD3	1.87	0.42
2:B:535:LEU:HA	2:B:535:LEU:HD23	1.79	0.42
2:B:558:LEU:O	2:B:561:TRP:N	2.53	0.42
2:B:570:VAL:HA	2:B:571:PRO:HD2	1.86	0.42
2:B:592:ASN:OD1	2:B:595:ARG:HG2	2.20	0.42
3:C:132:PRO:O	3:C:134:ILE:HG13	2.20	0.42
3:C:186:LEU:N	3:C:186:LEU:CD1	2.82	0.42
5:E:149:LEU:O	5:E:151:PRO:HD3	2.19	0.42
5:E:162:ARG:HH11	5:E:162:ARG:HG2	1.85	0.42
5:E:186:LEU:O	5:E:189:GLY:N	2.41	0.42
5:E:204:THR:CG2	5:E:205:SER:H	2.30	0.42
5:E:164:LEU:CD2	5:E:211:TYR:CD2	3.02	0.42
10:J:53:HIS:NE2	10:J:55:ASP:HA	2.34	0.42
10:J:1:MET:H1	10:J:56:LEU:HB2	1.85	0.42
1:A:973:ILE:CD1	1:A:1037:LEU:HA	2.45	0.42
1:A:1135:ARG:NH2	1:A:1284:MET:HG3	2.34	0.42
1:A:1141:THR:HG21	1:A:1205:LYS:HD3	1.99	0.42
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.80	0.42
1:A:160:GLN:O	1:A:160:GLN:OE1	2.38	0.42
1:A:298:PHE:HD2	1:A:299:HIS:CD2	2.38	0.42
1:A:316:GLN:CG	1:A:317:LYS:N	2.80	0.42
1:A:548:ASN:HD21	11:K:47:ARG:NH2	2.18	0.42
1:A:672:ASP:HB3	1:A:736:ASN:CG	2.40	0.42
1:A:856:THR:HB	1:A:865:GLN:HB2	2.01	0.42
2:B:1004:GLU:OE2	2:B:1064:TYR:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1201:LYS:HE2	2:B:1205:GLN:NE2	2.33	0.42
2:B:448:ILE:H	2:B:448:ILE:HG13	1.66	0.42
2:B:864:LYS:HG3	2:B:872:GLU:OE1	2.19	0.42
3:C:11:ARG:NH2	3:C:229:TYR:HB3	2.35	0.42
3:C:3:GLU:CD	3:C:4:GLU:HG3	2.40	0.42
4:D:218:GLU:O	4:D:219:THR:O	2.38	0.42
5:E:207:ARG:NH1	5:E:207:ARG:CB	2.83	0.42
5:E:213:ILE:HG12	5:E:214:CYS:N	2.35	0.42
1:A:1127:ASP:O	1:A:1128:GLN:C	2.58	0.42
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.34	0.42
1:A:1217:LYS:HE3	1:A:1217:LYS:HA	2.02	0.42
1:A:137:ALA:O	1:A:138:ILE:C	2.58	0.42
1:A:50:ILE:C	1:A:52:GLY:N	2.72	0.42
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.53	0.42
2:B:104:GLU:HG3	2:B:104:GLU:O	2.20	0.42
2:B:1079:LYS:CG	2:B:1080:LYS:N	2.83	0.42
2:B:231:PRO:HG2	2:B:231:PRO:O	2.20	0.42
2:B:707:PRO:CG	2:B:708:GLU:N	2.82	0.42
3:C:133:ILE:CD1	3:C:237:SER:N	2.82	0.42
8:H:56:THR:O	8:H:144:ILE:HA	2.19	0.42
11:K:67:PHE:C	11:K:68:PHE:CD2	2.93	0.42
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.56	0.41
1:A:1109:LYS:O	1:A:1109:LYS:HD2	2.20	0.41
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.55	0.41
1:A:254:GLU:HB3	1:A:255:SER:H	1.45	0.41
1:A:977:LYS:HB3	1:A:978:PRO:CD	2.48	0.41
2:B:1017:ILE:HA	2:B:1017:ILE:HD13	1.86	0.41
1:A:666:ILE:HD11	2:B:1086:PHE:CE1	2.54	0.41
2:B:25:ILE:HG21	2:B:658:ILE:CD1	2.45	0.41
2:B:293:PRO:C	2:B:294:ASP:O	2.56	0.41
2:B:277:LYS:HG2	2:B:336:ARG:HG2	2.01	0.41
2:B:498:THR:CG2	2:B:537:LYS:HB2	2.50	0.41
2:B:546:SER:OG	2:B:631:GLY:N	2.51	0.41
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.81	0.41
2:B:899:ILE:HG22	2:B:900:ALA:O	2.20	0.41
2:B:986:GLN:HE22	2:B:1022:THR:HG21	1.84	0.41
8:H:10:PHE:N	8:H:10:PHE:CD1	2.88	0.41
9:I:75:CYS:SG	9:I:78:CYS:SG	3.18	0.41
1:A:1036:ARG:NH1	1:A:1036:ARG:HG2	2.35	0.41
1:A:1259:MET:HE2	1:A:1263:ILE:CD1	2.48	0.41
1:A:84:ILE:HD13	1:A:270:LEU:HD13	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:GLN:HB2	1:A:430:TRP:CD1	2.55	0.41
1:A:463:ILE:HB	1:A:464:PRO:CD	2.48	0.41
1:A:666:ILE:HD11	2:B:1086:PHE:HE1	1.85	0.41
1:A:767:GLN:NE2	1:A:774:ARG:CB	2.75	0.41
2:B:225:VAL:HA	2:B:237:VAL:O	2.20	0.41
2:B:265:SER:O	2:B:266:ALA:HB3	2.20	0.41
2:B:457:LEU:O	2:B:461:LEU:HD13	2.21	0.41
3:C:133:ILE:HD12	3:C:237:SER:CA	2.49	0.41
3:C:203:GLN:CG	3:C:207:CYS:SG	3.06	0.41
3:C:259:LEU:HD21	11:K:91:CYS:HB3	2.02	0.41
5:E:63:ASN:HB3	5:E:64:PRO:CD	2.50	0.41
10:J:42:LYS:HD3	10:J:43:ARG:N	2.35	0.41
12:L:32:ALA:HB3	12:L:33:GLU:OE2	2.20	0.41
13:T:16:DT:H2''	13:T:17:DT:H5'	2.01	0.41
1:A:1140:HIS:N	1:A:1275:GLY:HA3	2.36	0.41
1:A:452:LYS:HB3	2:B:1141:HIS:CE1	2.55	0.41
2:B:292:ILE:HG23	2:B:325:GLN:O	2.20	0.41
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.56	0.41
2:B:835:GLN:HB2	2:B:835:GLN:HE21	1.52	0.41
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.20	0.41
3:C:133:ILE:CD1	3:C:237:SER:CA	2.95	0.41
5:E:33:GLU:OE1	5:E:33:GLU:N	2.51	0.41
7:G:9:LEU:HD23	7:G:30:LEU:HD12	2.02	0.41
1:A:1121:GLU:O	1:A:1122:PRO:C	2.59	0.41
1:A:1421:CYS:HA	1:A:1426:GLU:HG3	2.02	0.41
1:A:150:THR:HG22	1:A:150:THR:O	2.21	0.41
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.65	0.41
1:A:347:PHE:CE2	1:A:375:THR:HG22	2.56	0.41
1:A:446:ARG:CD	1:A:480:ALA:HB2	2.50	0.41
1:A:789:LYS:HD2	2:B:620:ARG:HH12	1.84	0.41
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.80	0.41
2:B:272:THR:HG23	2:B:279:ASP:OD1	2.20	0.41
2:B:36:ALA:O	2:B:39:ARG:HB2	2.21	0.41
2:B:757:PRO:HG2	2:B:984:HIS:HE1	1.86	0.41
2:B:831:SER:HB3	2:B:994:TYR:OH	2.20	0.41
2:B:996:ARG:CZ	3:C:175:ALA:H	2.34	0.41
3:C:36:VAL:CG2	3:C:251:LEU:HD13	2.48	0.41
4:D:204:ASP:O	4:D:208:GLU:HB2	2.20	0.41
4:D:27:LEU:HA	4:D:27:LEU:HD23	1.85	0.41
5:E:186:LEU:HA	5:E:186:LEU:HD23	1.76	0.41
1:A:1142:THR:O	1:A:1145:SER:OG	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.68	0.41
1:A:204:THR:C	1:A:206:GLU:N	2.74	0.41
1:A:913:LEU:HD13	1:A:981:LEU:O	2.21	0.41
2:B:1004:GLU:CG	10:J:42:LYS:HZ3	2.33	0.41
2:B:1050:ILE:HG22	2:B:1051:THR:N	2.35	0.41
2:B:23:ALA:O	2:B:24:PRO:O	2.39	0.41
2:B:301:ILE:CG2	2:B:314:LEU:HD11	2.49	0.41
2:B:458:LYS:O	2:B:459:TYR:C	2.59	0.41
2:B:515:HIS:CD2	2:B:517:THR:H	2.39	0.41
2:B:56:ASP:CB	2:B:57:TYR:HD1	2.26	0.41
2:B:778:MET:HE1	2:B:1094:ARG:CD	2.50	0.41
3:C:22:LEU:HD22	3:C:230:MET:HE2	2.03	0.41
4:D:126:ILE:HG21	4:D:145:MET:HB3	2.03	0.41
5:E:153:HIS:C	5:E:154:ILE:HG13	2.39	0.41
5:E:96:PHE:O	5:E:99:HIS:HB3	2.21	0.41
8:H:12:VAL:HG13	8:H:26:ILE:CG1	2.50	0.41
10:J:27:GLU:O	10:J:29:GLU:N	2.53	0.41
11:K:5:ASP:HB3	11:K:7:PHE:CE2	2.55	0.41
13:T:25:DG:C2'	13:T:26:DT:H72	2.50	0.41
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.56	0.41
1:A:1341:ILE:HG23	1:A:1342:GLU:H	1.84	0.41
1:A:262:LEU:O	1:A:266:LEU:HG	2.21	0.41
1:A:380:VAL:HG22	1:A:426:LEU:HD13	2.02	0.41
1:A:820:GLY:O	1:A:822:GLU:N	2.54	0.41
1:A:886:ILE:CG2	1:A:952:ALA:HB2	2.50	0.41
1:A:91:PHE:HB2	1:A:297:GLN:OE1	2.21	0.41
2:B:1045:SER:HB3	2:B:1046:PRO:HD2	2.03	0.41
2:B:1170:THR:O	2:B:1171:VAL:C	2.59	0.41
2:B:134:LYS:NZ	2:B:164:LYS:NZ	2.68	0.41
2:B:280:ILE:HD11	2:B:334:ILE:HG12	2.02	0.41
2:B:621:GLU:O	2:B:621:GLU:HG3	2.20	0.41
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.56	0.41
3:C:136:ASP:OD2	3:C:137:LYS:N	2.53	0.41
3:C:215:GLU:O	3:C:217:ASP:N	2.54	0.41
3:C:66:ARG:NH2	10:J:5:VAL:HG23	2.34	0.41
5:E:13:TRP:CE3	5:E:39:LEU:HD13	2.55	0.41
1:A:1342:GLU:HG2	5:E:198:ILE:HD13	2.02	0.41
6:F:97:ARG:NH1	6:F:97:ARG:HG3	2.35	0.41
1:A:710:LEU:HD22	9:I:96:SER:HA	2.03	0.41
12:L:47:ARG:HD3	12:L:52:GLY:HA2	2.02	0.41
15:P:5:C:H2'	15:P:6:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LYS:NZ	1:A:294:SER:HB3	2.35	0.41
1:A:34:LYS:H	1:A:34:LYS:HG2	1.63	0.41
1:A:51:GLY:HA2	1:A:56:PRO:HA	2.02	0.41
1:A:562:THR:HA	1:A:563:PRO:HD3	1.85	0.41
1:A:753:GLY:HA2	1:A:757:ASN:ND2	2.35	0.41
1:A:899:VAL:HG22	1:A:908:LEU:HD21	2.02	0.41
2:B:390:LEU:O	2:B:391:ASP:C	2.58	0.41
2:B:418:LYS:CG	2:B:422:LYS:HE3	2.50	0.41
2:B:629:ASP:HB3	2:B:632:ARG:NE	2.36	0.41
3:C:259:LEU:CD2	11:K:91:CYS:HB3	2.51	0.41
4:D:166:LEU:HD21	4:D:213:GLU:HB3	2.02	0.41
7:G:1:MET:HE3	7:G:80:LYS:H	1.85	0.41
8:H:106:GLU:C	8:H:108:SER:N	2.72	0.41
2:B:309:GLN:HG3	9:I:52:ILE:HD11	2.00	0.41
10:J:30:LEU:HD22	10:J:34:THR:CG2	2.50	0.41
1:A:1148:ILE:O	1:A:1148:ILE:HG22	2.21	0.41
1:A:1161:THR:CG2	1:A:1162:VAL:N	2.84	0.41
1:A:1171:GLN:H	1:A:1171:GLN:HG3	1.66	0.41
1:A:650:GLN:O	1:A:654:ASN:HB2	2.21	0.41
1:A:344:ARG:HD3	2:B:1118:PRO:O	2.21	0.41
2:B:27:ALA:O	2:B:29:ASP:N	2.54	0.41
2:B:618:ASP:OD1	2:B:621:GLU:HB3	2.20	0.41
2:B:67:SER:HB3	2:B:92:PHE:HD1	1.84	0.41
3:C:164:ALA:HA	3:C:167:HIS:O	2.21	0.41
5:E:99:HIS:ND1	5:E:103:LYS:HG3	2.36	0.41
7:G:92:VAL:HG21	7:G:102:GLN:HB2	2.03	0.41
7:G:122:ASN:HB2	7:G:131:GLN:HE21	1.85	0.41
4:D:32:GLU:HG3	7:G:5:LYS:HE2	2.03	0.41
9:I:56:ALA:O	9:I:57:GLY:O	2.39	0.41
12:L:30:ILE:HD11	12:L:59:ALA:HB2	2.01	0.41
1:A:1381:LEU:HA	1:A:1381:LEU:HD23	1.92	0.41
1:A:674:PRO:C	1:A:676:MET:N	2.75	0.41
1:A:739:ASP:N	1:A:739:ASP:OD1	2.53	0.41
2:B:105:SER:O	2:B:106:ASP:CB	2.69	0.41
2:B:1110:PRO:HB2	2:B:1119:VAL:HG11	2.03	0.41
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	2.03	0.41
2:B:408:LEU:N	2:B:408:LEU:CD1	2.84	0.41
2:B:722:ASP:HB3	2:B:723:VAL:H	1.62	0.41
2:B:809:MET:O	2:B:812:LEU:N	2.47	0.41
3:C:179:GLU:HG2	3:C:180:TYR:H	1.86	0.41
8:H:41:ASP:HB2	8:H:121:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:35:GLN:HB3	8:H:111:LEU:HD21	2.03	0.41
10:J:1:MET:H1	10:J:56:LEU:CA	2.33	0.41
1:A:1120:LEU:CD2	1:A:1125:ALA:HA	2.48	0.41
1:A:1313:LEU:C	1:A:1315:GLU:H	2.24	0.41
1:A:69:THR:O	1:A:70:CYS:C	2.59	0.41
1:A:705:LYS:O	1:A:706:HIS:C	2.60	0.41
1:A:907:THR:HG23	1:A:908:LEU:H	1.86	0.41
1:A:982:THR:N	1:A:985:ASP:HB2	2.36	0.41
2:B:129:PHE:CD2	2:B:166:PHE:HA	2.52	0.41
2:B:185:THR:O	2:B:188:ASP:HB2	2.21	0.41
2:B:241:ARG:CZ	2:B:241:ARG:HB3	2.51	0.41
2:B:496:ARG:HH11	2:B:496:ARG:HB3	1.86	0.41
2:B:860:MET:CG	2:B:861:ASP:N	2.84	0.41
2:B:906:SER:O	2:B:907:GLY:O	2.39	0.41
2:B:976:ILE:HD13	2:B:992:ILE:HA	2.03	0.41
3:C:58:LEU:HD12	3:C:145:CYS:HB2	2.01	0.41
3:C:43:THR:HG23	3:C:44:LEU:H	1.86	0.41
4:D:24:ALA:HB1	4:D:25:ALA:H	1.72	0.41
4:D:33:PHE:HE1	7:G:80:LYS:CD	2.33	0.41
4:D:36:LYS:HE2	4:D:44:GLU:OE1	2.20	0.41
5:E:164:LEU:HD22	5:E:211:TYR:CD2	2.56	0.41
7:G:56:ILE:O	7:G:57:GLN:HB2	2.20	0.41
9:I:65:ASP:HA	9:I:66:PRO:HD2	1.92	0.41
12:L:28:LYS:HB2	12:L:39:SER:HB2	2.03	0.41
1:A:1386:ARG:HD3	1:A:1403:GLU:HB3	2.03	0.41
1:A:202:LEU:HA	1:A:206:GLU:OE1	2.21	0.41
1:A:443:LEU:HA	1:A:443:LEU:HD23	1.79	0.41
1:A:688:LYS:CD	1:A:691:LEU:HD23	2.34	0.41
1:A:720:ARG:O	1:A:724:GLU:CB	2.68	0.41
2:B:1117:GLN:HE21	2:B:1199:ALA:HB2	1.85	0.41
2:B:571:PRO:O	2:B:574:SER:O	2.39	0.41
2:B:910:VAL:HG13	2:B:938:SER:HB3	2.01	0.41
2:B:975:GLN:O	2:B:990:ILE:HD12	2.20	0.41
3:C:239:PRO:O	3:C:241:ASP:N	2.54	0.41
3:C:44:LEU:HD21	3:C:159:ALA:HB3	2.03	0.41
4:D:155:ARG:NH1	4:D:155:ARG:CB	2.84	0.41
5:E:161:LYS:HD2	5:E:195:VAL:HG23	2.02	0.41
5:E:24:LYS:HB3	5:E:30:ILE:HB	2.03	0.41
8:H:63:LEU:HD11	8:H:141:TYR:CD2	2.55	0.41
12:L:33:GLU:CD	12:L:33:GLU:N	2.75	0.41
13:T:25:DG:H2'	13:T:26:DT:H72	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LYS:HE3	1:A:1411:GLU:CG	2.51	0.40
1:A:1395:GLY:O	1:A:1396:ALA:C	2.59	0.40
1:A:1412:ALA:HA	1:A:1417:GLU:HG3	2.03	0.40
1:A:1438:THR:HB	2:B:1144:ALA:CB	2.49	0.40
1:A:150:THR:HA	1:A:165:GLY:O	2.20	0.40
1:A:295:LEU:O	1:A:298:PHE:HB3	2.21	0.40
1:A:531:ILE:HG13	1:A:653:VAL:HG21	2.03	0.40
1:A:676:MET:O	1:A:677:ARG:C	2.60	0.40
1:A:709:THR:HG22	1:A:711:ARG:H	1.86	0.40
1:A:956:LEU:HD21	1:A:1017:LEU:HD23	2.03	0.40
1:A:992:ASP:O	1:A:995:GLU:HB2	2.21	0.40
2:B:1177:HIS:HB2	2:B:1179:GLN:HE21	1.80	0.40
2:B:331:LEU:CD2	2:B:353:LYS:HG2	2.51	0.40
2:B:282:ILE:HG21	2:B:382:ILE:HD11	2.03	0.40
2:B:224:GLN:HA	2:B:396:ASP:OD2	2.21	0.40
2:B:570:VAL:CG2	2:B:573:GLN:HB3	2.51	0.40
2:B:660:LYS:HG2	2:B:679:TYR:CD2	2.56	0.40
2:B:69:LEU:HB3	2:B:429:PHE:CD1	2.56	0.40
2:B:789:MET:HE1	2:B:953:LEU:HD22	2.01	0.40
3:C:260:LEU:O	3:C:263:THR:HB	2.21	0.40
5:E:124:VAL:C	5:E:126:SER:H	2.24	0.40
5:E:177:ARG:C	5:E:212:ARG:HD3	2.42	0.40
6:F:109:VAL:HG21	6:F:124:GLU:HA	2.02	0.40
9:I:2:THR:O	9:I:2:THR:HG23	2.21	0.40
2:B:780:VAL:HG21	10:J:56:LEU:HD11	2.04	0.40
1:A:369:SER:CB	11:K:2:ASN:OD1	2.66	0.40
1:A:1163:ILE:HG22	1:A:1165:GLU:HG2	2.04	0.40
1:A:219:PHE:HE1	1:A:230:ARG:NE	2.18	0.40
1:A:298:PHE:HD2	1:A:299:HIS:HD2	1.68	0.40
1:A:997:LEU:HD13	1:A:1018:PHE:HE2	1.84	0.40
2:B:229:ALA:CB	2:B:231:PRO:HD2	2.50	0.40
2:B:269:ILE:CG2	2:B:282:ILE:HD13	2.52	0.40
2:B:357:GLN:HA	2:B:374:LYS:NZ	2.36	0.40
2:B:880:THR:HG22	2:B:934:LYS:HG3	2.03	0.40
6:F:130:ILE:O	6:F:148:VAL:HG22	2.21	0.40
8:H:58:THR:HB	8:H:143:LEU:HD13	2.03	0.40
12:L:34:CYS:SG	12:L:51:CYS:SG	3.18	0.40
1:A:254:GLU:O	1:A:256:GLN:N	2.54	0.40
1:A:347:PHE:HE2	1:A:375:THR:HG22	1.86	0.40
1:A:798:GLY:HA2	1:A:815:PHE:HD1	1.86	0.40
1:A:983:ILE:HG23	1:A:983:ILE:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1095:LEU:C	2:B:1096:ARG:O	2.57	0.40
2:B:1159:ARG:HH11	2:B:1159:ARG:HB3	1.86	0.40
2:B:216:GLU:HA	2:B:406:LEU:HD23	2.03	0.40
2:B:307:ASP:OD2	2:B:310:MET:HE3	2.22	0.40
2:B:778:MET:HB2	2:B:1094:ARG:O	2.22	0.40
2:B:861:ASP:OD1	2:B:914:LYS:HD2	2.22	0.40
2:B:918:ILE:HD12	2:B:935:ARG:CZ	2.51	0.40
2:B:970:THR:HG22	2:B:971:THR:N	2.36	0.40
3:C:77:ILE:HD13	3:C:77:ILE:HA	1.74	0.40
4:D:130:LEU:O	4:D:132:GLN:N	2.53	0.40
4:D:167:LEU:HB3	4:D:177:VAL:HG13	2.03	0.40
4:D:53:SER:HA	4:D:56:ARG:HB3	2.04	0.40
8:H:99:GLY:HA3	8:H:118:PHE:CD2	2.57	0.40
9:I:10:CYS:O	9:I:11:ASN:C	2.59	0.40
11:K:94:ILE:O	11:K:98:LEU:HG	2.22	0.40
12:L:38:LEU:O	12:L:39:SER:CB	2.69	0.40
1:A:1169:ILE:HG13	1:A:1169:ILE:H	1.66	0.40
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.89	0.40
1:A:380:VAL:HG12	1:A:428:TYR:HA	2.03	0.40
1:A:6:TYR:CG	1:A:7:SER:N	2.88	0.40
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.39	0.40
2:B:300:HIS:O	2:B:303:TYR:CE2	2.73	0.40
2:B:304:ASP:OD1	2:B:306:ASN:N	2.36	0.40
2:B:789:MET:HE2	2:B:953:LEU:HD22	2.01	0.40
3:C:7:GLN:NE2	11:K:104:ASN:HD21	2.18	0.40
4:D:155:ARG:HH11	4:D:155:ARG:CB	2.35	0.40
5:E:55:ARG:HD2	5:E:113:GLN:HE21	1.86	0.40
5:E:28:TYR:HE1	5:E:78:LEU:HD13	1.84	0.40
5:E:92:THR:O	5:E:95:THR:HB	2.21	0.40
6:F:100:GLN:HA	6:F:103:MET:HG3	2.03	0.40
6:F:82:THR:HA	6:F:83:PRO:HD3	1.84	0.40
8:H:100:THR:CG2	8:H:101:ALA:N	2.84	0.40
8:H:128:ASN:C	8:H:128:ASN:HD22	2.25	0.40
14:N:4:DA:N3	14:N:5:DC:C5	2.89	0.40
1:A:1148:ILE:CG1	1:A:1198:ASP:HB2	2.51	0.40
1:A:130:ASP:O	1:A:131:SER:C	2.60	0.40
1:A:1393:ASN:O	1:A:1394:THR:C	2.59	0.40
1:A:1451:VAL:C	1:A:1453:TYR:N	2.73	0.40
1:A:279:LEU:HB3	1:A:289:ILE:HG13	2.04	0.40
1:A:514:PRO:O	1:A:515:GLN:C	2.59	0.40
1:A:543:LEU:O	1:A:544:ASP:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1074:ASN:HB2	2:B:1081:LEU:HD21	2.04	0.40
2:B:1116:ARG:HG3	2:B:1198:TYR:CE2	2.56	0.40
2:B:311:LEU:O	2:B:314:LEU:N	2.54	0.40
2:B:557:PHE:O	2:B:557:PHE:HD2	2.04	0.40
2:B:809:MET:HA	2:B:812:LEU:HD12	2.02	0.40
2:B:990:ILE:HG22	2:B:991:GLY:N	2.36	0.40
5:E:30:ILE:HG22	5:E:31:THR:O	2.22	0.40
6:F:152:ILE:HG22	6:F:153:VAL:N	2.37	0.40
7:G:129:SER:CB	7:G:138:THR:HG1	2.33	0.40
2:B:737:THR:HG21	9:I:70:ARG:HH21	1.86	0.40
10:J:31:ASP:OD1	10:J:34:THR:HB	2.21	0.40
11:K:102:LYS:O	11:K:106:GLU:HG3	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1406/1733 (81%)	1062 (76%)	240 (17%)	104 (7%)	1	11
2	B	1082/1224 (88%)	795 (74%)	188 (17%)	99 (9%)	1	8
3	C	264/318 (83%)	200 (76%)	45 (17%)	19 (7%)	1	11
4	D	174/221 (79%)	131 (75%)	29 (17%)	14 (8%)	1	10
5	E	212/215 (99%)	159 (75%)	40 (19%)	13 (6%)	1	15
6	F	85/155 (55%)	72 (85%)	12 (14%)	1 (1%)	13	50
7	G	169/171 (99%)	143 (85%)	20 (12%)	6 (4%)	3	26
8	H	130/146 (89%)	86 (66%)	23 (18%)	21 (16%)	0	2
9	I	117/122 (96%)	76 (65%)	31 (26%)	10 (8%)	1	9
10	J	63/70 (90%)	44 (70%)	10 (16%)	9 (14%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	112/120 (93%)	90 (80%)	19 (17%)	3 (3%)	5	33
12	L	44/70 (63%)	18 (41%)	16 (36%)	10 (23%)	0	1
All	All	3858/4565 (84%)	2876 (74%)	673 (17%)	309 (8%)	1	10

All (309) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	43	GLU
1	A	54	ASN
1	A	57	ARG
1	A	58	LEU
1	A	62	ASP
1	A	63	ARG
1	A	67	CYS
1	A	70	CYS
1	A	130	ASP
1	A	167	CYS
1	A	250	ILE
1	A	255	SER
1	A	257	ARG
1	A	286	HIS
1	A	318	SER
1	A	332	LYS
1	A	399	HIS
1	A	410	GLY
1	A	567	LYS
1	A	597	LEU
1	A	1002	GLY
1	A	1112	LYS
1	A	1114	PRO
1	A	1120	LEU
1	A	1122	PRO
1	A	1124	HIS
1	A	1223	ASP
1	A	1233	ASP
1	A	1242	VAL
1	A	1255	GLU
1	A	1281	ARG
1	A	1403	GLU
1	A	1405	THR

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Mol	Chain	Res	Type
1	A	1438	THR
2	B	21	GLU
2	B	58	THR
2	B	67	SER
2	B	68	THR
2	B	108	VAL
2	B	186	GLU
2	B	258	LEU
2	B	259	TYR
2	B	294	ASP
2	B	295	GLY
2	B	334	ILE
2	B	365	THR
2	B	367	LEU
2	B	391	ASP
2	B	435	THR
2	B	509	ALA
2	B	642	ASP
2	B	643	ASP
2	B	708	GLU
2	B	709	ASP
2	B	728	ARG
2	B	731	VAL
2	B	879	ARG
2	B	907	GLY
2	B	958	GLN
2	B	1046	PRO
2	B	1069	PHE
2	B	1155	SER
2	B	1156	ASP
2	B	1175	LEU
3	C	110	THR
3	C	141	GLY
3	C	149	LYS
3	C	184	ASN
3	C	209	TYR
3	C	215	GLU
3	C	216	GLY
4	D	5	THR
4	D	8	PHE
4	D	17	LYS
4	D	19	GLU

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Mol	Chain	Res	Type
4	D	52	LEU
4	D	119	ARG
4	D	218	GLU
5	E	45	LYS
5	E	106	GLN
5	E	115	ASN
5	E	129	PRO
7	G	139	ILE
8	H	82	PRO
8	H	107	VAL
8	H	128	ASN
8	H	140	ALA
9	I	11	ASN
9	I	62	ILE
9	I	78	CYS
10	J	2	ILE
10	J	6	ARG
10	J	55	ASP
10	J	64	ASN
12	L	50	ASP
12	L	53	HIS
12	L	59	ALA
12	L	60	ARG
1	A	41	MET
1	A	42	ASP
1	A	76	GLU
1	A	93	VAL
1	A	128	ILE
1	A	138	ILE
1	A	253	ASN
1	A	311	GLN
1	A	312	PRO
1	A	322	VAL
1	A	331	GLY
1	A	423	ASP
1	A	424	ILE
1	A	517	ASN
1	A	556	TRP
1	A	846	GLU
1	A	958	VAL
1	A	1123	GLY
1	A	1139	GLU

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Mol	Chain	Res	Type
1	A	1169	ILE
1	A	1221	LYS
1	A	1308	THR
1	A	1309	ASP
1	A	1314	SER
1	A	1448	GLU
2	B	24	PRO
2	B	28	GLU
2	B	65	GLU
2	B	124	TYR
2	B	206	ASN
2	B	257	LYS
2	B	291	ILE
2	B	369	GLY
2	B	448	ILE
2	B	449	ASN
2	B	450	ALA
2	B	467	GLY
2	B	468	GLU
2	B	531	GLN
2	B	591	ARG
2	B	641	GLU
2	B	734	HIS
2	B	751	VAL
2	B	848	ARG
2	B	992	ILE
2	B	1097	HIS
2	B	1103	ILE
2	B	1167	GLY
2	B	1171	VAL
2	B	1176	ASN
2	B	1181	GLU
2	B	1222	ARG
3	C	90	ASP
3	C	126	GLY
4	D	14	ARG
4	D	198	LEU
4	D	219	THR
5	E	74	ASP
5	E	130	ALA
8	H	17	PRO
8	H	32	THR

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Mol	Chain	Res	Type
8	H	59	ILE
8	H	62	SER
8	H	77	ARG
8	H	108	SER
8	H	134	ASN
9	I	57	GLY
9	I	79	HIS
9	I	106	CYS
10	J	28	ASP
11	K	53	ASP
12	L	27	LEU
12	L	28	LYS
12	L	35	SER
12	L	54	ARG
1	A	48	ALA
1	A	65	LEU
1	A	69	THR
1	A	126	LEU
1	A	169	ASN
1	A	314	ALA
1	A	317	LYS
1	A	400	PRO
1	A	453	MET
1	A	543	LEU
1	A	628	GLY
1	A	755	PHE
1	A	821	ARG
1	A	852	TYR
1	A	884	ASP
1	A	1140	HIS
1	A	1206	ASP
1	A	1270	ASN
1	A	1447	GLU
2	B	43	LEU
2	B	45	SER
2	B	245	GLU
2	B	266	ALA
2	B	282	ILE
2	B	466	TRP
2	B	655	LYS
2	B	705	MET
2	B	711	GLU

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Mol	Chain	Res	Type
2	B	746	SER
2	B	792	MET
2	B	810	GLU
2	B	906	SER
2	B	1075	GLY
2	B	1108	ARG
2	B	1157	ALA
3	C	132	PRO
3	C	213	PRO
3	C	237	SER
4	D	16	LYS
4	D	30	GLY
4	D	53	SER
5	E	36	GLU
5	E	95	THR
6	F	128	LYS
7	G	112	LYS
7	G	154	VAL
8	H	90	ALA
8	H	92	ASP
8	H	95	TYR
8	H	139	ASN
9	I	8	ARG
9	I	9	ASP
10	J	17	LYS
10	J	24	LEU
10	J	29	GLU
1	A	5	GLN
1	A	59	GLY
1	A	61	ILE
1	A	154	SER
1	A	256	GLN
1	A	415	LEU
1	A	591	PHE
1	A	604	GLY
1	A	1168	GLU
1	A	1316	VAL
1	A	1390	ASN
2	B	27	ALA
2	B	249	ARG
2	B	264	SER
2	B	323	VAL

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Mol	Chain	Res	Type
2	B	559	SER
2	B	575	PRO
2	B	594	ALA
2	B	636	PRO
2	B	738	PHE
2	B	1017	ILE
2	B	1035	ALA
2	B	1223	ASP
3	C	142	VAL
3	C	214	ASN
5	E	44	ALA
5	E	154	ILE
5	E	192	ARG
7	G	63	PRO
9	I	54	GLU
11	K	14	GLU
12	L	26	THR
12	L	55	ILE
1	A	35	ILE
1	A	66	LYS
1	A	219	PHE
1	A	308	ILE
1	A	871	ASP
1	A	885	THR
2	B	114	PRO
2	B	433	GLN
2	B	667	GLN
2	B	869	SER
3	C	208	GLU
3	C	240	VAL
4	D	131	GLU
5	E	51	GLY
8	H	12	VAL
8	H	47	PHE
10	J	14	VAL
1	A	598	LEU
1	A	780	VAL
1	A	1280	GLU
1	A	1297	GLU
2	B	56	ASP
2	B	115	GLN
2	B	260	GLY

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Mol	Chain	Res	Type
2	B	1214	PRO
5	E	73	PRO
8	H	21	ASN
8	H	44	VAL
8	H	81	PRO
8	H	83	GLN
11	K	107	THR
1	A	283	GLY
1	A	963	ILE
2	B	729	ILE
7	G	136	VAL
1	A	284	ALA
2	B	25	ILE
2	B	619	ILE
2	B	764	SER
3	C	172	PRO
9	I	59	VAL
2	B	55	VAL
3	C	182	PRO
1	A	1388	GLY
2	B	501	PRO
3	C	217	ASP
7	G	20	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1239/1520 (82%)	1099 (89%)	140 (11%)	6	27
2	B	958/1061 (90%)	845 (88%)	113 (12%)	5	25
3	C	234/274 (85%)	205 (88%)	29 (12%)	4	23
4	D	160/200 (80%)	134 (84%)	26 (16%)	2	13
5	E	196/197 (100%)	180 (92%)	16 (8%)	11	40
6	F	77/137 (56%)	70 (91%)	7 (9%)	9	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	152/152 (100%)	138 (91%)	14 (9%)	9	36
8	H	118/128 (92%)	105 (89%)	13 (11%)	6	29
9	I	113/116 (97%)	106 (94%)	7 (6%)	18	51
10	J	60/65 (92%)	53 (88%)	7 (12%)	5	26
11	K	99/102 (97%)	91 (92%)	8 (8%)	11	41
12	L	40/57 (70%)	35 (88%)	5 (12%)	4	23
All	All	3446/4009 (86%)	3061 (89%)	385 (11%)	6	27

All (385) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	18	GLN
1	A	34	LYS
1	A	36	ARG
1	A	37	PHE
1	A	41	MET
1	A	68	GLN
1	A	70	CYS
1	A	93	VAL
1	A	121	LEU
1	A	141	LEU
1	A	145	LYS
1	A	160	GLN
1	A	173	THR
1	A	185	TRP
1	A	200	ARG
1	A	207	ILE
1	A	208	LEU
1	A	213	HIS
1	A	221	SER
1	A	244	PRO
1	A	245	PRO
1	A	249	SER
1	A	261	ASP
1	A	265	LYS
1	A	297	GLN
1	A	302	THR
1	A	315	LEU
1	A	320	ARG

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Mol	Chain	Res	Type
1	A	322	VAL
1	A	324	SER
1	A	337	ARG
1	A	344	ARG
1	A	353	ILE
1	A	369	SER
1	A	385	ILE
1	A	394	ASN
1	A	408	ASP
1	A	425	GLN
1	A	434	ARG
1	A	438	ASP
1	A	443	LEU
1	A	445	ASN
1	A	449	SER
1	A	451	HIS
1	A	469	ARG
1	A	470	LEU
1	A	475	THR
1	A	479	ASN
1	A	481	ASP
1	A	493	GLN
1	A	505	CYS
1	A	512	VAL
1	A	524	VAL
1	A	538	ASP
1	A	562	THR
1	A	596	THR
1	A	597	LEU
1	A	618	GLU
1	A	635	ARG
1	A	666	ILE
1	A	670	ILE
1	A	672	ASP
1	A	685	GLU
1	A	690	VAL
1	A	710	LEU
1	A	737	LEU
1	A	738	LYS
1	A	758	ILE
1	A	768	GLN
1	A	774	ARG

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Mol	Chain	Res	Type
1	A	788	SER
1	A	805	LEU
1	A	816	HIS
1	A	821	ARG
1	A	827	THR
1	A	834	THR
1	A	838	GLN
1	A	855	THR
1	A	858	ASN
1	A	871	ASP
1	A	882	SER
1	A	903	ASN
1	A	907	THR
1	A	920	LEU
1	A	929	LEU
1	A	937	VAL
1	A	941	LYS
1	A	961	ARG
1	A	974	ASP
1	A	976	THR
1	A	978	PRO
1	A	983	ILE
1	A	987	VAL
1	A	1005	GLU
1	A	1029	ARG
1	A	1033	GLN
1	A	1060	PRO
1	A	1067	LEU
1	A	1095	THR
1	A	1110	ASN
1	A	1114	PRO
1	A	1116	LEU
1	A	1122	PRO
1	A	1124	HIS
1	A	1129	GLU
1	A	1145	SER
1	A	1160	SER
1	A	1165	GLU
1	A	1171	GLN
1	A	1193	LEU
1	A	1206	ASP
1	A	1217	LYS

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Mol	Chain	Res	Type
1	A	1230	GLU
1	A	1257	ASP
1	A	1264	GLU
1	A	1265	ASN
1	A	1276	VAL
1	A	1280	GLU
1	A	1288	ASP
1	A	1295	THR
1	A	1297	GLU
1	A	1299	VAL
1	A	1325	THR
1	A	1349	TYR
1	A	1353	TYR
1	A	1365	TYR
1	A	1366	ARG
1	A	1370	LEU
1	A	1385	THR
1	A	1393	ASN
1	A	1394	THR
1	A	1400	CYS
1	A	1410	PHE
1	A	1424	VAL
1	A	1426	GLU
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1451	VAL
2	B	20	ASP
2	B	25	ILE
2	B	46	GLN
2	B	57	TYR
2	B	61	ASP
2	B	98	THR
2	B	128	LEU
2	B	134	LYS
2	B	194	GLU
2	B	203	PHE
2	B	217	ARG
2	B	218	SER
2	B	225	VAL
2	B	241	ARG
2	B	249	ARG

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Mol	Chain	Res	Type
2	B	261	ARG
2	B	267	ARG
2	B	272	THR
2	B	298	LEU
2	B	299	GLU
2	B	303	TYR
2	B	336	ARG
2	B	364	ILE
2	B	368	GLU
2	B	371	GLU
2	B	376	PHE
2	B	393	LYS
2	B	396	ASP
2	B	401	PHE
2	B	425	THR
2	B	427	ASP
2	B	429	PHE
2	B	430	ARG
2	B	446	LEU
2	B	452	THR
2	B	455	SER
2	B	465	ASN
2	B	466	TRP
2	B	473	MET
2	B	475	SER
2	B	485	ARG
2	B	493	SER
2	B	496	ARG
2	B	498	THR
2	B	516	ASN
2	B	552	MET
2	B	557	PHE
2	B	570	VAL
2	B	603	LEU
2	B	615	MET
2	B	616	ILE
2	B	620	ARG
2	B	621	GLU
2	B	635	ARG
2	B	636	PRO
2	B	645	SER
2	B	648	HIS

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Mol	Chain	Res	Type
2	B	682	SER
2	B	694	ASP
2	B	705	MET
2	B	714	GLU
2	B	737	THR
2	B	743	ILE
2	B	786	ASN
2	B	790	ASP
2	B	805	THR
2	B	807	ARG
2	B	811	TYR
2	B	835	GLN
2	B	837	ASP
2	B	839	MET
2	B	857	ARG
2	B	868	MET
2	B	878	GLN
2	B	887	HIS
2	B	889	THR
2	B	895	ASP
2	B	915	THR
2	B	933	SER
2	B	944	THR
2	B	946	ASN
2	B	953	LEU
2	B	955	THR
2	B	956	THR
2	B	957	ASN
2	B	959	ASP
2	B	969	ARG
2	B	987	LYS
2	B	997	GLU
2	B	1006	ILE
2	B	1007	VAL
2	B	1046	PRO
2	B	1047	PHE
2	B	1049	ASP
2	B	1060	ARG
2	B	1084	GLN
2	B	1087	PHE
2	B	1092	TYR
2	B	1095	LEU

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Mol	Chain	Res	Type
2	B	1096	ARG
2	B	1112	GLN
2	B	1147	LEU
2	B	1150	ARG
2	B	1151	LEU
2	B	1159	ARG
2	B	1160	VAL
2	B	1169	MET
2	B	1172	ILE
2	B	1175	LEU
2	B	1178	ASN
2	B	1183	LYS
2	B	1185	CYS
2	B	1202	LEU
3	C	12	GLU
3	C	26	ASP
3	C	55	THR
3	C	56	THR
3	C	62	PHE
3	C	77	ILE
3	C	78	GLU
3	C	91	HIS
3	C	99	LEU
3	C	100	THR
3	C	104	PHE
3	C	106	GLU
3	C	115	SER
3	C	117	ASP
3	C	124	LEU
3	C	129	ILE
3	C	138	GLU
3	C	145	CYS
3	C	147	LEU
3	C	156	THR
3	C	166	GLU
3	C	170	TRP
3	C	177	GLU
3	C	186	LEU
3	C	190	ASP
3	C	238	ILE
3	C	240	VAL
3	C	259	LEU

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Mol	Chain	Res	Type
3	C	266	ASP
4	D	4	SER
4	D	11	ARG
4	D	12	ARG
4	D	16	LYS
4	D	17	LYS
4	D	18	VAL
4	D	22	GLU
4	D	26	THR
4	D	29	LEU
4	D	38	ILE
4	D	40	HIS
4	D	47	LEU
4	D	65	GLU
4	D	70	PHE
4	D	120	GLU
4	D	124	GLU
4	D	125	SER
4	D	126	ILE
4	D	128	VAL
4	D	169	SER
4	D	187	THR
4	D	200	ASN
4	D	213	GLU
4	D	219	THR
4	D	220	LEU
4	D	221	TYR
5	E	5	ASN
5	E	8	ASN
5	E	17	ARG
5	E	41	ASP
5	E	72	PHE
5	E	74	ASP
5	E	77	SER
5	E	78	LEU
5	E	83	CYS
5	E	99	HIS
5	E	110	PHE
5	E	115	ASN
5	E	123	LEU
5	E	131	THR
5	E	202	SER

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Mol	Chain	Res	Type
5	E	212	ARG
6	F	79	ARG
6	F	82	THR
6	F	90	ARG
6	F	112	GLU
6	F	116	ASP
6	F	119	ARG
6	F	153	VAL
7	G	1	MET
7	G	8	SER
7	G	13	LEU
7	G	21	ARG
7	G	24	GLN
7	G	51	TYR
7	G	53	ASN
7	G	74	TYR
7	G	93	SER
7	G	113	HIS
7	G	114	LEU
7	G	126	ASN
7	G	134	GLU
7	G	171	ILE
8	H	2	SER
8	H	10	PHE
8	H	53	ASP
8	H	61	SER
8	H	64	ASN
8	H	89	LEU
8	H	95	TYR
8	H	128	ASN
8	H	129	TYR
8	H	130	ARG
8	H	138	GLU
8	H	139	ASN
8	H	143	LEU
9	I	7	CYS
9	I	8	ARG
9	I	15	TYR
9	I	59	VAL
9	I	86	PHE
9	I	93	LYS
9	I	94	ASP

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Mol	Chain	Res	Type
10	J	7	CYS
10	J	13	VAL
10	J	22	LEU
10	J	28	ASP
10	J	43	ARG
10	J	44	TYR
10	J	48	ARG
11	K	12	LEU
11	K	42	LEU
11	K	47	ARG
11	K	70	ARG
11	K	76	GLN
11	K	78	THR
11	K	111	LEU
11	K	114	LEU
12	L	27	LEU
12	L	55	ILE
12	L	65	VAL
12	L	68	GLU
12	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	68	GLN
1	A	75	ASN
1	A	169	ASN
1	A	171	GLN
1	A	225	ASN
1	A	253	ASN
1	A	256	GLN
1	A	282	ASN
1	A	299	HIS
1	A	316	GLN
1	A	339	ASN
1	A	390	GLN
1	A	435	HIS
1	A	447	GLN
1	A	451	HIS
1	A	479	ASN
1	A	493	GLN

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Mol	Chain	Res	Type
1	A	503	GLN
1	A	517	ASN
1	A	603	ASN
1	A	650	GLN
1	A	698	GLN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	786	HIS
1	A	854	ASN
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	969	GLN
1	A	1048	ASN
1	A	1110	ASN
1	A	1187	GLN
1	A	1203	ASN
1	A	1258	HIS
1	A	1312	ASN
1	A	1354	ASN
1	A	1393	ASN
1	A	1432	GLN
2	B	178	ASN
2	B	236	HIS
2	B	366	GLN
2	B	465	ASN
2	B	484	ASN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	573	GLN
2	B	587	HIS
2	B	686	ASN
2	B	744	HIS
2	B	821	GLN
2	B	835	GLN
2	B	842	ASN
2	B	862	GLN
2	B	887	HIS
2	B	957	ASN

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Mol	Chain	Res	Type
2	B	975	GLN
2	B	986	GLN
2	B	1062	HIS
2	B	1065	GLN
2	B	1076	HIS
2	B	1084	GLN
2	B	1161	HIS
2	B	1179	GLN
2	B	1193	GLN
2	B	1205	GLN
3	C	65	HIS
3	C	73	GLN
3	C	79	GLN
3	C	91	HIS
3	C	112	ASN
4	D	39	ASN
4	D	40	HIS
4	D	138	ASN
4	D	165	GLN
5	E	3	GLN
5	E	101	GLN
5	E	104	ASN
5	E	113	GLN
5	E	143	ASN
5	E	147	HIS
6	F	100	GLN
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	128	ASN
8	H	131	ASN
8	H	137	GLN
9	I	12	ASN
9	I	108	HIS
10	J	53	HIS
10	J	64	ASN
11	K	104	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/17 (52%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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	$\# Z  > 2$
13	BRU	T	23	13,15	15,21,22	4.02	4 (26%)	17,30,33	3.98	4 (23%)

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
13	BRU	T	23	13,15	-	1/4/21/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	23	BRU	BR-C5	-14.02	1.50	1.90
13	T	23	BRU	C4-C5	5.17	1.45	1.38
13	T	23	BRU	C4-N3	3.57	1.39	1.33
13	T	23	BRU	C6-C5	-2.23	1.34	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	23	BRU	C4-N3-C2	14.05	127.01	115.14
13	T	23	BRU	C5-C4-N3	-6.94	115.33	123.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	23	BRU	C5-C6-N1	2.97	123.81	119.97
13	T	23	BRU	BR-C5-C6	2.56	123.13	117.31

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	T	23	BRU	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T	23	BRU	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1416/1733 (81%)	-0.27	10 (0%) 87 83	28, 72, 115, 145	0
2	B	1104/1224 (90%)	-0.22	8 (0%) 87 83	28, 85, 126, 140	0
3	C	266/318 (83%)	-0.24	1 (0%) 92 90	41, 71, 107, 125	0
4	D	178/221 (80%)	-0.11	0 100 100	52, 84, 120, 134	0
5	E	214/215 (99%)	-0.05	0 100 100	52, 103, 130, 138	0
6	F	87/155 (56%)	-0.56	0 100 100	32, 51, 81, 91	0
7	G	171/171 (100%)	-0.24	0 100 100	48, 71, 104, 117	0
8	H	134/146 (91%)	0.23	1 (0%) 87 83	79, 109, 127, 139	0
9	I	119/122 (97%)	0.03	3 (2%) 57 51	66, 106, 126, 144	0
10	J	65/70 (92%)	-0.39	0 100 100	49, 68, 95, 107	0
11	K	114/120 (95%)	-0.24	0 100 100	36, 76, 95, 112	0
12	L	46/70 (65%)	0.01	0 100 100	48, 111, 129, 130	0
13	T	16/26 (61%)	0.46	0 100 100	99, 137, 166, 166	0
14	N	5/13 (38%)	1.41	1 (20%) 1 1	143, 147, 156, 171	0
15	P	10/17 (58%)	0.64	1 (10%) 7 8	122, 129, 147, 153	0
All	All	3945/4621 (85%)	-0.20	25 (0%) 89 86	28, 80, 124, 171	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1455	PRO	4.0
2	B	918	ILE	3.3
9	I	120	GLN	3.0
15	P	1	C	2.9
14	N	1	DA	2.9
2	B	868	MET	2.8
1	A	155	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
9	I	119	THR	2.7
1	A	158	PRO	2.7
1	A	44	THR	2.6
1	A	253	ASN	2.5
1	A	154	SER	2.5
9	I	116	ASN	2.5
1	A	159	THR	2.5
1	A	195	ASP	2.4
2	B	867	GLY	2.3
2	B	733	HIS	2.3
2	B	709	ASP	2.2
2	B	870	ILE	2.2
3	C	3	GLU	2.1
2	B	250	PHE	2.1
1	A	149	GLU	2.0
1	A	256	GLN	2.0
2	B	433	GLN	2.0
8	H	126	GLU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
13	BRU	T	23	20/21	0.74	0.26	127,131,137,139	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
17	MG	A	2458	1/1	0.73	0.32	123,123,123,123	0
16	ZN	L	1071	1/1	0.91	0.08	111,111,111,111	0
16	ZN	I	1122	1/1	0.95	0.05	122,122,122,122	0
16	ZN	A	2456	1/1	0.97	0.05	86,86,86,86	0
16	ZN	J	1066	1/1	0.99	0.21	61,61,61,61	0
16	ZN	C	1269	1/1	0.99	0.10	49,49,49,49	0
16	ZN	I	1121	1/1	0.99	0.10	90,90,90,90	0
16	ZN	B	2225	1/1	0.99	0.17	54,54,54,54	0
16	ZN	A	2457	1/1	0.99	0.14	51,51,51,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.