



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:41 PM UTC

PDB ID : 3H3V / pdb_00003h3v
Title : Yeast RNAP II containing poly(A)-signal sequence in the active site
Authors : Dengl, S.; Cramer, P.
Deposited on : 2009-04-17
Resolution : 4.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

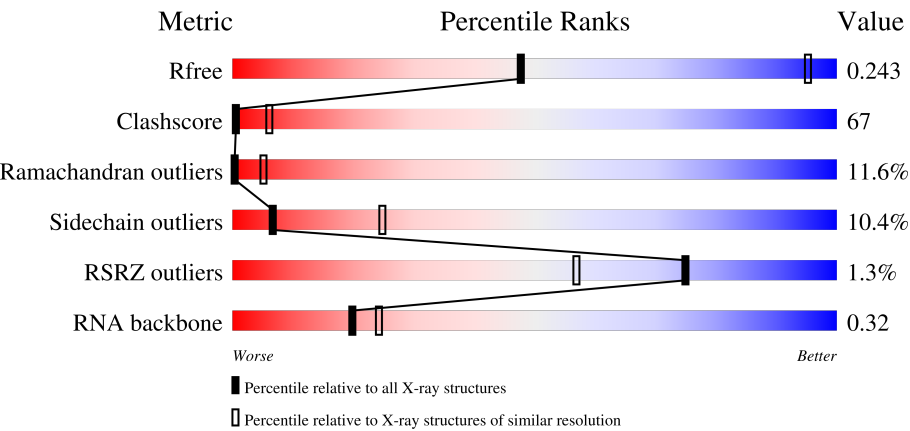
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



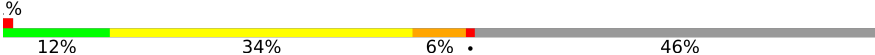
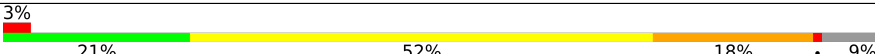
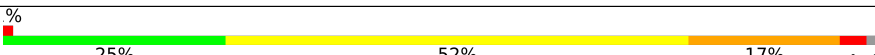
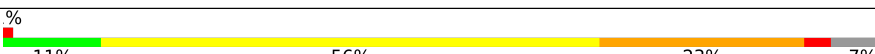
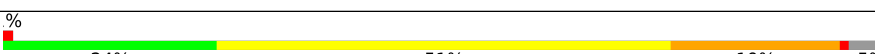
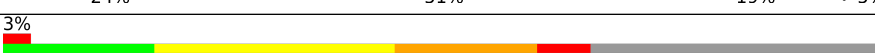
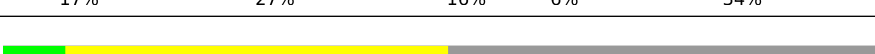
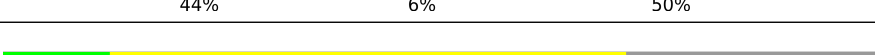
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)
RNA backbone	3983	1017 (4.84-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	B	1733	19% 47% 13% • 18%
2	C	1224	20% 53% 16% • 9%
3	D	318	18% 49% 15% • 16%
4	E	221	16% 44% 16% • 20%

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Mol	Chain	Length	Quality of chain
5	F	215	
6	G	155	
7	H	171	
8	I	146	
9	J	122	
10	K	70	
11	L	120	
12	M	70	
13	N	14	
14	P	16	
15	T	26	

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	B	1416	Total	C	N	O	S	0	0	0
			11140	7021	1946	2111	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1108	Total	C	N	O	S	0	0	0
			8810	5580	1541	1634	55			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	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	E	177	Total	C	N	O	S	0	0	0
			1427	882	256	287	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	F	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	G	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	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	I	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	7	Total	C	N	O	P	11	0	0
			138	67	26	39	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	8	Total	C	N	O	P	0	0	0
			168	77	33	51	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	18	Total	C	N	O	P	8	0	0
			365	177	60	111	17			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	B	2	Total	Zn	0	0
			2	2		
16	C	1	Total	Zn	0	0
			1	1		
16	D	1	Total	Zn	0	0
			1	1		
16	J	2	Total	Zn	0	0
			2	2		
16	K	1	Total	Zn	0	0
			1	1		
16	M	1	Total	Zn	0	0
			1	1		

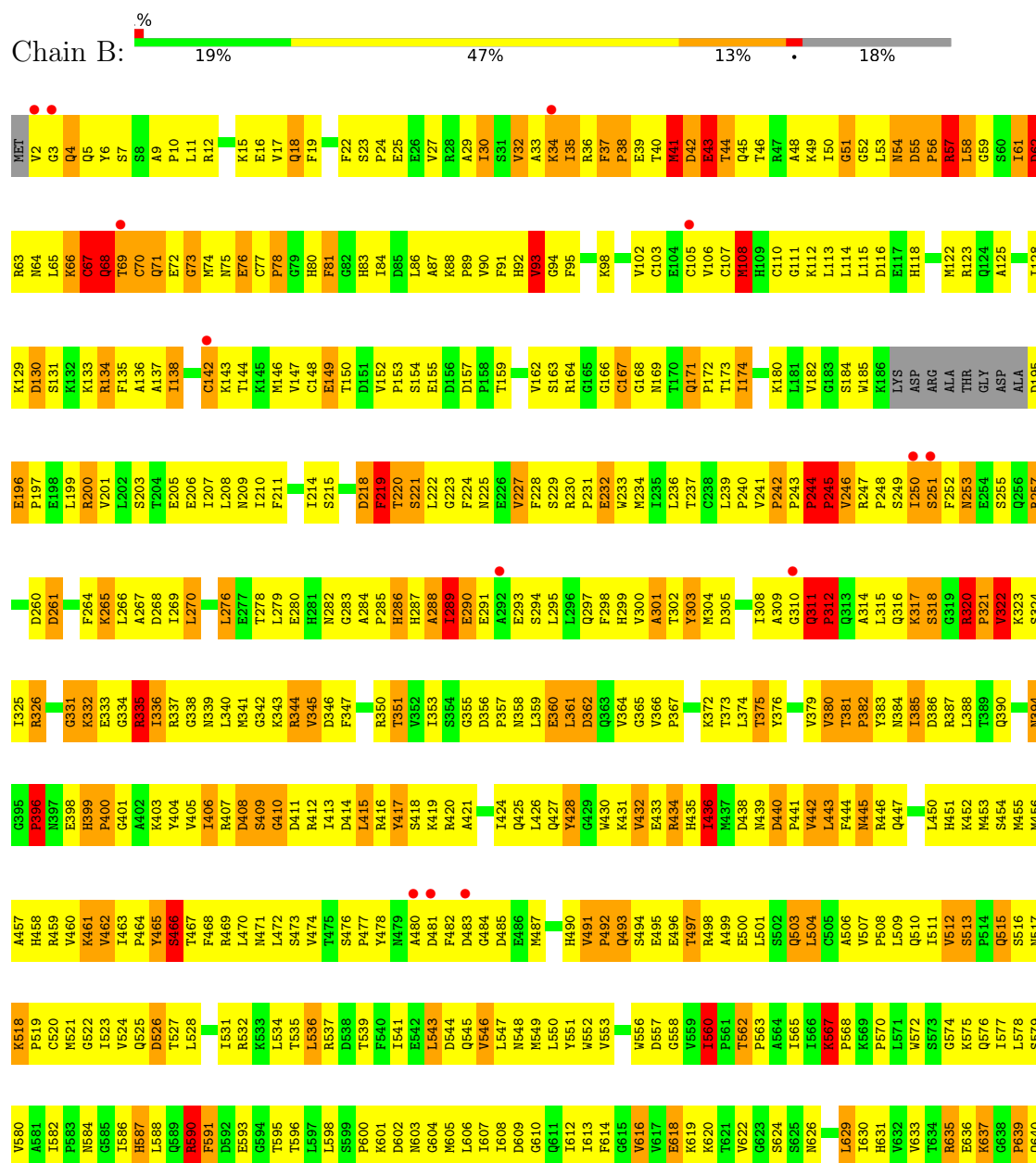
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

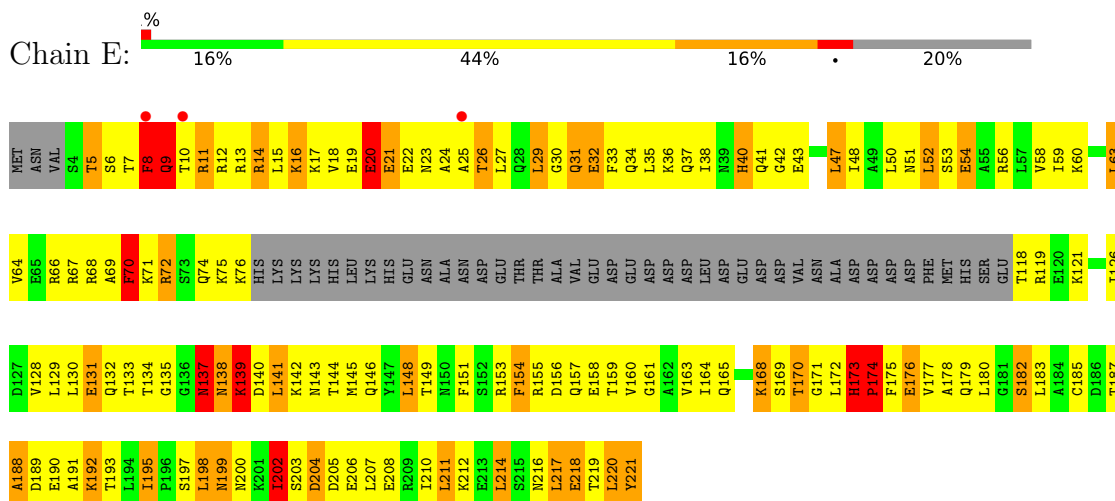
3 Residue-property plots

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

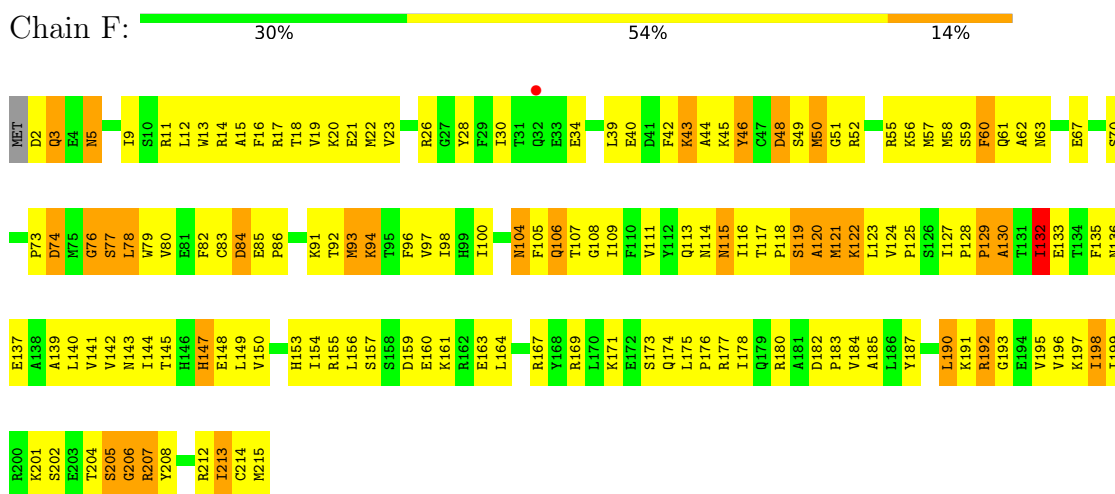
• Molecule 1: DNA-directed RNA polymerase II subunit RPB1



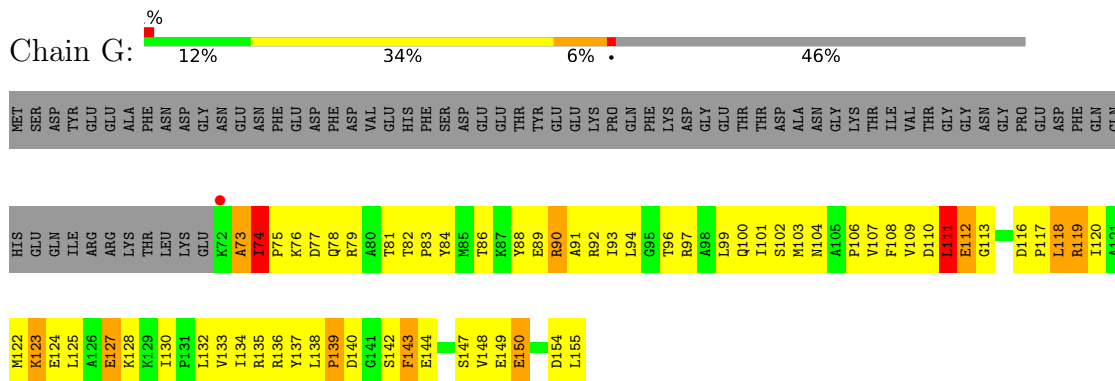




- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

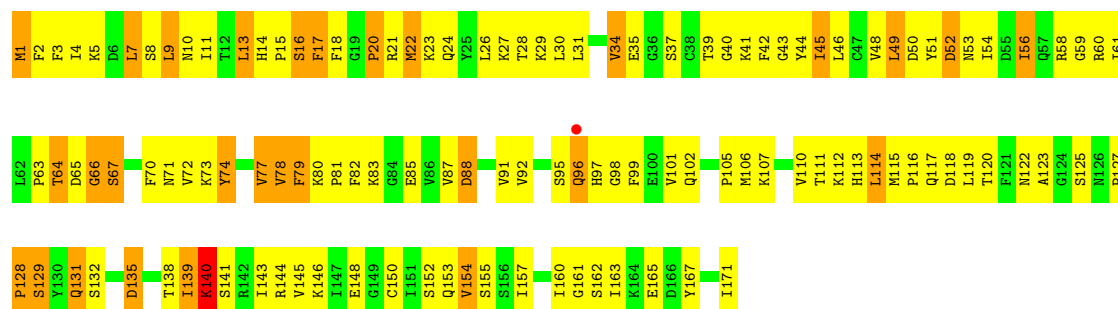


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

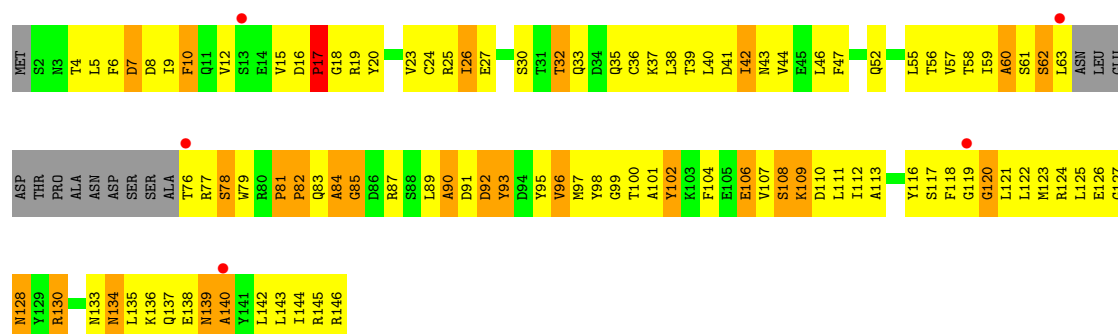
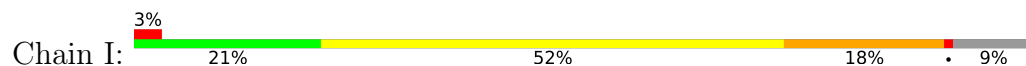


- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

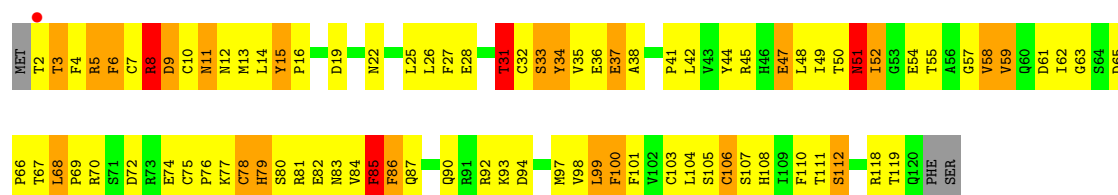




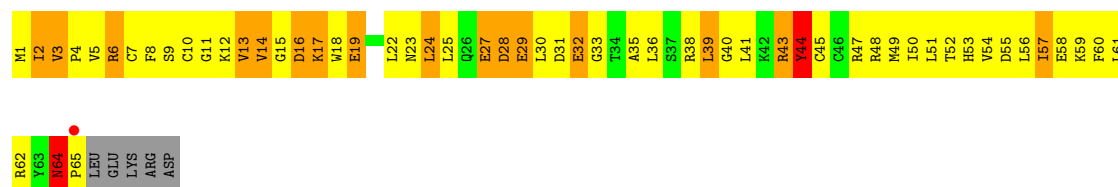
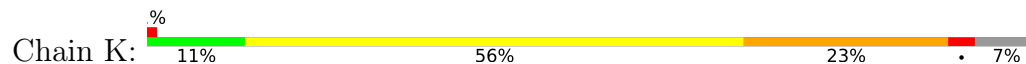
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



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



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

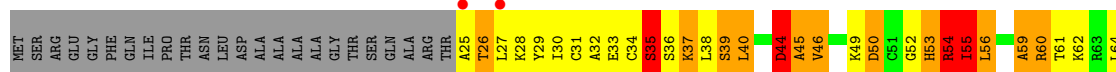


• Molecule 11: DNA-directed RNA polymerase II subunit RPB11





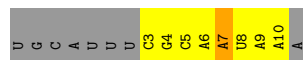
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



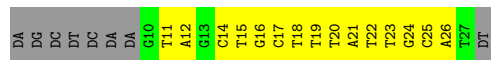
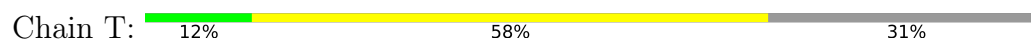
- Molecule 13: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*GP*CP*TP*GP*CP*TP*TP*TP*AP*TP*TP*GP*CP*AP*TP*T)-3'



- Molecule 14: 5'-D(*CP*AP*GP*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*CP*AP*AP*UP*AP*AP*A)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.47Å 391.62Å 284.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.00 50.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-4.00) 99.9 (50.00-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 4.00Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.205 , 0.241 0.215 , 0.243	Depositor DCC
R_{free} test set	16372 reflections (8.09%)	wwPDB-VP
Wilson B-factor (Å ²)	131.8	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 106.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.024 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	0.92	EDS
Total number of atoms	31777	wwPDB-VP
Average B, all atoms (Å ²)	138.0	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.54	0/11339	1.08	97/15334 (0.6%)
2	C	0.51	0/8981	1.04	52/12108 (0.4%)
3	D	0.53	0/2133	1.09	15/2891 (0.5%)
4	E	0.48	0/1437	1.14	17/1925 (0.9%)
5	F	0.48	0/1788	1.03	9/2406 (0.4%)
6	G	0.58	0/691	1.10	3/933 (0.3%)
7	H	0.52	0/1368	1.08	9/1844 (0.5%)
8	I	0.47	0/1086	1.03	4/1470 (0.3%)
9	J	0.48	0/989	1.02	8/1331 (0.6%)
10	K	0.53	0/541	0.96	1/727 (0.1%)
11	L	0.50	0/937	1.05	10/1265 (0.8%)
12	M	0.56	0/366	0.95	1/485 (0.2%)
13	N	0.42	0/154	0.78	0/235
14	P	0.40	0/188	0.96	0/291
15	T	0.10	0/407	0.30	0/627
All	All	0.51	0/32405	1.05	226/43872 (0.5%)

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
10	K	0	1

There are no bond length outliers.

All (226) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	56	PRO	N-CA-C	-16.32	97.71	114.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	173	HIS	CA-C-N	11.00	133.59	119.84
4	E	173	HIS	C-N-CA	11.00	133.59	119.84
2	C	574	SER	CA-C-N	9.87	129.24	118.97
2	C	574	SER	C-N-CA	9.87	129.24	118.97
4	E	26	THR	N-CA-C	-9.79	99.33	112.26
1	B	710	LEU	N-CA-C	-9.66	100.75	111.28
2	C	1184	GLY	N-CA-C	-9.35	103.96	115.08
2	C	807	ARG	N-CA-C	-9.02	101.37	112.38
1	B	288	ALA	N-CA-C	-8.97	99.72	113.89
8	I	85	GLY	N-CA-C	-8.93	101.54	113.24
2	C	473	MET	N-CA-C	-8.77	100.80	112.72
4	E	72	ARG	N-CA-C	-8.51	102.89	113.18
2	C	428	ILE	N-CA-C	-8.15	102.31	110.62
2	C	555	ILE	N-CA-C	-8.13	102.88	110.53
2	C	1163	CYS	N-CA-C	-8.04	96.94	109.25
1	B	1262	LYS	N-CA-C	-8.01	102.14	112.23
1	B	440	ASP	N-CA-C	-7.82	97.44	109.64
5	F	171	LYS	N-CA-C	-7.79	98.93	110.46
4	E	157	GLN	N-CA-C	-7.76	103.92	113.15
2	C	296	GLU	N-CA-C	-7.73	102.93	111.36
7	H	129	SER	N-CA-C	7.71	118.79	108.38
4	E	142	LYS	N-CA-C	-7.60	102.93	111.14
1	B	425	GLN	N-CA-C	-7.51	96.48	108.73
1	B	1376	THR	N-CA-C	7.47	119.21	111.14
1	B	452	LYS	N-CA-C	-7.43	102.87	112.23
1	B	567	LYS	CA-C-N	-7.43	110.56	119.84
1	B	567	LYS	C-N-CA	-7.43	110.56	119.84
1	B	562	THR	CA-C-N	7.41	127.46	119.90
1	B	562	THR	C-N-CA	7.41	127.46	119.90
4	E	54	GLU	N-CA-C	-7.39	103.52	112.54
3	D	39	ALA	N-CA-C	7.38	122.95	113.88
1	B	311	GLN	N-CA-C	7.38	126.11	109.81
1	B	983	ILE	N-CA-C	-7.36	103.12	110.62
2	C	609	ILE	N-CA-C	-7.34	100.13	109.30
1	B	938	LYS	N-CA-C	-7.31	103.30	111.71
9	J	112	SER	N-CA-C	-7.29	102.63	112.26
3	D	4	GLU	N-CA-C	7.26	122.07	112.13
1	B	81	PHE	N-CA-C	7.21	120.16	110.35
1	B	320	ARG	CA-C-N	7.21	128.86	119.84
1	B	320	ARG	C-N-CA	7.21	128.86	119.84
1	B	466	SER	N-CA-C	7.21	121.06	108.52
9	J	85	PHE	N-CA-C	7.00	120.03	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	637	LYS	N-CA-C	6.94	119.87	111.82
2	C	395	GLN	N-CA-C	-6.90	100.06	110.28
2	C	208	SER	N-CA-C	6.86	119.82	110.35
2	C	650	GLU	N-CA-C	6.84	118.79	108.46
2	C	934	LYS	N-CA-C	6.77	120.71	107.57
2	C	681	TRP	N-CA-C	-6.72	103.58	111.03
2	C	1223	ASP	CB-CA-C	-6.71	108.85	116.63
7	H	52	ASP	N-CA-C	6.68	120.53	112.38
4	E	154	PHE	N-CA-C	6.66	116.79	108.19
2	C	66	ASP	N-CA-C	-6.64	103.33	112.03
1	B	1421	CYS	N-CA-C	-6.63	104.49	112.58
3	D	193	TYR	N-CA-C	6.57	116.73	108.45
2	C	112	LEU	N-CA-C	6.57	119.76	110.50
3	D	244	VAL	N-CA-C	-6.54	107.50	113.71
4	E	70	PHE	N-CA-C	-6.48	105.25	113.02
1	B	413	ILE	CB-CA-C	-6.47	102.89	110.91
1	B	289	ILE	N-CA-C	-6.45	106.26	111.81
1	B	398	GLU	N-CA-C	-6.42	102.02	110.43
3	D	200	GLU	N-CA-C	6.39	118.32	111.36
3	D	41	ILE	CA-C-N	6.34	126.36	119.90
3	D	41	ILE	C-N-CA	6.34	126.36	119.90
11	L	58	PHE	N-CA-C	6.32	118.01	108.46
6	G	119	ARG	N-CA-C	-6.32	103.69	111.40
5	F	147	HIS	N-CA-C	6.25	119.42	110.10
1	B	582	ILE	CA-C-N	6.25	126.16	119.85
1	B	582	ILE	C-N-CA	6.25	126.16	119.85
4	E	38	ILE	N-CA-C	6.23	116.89	108.17
2	C	1078	GLY	N-CA-C	-6.21	106.19	114.95
4	E	171	GLY	N-CA-C	-6.20	106.39	115.63
1	B	108	MET	N-CA-C	-6.19	100.76	110.36
2	C	1009	ASP	N-CA-C	-6.16	103.89	112.45
2	C	1168	LEU	N-CA-C	6.15	118.77	109.41
2	C	1185	CYS	N-CA-C	-6.15	97.70	110.80
11	L	65	HIS	CA-C-N	6.14	127.52	119.84
11	L	65	HIS	C-N-CA	6.14	127.52	119.84
5	F	5	ASN	N-CA-C	-6.12	105.51	114.39
1	B	982	THR	N-CA-C	-6.12	102.45	110.53
3	D	7	GLN	N-CA-C	6.11	119.43	109.59
2	C	949	VAL	N-CA-C	-6.11	100.13	109.78
1	B	242	PRO	CA-C-N	6.10	126.66	120.38
1	B	242	PRO	C-N-CA	6.10	126.66	120.38
9	J	5	ARG	N-CA-C	6.06	118.62	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	293	GLU	N-CA-C	-6.05	105.73	113.23
1	B	1137	ALA	N-CA-C	-6.04	105.47	114.64
1	B	590	ARG	N-CA-C	6.03	118.43	108.48
5	F	119	SER	N-CA-C	-6.01	105.60	113.12
1	B	246	VAL	N-CA-C	-5.99	106.41	113.42
6	G	108	PHE	N-CA-C	5.99	120.21	113.02
7	H	22	MET	N-CA-C	-5.99	104.71	112.68
4	E	188	ALA	N-CA-C	-5.98	105.83	113.01
9	J	68	LEU	CA-C-N	5.98	126.17	120.31
9	J	68	LEU	C-N-CA	5.98	126.17	120.31
10	K	64	ASN	N-CA-C	5.97	123.00	109.81
1	B	857	ARG	N-CA-C	5.97	116.16	108.34
1	B	468	PHE	N-CA-C	-5.96	100.13	109.25
3	D	96	SER	N-CA-C	5.95	119.09	109.40
1	B	776	ALA	N-CA-C	5.94	119.14	110.17
1	B	143	LYS	N-CA-C	-5.92	105.89	113.23
1	B	896	ARG	N-CA-C	5.91	118.23	111.02
1	B	1422	ARG	N-CA-C	-5.90	105.91	113.23
7	H	42	PHE	N-CA-C	-5.89	107.08	114.56
2	C	817	LEU	CA-C-N	5.89	127.20	119.84
2	C	817	LEU	C-N-CA	5.89	127.20	119.84
1	B	344	ARG	N-CA-C	-5.88	100.96	110.32
4	E	138	ASN	N-CA-C	-5.88	104.25	112.25
2	C	366	GLN	N-CA-C	-5.87	105.43	113.30
3	D	38	ILE	N-CA-C	5.87	115.99	110.30
7	H	2	PHE	N-CA-C	-5.86	100.11	109.96
8	I	42	ILE	N-CA-C	5.82	117.06	108.45
2	C	805	THR	N-CA-C	5.81	117.61	108.96
1	B	1412	ALA	N-CA-C	-5.80	103.69	112.04
1	B	560	ILE	CA-C-N	5.80	125.56	119.76
1	B	560	ILE	C-N-CA	5.80	125.56	119.76
2	C	1025	HIS	N-CA-C	-5.80	104.65	110.97
1	B	301	ALA	N-CA-C	-5.79	103.69	112.04
6	G	127	GLU	N-CA-C	-5.79	105.41	112.88
2	C	1223	ASP	N-CA-C	5.79	117.87	108.08
1	B	171	GLN	CA-C-N	5.79	125.55	119.76
1	B	171	GLN	C-N-CA	5.79	125.55	119.76
3	D	41	ILE	N-CA-C	5.78	113.59	107.76
2	C	1099	VAL	N-CA-C	5.77	116.23	110.23
1	B	1445	ILE	CB-CA-C	-5.73	105.10	111.35
2	C	292	ILE	N-CA-C	5.72	121.24	108.88
1	B	55	ASP	CA-C-N	-5.72	115.00	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	ASP	C-N-CA	-5.72	115.00	120.83
1	B	1207	LEU	N-CA-C	5.72	117.76	109.07
2	C	1033	LYS	N-CA-C	-5.72	105.02	112.23
1	B	290	GLU	N-CA-C	-5.72	106.15	113.01
4	E	176	GLU	N-CA-C	-5.71	104.69	111.03
1	B	998	LEU	N-CA-C	5.70	117.51	108.67
3	D	11	ARG	N-CA-C	-5.67	103.31	108.75
1	B	412	ARG	N-CA-C	5.66	118.46	109.24
1	B	513	SER	N-CA-C	5.65	117.78	109.42
3	D	258	ILE	N-CA-C	-5.64	105.23	110.53
1	B	227	VAL	CB-CA-C	-5.63	106.11	111.06
11	L	55	LYS	N-CA-C	-5.63	106.41	113.28
2	C	427	ASP	N-CA-C	-5.63	98.81	110.80
11	L	75	ILE	N-CA-C	5.62	115.96	107.75
4	E	137	ASN	N-CA-C	-5.62	106.09	113.17
1	B	1209	MET	N-CA-C	-5.60	104.58	111.75
2	C	1008	PRO	N-CA-C	5.60	120.28	111.38
1	B	1277	GLU	N-CA-C	5.59	117.75	110.43
5	F	52	ARG	CA-C-N	5.58	125.90	119.93
5	F	52	ARG	C-N-CA	5.58	125.90	119.93
1	B	323	LYS	N-CA-C	5.58	117.56	108.63
2	C	192	LEU	N-CA-C	-5.57	106.52	113.38
2	C	851	PHE	N-CA-C	5.57	119.90	113.38
2	C	363	HIS	N-CA-C	-5.56	98.96	110.80
2	C	896	ASP	N-CA-C	-5.55	106.46	113.18
3	D	203	GLN	N-CA-C	-5.55	101.64	109.96
2	C	1191	ILE	N-CA-C	5.53	116.02	107.78
11	L	77	THR	N-CA-C	5.53	115.58	108.34
1	B	68	GLN	N-CA-C	-5.51	104.47	110.91
9	J	6	PHE	N-CA-C	-5.49	101.17	109.85
2	C	1045	SER	CA-C-N	5.46	126.67	119.84
2	C	1045	SER	C-N-CA	5.46	126.67	119.84
2	C	680	THR	N-CA-C	5.46	117.06	109.31
7	H	102	GLN	N-CA-C	5.46	118.24	107.98
1	B	683	ILE	N-CA-C	-5.45	105.78	110.74
1	B	553	VAL	CA-C-N	5.42	125.49	119.32
1	B	553	VAL	C-N-CA	5.42	125.49	119.32
7	H	78	VAL	N-CA-C	5.41	115.14	108.53
11	L	52	ASN	N-CA-C	-5.41	105.73	112.93
1	B	244	PRO	N-CA-C	5.41	117.30	110.70
2	C	882	THR	N-CA-C	5.39	118.65	111.75
1	B	689	LYS	N-CA-C	-5.38	105.97	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	95	ILE	N-CA-C	-5.37	105.27	110.42
3	D	215	GLU	N-CA-C	5.36	122.22	110.80
2	C	331	LEU	N-CA-C	-5.35	105.49	112.23
1	B	816	HIS	N-CA-C	-5.33	105.58	111.71
11	L	100	ALA	N-CA-C	-5.33	105.11	111.03
2	C	903	VAL	N-CA-C	5.33	120.42	109.34
1	B	536	LEU	N-CA-C	5.32	122.14	110.80
2	C	770	GLN	N-CA-C	-5.32	105.89	112.38
8	I	109	LYS	CB-CA-C	-5.31	108.88	115.89
1	B	769	SER	N-CA-C	5.31	117.14	109.07
1	B	931	GLU	N-CA-C	-5.30	105.68	111.82
1	B	362	ASP	N-CA-C	5.29	119.22	112.87
1	B	351	THR	CB-CA-C	-5.28	106.89	114.87
1	B	219	PHE	N-CA-C	-5.27	99.57	110.80
2	C	471	LYS	N-CA-C	5.27	122.03	110.80
2	C	432	MET	N-CA-C	-5.25	106.64	113.16
1	B	1076	ALA	N-CA-C	-5.24	106.04	112.90
1	B	1403	GLU	N-CA-C	5.23	121.94	110.80
1	B	1191	TRP	N-CA-C	5.22	117.26	108.96
5	F	63	ASN	N-CA-C	5.21	118.08	109.58
1	B	251	SER	N-CA-C	5.21	116.66	109.15
1	B	173	THR	N-CA-C	-5.21	102.14	109.96
1	B	432	VAL	CB-CA-C	-5.21	105.55	111.59
2	C	774	GLY	N-CA-C	-5.20	107.33	113.99
7	H	135	ASP	N-CA-C	5.20	118.20	110.14
1	B	970	THR	N-CA-C	-5.20	107.11	113.50
1	B	134	ARG	N-CA-C	-5.19	105.27	111.03
1	B	1291	VAL	CA-C-N	5.19	126.00	119.98
1	B	1291	VAL	C-N-CA	5.19	126.00	119.98
1	B	491	VAL	N-CA-C	5.18	113.58	107.77
1	B	1055	ARG	N-CA-C	-5.15	105.29	112.45
9	J	51	ASN	N-CA-C	-5.15	105.88	113.61
1	B	923	LEU	N-CA-C	5.14	117.78	111.82
1	B	1162	VAL	N-CA-C	-5.12	105.38	112.50
1	B	236	LEU	N-CA-C	5.12	117.08	109.25
1	B	539	THR	N-CA-C	5.12	117.09	108.96
9	J	31	THR	N-CA-C	-5.11	106.99	113.43
2	C	1199	ALA	N-CA-C	-5.11	107.02	113.20
1	B	1138	ILE	CB-CA-C	-5.10	105.91	110.91
7	H	131	GLN	N-CA-C	5.10	117.38	108.76
12	M	44	ASP	N-CA-C	-5.09	105.14	113.19
1	B	515	GLN	N-CA-C	-5.09	106.20	114.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	CYS	N-CA-C	5.06	119.03	113.21
1	B	218	ASP	N-CA-C	-5.06	105.42	112.45
1	B	1444	MET	N-CA-C	5.05	117.64	109.06
2	C	527	THR	CA-C-N	5.05	125.28	119.83
2	C	527	THR	C-N-CA	5.05	125.28	119.83
11	L	84	LYS	N-CA-C	-5.04	105.23	111.33
8	I	4	THR	N-CA-C	-5.03	102.11	109.81
4	E	195	ILE	CA-C-N	5.03	126.12	119.84
4	E	195	ILE	C-N-CA	5.03	126.12	119.84
1	B	30	ILE	N-CA-C	5.02	115.24	110.42
5	F	132	ILE	N-CA-C	5.02	115.70	108.48
1	B	1039	LYS	N-CA-C	-5.01	105.95	111.71
5	F	84	ASP	N-CA-C	-5.01	107.19	113.15
1	B	436	ILE	N-CA-C	-5.01	102.42	109.63
1	B	831	THR	N-CA-C	-5.00	107.25	113.55

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	K	44	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	11140	0	11215	1592	0
2	C	8810	0	8847	1339	0
3	D	2095	0	2051	319	0
4	E	1427	0	1451	186	0
5	F	1752	0	1776	189	0
6	G	679	0	701	108	0
7	H	1340	0	1357	192	0
8	I	1068	0	1040	167	0
9	J	971	0	929	129	0
10	K	532	0	542	131	0
11	L	919	0	929	140	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	M	364	0	388	57	0
13	N	138	0	80	8	0
14	P	168	0	88	15	0
15	T	365	0	208	48	0
16	B	2	0	0	0	0
16	C	1	0	0	0	0
16	D	1	0	0	0	0
16	J	2	0	0	0	0
16	K	1	0	0	0	0
16	M	1	0	0	0	0
17	B	1	0	0	0	0
All	All	31777	0	31602	4227	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 67.

All (4227) 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)
15:T:21:DA:C2'	15:T:22:DT:H5'	1.58	1.32
15:T:21:DA:H2''	15:T:22:DT:C5'	1.65	1.25
15:T:20:DT:C2'	15:T:21:DA:H5'	1.73	1.18
11:L:47:ARG:HB3	11:L:47:ARG:HH11	1.11	1.15
15:T:20:DT:H2'	15:T:21:DA:H5'	1.13	1.12
2:C:1072:MET:HE3	2:C:1085:ILE:HB	1.28	1.12
1:B:541:ILE:HD13	1:B:549:MET:HE1	1.22	1.11
3:D:101:LEU:HD13	3:D:118:LEU:HD23	1.31	1.10
2:C:622:LYS:HE2	9:J:59:VAL:HG22	1.21	1.08
1:B:590:ARG:HH21	1:B:620:LYS:HB3	1.10	1.08
4:E:134:THR:HG22	4:E:135:GLY:H	1.13	1.08
5:F:22:MET:HE3	5:F:26:ARG:HE	1.14	1.08
1:B:53:LEU:HD23	1:B:54:ASN:H	1.14	1.07
4:E:40:HIS:HB2	7:H:73:LYS:HZ2	1.19	1.07
1:B:356:ASP:HB2	1:B:469:ARG:HH12	1.19	1.07
1:B:981:LEU:HD21	1:B:1039:LYS:HA	1.35	1.06
2:C:839:MET:HG3	2:C:1010:LEU:HD12	1.37	1.06
1:B:353:ILE:HD13	1:B:487:MET:HE2	1.34	1.06
1:B:682:THR:HG23	1:B:728:LYS:HE3	1.30	1.06
2:C:1197:PRO:HG2	2:C:1200:ALA:HB2	1.38	1.06
12:M:32:ALA:HB3	12:M:55:ILE:HD12	1.36	1.06
7:H:13:LEU:HD21	7:H:17:PHE:HB2	1.32	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1076:ALA:HA	1:B:1079:MET:HE2	1.36	1.05
1:B:535:THR:HG21	1:B:616:VAL:HA	1.38	1.05
8:I:100:THR:HG23	8:I:138:GLU:HA	1.38	1.03
2:C:603:LEU:HD12	2:C:609:ILE:HG13	1.39	1.02
8:I:59:ILE:HG22	8:I:60:ALA:H	1.19	1.02
1:B:1445:ILE:H	1:B:1445:ILE:HD12	1.20	1.02
2:C:278:GLN:HG2	2:C:279:ASP:H	1.24	1.02
2:C:189:LEU:HA	2:C:192:LEU:HD12	1.40	1.02
1:B:443:LEU:HD21	1:B:455:MET:HB3	1.36	1.01
4:E:170:THR:HB	4:E:172:LEU:HG	1.43	1.00
2:C:516:ASN:N	2:C:516:ASN:HD22	1.58	1.00
2:C:577:ALA:HB1	2:C:589:VAL:HG11	1.41	1.00
1:B:901:LEU:HB2	1:B:926:GLN:HG2	1.42	1.00
1:B:1329:THR:H	1:B:1335:ILE:HD11	1.27	1.00
15:T:21:DA:C2'	15:T:22:DT:C5'	2.30	1.00
2:C:96:TYR:HB2	2:C:129:PHE:HB2	1.44	0.99
1:B:340:LEU:HD13	1:B:1429:ILE:HG23	1.42	0.99
6:G:111:LEU:H	6:G:111:LEU:HD12	1.26	0.99
3:D:57:VAL:HG11	10:K:60:PHE:HB3	1.44	0.99
1:B:1017:LEU:HB2	5:F:206:GLY:H	1.27	0.99
1:B:855:THR:HG21	1:B:857:ARG:HE	1.23	0.99
4:E:12:ARG:HH22	4:E:14:ARG:HG3	1.27	0.97
2:C:516:ASN:HD22	2:C:516:ASN:H	1.12	0.97
4:E:5:THR:HG22	7:H:8:SER:O	1.63	0.97
1:B:446:ARG:HD3	1:B:480:ALA:HB2	1.46	0.97
1:B:981:LEU:CD2	1:B:1039:LYS:HA	1.95	0.96
2:C:168:GLY:H	2:C:450:ALA:HB1	1.26	0.96
1:B:399:HIS:HB3	1:B:400:PRO:HD3	1.48	0.96
4:E:185:CYS:HB2	4:E:211:LEU:HD21	1.45	0.96
2:C:800:GLN:HG2	10:K:52:THR:CG2	1.96	0.96
1:B:768:GLN:HG2	1:B:816:HIS:HA	1.48	0.96
1:B:567:LYS:CD	1:B:568:PRO:HD2	1.96	0.95
1:B:1161:THR:HG22	1:B:1163:ILE:H	1.30	0.95
4:E:14:ARG:HH22	4:E:16:LYS:HZ1	1.14	0.95
1:B:40:THR:HG22	1:B:41:MET:HG3	1.45	0.95
1:B:55:ASP:C	1:B:57:ARG:H	1.69	0.95
2:C:121:ASN:HA	2:C:207:GLY:HA2	1.48	0.95
5:F:180:ARG:HH21	5:F:192:ARG:HB2	1.27	0.95
1:B:40:THR:HB	1:B:41:MET:HE2	1.45	0.95
2:C:728:ARG:HH12	2:C:1047:PHE:HB3	1.31	0.95
11:L:49:GLU:HG3	11:L:94:ILE:HG12	1.44	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:999:MET:HG3	2:C:1000:PRO:HD2	1.49	0.94
1:B:563:PRO:HG3	1:B:572:TRP:CZ2	2.01	0.94
1:B:567:LYS:CG	1:B:568:PRO:HD2	1.98	0.94
3:D:166:GLU:HG3	11:L:10:PHE:HZ	1.31	0.93
15:T:25:DC:H42	15:T:26:DA:N6	1.66	0.93
2:C:23:ALA:HB1	2:C:24:PRO:HD2	1.48	0.93
10:K:12:LYS:O	10:K:14:VAL:HG23	1.69	0.93
1:B:1006:ILE:HD11	5:F:163:GLU:HG3	1.48	0.93
1:B:1193:LEU:HD22	1:B:1260:LEU:HD11	1.51	0.93
12:M:49:LYS:O	12:M:50:ASP:HB2	1.65	0.93
1:B:37:PHE:HB2	1:B:52:GLY:HA3	1.51	0.93
8:I:23:VAL:HG22	8:I:43:ASN:HA	1.51	0.93
1:B:1424:VAL:HG13	1:B:1436:ILE:HD11	1.52	0.92
1:B:658:LEU:HD13	2:C:831:SER:H	1.33	0.92
1:B:524:VAL:HG12	1:B:525:GLN:H	1.34	0.92
1:B:754:SER:H	1:B:757:ASN:HD22	1.18	0.92
1:B:1002:GLY:HA3	1:B:1007:ILE:HG21	1.50	0.91
2:C:778:MET:HE2	2:C:1094:ARG:HG2	1.50	0.91
7:H:7:LEU:HB2	7:H:74:TYR:HE2	1.35	0.91
10:K:1:MET:H1	10:K:57:ILE:N	1.68	0.91
1:B:547:LEU:HB3	11:L:58:PHE:HE1	1.31	0.91
1:B:1208:THR:HG22	1:B:1210:GLY:H	1.35	0.91
1:B:41:MET:CB	1:B:49:LYS:HA	2.01	0.91
10:K:1:MET:N	10:K:57:ILE:H	1.68	0.91
2:C:515:HIS:H	2:C:518:HIS:HD2	1.13	0.91
15:T:25:DC:N4	15:T:26:DA:H62	1.67	0.91
4:E:40:HIS:HB2	7:H:73:LYS:NZ	1.86	0.91
2:C:483:LEU:HD11	2:C:491:THR:HG23	1.51	0.91
1:B:225:ASN:HD22	1:B:228:PHE:H	1.18	0.90
2:C:806:THR:HG22	2:C:808:ALA:H	1.37	0.90
1:B:1160:SER:HA	1:B:1170:ILE:HD13	1.53	0.90
11:L:47:ARG:HB3	11:L:47:ARG:NH1	1.85	0.90
6:G:90:ARG:HG3	6:G:91:ALA:N	1.85	0.90
2:C:821:GLN:HE22	2:C:851:PHE:HA	1.36	0.90
4:E:56:ARG:HD3	4:E:149:THR:HA	1.54	0.90
1:B:1341:ILE:HG23	1:B:1342:GLU:H	1.35	0.89
2:C:1156:ASP:HB3	2:C:1198:TYR:H	1.37	0.89
2:C:642:ASP:HA	2:C:649:LYS:HA	1.51	0.89
1:B:537:ARG:HD2	8:I:20:TYR:HE1	1.35	0.89
1:B:899:VAL:HG13	1:B:908:LEU:HD21	1.54	0.89
1:B:265:LYS:HG2	1:B:303:TYR:HA	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:CYS:HB3	1:B:167:CYS:SG	2.13	0.89
1:B:913:LEU:HD12	1:B:914:GLU:H	1.38	0.89
2:C:214:ALA:HB3	2:C:498:THR:HA	1.52	0.89
8:I:59:ILE:HG22	8:I:60:ALA:N	1.86	0.89
1:B:347:PHE:H	2:C:1107:ALA:HA	1.38	0.89
2:C:217:ARG:HE	2:C:405:ARG:HB2	1.37	0.89
2:C:810:GLU:HA	2:C:815:ARG:HH12	1.36	0.88
2:C:542:MET:HE2	2:C:743:ILE:HG13	1.53	0.88
2:C:792:MET:HE2	2:C:857:ARG:HH12	1.37	0.88
6:G:86:THR:OG1	6:G:89:GLU:HG3	1.74	0.88
5:F:19:VAL:O	5:F:23:VAL:HG23	1.73	0.88
1:B:470:LEU:HD23	1:B:470:LEU:H	1.38	0.88
1:B:534:LEU:O	1:B:574:GLY:HA3	1.74	0.88
2:C:34:ILE:HD13	2:C:747:MET:HE2	1.54	0.88
2:C:112:LEU:HD21	2:C:117:ALA:HB2	1.56	0.88
2:C:46:GLN:HG3	2:C:47:GLN:H	1.36	0.88
7:H:91:VAL:HB	7:H:139:ILE:O	1.72	0.88
15:T:18:DT:H2''	15:T:19:DT:H5'	1.56	0.88
1:B:356:ASP:HB2	1:B:469:ARG:NH1	1.87	0.88
1:B:779:PHE:CE1	1:B:785:PRO:HD3	2.08	0.88
1:B:590:ARG:HH21	1:B:620:LYS:CB	1.87	0.88
1:B:779:PHE:HE1	1:B:785:PRO:HD3	1.37	0.87
11:L:12:LEU:H	11:L:12:LEU:HD12	1.39	0.87
12:M:27:LEU:HD13	12:M:37:LYS:HE2	1.56	0.87
2:C:1159:ARG:NH1	2:C:1159:ARG:HB3	1.88	0.87
1:B:828:ALA:CB	2:C:530:GLY:HA2	2.04	0.87
1:B:1017:LEU:HB3	5:F:205:SER:HA	1.53	0.87
2:C:313:MET:HE3	2:C:386:LEU:HD22	1.55	0.87
5:F:156:LEU:HD12	5:F:195:VAL:HB	1.56	0.87
2:C:737:THR:HG21	9:J:66:PRO:HA	1.56	0.87
6:G:82:THR:HG22	6:G:84:TYR:H	1.36	0.87
2:C:847:ASP:HB3	3:D:167:HIS:NE2	1.90	0.87
2:C:1159:ARG:HB3	2:C:1159:ARG:HH11	1.38	0.86
10:K:44:TYR:HA	10:K:47:ARG:HB2	1.57	0.86
3:D:6:PRO:HB3	3:D:25:VAL:HG12	1.55	0.86
10:K:1:MET:H1	10:K:57:ILE:H	0.90	0.86
2:C:100:PRO:HD2	2:C:180:TYR:HE1	1.40	0.86
8:I:15:VAL:HG22	8:I:26:ILE:HD11	1.58	0.86
9:J:111:THR:HG22	9:J:112:SER:H	1.41	0.86
1:B:341:MET:HE2	1:B:843:LYS:NZ	1.91	0.86
2:C:654:ARG:H	2:C:657:HIS:HD2	1.21	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:LYS:HB3	8:I:96:VAL:H	1.41	0.86
1:B:568:PRO:HG2	8:I:46:LEU:HD22	1.58	0.86
1:B:1444:MET:HE1	6:G:135:ARG:HB2	1.57	0.85
2:C:393:LYS:HE3	2:C:393:LYS:HA	1.58	0.85
1:B:709:THR:HG22	1:B:711:ARG:H	1.39	0.85
2:C:387:LEU:O	2:C:392:ARG:HB2	1.76	0.85
2:C:1065:GLN:HG3	2:C:1067:ARG:H	1.39	0.85
8:I:59:ILE:CG2	8:I:60:ALA:H	1.89	0.85
2:C:856:PHE:HD2	2:C:967:ARG:HD2	1.41	0.85
4:E:56:ARG:HB2	4:E:148:LEU:HD22	1.59	0.85
10:K:57:ILE:HA	10:K:60:PHE:HD2	1.41	0.85
3:D:47:ASP:HA	12:M:69:ALA:HB3	1.57	0.85
1:B:53:LEU:HD23	1:B:54:ASN:N	1.92	0.85
2:C:1180:PHE:HB3	2:C:1191:ILE:CD1	2.06	0.85
15:T:20:DT:C2'	15:T:21:DA:C5'	2.54	0.85
1:B:321:PRO:O	1:B:322:VAL:HB	1.75	0.84
5:F:117:THR:HG22	5:F:119:SER:H	1.41	0.84
2:C:549:THR:HG22	2:C:550:ASP:H	1.41	0.84
7:H:18:PHE:HA	7:H:22:MET:HE3	1.58	0.84
1:B:265:LYS:HA	1:B:265:LYS:HE3	1.60	0.84
1:B:901:LEU:H	1:B:926:GLN:NE2	1.75	0.84
1:B:1094:VAL:HG13	1:B:1113:THR:HG21	1.58	0.84
1:B:172:PRO:HD3	1:B:185:TRP:NE1	1.93	0.84
3:D:39:ALA:HA	3:D:164:ALA:HB3	1.60	0.84
3:D:45:ALA:HA	3:D:72:LEU:HD12	1.59	0.84
4:E:63:LEU:HD12	4:E:129:LEU:HG	1.58	0.84
1:B:196:GLU:HG3	1:B:197:PRO:HD2	1.59	0.84
9:J:13:MET:HE3	9:J:14:LEU:H	1.40	0.84
2:C:521:LEU:HD22	2:C:633:VAL:HG12	1.58	0.84
2:C:261:ARG:HB3	2:C:261:ARG:NH1	1.93	0.83
2:C:1002:THR:HG23	2:C:1006:ILE:HG13	1.59	0.83
4:E:134:THR:HG22	4:E:135:GLY:N	1.93	0.83
2:C:579:ARG:HB2	2:C:586:TRP:NE1	1.92	0.83
7:H:30:LEU:HD13	7:H:72:VAL:HG11	1.61	0.83
1:B:567:LYS:HD3	8:I:95:TYR:CG	2.14	0.83
2:C:428:ILE:HG22	2:C:432:MET:HE2	1.60	0.83
4:E:47:LEU:HD11	7:H:3:PHE:CD2	2.13	0.83
2:C:210:LYS:HD3	2:C:481:GLN:O	1.78	0.83
2:C:825:VAL:HG12	2:C:826:ALA:N	1.93	0.83
2:C:770:GLN:OE1	2:C:983:ARG:HA	1.78	0.83
9:J:85:PHE:H	9:J:85:PHE:HD2	1.24	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1341:ILE:HG23	1:B:1342:GLU:N	1.93	0.83
2:C:899:ILE:HD11	2:C:911:ILE:HA	1.59	0.82
11:L:65:HIS:HD2	11:L:67:PHE:H	1.25	0.82
1:B:598:LEU:HA	8:I:122:LEU:HD13	1.59	0.82
2:C:1072:MET:CE	2:C:1085:ILE:HB	2.08	0.82
5:F:22:MET:HE3	5:F:26:ARG:NE	1.94	0.82
1:B:244:PRO:HB2	1:B:245:PRO:HD3	1.60	0.82
2:C:773:MET:CE	2:C:985:GLY:HA2	2.08	0.82
5:F:93:MET:HE3	5:F:123:LEU:HB2	1.58	0.82
1:B:679:ILE:HG12	1:B:732:LEU:HD12	1.62	0.82
3:D:7:GLN:HG2	11:L:104:ASN:HD22	1.44	0.82
2:C:762:ASN:HD21	2:C:1024:ALA:HB3	1.44	0.82
6:G:132:LEU:HD11	7:H:61:ILE:HD11	1.62	0.82
1:B:341:MET:HE2	1:B:843:LYS:HZ1	1.45	0.82
10:K:48:ARG:HD2	10:K:49:MET:N	1.95	0.82
1:B:528:LEU:HD23	1:B:751:SER:HB3	1.62	0.81
2:C:953:LEU:HD21	2:C:965:LYS:HB2	1.62	0.81
1:B:353:ILE:CD1	1:B:487:MET:HE2	2.09	0.81
2:C:520:GLY:H	2:C:748:ILE:HG22	1.45	0.81
11:L:113:THR:O	11:L:114:LEU:HB2	1.79	0.81
6:G:118:LEU:HD12	6:G:118:LEU:O	1.79	0.81
11:L:21:ILE:HG12	11:L:33:ILE:HG12	1.60	0.81
1:B:1116:LEU:HB3	1:B:1308:THR:HG21	1.63	0.81
2:C:102:VAL:HG21	2:C:112:LEU:HD22	1.61	0.81
2:C:359:GLU:O	2:C:362:PRO:HD3	1.79	0.81
4:E:47:LEU:HD11	7:H:3:PHE:HD2	1.42	0.81
15:T:18:DT:C2'	15:T:19:DT:H5'	2.09	0.81
1:B:12:ARG:O	2:C:1194:ILE:HG22	1.81	0.81
2:C:952:VAL:HG22	2:C:966:VAL:HG13	1.62	0.81
8:I:55:LEU:HD22	8:I:144:ILE:CG2	2.10	0.81
2:C:579:ARG:HB2	2:C:586:TRP:HE1	1.43	0.81
8:I:135:LEU:HD13	8:I:137:GLN:HE21	1.45	0.81
1:B:849:MET:CE	1:B:1061:GLY:HA2	2.09	0.81
10:K:3:VAL:HG21	10:K:18:TRP:HB2	1.62	0.81
2:C:244:LEU:HD21	2:C:366:GLN:NE2	1.96	0.80
3:D:46:ILE:HG23	3:D:157:CYS:HB3	1.63	0.80
3:D:238:ILE:CG2	3:D:242:GLN:HB2	2.11	0.80
1:B:855:THR:CG2	1:B:857:ARG:HE	1.94	0.80
2:C:37:PHE:CE1	2:C:41:LYS:HG3	2.17	0.80
7:H:106:MET:HG2	7:H:107:LYS:N	1.96	0.80
9:J:50:THR:HG23	9:J:52:ILE:HG23	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:210:LYS:HE2	2:C:462:ALA:HA	1.62	0.80
1:B:929:LEU:HD21	1:B:983:ILE:HG21	1.62	0.80
1:B:1148:ILE:HD11	1:B:1198:ASP:HA	1.64	0.80
2:C:217:ARG:HD2	2:C:217:ARG:C	2.06	0.80
1:B:783:THR:HG21	1:B:815:PHE:CZ	2.16	0.80
1:B:993:LEU:HD23	1:B:1022:LEU:HD21	1.62	0.80
12:M:27:LEU:HB3	12:M:37:LYS:HD3	1.64	0.80
1:B:1226:VAL:HG22	1:B:1240:CYS:HB3	1.62	0.80
2:C:254:LEU:HD23	2:C:381:MET:HE1	1.64	0.80
1:B:440:ASP:H	1:B:460:VAL:HG12	1.47	0.79
1:B:913:LEU:HD12	1:B:914:GLU:N	1.96	0.79
1:B:1343:ALA:HB2	5:F:150:VAL:HG22	1.63	0.79
8:I:81:PRO:HB2	8:I:82:PRO:HD2	1.64	0.79
15:T:24:DG:H3'	15:T:25:DC:H5''	1.65	0.79
1:B:743:VAL:O	1:B:747:VAL:HG23	1.82	0.79
1:B:1242:VAL:HG12	1:B:1243:VAL:H	1.45	0.79
2:C:169:ARG:HB2	2:C:454:THR:HG23	1.65	0.79
2:C:1069:PHE:HD1	2:C:1069:PHE:H	1.27	0.79
2:C:1085:ILE:HD12	2:C:1085:ILE:N	1.97	0.79
3:D:67:LEU:HD11	3:D:155:LEU:HD13	1.64	0.79
5:F:153:HIS:HB3	5:F:196:VAL:CG1	2.11	0.79
2:C:1147:LEU:O	2:C:1151:LEU:HD13	1.80	0.79
3:D:70:ILE:HG12	3:D:142:VAL:HG11	1.64	0.79
1:B:1373:ASP:HA	1:B:1376:THR:HG22	1.65	0.79
5:F:80:VAL:HG22	5:F:109:ILE:HD12	1.64	0.79
2:C:770:GLN:CD	2:C:983:ARG:HA	2.08	0.79
7:H:45:ILE:HA	7:H:78:VAL:HG12	1.64	0.79
5:F:135:PHE:HB3	5:F:140:LEU:HD11	1.64	0.79
2:C:1098:MET:HE3	2:C:1098:MET:H	1.46	0.79
1:B:973:ILE:HD11	1:B:1038:THR:HG23	1.64	0.79
2:C:756:ILE:O	2:C:759:PRO:HD3	1.83	0.79
5:F:180:ARG:NH2	5:F:192:ARG:HB2	1.96	0.79
2:C:515:HIS:HD2	2:C:517:THR:H	1.28	0.79
2:C:593:PRO:HG2	2:C:617:ARG:NH2	1.97	0.78
3:D:44:LEU:HB2	3:D:77:ILE:HD11	1.63	0.78
5:F:198:ILE:HD11	5:F:212:ARG:HG3	1.63	0.78
9:J:93:LYS:H	9:J:93:LYS:HD2	1.46	0.78
1:B:1317:MET:HE2	1:B:1327:ILE:HG21	1.66	0.78
2:C:847:ASP:HB3	3:D:167:HIS:CD2	2.17	0.78
5:F:78:LEU:HD21	5:F:80:VAL:HG23	1.66	0.78
1:B:741:ASN:C	1:B:741:ASN:HD22	1.89	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:767:GLN:NE2	1:B:774:ARG:HB3	1.99	0.78
1:B:180:LYS:NZ	1:B:294:SER:HB3	1.99	0.78
2:C:167:ILE:HG22	2:C:453:ILE:HD11	1.64	0.78
2:C:1084:GLN:NE2	2:C:1084:GLN:H	1.81	0.78
8:I:17:PRO:HB3	8:I:24:CYS:SG	2.24	0.78
15:T:21:DA:H2''	15:T:22:DT:H5'	0.82	0.78
2:C:800:GLN:HG2	10:K:52:THR:HG22	1.64	0.78
4:E:159:THR:O	4:E:163:VAL:HG23	1.84	0.78
11:L:47:ARG:HH11	11:L:47:ARG:CB	1.95	0.78
2:C:516:ASN:H	2:C:516:ASN:ND2	1.72	0.78
3:D:32:SER:O	3:D:36:VAL:HG23	1.84	0.78
7:H:14:HIS:CD2	7:H:16:SER:HB2	2.19	0.78
1:B:845:LEU:HD22	1:B:1374:VAL:HG21	1.65	0.78
1:B:857:ARG:HD3	1:B:861:GLY:O	1.83	0.78
1:B:1148:ILE:HG12	9:J:49:ILE:HD12	1.65	0.78
1:B:1325:THR:HG22	1:B:1325:THR:O	1.83	0.78
2:C:25:ILE:HD11	2:C:653:VAL:O	1.82	0.78
2:C:167:ILE:HG22	2:C:453:ILE:CD1	2.14	0.78
2:C:542:MET:HE3	2:C:636:PRO:HG2	1.65	0.78
2:C:29:ASP:HB3	2:C:658:ILE:HD13	1.65	0.78
5:F:202:SER:OG	5:F:204:THR:HG22	1.83	0.78
8:I:42:ILE:HG23	8:I:95:TYR:HE1	1.47	0.78
1:B:341:MET:HE1	2:C:1135:ARG:NH1	1.99	0.77
2:C:329:THR:HA	2:C:332:ASP:HB3	1.67	0.77
3:D:43:THR:HG22	3:D:44:LEU:H	1.47	0.77
1:B:608:ILE:HB	1:B:613:ILE:HD11	1.65	0.77
1:B:1193:LEU:HD22	1:B:1260:LEU:CD1	2.14	0.77
2:C:798:TYR:HE2	3:D:62:PHE:CE2	2.03	0.77
3:D:147:LEU:HB2	3:D:151:GLN:HB2	1.65	0.77
3:D:196:ASP:HB3	3:D:199:LYS:HB2	1.65	0.77
8:I:89:LEU:C	8:I:91:ASP:H	1.92	0.77
2:C:1099:VAL:HG13	2:C:1100:ASP:N	1.98	0.77
5:F:94:LYS:NZ	5:F:98:ILE:HD11	1.99	0.77
1:B:667:GLY:HA3	3:D:192:TRP:CH2	2.19	0.77
1:B:836:TYR:CE2	1:B:840:ARG:HD2	2.18	0.77
2:C:830:TYR:CE2	2:C:1000:PRO:HD3	2.18	0.77
2:C:1181:GLU:HG3	2:C:1188:LYS:HE3	1.67	0.77
4:E:134:THR:CG2	4:E:135:GLY:H	1.96	0.77
4:E:202:ILE:HG21	4:E:207:LEU:HB2	1.66	0.77
10:K:4:PRO:HD3	10:K:53:HIS:CD2	2.20	0.77
3:D:175:ALA:HB2	10:K:10:CYS:HB2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:76:LYS:C	6:G:79:ARG:HD2	2.10	0.77
1:B:885:THR:O	1:B:940:ARG:HD2	1.83	0.77
2:C:261:ARG:HB3	2:C:261:ARG:HH11	1.47	0.77
2:C:794:ASN:O	2:C:795:ILE:HD12	1.85	0.77
3:D:47:ASP:HA	12:M:69:ALA:CB	2.14	0.77
7:H:15:PRO:HA	7:H:18:PHE:CD1	2.20	0.77
3:D:163:ILE:HD13	3:D:163:ILE:N	1.98	0.77
4:E:71:LYS:HG2	4:E:74:GLN:HE21	1.50	0.77
7:H:14:HIS:ND1	7:H:15:PRO:HD2	2.00	0.77
1:B:524:VAL:HG12	1:B:525:GLN:N	2.00	0.77
2:C:589:VAL:HG12	2:C:590:HIS:H	1.50	0.77
2:C:773:MET:HE1	2:C:985:GLY:HA2	1.65	0.77
2:C:828:ALA:HB2	2:C:1085:ILE:HG23	1.67	0.77
1:B:763:ALA:O	1:B:803:SER:HB3	1.84	0.76
2:C:563:MET:CE	2:C:580:VAL:HB	2.15	0.76
2:C:825:VAL:CG1	2:C:826:ALA:H	1.96	0.76
5:F:56:LYS:HE3	5:F:84:ASP:HB2	1.67	0.76
1:B:1116:LEU:HB3	1:B:1308:THR:CG2	2.15	0.76
7:H:115:MET:HB2	7:H:116:PRO:HD2	1.66	0.76
14:P:3:C:H2'	14:P:4:G:C8	2.20	0.76
2:C:975:GLN:O	2:C:990:ILE:HD12	1.85	0.76
3:D:67:LEU:HD11	3:D:155:LEU:CD1	2.15	0.76
7:H:143:ILE:HG22	7:H:144:ARG:N	2.00	0.76
9:J:58:VAL:HG13	9:J:62:ILE:HD12	1.68	0.76
1:B:1030:ARG:HG3	1:B:1034:GLU:OE2	1.84	0.76
6:G:77:ASP:O	6:G:78:GLN:HB2	1.83	0.76
1:B:1189:SER:O	1:B:1241:ARG:HD3	1.86	0.76
2:C:33:VAL:HG21	2:C:638:PHE:HZ	1.51	0.76
6:G:89:GLU:O	6:G:93:ILE:HG13	1.85	0.76
1:B:816:HIS:CD2	2:C:764:SER:HB2	2.21	0.76
7:H:139:ILE:HG22	7:H:140:LYS:H	1.50	0.76
1:B:866:PHE:C	1:B:867:ILE:HD12	2.11	0.76
2:C:100:PRO:HD2	2:C:180:TYR:CE1	2.20	0.76
2:C:825:VAL:CG1	2:C:826:ALA:N	2.48	0.76
2:C:874:PHE:HA	2:C:913:GLY:O	1.85	0.76
3:D:66:ARG:NH1	10:K:2:ILE:HG21	2.01	0.76
1:B:1015:VAL:HG12	1:B:1019:CYS:SG	2.25	0.76
3:D:254:LYS:O	3:D:258:ILE:HD13	1.85	0.76
8:I:38:LEU:HD12	8:I:124:ARG:O	1.86	0.76
11:L:21:ILE:CG2	11:L:31:VAL:HG11	2.16	0.76
2:C:69:LEU:HD11	2:C:425:THR:HG23	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:235:SER:HB3	2:C:258:LEU:HG	1.68	0.75
2:C:792:MET:HE2	2:C:857:ARG:NH1	2.02	0.75
3:D:6:PRO:HB2	11:L:101:LEU:HD12	1.68	0.75
3:D:133:ILE:HD11	3:D:237:SER:HA	1.67	0.75
7:H:4:ILE:HG12	7:H:77:VAL:HG23	1.66	0.75
3:D:76:ASP:OD2	3:D:128:ASN:N	2.19	0.75
13:N:2:DA:H2'	13:N:3:DG:C8	2.20	0.75
2:C:603:LEU:HD13	2:C:608:ASP:HB2	1.68	0.75
1:B:230:ARG:H	1:B:233:TRP:HE3	1.28	0.75
1:B:590:ARG:NH2	1:B:620:LYS:HB3	1.95	0.75
2:C:39:ARG:NH2	2:C:665:GLU:HG2	2.01	0.75
2:C:879:ARG:NH1	2:C:883:LEU:HD13	2.00	0.75
1:B:382:PRO:HD3	1:B:428:TYR:CE2	2.21	0.75
1:B:1143:LEU:O	1:B:1146:VAL:HG23	1.87	0.75
1:B:447:GLN:HE22	15:T:20:DT:H4'	1.52	0.75
1:B:668:ASP:HB3	1:B:741:ASN:HD21	1.52	0.75
7:H:9:LEU:HD23	7:H:30:LEU:HD12	1.69	0.75
10:K:1:MET:H3	10:K:56:LEU:N	1.84	0.75
1:B:1424:VAL:HG13	1:B:1436:ILE:CD1	2.16	0.75
10:K:14:VAL:O	10:K:14:VAL:HG12	1.85	0.75
1:B:1438:THR:HB	2:C:1144:ALA:HB3	1.66	0.75
2:C:616:ILE:HD12	2:C:616:ILE:N	2.00	0.75
3:D:208:GLU:O	3:D:210:GLU:N	2.20	0.75
1:B:1004:ASN:ND2	5:F:167:ARG:HD2	2.01	0.74
1:B:1394:THR:HG22	1:B:1395:GLY:H	1.52	0.74
1:B:518:LYS:HE2	1:B:624:SER:O	1.87	0.74
1:B:946:VAL:HG13	5:F:201:LYS:HB3	1.67	0.74
1:B:1402:PHE:CE1	1:B:1403:GLU:HG3	2.21	0.74
2:C:29:ASP:HB3	2:C:658:ILE:CD1	2.16	0.74
2:C:1196:ILE:HD12	2:C:1200:ALA:HB3	1.68	0.74
7:H:44:TYR:HE1	7:H:157:ILE:H	1.34	0.74
9:J:14:LEU:HA	9:J:28:GLU:O	1.86	0.74
1:B:416:ARG:C	1:B:417:TYR:HD2	1.95	0.74
1:B:537:ARG:HD2	8:I:20:TYR:CE1	2.21	0.74
1:B:1208:THR:HB	1:B:1211:GLN:HG3	1.70	0.74
7:H:88:ASP:HB3	7:H:144:ARG:HA	1.68	0.74
9:J:51:ASN:O	9:J:54:GLU:HG3	1.87	0.74
1:B:567:LYS:HD2	1:B:568:PRO:HD2	1.66	0.74
3:D:166:GLU:HG3	11:L:10:PHE:CZ	2.19	0.74
9:J:25:LEU:HB3	9:J:38:ALA:HB2	1.69	0.74
1:B:1116:LEU:N	1:B:1308:THR:HG22	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:45:ALA:O	3:D:159:ALA:HA	1.86	0.74
2:C:69:LEU:HB3	2:C:429:PHE:HE1	1.51	0.74
4:E:144:THR:O	4:E:148:LEU:HB2	1.87	0.74
1:B:55:ASP:C	1:B:57:ARG:N	2.37	0.74
2:C:1007:VAL:HG22	2:C:1008:PRO:HD2	1.69	0.74
5:F:23:VAL:HG13	5:F:78:LEU:HD13	1.68	0.74
2:C:402:GLY:HA3	2:C:695:ALA:HB3	1.70	0.74
5:F:145:THR:HG21	5:F:187:TYR:CE2	2.23	0.74
10:K:23:ASN:C	10:K:25:LEU:H	1.93	0.74
11:L:46:ILE:O	11:L:50:LEU:HB2	1.87	0.74
1:B:4:GLN:O	1:B:5:GLN:HB2	1.86	0.74
1:B:388:LEU:HD23	1:B:432:VAL:HB	1.68	0.74
3:D:38:ILE:HA	3:D:173:ALA:HB2	1.68	0.74
7:H:1:MET:SD	7:H:79:PHE:HD1	2.10	0.74
1:B:547:LEU:HB3	11:L:58:PHE:CE1	2.20	0.73
5:F:16:PHE:CZ	5:F:20:LYS:HE2	2.23	0.73
1:B:1394:THR:HG21	1:B:1398:MET:SD	2.27	0.73
2:C:731:VAL:HG12	2:C:732:SER:H	1.53	0.73
1:B:23:SER:HA	1:B:233:TRP:NE1	2.03	0.73
1:B:343:LYS:HZ2	2:C:1151:LEU:HB3	1.52	0.73
1:B:1329:THR:HG22	1:B:1331:SER:H	1.53	0.73
2:C:102:VAL:CG2	2:C:112:LEU:HD22	2.18	0.73
2:C:185:THR:O	2:C:188:ASP:HB2	1.88	0.73
4:E:12:ARG:NH2	4:E:14:ARG:HG3	2.00	0.73
6:G:90:ARG:HD3	6:G:155:LEU:HD12	1.70	0.73
1:B:659:HIS:HA	2:C:1074:ASN:HD22	1.53	0.73
1:B:682:THR:CG2	1:B:728:LYS:HE3	2.16	0.73
2:C:274:PRO:HG2	2:C:359:GLU:HB3	1.70	0.73
2:C:847:ASP:C	2:C:849:GLY:H	1.94	0.73
9:J:82:GLU:O	9:J:104:LEU:HG	1.88	0.73
6:G:73:ALA:HA	6:G:143:PHE:HE1	1.54	0.73
7:H:139:ILE:HG22	7:H:140:LYS:N	2.01	0.73
11:L:65:HIS:CD2	11:L:67:PHE:H	2.05	0.73
1:B:41:MET:HB2	1:B:49:LYS:HA	1.69	0.73
1:B:903:ASN:HD22	1:B:904:THR:N	1.87	0.73
2:C:810:GLU:HA	2:C:815:ARG:NH1	2.02	0.73
11:L:49:GLU:HG3	11:L:94:ILE:CG1	2.19	0.73
1:B:1114:PRO:HB2	1:B:1311:VAL:HG23	1.71	0.73
5:F:94:LYS:HZ3	5:F:98:ILE:HD11	1.54	0.73
5:F:78:LEU:HA	5:F:107:THR:HB	1.71	0.73
1:B:722:LEU:H	1:B:722:LEU:HD12	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1028:THR:O	1:B:1032:LEU:HD12	1.88	0.72
2:C:758:PHE:HB3	2:C:761:HIS:HD2	1.53	0.72
1:B:855:THR:HG21	1:B:857:ARG:NE	2.03	0.72
1:B:1208:THR:O	1:B:1212:VAL:HG23	1.90	0.72
2:C:902:GLY:O	12:M:65:VAL:HG11	1.88	0.72
8:I:84:ALA:HA	8:I:87:ARG:HB2	1.70	0.72
10:K:64:ASN:HB3	10:K:65:PRO:CD	2.19	0.72
1:B:339:ASN:HB3	2:C:1117:GLN:HE22	1.54	0.72
2:C:378:LEU:HD12	2:C:378:LEU:O	1.89	0.72
15:T:20:DT:H2'	15:T:21:DA:C5'	2.06	0.72
1:B:90:VAL:CG1	1:B:297:GLN:HA	2.20	0.72
1:B:965:GLN:O	1:B:968:GLN:HB2	1.90	0.72
2:C:295:GLY:H	2:C:298:LEU:HD23	1.54	0.72
6:G:119:ARG:HH11	6:G:119:ARG:HG3	1.53	0.72
8:I:40:LEU:HD22	8:I:123:MET:HE3	1.69	0.72
1:B:56:PRO:HD2	1:B:58:LEU:HG	1.71	0.72
1:B:269:ILE:HD13	1:B:300:VAL:HG22	1.71	0.72
1:B:709:THR:HB	1:B:712:GLU:HG3	1.70	0.72
1:B:1127:ASP:CG	1:B:1130:GLN:HB2	2.14	0.72
1:B:1369:ALA:O	1:B:1372:VAL:HG12	1.88	0.72
2:C:642:ASP:HB3	2:C:649:LYS:CG	2.20	0.72
3:D:66:ARG:NH2	10:K:3:VAL:O	2.23	0.72
8:I:130:ARG:HB3	8:I:134:ASN:H	1.53	0.72
1:B:215:SER:HB3	1:B:218:ASP:HB2	1.69	0.72
1:B:965:GLN:HA	1:B:968:GLN:HG3	1.72	0.72
11:L:53:ASP:OD1	11:L:55:LYS:HB2	1.90	0.72
13:N:3:DG:H2''	13:N:4:DC:OP2	1.88	0.72
1:B:71:GLN:HE22	2:C:1176:ASN:ND2	1.88	0.72
2:C:882:THR:HG22	2:C:884:ARG:H	1.53	0.72
7:H:143:ILE:HG22	7:H:144:ARG:H	1.54	0.72
11:L:21:ILE:HG23	11:L:31:VAL:HG11	1.70	0.72
6:G:109:VAL:HG12	6:G:110:ASP:N	2.05	0.72
12:M:53:HIS:HB3	12:M:55:ILE:HD13	1.71	0.72
2:C:798:TYR:CE2	3:D:62:PHE:HE2	2.08	0.72
2:C:865:LYS:NZ	2:C:869:SER:HA	2.03	0.72
8:I:93:TYR:HB3	8:I:144:ILE:O	1.89	0.72
12:M:40:LEU:HD13	12:M:44:ASP:HB3	1.71	0.72
1:B:41:MET:HB3	1:B:49:LYS:HA	1.71	0.71
1:B:427:GLN:HG3	1:B:430:TRP:CE2	2.25	0.71
7:H:79:PHE:HE2	7:H:105:PRO:HG2	1.54	0.71
10:K:44:TYR:H	10:K:44:TYR:HD2	1.36	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:993:LEU:CD2	1:B:1022:LEU:HD21	2.20	0.71
1:B:639:PRO:HG2	1:B:640:GLN:H	1.53	0.71
2:C:910:VAL:HG12	2:C:912:ILE:H	1.55	0.71
4:E:128:VAL:O	4:E:132:GLN:HG3	1.90	0.71
1:B:144:THR:O	1:B:146:MET:HE2	1.90	0.71
1:B:567:LYS:CB	8:I:95:TYR:HA	2.20	0.71
1:B:586:ILE:HG22	1:B:587:HIS:N	2.05	0.71
1:B:1342:GLU:OE2	5:F:212:ARG:NH1	2.24	0.71
2:C:351:TYR:O	2:C:355:ILE:HG13	1.90	0.71
2:C:642:ASP:HB3	2:C:649:LYS:HG3	1.72	0.71
7:H:7:LEU:HD12	7:H:74:TYR:OH	1.90	0.71
8:I:63:LEU:C	8:I:90:ALA:HB3	2.16	0.71
1:B:1261:LYS:HE3	9:J:44:TYR:CD2	2.26	0.71
2:C:819:ALA:HB1	2:C:1093:GLN:HE21	1.56	0.71
3:D:238:ILE:HG23	3:D:242:GLN:HB2	1.71	0.71
4:E:14:ARG:HH22	4:E:16:LYS:NZ	1.86	0.71
5:F:23:VAL:HB	5:F:30:ILE:HD11	1.71	0.71
1:B:873:MET:HE3	1:B:957:PRO:HG3	1.72	0.71
1:B:1017:LEU:CB	5:F:205:SER:HA	2.19	0.71
2:C:175:ARG:HG2	2:C:175:ARG:HH11	1.56	0.71
2:C:758:PHE:HB3	2:C:761:HIS:CD2	2.25	0.71
2:C:794:ASN:C	2:C:795:ILE:HD12	2.15	0.71
2:C:1201:LYS:HE3	2:C:1205:GLN:OE1	1.90	0.71
8:I:127:GLY:O	8:I:128:ASN:HB2	1.91	0.71
1:B:1312:ASN:O	1:B:1316:VAL:HG23	1.89	0.71
2:C:642:ASP:HB3	2:C:649:LYS:CD	2.20	0.71
2:C:879:ARG:HH12	2:C:883:LEU:HD13	1.56	0.71
2:C:1182:CYS:O	2:C:1182:CYS:SG	2.48	0.71
1:B:67:CYS:O	1:B:70:CYS:HB3	1.91	0.71
1:B:657:LEU:HD12	1:B:657:LEU:O	1.91	0.71
2:C:69:LEU:HB3	2:C:429:PHE:CE1	2.25	0.71
5:F:16:PHE:CE2	5:F:20:LYS:HE2	2.24	0.71
7:H:15:PRO:HA	7:H:18:PHE:CE1	2.26	0.71
1:B:567:LYS:HB3	8:I:96:VAL:N	2.05	0.70
2:C:1187:ASN:O	2:C:1188:LYS:HB2	1.90	0.70
7:H:80:LYS:HD3	7:H:80:LYS:N	2.06	0.70
1:B:49:LYS:HZ1	1:B:61:ILE:H	1.39	0.70
1:B:483:ASP:HB2	2:C:987:LYS:HG3	1.73	0.70
1:B:541:ILE:CD1	1:B:549:MET:HE1	2.13	0.70
1:B:710:LEU:HD13	9:J:94:ASP:O	1.90	0.70
1:B:827:THR:HG22	1:B:828:ALA:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1261:LYS:HA	1:B:1264:GLU:HB3	1.73	0.70
2:C:168:GLY:N	2:C:450:ALA:HB1	2.04	0.70
7:H:7:LEU:HB2	7:H:74:TYR:CE2	2.24	0.70
1:B:53:LEU:HD22	1:B:54:ASN:ND2	2.06	0.70
1:B:92:HIS:O	1:B:94:GLY:N	2.24	0.70
1:B:496:GLU:HG2	6:G:99:LEU:HD22	1.73	0.70
2:C:276:ILE:HG22	2:C:278:GLN:O	1.90	0.70
3:D:194:GLU:O	3:D:195:GLN:HG3	1.91	0.70
12:M:40:LEU:HD22	12:M:44:ASP:CG	2.17	0.70
1:B:50:ILE:C	1:B:52:GLY:H	2.00	0.70
2:C:190:TYR:CE2	10:K:62:ARG:HB3	2.26	0.70
4:E:71:LYS:HG2	4:E:74:GLN:NE2	2.06	0.70
7:H:117:GLN:C	7:H:119:LEU:H	1.98	0.70
8:I:81:PRO:CB	8:I:82:PRO:HD2	2.21	0.70
8:I:102:TYR:OH	8:I:122:LEU:HD22	1.91	0.70
1:B:49:LYS:HZ1	1:B:61:ILE:N	1.89	0.70
1:B:728:LYS:O	1:B:732:LEU:HG	1.91	0.70
2:C:190:TYR:CD2	10:K:62:ARG:HB3	2.26	0.70
3:D:244:VAL:O	3:D:248:ILE:HG13	1.90	0.70
15:T:21:DA:H2'	15:T:22:DT:C5'	2.21	0.70
1:B:87:ALA:HB3	1:B:276:LEU:HD23	1.73	0.70
2:C:90:ILE:HD12	2:C:432:MET:SD	2.32	0.70
2:C:102:VAL:HG13	2:C:958:GLN:HE21	1.56	0.70
3:D:74:SER:HB3	3:D:77:ILE:HG12	1.74	0.70
6:G:111:LEU:H	6:G:111:LEU:CD1	2.03	0.70
9:J:111:THR:HG22	9:J:112:SER:N	2.06	0.70
1:B:340:LEU:HD13	1:B:1429:ILE:CG2	2.20	0.70
1:B:53:LEU:CD2	1:B:54:ASN:H	2.00	0.70
1:B:351:THR:HB	2:C:1103:ILE:HD12	1.74	0.70
1:B:567:LYS:HG3	1:B:568:PRO:HD2	1.73	0.70
1:B:886:ILE:HG23	1:B:887:GLY:N	2.06	0.70
1:B:886:ILE:HD12	1:B:943:LEU:HB3	1.72	0.70
8:I:100:THR:OG1	8:I:138:GLU:HG3	1.90	0.70
1:B:105:CYS:O	1:B:114:LEU:HG	1.92	0.70
1:B:1445:ILE:H	1:B:1445:ILE:CD1	2.00	0.70
2:C:955:THR:CG2	2:C:956:THR:N	2.54	0.70
3:D:242:GLN:C	3:D:244:VAL:H	1.99	0.70
1:B:382:PRO:HB3	1:B:428:TYR:CE2	2.26	0.69
1:B:567:LYS:HD3	8:I:95:TYR:CD2	2.27	0.69
1:B:600:PRO:HG2	1:B:601:LYS:H	1.56	0.69
1:B:1208:THR:HG22	1:B:1210:GLY:N	2.04	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:881:GLN:HE22	1:B:960:ILE:H	1.39	0.69
1:B:915:SER:O	1:B:919:ILE:HG13	1.91	0.69
1:B:1063:MET:CG	1:B:1436:ILE:HG23	2.22	0.69
2:C:542:MET:CE	2:C:743:ILE:HG13	2.22	0.69
2:C:654:ARG:H	2:C:657:HIS:CD2	2.08	0.69
2:C:1122:ARG:HB3	15:T:22:DT:OP1	1.91	0.69
3:D:56:THR:HG22	3:D:58:LEU:HD23	1.73	0.69
3:D:184:ASN:HD21	3:D:187:LYS:HA	1.56	0.69
3:D:209:TYR:HD1	3:D:209:TYR:H	1.40	0.69
11:L:45:LEU:HG	11:L:94:ILE:HD13	1.73	0.69
1:B:91:PHE:H	1:B:297:GLN:HE22	1.40	0.69
1:B:382:PRO:HB3	1:B:428:TYR:HE2	1.57	0.69
1:B:1436:ILE:HD13	2:C:1139:ILE:HG23	1.73	0.69
2:C:1085:ILE:HD12	2:C:1085:ILE:H	1.57	0.69
1:B:853:ASP:O	1:B:854:ASN:HB2	1.91	0.69
2:C:52:ASN:OD1	2:C:177:LYS:HB2	1.92	0.69
7:H:39:THR:HG22	7:H:41:LYS:H	1.57	0.69
11:L:29:ASN:O	11:L:76:GLN:HG3	1.92	0.69
3:D:179:GLU:HG2	3:D:180:TYR:N	2.07	0.69
5:F:135:PHE:HD2	5:F:140:LEU:HD21	1.56	0.69
1:B:49:LYS:NZ	1:B:61:ILE:HG13	2.07	0.69
2:C:378:LEU:O	2:C:382:ILE:HG13	1.92	0.69
2:C:916:THR:O	2:C:935:ARG:HG2	1.92	0.69
2:C:1007:VAL:CG2	2:C:1008:PRO:HD2	2.22	0.69
7:H:145:VAL:HG12	7:H:146:LYS:N	2.08	0.69
1:B:535:THR:CG2	1:B:616:VAL:HA	2.20	0.69
1:B:1445:ILE:HG12	7:H:18:PHE:CE2	2.27	0.69
2:C:210:LYS:HD2	2:C:480:SER:OG	1.91	0.69
2:C:728:ARG:NH1	2:C:1047:PHE:HB3	2.07	0.69
2:C:910:VAL:HG12	2:C:911:ILE:N	2.07	0.69
7:H:59:GLY:HA3	7:H:70:PHE:CD2	2.28	0.69
11:L:50:LEU:HD11	11:L:75:ILE:HD13	1.75	0.69
12:M:32:ALA:HB3	12:M:55:ILE:CD1	2.18	0.69
1:B:738:LYS:HB2	1:B:740:LEU:HG	1.74	0.69
1:B:845:LEU:HB3	1:B:848:ILE:HD12	1.75	0.69
2:C:800:GLN:HG2	10:K:52:THR:HG21	1.73	0.69
2:C:1084:GLN:H	2:C:1084:GLN:HE21	1.40	0.69
5:F:14:ARG:HH21	5:F:141:VAL:HG12	1.57	0.69
6:G:109:VAL:HG12	6:G:110:ASP:H	1.57	0.69
7:H:61:ILE:HG23	7:H:66:GLY:O	1.93	0.69
11:L:58:PHE:HE2	11:L:74:ARG:HE	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:LYS:HB3	8:I:95:TYR:HA	1.74	0.69
2:C:100:PRO:HG3	2:C:172:ILE:HD12	1.74	0.69
2:C:906:SER:O	2:C:941:LEU:HD23	1.93	0.69
3:D:163:ILE:HD13	3:D:163:ILE:H	1.55	0.69
13:N:2:DA:H2''	13:N:3:DG:O5'	1.93	0.69
1:B:182:VAL:HG22	1:B:201:VAL:HA	1.74	0.69
1:B:1063:MET:SD	1:B:1436:ILE:HG23	2.33	0.69
15:T:25:DC:H42	15:T:26:DA:H62	1.24	0.69
1:B:469:ARG:HB3	1:B:469:ARG:HH11	1.57	0.68
1:B:844:ALA:O	1:B:845:LEU:HD23	1.92	0.68
3:D:69:LEU:HD12	3:D:69:LEU:N	2.08	0.68
3:D:241:ASP:O	3:D:245:VAL:HG23	1.93	0.68
1:B:86:LEU:HG	1:B:237:THR:O	1.93	0.68
1:B:768:GLN:CG	1:B:816:HIS:HA	2.22	0.68
2:C:361:LEU:HD21	2:C:377:PHE:CD2	2.28	0.68
8:I:24:CYS:HB2	8:I:44:VAL:HG21	1.75	0.68
8:I:42:ILE:HG23	8:I:95:TYR:CE1	2.28	0.68
1:B:374:LEU:C	1:B:436:ILE:HD11	2.17	0.68
1:B:683:ILE:HG21	1:B:801:GLU:HG3	1.74	0.68
2:C:57:TYR:N	2:C:57:TYR:HD1	1.92	0.68
2:C:174:LEU:HD22	2:C:202:TYR:CE1	2.29	0.68
2:C:295:GLY:N	2:C:298:LEU:HD23	2.09	0.68
2:C:461:LEU:HD12	2:C:461:LEU:N	2.08	0.68
1:B:244:PRO:O	1:B:246:VAL:N	2.27	0.68
2:C:539:LEU:H	2:C:539:LEU:HD12	1.59	0.68
15:T:21:DA:C2'	15:T:22:DT:O5'	2.41	0.68
1:B:637:LYS:HB3	1:B:641:VAL:HG11	1.75	0.68
2:C:189:LEU:HD12	2:C:196:PRO:HA	1.74	0.68
6:G:82:THR:HG22	6:G:84:TYR:N	2.08	0.68
6:G:111:LEU:HD12	6:G:111:LEU:N	2.06	0.68
1:B:19:PHE:O	1:B:1416:ALA:HA	1.94	0.68
1:B:351:THR:HB	2:C:1103:ILE:CD1	2.24	0.68
2:C:53:GLN:HG2	2:C:547:VAL:CG2	2.24	0.68
2:C:569:TYR:CE1	2:C:589:VAL:HG21	2.29	0.68
2:C:570:VAL:HB	2:C:573:GLN:HB3	1.74	0.68
2:C:579:ARG:HH11	2:C:579:ARG:HG2	1.58	0.68
2:C:798:TYR:CE2	3:D:62:PHE:CE2	2.81	0.68
2:C:1095:LEU:H	2:C:1095:LEU:HD12	1.59	0.68
1:B:34:LYS:HG2	1:B:36:ARG:NH2	2.09	0.68
1:B:92:HIS:HB3	1:B:95:PHE:HB2	1.76	0.68
1:B:215:SER:HB3	1:B:218:ASP:OD2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:25:ILE:HD12	2:C:651:LEU:HD13	1.76	0.68
2:C:243:ALA:CB	2:C:251:ILE:HG12	2.24	0.68
2:C:651:LEU:HD11	2:C:707:PRO:CB	2.24	0.68
5:F:114:ASN:O	5:F:115:ASN:HB3	1.94	0.68
12:M:38:LEU:O	12:M:39:SER:HB3	1.93	0.68
2:C:361:LEU:HD21	2:C:377:PHE:HD2	1.58	0.68
3:D:18:VAL:HG23	3:D:240:VAL:HB	1.76	0.68
2:C:405:ARG:NE	2:C:632:ARG:HG3	2.09	0.68
2:C:955:THR:HG22	2:C:956:THR:N	2.08	0.68
2:C:1180:PHE:HB3	2:C:1191:ILE:HD12	1.75	0.68
1:B:1341:ILE:CG2	1:B:1342:GLU:H	2.06	0.67
2:C:380:TYR:O	2:C:384:ARG:HG2	1.95	0.67
2:C:398:ARG:HG3	2:C:398:ARG:HH11	1.59	0.67
2:C:589:VAL:HG12	2:C:590:HIS:N	2.09	0.67
2:C:619:ILE:HD12	9:J:65:ASP:HB2	1.76	0.67
3:D:142:VAL:H	10:K:16:ASP:HB3	1.58	0.67
3:D:144:ILE:HG22	3:D:145:CYS:N	2.09	0.67
1:B:93:VAL:HG22	1:B:301:ALA:HA	1.76	0.67
1:B:973:ILE:CD1	1:B:1038:THR:HG23	2.24	0.67
1:B:1198:ASP:HB3	1:B:1201:ALA:HB3	1.74	0.67
1:B:1263:ILE:O	1:B:1267:MET:HG3	1.94	0.67
1:B:1373:ASP:O	1:B:1376:THR:HG22	1.94	0.67
7:H:9:LEU:HD12	7:H:10:ASN:N	2.10	0.67
1:B:446:ARG:HB2	1:B:487:MET:SD	2.34	0.67
2:C:622:LYS:HE2	9:J:59:VAL:CG2	2.13	0.67
8:I:89:LEU:HB3	8:I:91:ASP:OD1	1.94	0.67
10:K:44:TYR:HD2	10:K:44:TYR:N	1.93	0.67
1:B:34:LYS:H	1:B:34:LYS:HD3	1.59	0.67
1:B:40:THR:CB	1:B:41:MET:HE2	2.24	0.67
1:B:444:PHE:HB3	1:B:458:HIS:CD2	2.29	0.67
1:B:1152:ILE:HG23	1:B:1193:LEU:HD13	1.76	0.67
2:C:255:GLN:O	2:C:271:ALA:HB1	1.93	0.67
2:C:542:MET:SD	2:C:747:MET:HE3	2.34	0.67
1:B:821:ARG:HD2	1:B:825:ILE:HD11	1.77	0.67
1:B:973:ILE:HG21	1:B:1036:ARG:O	1.95	0.67
2:C:291:ILE:HD11	2:C:375:ALA:HB1	1.76	0.67
4:E:12:ARG:HH22	4:E:14:ARG:CG	2.02	0.67
5:F:13:TRP:O	5:F:16:PHE:HB3	1.95	0.67
2:C:777:ALA:HA	2:C:1095:LEU:HA	1.75	0.67
5:F:182:ASP:HB3	5:F:185:ALA:HB2	1.75	0.67
1:B:519:PRO:HD3	1:B:631:HIS:HD1	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:185:THR:H	2:C:188:ASP:HB2	1.60	0.67
3:D:17:ASN:N	3:D:240:VAL:HG11	2.10	0.67
5:F:161:LYS:HD2	5:F:195:VAL:HG23	1.76	0.67
1:B:577:ILE:O	1:B:580:VAL:HG23	1.94	0.67
2:C:1099:VAL:HG22	2:C:1103:ILE:HD13	1.74	0.67
3:D:5:GLY:O	3:D:7:GLN:HG3	1.95	0.67
1:B:61:ILE:HG22	1:B:62:ASP:H	1.58	0.67
1:B:1211:GLN:O	1:B:1214:GLU:HB2	1.95	0.67
2:C:1099:VAL:CG1	2:C:1100:ASP:N	2.58	0.67
4:E:47:LEU:HD13	4:E:48:ILE:N	2.10	0.67
4:E:153:ARG:HB3	4:E:154:PHE:CE1	2.30	0.67
7:H:96:GLN:HG3	7:H:97:HIS:CD2	2.30	0.67
1:B:470:LEU:HD13	1:B:487:MET:HE1	1.77	0.67
2:C:842:ASN:O	2:C:846:ILE:HG13	1.95	0.67
5:F:191:LYS:O	5:F:193:GLY:N	2.27	0.67
7:H:145:VAL:HG12	7:H:146:LYS:H	1.60	0.67
1:B:567:LYS:CD	8:I:95:TYR:HA	2.25	0.66
2:C:911:ILE:HD11	2:C:941:LEU:HD13	1.76	0.66
3:D:46:ILE:HD12	3:D:67:LEU:HB3	1.77	0.66
5:F:213:ILE:HG12	5:F:214:CYS:N	2.09	0.66
7:H:111:THR:HG22	7:H:113:HIS:H	1.59	0.66
1:B:590:ARG:O	1:B:591:PHE:HB2	1.93	0.66
1:B:794:PRO:HG2	1:B:795:GLU:OE2	1.95	0.66
5:F:15:ALA:HA	5:F:140:LEU:O	1.95	0.66
7:H:51:TYR:O	7:H:54:ILE:HG13	1.96	0.66
10:K:36:LEU:HB2	10:K:47:ARG:HH12	1.59	0.66
1:B:29:ALA:HB1	2:C:1184:GLY:HA3	1.77	0.66
1:B:54:ASN:C	1:B:56:PRO:HD3	2.20	0.66
1:B:67:CYS:C	1:B:68:GLN:HG3	2.21	0.66
1:B:1227:ILE:HG22	1:B:1228:TRP:N	2.09	0.66
2:C:101:MET:HB3	2:C:109:THR:HG22	1.76	0.66
1:B:399:HIS:CB	1:B:400:PRO:HD3	2.24	0.66
1:B:1325:THR:O	5:F:148:GLU:HB2	1.95	0.66
1:B:1445:ILE:HD12	1:B:1445:ILE:N	2.02	0.66
2:C:687:GLU:O	2:C:689:LEU:HG	1.96	0.66
2:C:746:SER:HB2	2:C:1046:PRO:HG2	1.76	0.66
4:E:24:ALA:C	4:E:26:THR:H	2.04	0.66
4:E:170:THR:CB	4:E:172:LEU:HG	2.22	0.66
8:I:27:GLU:HG2	8:I:39:THR:HG23	1.77	0.66
1:B:765:VAL:HG12	1:B:766:GLY:N	2.09	0.66
1:B:903:ASN:HD22	1:B:904:THR:H	1.41	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:826:ALA:HB2	2:C:1008:PRO:HB3	1.77	0.66
3:D:176:ILE:HG22	3:D:177:GLU:N	2.09	0.66
8:I:15:VAL:HG22	8:I:26:ILE:CD1	2.26	0.66
1:B:56:PRO:O	1:B:57:ARG:HD2	1.96	0.66
1:B:285:PRO:HG2	1:B:288:ALA:HB3	1.77	0.66
2:C:243:ALA:HB2	2:C:251:ILE:HG12	1.78	0.66
8:I:89:LEU:O	8:I:91:ASP:N	2.26	0.66
9:J:7:CYS:HB3	9:J:14:LEU:HD21	1.77	0.66
15:T:14:DC:H2''	15:T:15:DT:H71	1.77	0.66
1:B:406:ILE:HG13	1:B:431:LYS:HB3	1.78	0.66
1:B:418:SER:O	1:B:420:ARG:N	2.28	0.66
2:C:20:ASP:C	2:C:22:SER:H	2.02	0.66
9:J:80:SER:HB2	9:J:103:CYS:SG	2.36	0.66
11:L:61:TYR:C	11:L:61:TYR:CD2	2.70	0.66
1:B:690:VAL:HG11	1:B:794:PRO:HD3	1.78	0.66
1:B:852:TYR:CD2	1:B:1060:PRO:HB2	2.31	0.66
1:B:899:VAL:CG1	1:B:908:LEU:HD21	2.24	0.66
2:C:792:MET:CE	2:C:857:ARG:HH12	2.08	0.66
2:C:1016:ALA:O	2:C:1020:ARG:HG3	1.96	0.66
6:G:97:ARG:O	6:G:101:ILE:HG13	1.96	0.66
8:I:98:TYR:HE1	8:I:139:ASN:HA	1.61	0.66
1:B:70:CYS:O	1:B:72:GLU:HG2	1.96	0.66
1:B:382:PRO:HD3	1:B:428:TYR:CD2	2.30	0.66
1:B:606:LEU:HB3	1:B:614:PHE:CE2	2.31	0.66
1:B:1074:GLU:C	1:B:1076:ALA:H	2.02	0.66
1:B:1242:VAL:O	1:B:1243:VAL:HB	1.96	0.66
2:C:278:GLN:HG2	2:C:279:ASP:N	2.05	0.66
2:C:850:LEU:HD12	2:C:851:PHE:N	2.11	0.66
2:C:1202:LEU:O	2:C:1206:GLU:HG3	1.95	0.66
6:G:73:ALA:HA	6:G:143:PHE:CE1	2.30	0.66
12:M:32:ALA:H	12:M:55:ILE:HG13	1.60	0.66
1:B:332:LYS:HA	1:B:337:ARG:HD2	1.78	0.66
1:B:567:LYS:HD3	8:I:95:TYR:HA	1.78	0.66
2:C:20:ASP:O	2:C:22:SER:N	2.28	0.66
2:C:1180:PHE:HB3	2:C:1191:ILE:HD13	1.77	0.66
3:D:147:LEU:HD23	3:D:147:LEU:N	2.09	0.66
4:E:40:HIS:CB	7:H:73:LYS:NZ	2.58	0.66
4:E:53:SER:H	4:E:148:LEU:CD2	2.09	0.66
8:I:40:LEU:HD13	8:I:123:MET:HB2	1.78	0.66
1:B:441:PRO:HG3	1:B:498:ARG:HB2	1.77	0.65
2:C:63:ILE:O	2:C:67:SER:HB3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:327:ARG:O	2:C:331:LEU:HD13	1.95	0.65
2:C:990:ILE:HG22	2:C:991:GLY:N	2.10	0.65
1:B:239:LEU:HD12	1:B:240:PRO:HD2	1.77	0.65
1:B:869:GLY:O	5:F:204:THR:HG21	1.96	0.65
2:C:1079:LYS:HG2	2:C:1080:LYS:H	1.61	0.65
3:D:179:GLU:HG2	3:D:180:TYR:H	1.61	0.65
3:D:253:LYS:O	3:D:256:ALA:HB3	1.96	0.65
7:H:66:GLY:O	7:H:67:SER:C	2.38	0.65
1:B:714:PHE:O	1:B:718:VAL:HG23	1.97	0.65
1:B:870:GLU:HG2	5:F:208:TYR:CG	2.31	0.65
2:C:563:MET:HE3	2:C:580:VAL:HB	1.76	0.65
5:F:48:ASP:CG	5:F:49:SER:H	2.03	0.65
5:F:61:GLN:HB2	5:F:79:TRP:HE3	1.61	0.65
1:B:103:CYS:SG	1:B:108:MET:HE1	2.36	0.65
1:B:308:ILE:HG22	1:B:309:ALA:H	1.60	0.65
1:B:443:LEU:CD2	1:B:455:MET:HB3	2.20	0.65
1:B:590:ARG:HB2	1:B:590:ARG:HH11	1.61	0.65
1:B:920:LEU:HD23	1:B:921:GLY:N	2.10	0.65
2:C:745:PRO:C	2:C:747:MET:H	2.04	0.65
2:C:1001:PHE:CD2	3:D:34:ARG:NH2	2.65	0.65
3:D:165:LYS:O	11:L:6:ARG:NH1	2.30	0.65
11:L:55:LYS:HD2	11:L:81:TYR:CD1	2.32	0.65
1:B:919:ILE:HG21	1:B:983:ILE:HD11	1.78	0.65
1:B:40:THR:C	1:B:41:MET:HG3	2.22	0.65
1:B:90:VAL:HG11	1:B:297:GLN:HA	1.79	0.65
1:B:298:PHE:CZ	1:B:314:ALA:HB2	2.32	0.65
1:B:298:PHE:HZ	1:B:314:ALA:HB2	1.61	0.65
1:B:310:GLY:O	1:B:312:PRO:HD2	1.97	0.65
2:C:217:ARG:NE	2:C:405:ARG:HB2	2.10	0.65
2:C:1160:VAL:HG11	2:C:1169:MET:SD	2.36	0.65
3:D:251:LEU:HD12	3:D:251:LEU:O	1.95	0.65
7:H:65:ASP:O	7:H:67:SER:N	2.29	0.65
10:K:2:ILE:HG22	10:K:3:VAL:O	1.96	0.65
3:D:43:THR:HG22	3:D:44:LEU:N	2.12	0.65
3:D:184:ASN:ND2	3:D:187:LYS:HA	2.12	0.65
6:G:135:ARG:HG2	6:G:137:TYR:CE1	2.31	0.65
1:B:418:SER:C	1:B:420:ARG:H	2.04	0.65
1:B:709:THR:HG22	1:B:711:ARG:N	2.12	0.65
1:B:1450:LEU:HG	1:B:1450:LEU:O	1.96	0.65
2:C:314:LEU:H	2:C:314:LEU:HD12	1.61	0.65
2:C:705:MET:HE3	2:C:705:MET:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1002:THR:O	2:C:1004:GLU:N	2.29	0.65
2:C:1079:LYS:HA	3:D:27:LEU:HD21	1.79	0.65
7:H:115:MET:HB3	7:H:163:ILE:HD11	1.78	0.65
8:I:139:ASN:O	8:I:140:ALA:HB2	1.97	0.65
10:K:5:VAL:HG12	10:K:6:ARG:HG3	1.77	0.65
1:B:34:LYS:HG2	1:B:36:ARG:HH21	1.60	0.65
1:B:49:LYS:HE2	1:B:61:ILE:HD12	1.77	0.65
1:B:560:ILE:HG13	8:I:78:SER:HB2	1.78	0.65
2:C:1084:GLN:NE2	2:C:1084:GLN:N	2.44	0.65
2:C:1096:ARG:O	2:C:1097:HIS:HB2	1.97	0.65
3:D:214:ASN:HB3	3:D:217:ASP:OD2	1.96	0.65
8:I:43:ASN:ND2	8:I:46:LEU:HD12	2.11	0.65
1:B:311:GLN:O	1:B:312:PRO:C	2.40	0.65
1:B:1050:GLU:HG2	1:B:1051:ALA:N	2.12	0.65
1:B:1411:GLU:HA	1:B:1414:ALA:HB3	1.78	0.65
2:C:658:ILE:HG22	2:C:662:MET:HE2	1.78	0.65
2:C:770:GLN:HG2	2:C:983:ARG:O	1.97	0.65
2:C:918:ILE:HD12	2:C:935:ARG:NH1	2.12	0.65
2:C:953:LEU:HD23	2:C:953:LEU:O	1.97	0.65
2:C:1138:MET:HE3	2:C:1143:ALA:HB3	1.79	0.65
1:B:353:ILE:HG21	1:B:487:MET:HG3	1.78	0.64
5:F:17:ARG:O	5:F:21:GLU:HG3	1.96	0.64
9:J:26:LEU:HD23	9:J:37:GLU:HA	1.78	0.64
1:B:78:PRO:HA	2:C:1201:LYS:HZ2	1.63	0.64
1:B:591:PHE:HA	1:B:595:THR:HG21	1.80	0.64
2:C:301:ILE:HG21	2:C:314:LEU:HD21	1.79	0.64
2:C:651:LEU:HD11	2:C:707:PRO:HB2	1.79	0.64
2:C:1166:CYS:HB2	2:C:1215:ARG:NH1	2.12	0.64
1:B:305:ASP:OD1	1:B:326:ARG:HD2	1.98	0.64
1:B:659:HIS:HA	2:C:1074:ASN:ND2	2.13	0.64
1:B:694:THR:O	1:B:698:GLN:HG3	1.96	0.64
2:C:210:LYS:HE2	2:C:462:ALA:CA	2.26	0.64
2:C:574:SER:HB3	2:C:577:ALA:HB2	1.79	0.64
5:F:67:GLU:O	5:F:70:SER:HB3	1.96	0.64
7:H:35:GLU:OE2	7:H:48:VAL:HG23	1.96	0.64
11:L:57:LEU:HD12	11:L:77:THR:O	1.97	0.64
1:B:504:LEU:HD11	6:G:91:ALA:HB1	1.78	0.64
1:B:1289:ARG:HD2	1:B:1303:GLU:OE2	1.97	0.64
2:C:496:ARG:O	2:C:539:LEU:HD12	1.97	0.64
2:C:880:THR:HG21	2:C:934:LYS:HE3	1.80	0.64
7:H:110:VAL:HG22	7:H:161:GLY:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ARG:NH2	14:P:3:C:H1'	2.12	0.64
1:B:343:LYS:NZ	2:C:1151:LEU:HB3	2.12	0.64
1:B:705:LYS:HB2	1:B:708:MET:HE3	1.77	0.64
1:B:896:ARG:NH2	1:B:1030:ARG:HH21	1.96	0.64
1:B:960:ILE:O	1:B:963:ILE:HG22	1.98	0.64
1:B:1315:GLU:C	1:B:1317:MET:H	2.04	0.64
1:B:1348:LEU:HG	1:B:1372:VAL:CG2	2.27	0.64
2:C:57:TYR:N	2:C:57:TYR:CD1	2.63	0.64
2:C:953:LEU:CD2	2:C:965:LYS:HB2	2.28	0.64
3:D:61:GLU:HA	3:D:64:ALA:HB3	1.80	0.64
4:E:180:LEU:HD23	4:E:195:ILE:HD12	1.77	0.64
5:F:2:ASP:O	5:F:3:GLN:HG2	1.98	0.64
7:H:43:GLY:HA3	7:H:80:LYS:HB3	1.78	0.64
1:B:427:GLN:HG3	1:B:430:TRP:CZ2	2.32	0.64
1:B:961:ARG:HG3	1:B:961:ARG:HH11	1.62	0.64
1:B:1121:GLU:HG3	1:B:1122:PRO:HD2	1.78	0.64
2:C:801:LYS:O	10:K:52:THR:CG2	2.45	0.64
2:C:801:LYS:O	10:K:52:THR:HG23	1.96	0.64
3:D:261:ALA:HA	3:D:264:GLN:OE1	1.98	0.64
8:I:40:LEU:HD13	8:I:123:MET:HE3	1.78	0.64
1:B:358:ASN:C	1:B:359:LEU:HD23	2.23	0.64
1:B:834:THR:HG21	1:B:1077:THR:HA	1.77	0.64
2:C:825:VAL:HG12	2:C:826:ALA:H	1.58	0.64
2:C:1079:LYS:HG2	2:C:1080:LYS:N	2.13	0.64
4:E:131:GLU:O	4:E:132:GLN:HG2	1.97	0.64
4:E:204:ASP:O	4:E:208:GLU:HB2	1.98	0.64
8:I:95:TYR:HE2	8:I:97:MET:CG	2.11	0.64
1:B:69:THR:O	1:B:71:GLN:N	2.30	0.64
1:B:444:PHE:HB3	1:B:458:HIS:HD2	1.63	0.64
2:C:269:ILE:HG21	2:C:282:ILE:HD13	1.79	0.64
5:F:23:VAL:O	5:F:28:TYR:HB2	1.97	0.64
10:K:35:ALA:O	10:K:39:LEU:HD12	1.97	0.64
12:M:39:SER:O	12:M:40:LEU:HG	1.98	0.64
1:B:138:ILE:HG21	1:B:222:LEU:HD21	1.79	0.64
1:B:768:GLN:HG2	1:B:816:HIS:CA	2.26	0.64
2:C:114:PRO:HG3	2:C:181:LEU:HD11	1.80	0.64
3:D:248:ILE:HD13	11:L:101:LEU:HD23	1.80	0.64
4:E:164:ILE:HG22	4:E:168:LYS:HG3	1.78	0.64
1:B:883:LEU:O	1:B:886:ILE:HG22	1.97	0.64
2:C:577:ALA:CB	2:C:589:VAL:HG11	2.20	0.64
2:C:652:LYS:HB3	2:C:689:LEU:HD23	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:661:LEU:HD23	2:C:679:TYR:O	1.97	0.64
2:C:956:THR:CG2	2:C:960:GLY:HA2	2.28	0.64
4:E:146:GLN:O	4:E:149:THR:HG22	1.97	0.64
10:K:1:MET:N	10:K:56:LEU:N	2.45	0.64
1:B:477:PRO:HG2	1:B:521:MET:HG2	1.80	0.63
1:B:853:ASP:OD1	1:B:855:THR:N	2.31	0.63
1:B:1119:TYR:HA	1:B:1305:VAL:HG13	1.79	0.63
2:C:113:TYR:HE2	2:C:192:LEU:HD22	1.63	0.63
2:C:355:ILE:O	2:C:359:GLU:HB2	1.98	0.63
2:C:797:TYR:HB2	2:C:852:ARG:O	1.98	0.63
2:C:1022:THR:HG23	2:C:1022:THR:O	1.98	0.63
7:H:106:MET:HG2	7:H:107:LYS:H	1.60	0.63
1:B:184:SER:HB3	1:B:199:LEU:CD2	2.28	0.63
1:B:675:THR:O	1:B:679:ILE:HG13	1.97	0.63
1:B:1225:PHE:CZ	1:B:1227:ILE:HD11	2.33	0.63
2:C:780:VAL:HG21	10:K:56:LEU:HD11	1.79	0.63
1:B:381:THR:C	1:B:383:TYR:H	2.06	0.63
1:B:883:LEU:HD11	1:B:1017:LEU:HD11	1.81	0.63
2:C:65:GLU:OE2	2:C:247:GLY:HA2	1.95	0.63
8:I:99:GLY:HA3	8:I:118:PHE:HA	1.81	0.63
1:B:93:VAL:HG23	1:B:304:MET:HE3	1.81	0.63
2:C:899:ILE:CD1	2:C:911:ILE:HA	2.27	0.63
10:K:48:ARG:HE	10:K:49:MET:HE2	1.63	0.63
15:T:11:DT:H2"	15:T:12:DA:OP2	1.99	0.63
1:B:881:GLN:NE2	1:B:958:VAL:O	2.32	0.63
1:B:1120:LEU:HD13	1:B:1120:LEU:H	1.64	0.63
2:C:310:MET:O	2:C:313:MET:HB2	1.99	0.63
2:C:461:LEU:HD12	2:C:461:LEU:H	1.64	0.63
2:C:865:LYS:HB2	2:C:961:LEU:HD21	1.81	0.63
3:D:8:VAL:HG11	11:L:105:PHE:HD1	1.63	0.63
6:G:73:ALA:O	6:G:74:ILE:HG13	1.98	0.63
6:G:119:ARG:HG3	6:G:119:ARG:NH1	2.13	0.63
7:H:15:PRO:HG3	7:H:66:GLY:HA3	1.79	0.63
1:B:287:HIS:HA	1:B:290:GLU:HG2	1.81	0.63
1:B:372:LYS:HA	1:B:435:HIS:ND1	2.13	0.63
1:B:901:LEU:O	1:B:921:GLY:N	2.31	0.63
1:B:996:ASN:O	1:B:998:LEU:N	2.29	0.63
2:C:431:TYR:CD1	2:C:447:ALA:HB2	2.34	0.63
2:C:844:SER:HB3	2:C:848:ARG:HH12	1.64	0.63
4:E:27:LEU:HD13	4:E:173:HIS:HB2	1.81	0.63
6:G:79:ARG:HB3	6:G:144:GLU:CD	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:43:ARG:H	10:K:43:ARG:HD3	1.63	0.63
1:B:107:CYS:HA	1:B:171:GLN:OE1	1.98	0.63
1:B:1022:LEU:HD11	1:B:1026:LEU:HD12	1.81	0.63
1:B:1042:PHE:CE2	1:B:1046:LEU:HD11	2.33	0.63
2:C:510:LYS:CG	2:C:511:PRO:HD3	2.28	0.63
4:E:173:HIS:O	4:E:175:PHE:N	2.31	0.63
5:F:13:TRP:CE3	5:F:39:LEU:HD13	2.34	0.63
7:H:106:MET:CG	7:H:107:LYS:N	2.60	0.63
8:I:95:TYR:CE2	8:I:97:MET:HG3	2.33	0.63
1:B:32:VAL:HG21	1:B:68:GLN:HE21	1.64	0.63
1:B:185:TRP:CZ3	1:B:200:ARG:HG2	2.34	0.63
1:B:325:ILE:HG22	2:C:1210:MET:HE2	1.81	0.63
1:B:399:HIS:HB3	1:B:400:PRO:CD	2.27	0.63
1:B:535:THR:HG21	1:B:616:VAL:CA	2.24	0.63
1:B:751:SER:O	1:B:752:LYS:HB2	1.96	0.63
1:B:899:VAL:HB	1:B:929:LEU:HD12	1.80	0.63
2:C:105:SER:O	2:C:106:ASP:HB2	1.98	0.63
2:C:113:TYR:CE2	2:C:192:LEU:HD22	2.34	0.63
2:C:1020:ARG:HB2	2:C:1022:THR:HG22	1.79	0.63
3:D:164:ALA:HA	3:D:167:HIS:O	1.99	0.63
1:B:134:ARG:HD2	1:B:221:SER:O	1.99	0.63
2:C:515:HIS:H	2:C:518:HIS:CD2	2.05	0.63
2:C:842:ASN:ND2	2:C:845:SER:OG	2.31	0.63
3:D:18:VAL:CG2	3:D:240:VAL:HB	2.28	0.63
3:D:45:ALA:HA	3:D:72:LEU:CD1	2.28	0.63
4:E:29:LEU:HD13	7:H:82:PHE:CZ	2.34	0.63
5:F:55:ARG:C	5:F:57:MET:H	2.05	0.63
1:B:445:ASN:HB2	1:B:454:SER:O	1.98	0.62
1:B:1074:GLU:HB3	1:B:1075:PRO:HD3	1.81	0.62
1:B:1336:MET:HE3	1:B:1381:LEU:HG	1.81	0.62
2:C:305:VAL:O	2:C:305:VAL:HG12	1.98	0.62
2:C:334:ILE:O	2:C:334:ILE:HG22	1.99	0.62
2:C:580:VAL:HG22	2:C:624:LEU:HB3	1.81	0.62
2:C:821:GLN:NE2	2:C:851:PHE:HA	2.13	0.62
3:D:8:VAL:HG21	11:L:105:PHE:HA	1.80	0.62
7:H:15:PRO:CG	7:H:66:GLY:HA3	2.29	0.62
11:L:21:ILE:HG23	11:L:31:VAL:CG1	2.28	0.62
11:L:31:VAL:HG12	11:L:32:VAL:N	2.14	0.62
1:B:78:PRO:HA	2:C:1201:LYS:NZ	2.14	0.62
1:B:902:LEU:HG	1:B:926:GLN:HG3	1.81	0.62
1:B:963:ILE:HD11	1:B:1048:ASN:CB	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:37:PHE:HE2	2:C:542:MET:HA	1.63	0.62
2:C:880:THR:HB	2:C:934:LYS:HD2	1.80	0.62
6:G:75:PRO:C	6:G:77:ASP:H	2.07	0.62
1:B:55:ASP:CG	1:B:55:ASP:O	2.41	0.62
1:B:69:THR:C	1:B:71:GLN:H	2.07	0.62
1:B:519:PRO:HD3	1:B:631:HIS:ND1	2.14	0.62
2:C:193:LYS:NZ	12:M:32:ALA:HB1	2.15	0.62
2:C:365:THR:HG23	2:C:367:LEU:H	1.65	0.62
2:C:515:HIS:O	2:C:518:HIS:HB2	2.00	0.62
2:C:579:ARG:HG2	2:C:579:ARG:NH1	2.14	0.62
2:C:850:LEU:HD12	2:C:851:PHE:H	1.65	0.62
9:J:50:THR:CG2	9:J:52:ILE:HG23	2.27	0.62
10:K:44:TYR:N	10:K:44:TYR:CD2	2.64	0.62
1:B:252:PHE:O	1:B:253:ASN:HB2	1.98	0.62
1:B:513:SER:OG	1:B:515:GLN:HG2	1.99	0.62
1:B:684:ALA:O	1:B:687:LYS:HB2	2.00	0.62
2:C:314:LEU:O	2:C:317:CYS:HB3	1.98	0.62
2:C:810:GLU:CA	2:C:815:ARG:HH12	2.09	0.62
2:C:843:GLN:O	2:C:846:ILE:N	2.32	0.62
4:E:175:PHE:HZ	7:H:85:GLU:HG3	1.63	0.62
1:B:719:VAL:HG12	1:B:723:ASN:HD21	1.65	0.62
1:B:1334:ASP:C	1:B:1336:MET:H	2.07	0.62
1:B:1436:ILE:O	1:B:1437:GLY:C	2.43	0.62
2:C:192:LEU:O	2:C:193:LYS:HB2	1.99	0.62
2:C:839:MET:HG3	2:C:1010:LEU:CD1	2.22	0.62
3:D:31:ASN:OD1	3:D:34:ARG:HD3	1.98	0.62
3:D:100:THR:HG22	3:D:101:LEU:N	2.14	0.62
3:D:235:VAL:HG12	10:K:13:VAL:CG2	2.29	0.62
6:G:75:PRO:HG2	6:G:77:ASP:O	1.99	0.62
6:G:132:LEU:HD11	7:H:61:ILE:CD1	2.30	0.62
9:J:35:VAL:HG12	9:J:36:GLU:N	2.14	0.62
1:B:1224:LEU:HD11	1:B:1240:CYS:HB2	1.82	0.62
1:B:1325:THR:HG23	5:F:148:GLU:N	2.14	0.62
1:B:1441:PHE:CZ	6:G:89:GLU:HA	2.34	0.62
3:D:36:VAL:HG21	3:D:251:LEU:HB2	1.80	0.62
1:B:2:VAL:HG11	2:C:1157:ALA:HB1	1.82	0.62
1:B:11:LEU:HD12	2:C:1193:GLN:O	2.00	0.62
1:B:35:ILE:O	1:B:35:ILE:HG22	1.99	0.62
1:B:35:ILE:O	1:B:84:ILE:HG13	2.00	0.62
1:B:863:VAL:HG11	1:B:866:PHE:CE2	2.34	0.62
1:B:1029:ARG:HD2	1:B:1033:GLN:NE2	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1102:LYS:HG2	1:B:1106:ASN:HD21	1.64	0.62
1:B:1349:TYR:CA	1:B:1372:VAL:HG21	2.29	0.62
2:C:526:GLU:HG2	2:C:538:ASN:HD22	1.64	0.62
2:C:859:TYR:OH	2:C:941:LEU:HD12	1.99	0.62
7:H:122:ASN:HD22	7:H:125:SER:HB3	1.64	0.62
8:I:127:GLY:HA3	8:I:130:ARG:HH22	1.64	0.62
9:J:8:ARG:O	9:J:9:ASP:HB2	2.00	0.62
1:B:222:LEU:O	1:B:224:PHE:N	2.33	0.62
1:B:316:GLN:HB2	1:B:322:VAL:HG23	1.82	0.62
1:B:401:GLY:C	1:B:435:HIS:CD2	2.78	0.62
2:C:115:GLN:HG2	2:C:193:LYS:HB2	1.81	0.62
2:C:220:GLY:O	2:C:222:ILE:HG13	2.00	0.62
2:C:604:ARG:NH1	2:C:691:GLU:OE2	2.33	0.62
3:D:163:ILE:HD11	11:L:10:PHE:CE1	2.34	0.62
4:E:34:GLN:C	4:E:36:LYS:H	2.07	0.62
1:B:57:ARG:HG2	1:B:57:ARG:HH11	1.64	0.62
1:B:110:CYS:SG	1:B:111:GLY:N	2.72	0.62
1:B:809:THR:HG23	1:B:812:GLU:OE1	2.00	0.62
1:B:1430:LEU:O	2:C:1196:ILE:HG22	2.00	0.62
2:C:205:ILE:HD12	2:C:205:ILE:N	2.14	0.62
2:C:364:ILE:HG12	2:C:585:VAL:HG13	1.80	0.62
4:E:30:GLY:O	4:E:32:GLU:N	2.33	0.62
7:H:106:MET:CG	7:H:107:LYS:H	2.12	0.62
1:B:2:VAL:CG1	2:C:1157:ALA:HB1	2.29	0.62
1:B:55:ASP:N	1:B:56:PRO:HD3	2.15	0.62
1:B:148:CYS:O	1:B:168:GLY:HA2	2.00	0.62
1:B:849:MET:HE3	1:B:1061:GLY:HA2	1.80	0.62
1:B:1153:TYR:CE1	9:J:42:LEU:HD13	2.35	0.62
2:C:405:ARG:HE	2:C:629:ASP:HB3	1.64	0.62
2:C:467:GLY:N	2:C:475:SER:HB3	2.15	0.62
2:C:1181:GLU:CG	2:C:1188:LYS:HE3	2.30	0.62
4:E:7:THR:HG21	4:E:32:GLU:OE2	2.00	0.62
5:F:153:HIS:HB3	5:F:196:VAL:HG11	1.82	0.62
2:C:36:ALA:HA	2:C:39:ARG:HD2	1.81	0.61
3:D:33:LEU:HG	3:D:37:MET:HE2	1.82	0.61
3:D:147:LEU:HD12	3:D:151:GLN:O	2.00	0.61
3:D:148:ARG:HD3	3:D:149:LYS:HG3	1.82	0.61
5:F:15:ALA:O	5:F:19:VAL:HG23	2.00	0.61
1:B:38:PRO:HA	1:B:270:LEU:HD23	1.81	0.61
1:B:50:ILE:O	1:B:52:GLY:N	2.33	0.61
1:B:180:LYS:HZ2	1:B:294:SER:HB3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:LYS:HD3	1:B:302:THR:HG22	1.82	0.61
1:B:1074:GLU:HB3	1:B:1075:PRO:CD	2.29	0.61
2:C:294:ASP:O	2:C:296:GLU:N	2.29	0.61
2:C:309:GLN:HG3	9:J:52:ILE:HD13	1.82	0.61
2:C:519:TRP:CH2	2:C:748:ILE:HD13	2.36	0.61
2:C:737:THR:CG2	9:J:66:PRO:HA	2.29	0.61
2:C:792:MET:H	2:C:857:ARG:HA	1.64	0.61
4:E:60:LYS:O	4:E:64:VAL:HG23	1.99	0.61
9:J:50:THR:HG23	9:J:52:ILE:CG2	2.30	0.61
1:B:215:SER:HB3	1:B:218:ASP:CB	2.30	0.61
1:B:1155:ASP:OD2	1:B:1161:THR:HA	1.99	0.61
2:C:172:ILE:HD13	2:C:178:ASN:HD22	1.63	0.61
2:C:583:ASN:OD1	2:C:628:THR:HG22	2.00	0.61
2:C:1072:MET:HB2	2:C:1085:ILE:HD13	1.82	0.61
9:J:62:ILE:O	9:J:62:ILE:HG12	1.99	0.61
1:B:885:THR:O	1:B:885:THR:HG22	1.99	0.61
1:B:899:VAL:HG13	1:B:908:LEU:CD2	2.30	0.61
2:C:1169:MET:CE	2:C:1201:LYS:HA	2.30	0.61
3:D:31:ASN:O	3:D:34:ARG:HB3	2.00	0.61
7:H:7:LEU:HD12	7:H:74:TYR:HH	1.65	0.61
7:H:80:LYS:HD3	7:H:80:LYS:H	1.65	0.61
1:B:184:SER:HB3	1:B:199:LEU:HD23	1.82	0.61
2:C:108:VAL:HG12	2:C:109:THR:H	1.66	0.61
2:C:593:PRO:HG2	2:C:617:ARG:HH21	1.64	0.61
2:C:910:VAL:HG12	2:C:911:ILE:H	1.63	0.61
4:E:153:ARG:C	4:E:154:PHE:CD1	2.78	0.61
10:K:64:ASN:HB3	10:K:65:PRO:HD3	1.81	0.61
1:B:18:GLN:HB2	2:C:1215:ARG:HB2	1.82	0.61
1:B:88:LYS:HE3	1:B:280:GLU:OE2	2.00	0.61
1:B:1348:LEU:HG	1:B:1372:VAL:HG23	1.83	0.61
2:C:542:MET:HE3	2:C:636:PRO:CG	2.31	0.61
2:C:745:PRO:O	2:C:747:MET:N	2.34	0.61
2:C:1012:ILE:HD13	2:C:1092:TYR:OH	1.99	0.61
2:C:1182:CYS:O	2:C:1183:LYS:O	2.19	0.61
2:C:1196:ILE:HD12	2:C:1200:ALA:CB	2.30	0.61
3:D:116:LYS:HD3	3:D:140:ASN:HB3	1.82	0.61
4:E:207:LEU:O	4:E:211:LEU:HB2	2.01	0.61
1:B:401:GLY:C	1:B:435:HIS:HD2	2.09	0.61
1:B:1444:MET:CG	7:H:60:ARG:HA	2.31	0.61
2:C:244:LEU:HD11	2:C:366:GLN:HE22	1.65	0.61
2:C:390:LEU:O	2:C:392:ARG:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:33:PHE:CE1	7:H:80:LYS:HE3	2.36	0.61
7:H:37:SER:OG	7:H:45:ILE:HB	2.01	0.61
1:B:317:LYS:O	1:B:318:SER:HB3	1.99	0.61
1:B:417:TYR:HD2	1:B:417:TYR:N	1.99	0.61
2:C:204:ILE:C	2:C:205:ILE:HD12	2.25	0.61
2:C:287:ARG:HG2	2:C:292:ILE:HA	1.83	0.61
3:D:238:ILE:HG22	3:D:243:VAL:HG23	1.82	0.61
11:L:10:PHE:CD2	11:L:10:PHE:N	2.68	0.61
1:B:152:VAL:HG13	1:B:153:PRO:HD2	1.82	0.61
1:B:222:LEU:O	1:B:224:PHE:HD1	1.83	0.61
1:B:596:THR:C	1:B:598:LEU:H	2.08	0.61
1:B:890:ASP:H	1:B:1296:GLY:HA3	1.65	0.61
2:C:868:MET:O	2:C:870:ILE:HG13	2.00	0.61
2:C:884:ARG:HB2	2:C:935:ARG:HA	1.83	0.61
2:C:884:ARG:O	2:C:936:ASP:HB3	1.99	0.61
7:H:26:LEU:HD11	7:H:70:PHE:CD1	2.36	0.61
10:K:8:PHE:H	10:K:49:MET:CE	2.13	0.61
1:B:57:ARG:HG2	1:B:57:ARG:NH1	2.15	0.61
1:B:224:PHE:CD2	1:B:231:PRO:HG3	2.36	0.61
1:B:266:LEU:HD21	1:B:303:TYR:CE1	2.36	0.61
1:B:503:GLN:C	1:B:504:LEU:HD12	2.25	0.61
1:B:545:GLN:C	1:B:547:LEU:N	2.56	0.61
1:B:567:LYS:HD2	1:B:568:PRO:CD	2.31	0.61
1:B:666:ILE:HD11	2:C:1067:ARG:O	2.01	0.61
2:C:44:VAL:CG1	2:C:199:MET:HG2	2.30	0.61
2:C:510:LYS:HG3	2:C:511:PRO:HD3	1.82	0.61
2:C:1079:LYS:CA	3:D:27:LEU:HD21	2.31	0.61
2:C:1169:MET:HE1	2:C:1201:LYS:HA	1.82	0.61
3:D:22:LEU:HD21	3:D:25:VAL:HG11	1.81	0.61
8:I:44:VAL:O	8:I:44:VAL:HG12	2.00	0.61
9:J:82:GLU:HB3	9:J:104:LEU:CD1	2.31	0.61
1:B:53:LEU:CD2	1:B:54:ASN:HD22	2.14	0.60
1:B:115:LEU:O	1:B:122:MET:HE2	2.00	0.60
1:B:1325:THR:HG23	5:F:148:GLU:H	1.63	0.60
1:B:1404:GLU:HB2	1:B:1408:ILE:HG13	1.82	0.60
2:C:288:ALA:HB1	2:C:331:LEU:HD12	1.83	0.60
4:E:205:ASP:O	4:E:208:GLU:HB3	2.00	0.60
5:F:157:SER:OG	5:F:160:GLU:HG3	2.01	0.60
1:B:265:LYS:HG2	1:B:303:TYR:CA	2.30	0.60
1:B:806:ARG:HH12	2:C:729:ILE:HD11	1.66	0.60
4:E:8:PHE:CE2	7:H:73:LYS:HD3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:16:LYS:NZ	4:E:16:LYS:HB3	2.15	0.60
1:B:364:VAL:HG13	1:B:364:VAL:O	2.00	0.60
1:B:446:ARG:CD	1:B:480:ALA:HB2	2.25	0.60
1:B:500:GLU:OE2	1:B:1438:THR:HG21	2.01	0.60
1:B:635:ARG:HA	1:B:635:ARG:HH11	1.64	0.60
1:B:1042:PHE:HE2	1:B:1046:LEU:HD11	1.66	0.60
2:C:603:LEU:HD13	2:C:608:ASP:CB	2.30	0.60
2:C:642:ASP:HB3	2:C:649:LYS:HD2	1.84	0.60
2:C:735:ALA:O	2:C:738:PHE:HE1	1.84	0.60
2:C:1220:ARG:NH1	2:C:1220:ARG:HB3	2.16	0.60
1:B:92:HIS:O	1:B:95:PHE:N	2.34	0.60
1:B:93:VAL:HG13	1:B:301:ALA:HB1	1.83	0.60
2:C:493:SER:HA	2:C:751:VAL:HG21	1.83	0.60
2:C:758:PHE:HZ	2:C:1031:LEU:HD22	1.67	0.60
3:D:39:ALA:CA	3:D:164:ALA:HB3	2.31	0.60
4:E:40:HIS:ND1	4:E:41:GLN:HG3	2.16	0.60
6:G:89:GLU:HB3	6:G:134:ILE:CD1	2.32	0.60
1:B:93:VAL:HG21	1:B:301:ALA:O	2.01	0.60
1:B:1151:GLU:HA	9:J:44:TYR:O	2.01	0.60
1:B:1443:VAL:O	1:B:1444:MET:HG3	2.02	0.60
2:C:37:PHE:HE1	2:C:41:LYS:HG3	1.64	0.60
2:C:311:LEU:O	2:C:312:GLU:C	2.44	0.60
2:C:497:ARG:NH2	2:C:775:LYS:NZ	2.49	0.60
2:C:1017:ILE:H	2:C:1018:PRO:CD	2.15	0.60
3:D:254:LYS:C	3:D:256:ALA:H	2.09	0.60
15:T:15:DT:H2''	15:T:16:DG:OP2	2.00	0.60
15:T:24:DG:H5'	15:T:25:DC:OP2	2.02	0.60
1:B:741:ASN:HD22	1:B:742:ASN:N	2.00	0.60
2:C:821:GLN:HE22	2:C:851:PHE:CA	2.13	0.60
10:K:48:ARG:HD2	10:K:48:ARG:C	2.27	0.60
1:B:647:GLY:O	1:B:651:LYS:HG3	2.01	0.60
1:B:1227:ILE:HG22	1:B:1228:TRP:H	1.66	0.60
1:B:1329:THR:HG22	1:B:1331:SER:N	2.17	0.60
2:C:217:ARG:HD2	2:C:217:ARG:O	2.00	0.60
2:C:563:MET:HE1	2:C:580:VAL:HB	1.82	0.60
2:C:878:GLN:HA	2:C:885:MET:SD	2.42	0.60
1:B:350:ARG:HB2	2:C:1128:LEU:HD11	1.83	0.60
1:B:871:ASP:OD2	1:B:873:MET:HB2	2.02	0.60
1:B:1001:ARG:O	1:B:1002:GLY:O	2.19	0.60
1:B:1101:LEU:HD11	1:B:1105:LEU:HD11	1.83	0.60
2:C:117:ALA:HB1	2:C:122:LEU:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:215:GLN:HA	2:C:215:GLN:NE2	2.17	0.60
2:C:879:ARG:HD3	2:C:883:LEU:HD22	1.84	0.60
2:C:1106:ARG:HD2	2:C:1125:ASP:O	2.01	0.60
7:H:91:VAL:HG23	7:H:141:SER:O	2.02	0.60
8:I:118:PHE:C	8:I:120:GLY:H	2.10	0.60
1:B:1161:THR:HG22	1:B:1163:ILE:HG13	1.82	0.60
2:C:983:ARG:HD2	2:C:1091:TYR:HB3	1.84	0.60
2:C:992:ILE:HD11	11:L:66:PRO:HB2	1.84	0.60
4:E:145:MET:O	4:E:149:THR:HB	2.01	0.60
5:F:157:SER:C	5:F:159:ASP:H	2.09	0.60
9:J:106:CYS:SG	9:J:108:HIS:HB2	2.42	0.60
2:C:67:SER:HB2	2:C:92:PHE:HD1	1.67	0.59
2:C:273:LEU:HD12	2:C:276:ILE:HD11	1.84	0.59
2:C:281:PRO:HG2	2:C:284:ILE:HG13	1.83	0.59
2:C:562:GLY:O	2:C:590:HIS:ND1	2.31	0.59
2:C:1181:GLU:HG3	2:C:1188:LYS:CE	2.32	0.59
7:H:1:MET:SD	7:H:79:PHE:CD1	2.95	0.59
1:B:339:ASN:HB3	2:C:1117:GLN:NE2	2.17	0.59
2:C:496:ARG:HH12	2:C:539:LEU:HB2	1.66	0.59
2:C:847:ASP:C	2:C:849:GLY:N	2.56	0.59
4:E:64:VAL:HG22	4:E:129:LEU:HD22	1.83	0.59
8:I:102:TYR:CD2	8:I:102:TYR:N	2.70	0.59
1:B:351:THR:CG2	2:C:1103:ILE:HG13	2.32	0.59
1:B:567:LYS:HB2	1:B:568:PRO:CD	2.32	0.59
1:B:925:LEU:HD13	1:B:983:ILE:HD12	1.83	0.59
1:B:986:ILE:HD12	1:B:1032:LEU:HD11	1.84	0.59
1:B:1027:ALA:O	1:B:1031:VAL:HG23	2.02	0.59
2:C:373:ARG:HA	2:C:566:LEU:HD23	1.84	0.59
2:C:778:MET:CE	2:C:1094:ARG:HG2	2.28	0.59
2:C:841:MET:HE1	2:C:980:PHE:CE1	2.37	0.59
2:C:882:THR:HG22	2:C:884:ARG:HB2	1.83	0.59
2:C:980:PHE:HD2	2:C:1094:ARG:HA	1.67	0.59
3:D:138:GLU:N	3:D:138:GLU:OE1	2.36	0.59
5:F:118:PRO:O	5:F:122:LYS:HG3	2.02	0.59
7:H:23:LYS:HG3	7:H:56:ILE:HD13	1.85	0.59
7:H:79:PHE:HZ	7:H:106:MET:HE2	1.67	0.59
8:I:81:PRO:CB	8:I:82:PRO:CD	2.80	0.59
1:B:466:SER:HB3	11:L:2:ASN:ND2	2.17	0.59
1:B:829:VAL:C	1:B:831:THR:H	2.10	0.59
1:B:1129:GLU:HG3	1:B:1132:LYS:HD2	1.83	0.59
1:B:1143:LEU:HB2	1:B:1271:ILE:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1420:ASP:HB3	1:B:1422:ARG:HG3	1.83	0.59
2:C:286:PHE:CD1	2:C:297:ILE:HG23	2.38	0.59
2:C:519:TRP:HE1	2:C:635:ARG:NH2	2.00	0.59
2:C:843:GLN:O	2:C:844:SER:C	2.45	0.59
2:C:956:THR:HG23	2:C:960:GLY:HA2	1.84	0.59
3:D:112:ASN:HB3	3:D:114:TYR:CE1	2.38	0.59
10:K:28:ASP:O	10:K:30:LEU:HG	2.01	0.59
1:B:445:ASN:HB2	1:B:455:MET:HA	1.84	0.59
1:B:608:ILE:C	1:B:610:GLY:H	2.10	0.59
2:C:600:LEU:O	2:C:609:ILE:HD12	2.02	0.59
2:C:782:LEU:HD12	2:C:788:ARG:HH11	1.66	0.59
3:D:73:GLN:NE2	3:D:75:MET:HB2	2.18	0.59
4:E:54:GLU:O	4:E:58:VAL:HG23	2.03	0.59
5:F:78:LEU:HD23	5:F:78:LEU:C	2.28	0.59
1:B:629:LEU:HD22	1:B:633:VAL:HG23	1.83	0.59
1:B:994:GLN:O	1:B:996:ASN:N	2.35	0.59
1:B:1017:LEU:HB2	5:F:206:GLY:N	2.09	0.59
1:B:1120:LEU:HD23	1:B:1124:HIS:O	2.02	0.59
9:J:59:VAL:C	9:J:61:ASP:H	2.10	0.59
1:B:195:ASP:O	1:B:196:GLU:HB3	2.01	0.59
1:B:230:ARG:HB2	1:B:233:TRP:CE3	2.38	0.59
1:B:1193:LEU:HB2	1:B:1260:LEU:HD11	1.83	0.59
1:B:1341:ILE:CG2	1:B:1342:GLU:N	2.63	0.59
1:B:1420:ASP:O	1:B:1421:CYS:HB2	2.02	0.59
2:C:402:GLY:CA	2:C:695:ALA:HB3	2.32	0.59
2:C:806:THR:HG23	2:C:1046:PRO:HD3	1.85	0.59
2:C:982:SER:HB3	2:C:1092:TYR:HE2	1.66	0.59
2:C:1099:VAL:CG1	2:C:1100:ASP:H	2.15	0.59
7:H:31:LEU:CD2	7:H:48:VAL:HG21	2.33	0.59
10:K:16:ASP:OD1	10:K:17:LYS:HD2	2.02	0.59
1:B:629:LEU:O	1:B:633:VAL:HG23	2.03	0.59
1:B:1041:ALA:O	1:B:1045:VAL:HG23	2.02	0.59
1:B:1213:GLY:O	1:B:1214:GLU:C	2.45	0.59
2:C:610:ASN:HB3	2:C:613:VAL:HG23	1.84	0.59
2:C:982:SER:HB3	2:C:1092:TYR:CE2	2.37	0.59
3:D:35:ARG:NH1	11:L:41:THR:H	1.99	0.59
4:E:195:ILE:HG22	4:E:198:LEU:HG	1.84	0.59
10:K:14:VAL:HG12	10:K:50:ILE:HD11	1.84	0.59
10:K:23:ASN:C	10:K:25:LEU:N	2.60	0.59
1:B:92:HIS:HD2	1:B:304:MET:HE1	1.67	0.59
1:B:144:THR:O	1:B:146:MET:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:901:LEU:HG	1:B:926:GLN:HE21	1.68	0.59
1:B:979:SER:OG	1:B:980:ASP:N	2.32	0.59
1:B:1148:ILE:HG23	9:J:49:ILE:HB	1.84	0.59
2:C:100:PRO:CD	2:C:180:TYR:HE1	2.12	0.59
2:C:604:ARG:HA	2:C:609:ILE:O	2.03	0.59
9:J:69:PRO:HG2	9:J:85:PHE:CD2	2.38	0.59
1:B:477:PRO:CG	1:B:521:MET:HG2	2.33	0.59
1:B:901:LEU:H	1:B:926:GLN:CD	2.10	0.59
1:B:1076:ALA:CA	1:B:1079:MET:HE2	2.22	0.59
2:C:449:ASN:C	2:C:451:LYS:H	2.10	0.59
2:C:797:TYR:OH	2:C:971:THR:HG21	2.03	0.59
8:I:98:TYR:CE1	8:I:139:ASN:HA	2.38	0.59
11:L:55:LYS:HD2	11:L:81:TYR:HD1	1.68	0.59
1:B:1050:GLU:O	1:B:1053:PHE:N	2.36	0.58
2:C:171:PRO:HD2	2:C:457:LEU:HD13	1.85	0.58
2:C:280:ILE:HB	2:C:285:ILE:HD11	1.83	0.58
2:C:331:LEU:O	2:C:334:ILE:HB	2.03	0.58
2:C:1181:GLU:H	2:C:1188:LYS:HG2	1.69	0.58
6:G:111:LEU:O	6:G:113:GLY:N	2.36	0.58
10:K:22:LEU:O	10:K:22:LEU:HD12	2.02	0.58
1:B:679:ILE:HG12	1:B:732:LEU:CD1	2.33	0.58
2:C:126:SER:OG	2:C:172:ILE:HD11	2.03	0.58
2:C:833:TYR:N	2:C:833:TYR:HD1	2.02	0.58
2:C:955:THR:CG2	2:C:956:THR:H	2.14	0.58
2:C:1167:GLY:HA3	2:C:1216:LEU:H	1.68	0.58
7:H:129:SER:HB3	7:H:138:THR:OG1	2.03	0.58
12:M:30:ILE:HG22	12:M:31:CYS:N	2.17	0.58
1:B:849:MET:HE1	1:B:1061:GLY:HA2	1.84	0.58
1:B:901:LEU:HD22	1:B:919:ILE:HG22	1.83	0.58
1:B:932:GLU:OE1	1:B:987:VAL:HG22	2.03	0.58
2:C:102:VAL:HG13	2:C:958:GLN:NE2	2.18	0.58
7:H:114:LEU:HG	7:H:162:SER:HB3	1.84	0.58
1:B:224:PHE:CE2	1:B:234:MET:HE2	2.39	0.58
1:B:886:ILE:CG2	1:B:887:GLY:N	2.66	0.58
2:C:98:THR:HG23	2:C:127:GLY:O	2.03	0.58
2:C:193:LYS:HZ2	12:M:32:ALA:HB1	1.69	0.58
2:C:731:VAL:HG12	2:C:732:SER:N	2.18	0.58
2:C:745:PRO:C	2:C:747:MET:N	2.60	0.58
2:C:885:MET:HA	2:C:936:ASP:HB3	1.85	0.58
5:F:42:PHE:CZ	5:F:58:MET:HE3	2.38	0.58
7:H:138:THR:CG2	7:H:139:ILE:HG13	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:118:PHE:O	8:I:120:GLY:N	2.35	0.58
1:B:35:ILE:HB	1:B:83:HIS:O	2.02	0.58
1:B:335:ARG:HH11	2:C:1202:LEU:HD13	1.66	0.58
1:B:446:ARG:HB2	1:B:487:MET:HG2	1.86	0.58
1:B:469:ARG:NH1	1:B:469:ARG:HB3	2.19	0.58
2:C:273:LEU:HB2	2:C:276:ILE:CD1	2.34	0.58
2:C:361:LEU:HD11	2:C:381:MET:HE1	1.86	0.58
2:C:701:ILE:HD11	2:C:703:ILE:HD11	1.84	0.58
2:C:755:ILE:CG2	2:C:809:MET:HE3	2.33	0.58
2:C:806:THR:HB	2:C:809:MET:HG3	1.84	0.58
2:C:811:TYR:N	2:C:811:TYR:CD1	2.70	0.58
2:C:880:THR:O	2:C:881:ASN:HB2	2.02	0.58
3:D:98:VAL:HG12	3:D:99:LEU:N	2.18	0.58
1:B:49:LYS:HZ1	1:B:61:ILE:HG13	1.66	0.58
1:B:545:GLN:C	1:B:547:LEU:H	2.09	0.58
1:B:947:PHE:HE2	1:B:954:TRP:CD2	2.22	0.58
2:C:978:ASP:OD2	2:C:1098:MET:HG2	2.03	0.58
2:C:1163:CYS:SG	2:C:1165:ILE:HB	2.44	0.58
3:D:98:VAL:HG12	3:D:99:LEU:H	1.67	0.58
7:H:45:ILE:HD13	7:H:78:VAL:CG1	2.34	0.58
1:B:403:LYS:O	1:B:415:LEU:HB2	2.03	0.58
1:B:675:THR:OG1	1:B:736:ASN:ND2	2.37	0.58
1:B:787:PHE:CE1	1:B:796:SER:HA	2.38	0.58
1:B:1299:VAL:HG12	1:B:1300:LYS:H	1.68	0.58
2:C:118:ARG:HG2	2:C:204:ILE:HD13	1.86	0.58
1:B:41:MET:HB3	1:B:50:ILE:H	1.69	0.58
1:B:567:LYS:CB	1:B:568:PRO:CD	2.81	0.58
1:B:858:ASN:HD22	1:B:858:ASN:C	2.11	0.58
1:B:997:LEU:HD13	1:B:1018:PHE:HE2	1.69	0.58
2:C:313:MET:O	2:C:316:PRO:HD2	2.03	0.58
2:C:843:GLN:O	2:C:846:ILE:HB	2.03	0.58
3:D:172:PRO:O	3:D:235:VAL:CG2	2.52	0.58
4:E:14:ARG:NH2	4:E:16:LYS:HZ1	1.94	0.58
5:F:42:PHE:CE1	5:F:58:MET:HE3	2.39	0.58
5:F:127:ILE:HG13	5:F:127:ILE:O	2.04	0.58
11:L:65:HIS:CD2	11:L:65:HIS:C	2.82	0.58
1:B:7:SER:HB3	2:C:1193:GLN:OE1	2.04	0.58
1:B:84:ILE:HG22	1:B:239:LEU:HB3	1.85	0.58
1:B:215:SER:HB3	1:B:218:ASP:CG	2.29	0.58
1:B:652:VAL:HG12	1:B:653:VAL:N	2.18	0.58
1:B:798:GLY:HA2	1:B:815:PHE:HD1	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1317:MET:O	1:B:1322:ILE:HD11	2.03	0.58
2:C:121:ASN:HA	2:C:207:GLY:CA	2.28	0.58
2:C:184:ALA:HB1	2:C:188:ASP:HB3	1.85	0.58
2:C:398:ARG:HG3	2:C:398:ARG:NH1	2.18	0.58
2:C:521:LEU:HB3	2:C:633:VAL:HG11	1.86	0.58
2:C:642:ASP:C	2:C:644:GLU:H	2.11	0.58
2:C:857:ARG:HD2	2:C:945:GLU:OE1	2.03	0.58
2:C:1172:ILE:O	2:C:1172:ILE:HG22	2.03	0.58
4:E:5:THR:HG23	7:H:9:LEU:HB2	1.86	0.58
5:F:111:VAL:HG12	5:F:137:GLU:HG2	1.86	0.58
7:H:1:MET:O	7:H:3:PHE:CE1	2.57	0.58
11:L:42:LEU:O	11:L:46:ILE:HG13	2.04	0.58
1:B:499:ALA:O	1:B:503:GLN:HB2	2.04	0.58
1:B:981:LEU:HD23	1:B:1039:LYS:HA	1.85	0.58
1:B:1118:VAL:HG23	1:B:1306:LEU:HB2	1.85	0.58
2:C:310:MET:O	2:C:314:LEU:HD12	2.04	0.58
2:C:471:LYS:O	2:C:472:ALA:CB	2.52	0.58
3:D:38:ILE:HA	3:D:173:ALA:CB	2.33	0.58
1:B:913:LEU:HD23	1:B:919:ILE:HD12	1.84	0.57
1:B:986:ILE:HG22	1:B:987:VAL:N	2.18	0.57
2:C:244:LEU:O	2:C:249:ARG:HG2	2.03	0.57
2:C:862:GLN:HG2	2:C:963:PHE:HD1	1.69	0.57
1:B:63:ARG:HA	1:B:74:MET:SD	2.44	0.57
1:B:438:ASP:OD1	1:B:461:LYS:HA	2.04	0.57
1:B:584:ASN:HA	1:B:609:ASP:O	2.04	0.57
1:B:711:ARG:NH2	9:J:87:GLN:OE1	2.38	0.57
1:B:756:ILE:O	1:B:759:ALA:HB3	2.04	0.57
2:C:56:ASP:HB3	2:C:57:TYR:CD1	2.38	0.57
2:C:63:ILE:HA	2:C:421:PHE:CE2	2.39	0.57
2:C:129:PHE:CE2	2:C:166:PHE:HD1	2.22	0.57
2:C:459:TYR:CE1	2:C:469:GLN:HG2	2.39	0.57
2:C:617:ARG:HA	2:C:624:LEU:HD12	1.87	0.57
3:D:6:PRO:CB	3:D:25:VAL:HG12	2.33	0.57
3:D:232:VAL:HG21	3:D:244:VAL:HG22	1.86	0.57
7:H:127:PRO:HG3	7:H:139:ILE:HD12	1.86	0.57
9:J:99:LEU:HD23	9:J:99:LEU:N	2.19	0.57
11:L:18:LYS:NZ	11:L:38:GLU:HG2	2.19	0.57
1:B:814:PHE:O	1:B:818:MET:HG3	2.04	0.57
1:B:1057:VAL:HG12	1:B:1058:VAL:N	2.19	0.57
1:B:1402:PHE:CD1	1:B:1403:GLU:HG3	2.38	0.57
11:L:68:PHE:HD1	11:L:70:ARG:NH1	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ILE:HG21	1:B:222:LEU:CD2	2.33	0.57
1:B:1127:ASP:OD1	1:B:1130:GLN:HB2	2.04	0.57
1:B:1138:ILE:HG21	1:B:1316:VAL:HG13	1.87	0.57
1:B:1205:LYS:O	1:B:1207:LEU:HG	2.03	0.57
1:B:1230:GLU:O	1:B:1232:ASN:N	2.38	0.57
2:C:199:MET:HE2	2:C:492:LEU:CD2	2.35	0.57
2:C:388:CYS:O	2:C:390:LEU:N	2.36	0.57
2:C:446:LEU:HG	2:C:446:LEU:O	2.03	0.57
2:C:750:GLY:O	2:C:751:VAL:C	2.46	0.57
2:C:1192:TYR:CD1	2:C:1192:TYR:N	2.73	0.57
4:E:66:ARG:HD2	4:E:133:THR:HB	1.84	0.57
1:B:147:VAL:O	1:B:149:GLU:HG3	2.04	0.57
1:B:417:TYR:N	1:B:417:TYR:CD2	2.72	0.57
1:B:1373:ASP:HA	1:B:1376:THR:CG2	2.33	0.57
2:C:834:ASN:HB3	2:C:840:ILE:HG13	1.85	0.57
2:C:882:THR:CG2	2:C:884:ARG:HB2	2.35	0.57
3:D:31:ASN:HA	3:D:34:ARG:HB3	1.86	0.57
3:D:208:GLU:C	3:D:210:GLU:H	2.13	0.57
9:J:15:TYR:N	9:J:15:TYR:CD1	2.71	0.57
1:B:180:LYS:HZ1	1:B:294:SER:HB3	1.65	0.57
1:B:416:ARG:C	1:B:417:TYR:CD2	2.80	0.57
1:B:593:GLU:C	1:B:595:THR:H	2.12	0.57
1:B:1323:ASP:C	1:B:1325:THR:H	2.12	0.57
3:D:43:THR:CG2	3:D:44:LEU:H	2.10	0.57
4:E:16:LYS:HG2	4:E:18:VAL:HG12	1.86	0.57
4:E:37:GLN:OE1	7:H:5:LYS:HD2	2.05	0.57
5:F:178:ILE:HB	5:F:212:ARG:HD3	1.85	0.57
13:N:2:DA:C2'	13:N:3:DG:C8	2.88	0.57
1:B:71:GLN:HG3	1:B:72:GLU:N	2.19	0.57
1:B:726:ARG:O	1:B:729:ALA:HB3	2.04	0.57
1:B:984:LYS:HG2	1:B:988:LEU:HD12	1.86	0.57
2:C:44:VAL:O	2:C:45:SER:C	2.48	0.57
2:C:273:LEU:HD22	2:C:360:PHE:HD1	1.69	0.57
2:C:363:HIS:O	2:C:364:ILE:HB	2.04	0.57
2:C:803:LEU:HD12	2:C:1032:SER:HB3	1.86	0.57
2:C:1197:PRO:O	2:C:1200:ALA:HB3	2.04	0.57
1:B:35:ILE:HA	1:B:52:GLY:O	2.04	0.57
1:B:87:ALA:CB	1:B:276:LEU:HD23	2.35	0.57
1:B:320:ARG:HH22	14:P:3:C:H1'	1.67	0.57
1:B:445:ASN:HA	1:B:478:TYR:HE2	1.70	0.57
2:C:582:VAL:HB	2:C:587:HIS:CD2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:242:GLN:C	3:D:244:VAL:N	2.63	0.57
7:H:83:LYS:HE2	7:H:150:CYS:H	1.68	0.57
10:K:23:ASN:O	10:K:25:LEU:N	2.38	0.57
12:M:27:LEU:HB3	12:M:37:LYS:CD	2.34	0.57
1:B:567:LYS:HB3	8:I:95:TYR:CA	2.34	0.57
1:B:667:GLY:HA3	3:D:192:TRP:HH2	1.69	0.57
1:B:1198:ASP:HB3	1:B:1201:ALA:CB	2.34	0.57
2:C:1069:PHE:N	2:C:1069:PHE:CD1	2.73	0.57
8:I:128:ASN:H	8:I:130:ARG:NH2	2.02	0.57
1:B:84:ILE:HD11	1:B:270:LEU:HD13	1.87	0.57
1:B:346:ASP:HB3	2:C:1108:ARG:H	1.70	0.57
1:B:436:ILE:HD13	1:B:436:ILE:N	2.19	0.57
1:B:903:ASN:ND2	1:B:904:THR:N	2.52	0.57
1:B:903:ASN:O	1:B:907:THR:HB	2.05	0.57
1:B:1276:VAL:HB	1:B:1279:ILE:HD12	1.86	0.57
2:C:176:SER:O	2:C:182:SER:HB3	2.05	0.57
3:D:74:SER:HB3	3:D:77:ILE:CG1	2.34	0.57
5:F:100:ILE:HG23	5:F:105:PHE:CD1	2.39	0.57
7:H:154:VAL:HG12	7:H:155:SER:N	2.20	0.57
11:L:17:SER:O	11:L:18:LYS:C	2.45	0.57
14:P:5:C:H2'	14:P:6:A:C8	2.40	0.57
1:B:37:PHE:N	1:B:37:PHE:HD1	2.03	0.56
1:B:1373:ASP:CA	1:B:1376:THR:HG22	2.34	0.56
2:C:240:ILE:CG2	2:C:254:LEU:HB3	2.35	0.56
2:C:345:LYS:O	2:C:347:LYS:HG2	2.05	0.56
2:C:433:GLN:O	2:C:434:ARG:HG3	2.05	0.56
9:J:92:ARG:HG2	9:J:94:ASP:OD1	2.05	0.56
14:P:6:A:H2'	14:P:7:A:C8	2.40	0.56
1:B:107:CYS:HA	1:B:171:GLN:CD	2.30	0.56
2:C:780:VAL:HG12	2:C:782:LEU:O	2.05	0.56
3:D:31:ASN:O	3:D:32:SER:C	2.48	0.56
8:I:89:LEU:C	8:I:91:ASP:N	2.60	0.56
12:M:25:ALA:O	12:M:26:THR:HB	2.05	0.56
1:B:22:PHE:CD1	2:C:1213:THR:HG22	2.40	0.56
1:B:90:VAL:HG13	1:B:297:GLN:HA	1.86	0.56
1:B:590:ARG:HD3	1:B:604:GLY:HA2	1.87	0.56
1:B:663:SER:OG	1:B:664:THR:N	2.36	0.56
1:B:714:PHE:CG	9:J:97:MET:HE1	2.39	0.56
1:B:719:VAL:CG1	1:B:723:ASN:HD21	2.18	0.56
1:B:881:GLN:NE2	1:B:959:ASN:HA	2.21	0.56
1:B:881:GLN:O	1:B:953:ASN:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:901:LEU:HA	1:B:907:THR:OG1	2.06	0.56
1:B:984:LYS:O	1:B:988:LEU:HB2	2.06	0.56
1:B:1072:ILE:HD11	1:B:1368:MET:HA	1.86	0.56
1:B:1373:ASP:O	1:B:1376:THR:N	2.39	0.56
2:C:129:PHE:HE2	2:C:166:PHE:HD1	1.54	0.56
2:C:129:PHE:HE2	2:C:166:PHE:CD1	2.22	0.56
2:C:180:TYR:HD1	2:C:180:TYR:H	1.53	0.56
2:C:332:ASP:C	2:C:334:ILE:H	2.13	0.56
2:C:1002:THR:O	2:C:1005:GLY:N	2.37	0.56
3:D:20:PHE:HE1	3:D:22:LEU:HB2	1.71	0.56
3:D:116:LYS:O	3:D:118:LEU:N	2.37	0.56
3:D:137:LYS:HB3	3:D:138:GLU:OE1	2.04	0.56
3:D:249:ASP:O	3:D:252:GLN:HB3	2.05	0.56
4:E:64:VAL:O	4:E:67:ARG:N	2.38	0.56
7:H:13:LEU:O	7:H:67:SER:HA	2.05	0.56
7:H:23:LYS:HG3	7:H:56:ILE:CD1	2.35	0.56
7:H:26:LEU:HD12	7:H:56:ILE:HG21	1.86	0.56
7:H:129:SER:CB	7:H:138:THR:OG1	2.52	0.56
9:J:2:THR:O	9:J:3:THR:C	2.48	0.56
9:J:119:THR:HG22	9:J:119:THR:O	2.04	0.56
1:B:34:LYS:HD3	1:B:34:LYS:N	2.20	0.56
1:B:334:GLY:O	1:B:336:ILE:N	2.39	0.56
1:B:494:SER:O	1:B:497:THR:HB	2.05	0.56
1:B:719:VAL:HG12	1:B:723:ASN:ND2	2.20	0.56
1:B:751:SER:O	1:B:752:LYS:CB	2.53	0.56
1:B:1130:GLN:O	1:B:1134:ILE:HG13	2.04	0.56
1:B:1444:MET:HG2	7:H:60:ARG:HA	1.87	0.56
2:C:278:GLN:CG	2:C:279:ASP:H	2.06	0.56
2:C:838:SER:HA	2:C:989:THR:O	2.05	0.56
2:C:999:MET:HG2	2:C:1007:VAL:HG22	1.86	0.56
2:C:1187:ASN:O	2:C:1188:LYS:CB	2.54	0.56
3:D:258:ILE:HG23	11:L:19:LEU:HD11	1.88	0.56
4:E:198:LEU:O	4:E:200:ASN:N	2.38	0.56
5:F:5:ASN:O	5:F:9:ILE:HG13	2.05	0.56
5:F:147:HIS:HD2	5:F:149:LEU:HB2	1.70	0.56
8:I:36:CYS:HA	8:I:126:GLU:O	2.05	0.56
10:K:14:VAL:CG1	10:K:50:ILE:HD11	2.36	0.56
10:K:57:ILE:HA	10:K:60:PHE:CD2	2.30	0.56
11:L:19:LEU:HD22	11:L:33:ILE:CG2	2.36	0.56
1:B:211:PHE:HA	1:B:214:ILE:HG13	1.88	0.56
1:B:225:ASN:ND2	1:B:227:VAL:H	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:VAL:CG1	1:B:525:GLN:H	2.12	0.56
1:B:586:ILE:CG2	1:B:587:HIS:N	2.68	0.56
1:B:1120:LEU:CD1	1:B:1120:LEU:N	2.68	0.56
2:C:496:ARG:HB3	2:C:496:ARG:NH1	2.20	0.56
2:C:1099:VAL:HG13	2:C:1100:ASP:H	1.70	0.56
1:B:98:LYS:HE2	1:B:224:PHE:CZ	2.40	0.56
2:C:459:TYR:CZ	2:C:469:GLN:HG2	2.41	0.56
2:C:1183:LYS:C	2:C:1185:CYS:H	2.12	0.56
6:G:99:LEU:CD1	6:G:103:MET:HE2	2.35	0.56
1:B:37:PHE:N	1:B:37:PHE:CD1	2.74	0.56
1:B:69:THR:C	1:B:71:GLN:N	2.61	0.56
1:B:347:PHE:CE2	1:B:375:THR:HG23	2.40	0.56
1:B:382:PRO:CB	1:B:428:TYR:HE2	2.17	0.56
2:C:56:ASP:HB3	2:C:57:TYR:HD1	1.71	0.56
2:C:102:VAL:HG23	2:C:112:LEU:HB2	1.86	0.56
2:C:212:LEU:HD12	2:C:409:ALA:HB1	1.87	0.56
2:C:957:ASN:HB3	2:C:961:LEU:H	1.70	0.56
4:E:59:ILE:HG21	4:E:145:MET:SD	2.46	0.56
5:F:156:LEU:HA	5:F:160:GLU:OE1	2.04	0.56
11:L:46:ILE:O	11:L:46:ILE:HG22	2.06	0.56
1:B:18:GLN:NE2	1:B:228:PHE:CE1	2.74	0.56
1:B:37:PHE:HB2	1:B:52:GLY:CA	2.30	0.56
1:B:527:THR:HG21	1:B:650:GLN:HA	1.87	0.56
1:B:693:VAL:HG21	1:B:721:PHE:HE1	1.70	0.56
1:B:1114:PRO:HG2	1:B:1115:SER:H	1.70	0.56
1:B:1349:TYR:HA	1:B:1372:VAL:HG21	1.87	0.56
2:C:422:LYS:O	2:C:426:LYS:HG2	2.05	0.56
2:C:423:LYS:HE2	2:C:470:LYS:HZ1	1.70	0.56
2:C:542:MET:HB3	2:C:636:PRO:HD2	1.87	0.56
2:C:616:ILE:HG23	2:C:700:SER:OG	2.06	0.56
2:C:758:PHE:CE1	2:C:1027:ILE:HG22	2.41	0.56
8:I:100:THR:HG22	8:I:101:ALA:N	2.21	0.56
2:C:185:THR:O	2:C:186:GLU:C	2.49	0.56
2:C:215:GLN:OE1	2:C:479:VAL:HG22	2.06	0.56
2:C:411:PRO:O	2:C:414:ALA:HB3	2.06	0.56
2:C:521:LEU:HD13	2:C:633:VAL:HB	1.87	0.56
3:D:56:THR:CG2	3:D:58:LEU:HD23	2.36	0.56
6:G:90:ARG:CG	6:G:91:ALA:N	2.63	0.56
8:I:18:GLY:O	8:I:19:ARG:HB2	2.05	0.56
10:K:7:CYS:SG	10:K:49:MET:HE3	2.45	0.56
1:B:116:ASP:C	1:B:118:HIS:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:PRO:HA	1:B:463:ILE:O	2.05	0.56
1:B:779:PHE:O	1:B:780:VAL:C	2.49	0.56
2:C:221:ASN:N	2:C:241:ARG:O	2.31	0.56
5:F:93:MET:SD	5:F:97:VAL:HG23	2.46	0.56
7:H:13:LEU:HD12	7:H:26:LEU:HD21	1.88	0.56
11:L:58:PHE:HE2	11:L:74:ARG:NE	2.04	0.56
11:L:109:TRP:O	11:L:112:GLN:HB2	2.06	0.56
1:B:347:PHE:N	2:C:1107:ALA:HA	2.17	0.55
2:C:423:LYS:HE2	2:C:470:LYS:NZ	2.21	0.55
2:C:758:PHE:CE2	2:C:1044:ALA:HA	2.40	0.55
2:C:833:TYR:N	2:C:833:TYR:CD1	2.70	0.55
2:C:871:THR:HG22	2:C:872:GLU:N	2.21	0.55
2:C:871:THR:HG22	2:C:872:GLU:O	2.06	0.55
2:C:906:SER:HA	2:C:946:ASN:HB2	1.86	0.55
2:C:956:THR:HG22	2:C:957:ASN:O	2.07	0.55
2:C:1151:LEU:N	2:C:1151:LEU:CD1	2.68	0.55
4:E:183:LEU:HD22	7:H:144:ARG:NH2	2.21	0.55
6:G:75:PRO:C	6:G:77:ASP:N	2.63	0.55
1:B:230:ARG:N	1:B:233:TRP:CE3	2.62	0.55
1:B:315:LEU:HD12	2:C:471:LYS:HB3	1.88	0.55
1:B:441:PRO:CG	1:B:498:ARG:HB2	2.36	0.55
1:B:698:GLN:HA	9:J:97:MET:O	2.06	0.55
1:B:808:LEU:HD23	1:B:813:PHE:HA	1.88	0.55
1:B:857:ARG:NH2	6:G:139:PRO:HG3	2.21	0.55
1:B:1152:ILE:HG22	1:B:1192:LEU:O	2.07	0.55
2:C:658:ILE:CG2	2:C:662:MET:HE2	2.36	0.55
2:C:1047:PHE:CD1	2:C:1047:PHE:N	2.74	0.55
2:C:1156:ASP:HB3	2:C:1198:TYR:N	2.17	0.55
3:D:48:SER:HB3	3:D:158:VAL:HB	1.87	0.55
7:H:79:PHE:CE2	7:H:105:PRO:HG2	2.37	0.55
1:B:53:LEU:CD2	1:B:54:ASN:ND2	2.68	0.55
1:B:224:PHE:CG	1:B:231:PRO:HG3	2.41	0.55
1:B:666:ILE:N	1:B:666:ILE:HD12	2.21	0.55
1:B:1226:VAL:HG22	1:B:1240:CYS:CB	2.33	0.55
1:B:1242:VAL:HG12	1:B:1243:VAL:N	2.19	0.55
1:B:1325:THR:O	1:B:1325:THR:CG2	2.54	0.55
2:C:38:PHE:CD1	2:C:811:TYR:CD2	2.94	0.55
2:C:577:ALA:HB1	2:C:589:VAL:CG1	2.27	0.55
3:D:75:MET:HE2	3:D:239:PRO:HD3	1.87	0.55
5:F:135:PHE:CD2	5:F:140:LEU:HD21	2.38	0.55
6:G:82:THR:CG2	6:G:84:TYR:H	2.16	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:55:THR:O	9:J:55:THR:HG22	2.06	0.55
1:B:341:MET:CE	1:B:843:LYS:NZ	2.66	0.55
1:B:541:ILE:HG21	1:B:549:MET:CE	2.36	0.55
1:B:1149:ALA:HB2	9:J:47:GLU:HA	1.88	0.55
1:B:1266:THR:O	1:B:1270:ASN:HB2	2.06	0.55
2:C:418:LYS:HE2	2:C:422:LYS:NZ	2.21	0.55
2:C:757:PRO:HG3	2:C:1028:GLU:OE2	2.06	0.55
2:C:986:GLN:OE1	2:C:986:GLN:HA	2.05	0.55
15:T:21:DA:H2'	15:T:22:DT:O5'	2.03	0.55
1:B:33:ALA:HB1	1:B:56:PRO:HB2	1.89	0.55
1:B:853:ASP:OD1	1:B:853:ASP:C	2.49	0.55
1:B:942:PHE:C	1:B:942:PHE:CD2	2.84	0.55
1:B:1210:GLY:O	1:B:1214:GLU:HG2	2.06	0.55
1:B:1261:LYS:CA	1:B:1264:GLU:HB3	2.36	0.55
1:B:1319:VAL:HG13	1:B:1320:PRO:HD2	1.88	0.55
2:C:25:ILE:HG22	2:C:29:ASP:CB	2.36	0.55
2:C:552:MET:HA	2:C:555:ILE:HB	1.89	0.55
2:C:708:GLU:O	2:C:710:LEU:N	2.39	0.55
2:C:865:LYS:HZ2	2:C:869:SER:HA	1.69	0.55
4:E:69:ALA:HA	4:E:72:ARG:HG3	1.88	0.55
5:F:153:HIS:CE1	5:F:184:VAL:HG11	2.41	0.55
7:H:31:LEU:HD22	7:H:48:VAL:HG21	1.89	0.55
9:J:5:ARG:O	9:J:14:LEU:HG	2.07	0.55
9:J:13:MET:CE	9:J:14:LEU:H	2.13	0.55
1:B:244:PRO:HB2	1:B:245:PRO:CD	2.32	0.55
1:B:322:VAL:O	1:B:322:VAL:HG12	2.07	0.55
1:B:754:SER:O	1:B:755:PHE:C	2.49	0.55
1:B:1280:GLU:O	1:B:1282:VAL:HG23	2.06	0.55
2:C:483:LEU:HD21	2:C:491:THR:HG23	1.89	0.55
3:D:182:PRO:HG3	3:D:206:ASN:O	2.06	0.55
6:G:130:ILE:O	6:G:148:VAL:HG21	2.06	0.55
1:B:230:ARG:N	1:B:233:TRP:HE3	2.02	0.55
1:B:545:GLN:O	1:B:547:LEU:N	2.40	0.55
1:B:1002:GLY:HA3	1:B:1007:ILE:CG2	2.30	0.55
2:C:51:PHE:CD2	2:C:173:MET:HB3	2.41	0.55
2:C:221:ASN:OD1	2:C:242:SER:HA	2.06	0.55
2:C:273:LEU:HD22	2:C:360:PHE:CD1	2.42	0.55
2:C:315:LYS:N	2:C:316:PRO:HD2	2.21	0.55
5:F:147:HIS:CD2	5:F:149:LEU:H	2.25	0.55
7:H:153:GLN:HG3	7:H:154:VAL:HG23	1.87	0.55
1:B:61:ILE:HG22	1:B:62:ASP:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:ILE:HG12	1:B:521:MET:HE3	1.88	0.55
1:B:942:PHE:C	1:B:942:PHE:HD2	2.15	0.55
1:B:1351:GLU:O	1:B:1355:VAL:HG23	2.07	0.55
2:C:508:LEU:O	2:C:509:ALA:HB3	2.07	0.55
2:C:520:GLY:N	2:C:748:ILE:HG22	2.19	0.55
2:C:583:ASN:HD21	2:C:628:THR:CG2	2.20	0.55
2:C:637:LEU:HD21	2:C:742:GLU:OE2	2.07	0.55
2:C:973:ILE:HG23	2:C:974:PRO:HD2	1.88	0.55
2:C:1008:PRO:HB2	2:C:1010:LEU:O	2.07	0.55
3:D:20:PHE:CZ	3:D:230:MET:HE3	2.42	0.55
5:F:78:LEU:HD21	5:F:80:VAL:CG2	2.37	0.55
1:B:150:THR:HG23	1:B:166:GLY:HA2	1.89	0.55
1:B:1149:ALA:CB	9:J:47:GLU:HA	2.36	0.55
2:C:60:GLN:HE22	2:C:94:LYS:HA	1.72	0.55
2:C:820:GLY:C	2:C:821:GLN:HG3	2.31	0.55
3:D:80:LEU:HD22	3:D:129:ILE:HD13	1.88	0.55
5:F:43:LYS:O	5:F:45:LYS:N	2.40	0.55
7:H:81:PRO:HG3	7:H:106:MET:SD	2.46	0.55
7:H:143:ILE:CG2	7:H:144:ARG:H	2.20	0.55
8:I:130:ARG:HA	8:I:133:ASN:HB2	1.89	0.55
8:I:139:ASN:O	8:I:140:ALA:CB	2.55	0.55
11:L:93:SER:O	11:L:97:LYS:HG3	2.06	0.55
1:B:407:ARG:HG2	1:B:430:TRP:CZ2	2.41	0.55
1:B:682:THR:HG23	1:B:728:LYS:CE	2.22	0.55
1:B:828:ALA:HB3	2:C:530:GLY:HA2	1.87	0.55
1:B:992:ASP:O	1:B:993:LEU:C	2.49	0.55
2:C:247:GLY:H	2:C:418:LYS:HZ1	1.53	0.55
2:C:654:ARG:N	2:C:657:HIS:HD2	1.96	0.55
2:C:865:LYS:HZ3	2:C:869:SER:HA	1.70	0.55
3:D:11:ARG:HD3	3:D:209:TYR:OH	2.07	0.55
4:E:35:LEU:HA	4:E:47:LEU:HB2	1.89	0.55
5:F:121:MET:O	5:F:124:VAL:HG23	2.07	0.55
1:B:185:TRP:HZ3	1:B:200:ARG:HG2	1.71	0.54
1:B:503:GLN:HE21	6:G:90:ARG:HH21	1.54	0.54
1:B:586:ILE:HG22	1:B:587:HIS:H	1.69	0.54
2:C:656:GLY:O	2:C:657:HIS:C	2.50	0.54
2:C:1103:ILE:O	2:C:1122:ARG:NH1	2.40	0.54
3:D:212:PRO:HB3	3:D:213:PRO:HD2	1.89	0.54
4:E:5:THR:CG2	7:H:9:LEU:HB2	2.36	0.54
8:I:59:ILE:O	8:I:60:ALA:HB3	2.06	0.54
1:B:29:ALA:HB1	2:C:1184:GLY:CA	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ALA:HB3	1:B:276:LEU:CD2	2.37	0.54
1:B:172:PRO:HB3	1:B:185:TRP:CD2	2.42	0.54
1:B:206:GLU:O	1:B:210:ILE:HG13	2.07	0.54
1:B:709:THR:HG22	1:B:710:LEU:N	2.22	0.54
1:B:827:THR:CG2	1:B:828:ALA:N	2.70	0.54
2:C:361:LEU:HD21	2:C:377:PHE:HB3	1.88	0.54
3:D:34:ARG:O	3:D:38:ILE:HG13	2.07	0.54
3:D:44:LEU:HG	3:D:159:ALA:HB1	1.88	0.54
3:D:46:ILE:CG2	3:D:157:CYS:HB3	2.35	0.54
3:D:173:ALA:O	3:D:174:ALA:HB3	2.06	0.54
7:H:3:PHE:CD1	7:H:80:LYS:NZ	2.75	0.54
7:H:52:ASP:C	7:H:53:ASN:HD22	2.14	0.54
8:I:107:VAL:O	8:I:108:SER:O	2.25	0.54
1:B:54:ASN:HD21	1:B:247:ARG:HH12	1.55	0.54
1:B:374:LEU:CB	1:B:436:ILE:HD11	2.37	0.54
2:C:485:ARG:NH2	2:C:782:LEU:HD11	2.22	0.54
2:C:942:ARG:O	2:C:944:THR:N	2.41	0.54
5:F:163:GLU:O	5:F:164:LEU:C	2.49	0.54
6:G:89:GLU:OE2	6:G:134:ILE:HG21	2.07	0.54
12:M:38:LEU:CD1	12:M:49:LYS:HG2	2.38	0.54
1:B:172:PRO:HD3	1:B:185:TRP:CE2	2.43	0.54
1:B:347:PHE:HE2	1:B:375:THR:HG23	1.73	0.54
1:B:356:ASP:CB	1:B:469:ARG:HH12	2.08	0.54
1:B:498:ARG:HA	1:B:501:LEU:HD12	1.88	0.54
1:B:765:VAL:HG23	1:B:802:ASN:O	2.07	0.54
1:B:896:ARG:NH2	1:B:1030:ARG:NH2	2.56	0.54
1:B:1349:TYR:HE1	1:B:1368:MET:HE3	1.72	0.54
2:C:1095:LEU:HD12	2:C:1095:LEU:N	2.22	0.54
3:D:254:LYS:C	3:D:256:ALA:N	2.65	0.54
4:E:53:SER:H	4:E:148:LEU:HD21	1.72	0.54
4:E:137:ASN:H	4:E:137:ASN:ND2	2.04	0.54
8:I:40:LEU:HD22	8:I:123:MET:CE	2.37	0.54
8:I:135:LEU:HD13	8:I:137:GLN:NE2	2.19	0.54
9:J:35:VAL:HG12	9:J:36:GLU:H	1.73	0.54
11:L:19:LEU:HD21	11:L:35:PHE:CE2	2.42	0.54
15:T:19:DT:H2'	15:T:20:DT:C6	2.42	0.54
1:B:18:GLN:CB	2:C:1215:ARG:HB2	2.37	0.54
1:B:1394:THR:HG22	1:B:1395:GLY:N	2.21	0.54
2:C:312:GLU:O	2:C:315:LYS:HB2	2.07	0.54
2:C:693:ILE:HD11	2:C:740:HIS:CD2	2.43	0.54
2:C:785:TYR:C	2:C:785:TYR:CD1	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:984:HIS:NE2	2:C:1025:HIS:HA	2.23	0.54
3:D:174:ALA:O	3:D:175:ALA:HB2	2.08	0.54
4:E:160:VAL:O	4:E:164:ILE:HG13	2.06	0.54
6:G:86:THR:HG23	6:G:89:GLU:OE1	2.08	0.54
9:J:34:TYR:CD2	9:J:35:VAL:N	2.75	0.54
1:B:40:THR:HB	1:B:41:MET:CE	2.27	0.54
1:B:68:GLN:C	1:B:70:CYS:H	2.15	0.54
1:B:149:GLU:HB2	1:B:164:ARG:HH21	1.72	0.54
1:B:500:GLU:OE2	2:C:1145:SER:HB2	2.06	0.54
1:B:853:ASP:OD1	1:B:855:THR:HG22	2.08	0.54
1:B:1144:LYS:HD2	1:B:1268:LEU:O	2.08	0.54
2:C:314:LEU:O	2:C:318:VAL:HG23	2.08	0.54
2:C:642:ASP:CB	2:C:649:LYS:HG3	2.38	0.54
2:C:1001:PHE:CZ	2:C:1073:TYR:HB2	2.42	0.54
3:D:175:ALA:HB3	10:K:43:ARG:HH22	1.71	0.54
3:D:255:VAL:HG12	11:L:91:CYS:HB3	1.90	0.54
10:K:27:GLU:C	10:K:29:GLU:H	2.16	0.54
1:B:91:PHE:N	1:B:297:GLN:HE22	2.04	0.54
1:B:360:GLU:O	1:B:361:LEU:C	2.51	0.54
1:B:472:LEU:HD11	2:C:835:GLN:NE2	2.22	0.54
1:B:809:THR:H	1:B:812:GLU:HB2	1.71	0.54
1:B:872:GLY:C	1:B:1058:VAL:HG23	2.33	0.54
1:B:1375:MET:HE3	1:B:1384:VAL:HG23	1.88	0.54
2:C:393:LYS:HA	2:C:393:LYS:CE	2.35	0.54
2:C:1001:PHE:CE2	3:D:34:ARG:CZ	2.91	0.54
2:C:1084:GLN:OE1	3:D:189:THR:HG22	2.08	0.54
3:D:35:ARG:HA	3:D:38:ILE:HD12	1.89	0.54
4:E:118:THR:HB	4:E:121:LYS:CB	2.38	0.54
4:E:141:LEU:HD12	4:E:141:LEU:O	2.07	0.54
4:E:207:LEU:O	4:E:207:LEU:HD12	2.08	0.54
4:E:216:ASN:C	4:E:218:GLU:N	2.64	0.54
6:G:116:ASP:O	6:G:120:ILE:HG13	2.07	0.54
7:H:14:HIS:CD2	7:H:16:SER:CB	2.91	0.54
9:J:11:ASN:C	9:J:12:ASN:HD22	2.15	0.54
9:J:93:LYS:H	9:J:93:LYS:CD	2.18	0.54
15:T:25:DC:N4	15:T:26:DA:N6	2.34	0.54
1:B:224:PHE:CZ	1:B:234:MET:HE2	2.43	0.54
1:B:367:PRO:HB3	1:B:466:SER:HA	1.89	0.54
1:B:471:ASN:OD1	1:B:472:LEU:N	2.41	0.54
1:B:639:PRO:HG2	1:B:640:GLN:N	2.22	0.54
1:B:834:THR:HG21	1:B:1077:THR:CA	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:977:LYS:HB3	1:B:978:PRO:HD2	1.89	0.54
1:B:1079:MET:HE3	1:B:1098:VAL:HG22	1.88	0.54
1:B:1344:GLY:O	1:B:1345:ARG:C	2.51	0.54
2:C:357:GLN:O	2:C:366:GLN:HA	2.08	0.54
2:C:601:ARG:O	2:C:605:ARG:HG3	2.08	0.54
2:C:651:LEU:HD11	2:C:707:PRO:HB3	1.89	0.54
2:C:1183:LYS:O	2:C:1183:LYS:HE3	2.06	0.54
3:D:133:ILE:HD13	3:D:236:GLY:C	2.32	0.54
5:F:213:ILE:HG12	5:F:214:CYS:H	1.69	0.54
10:K:35:ALA:C	10:K:39:LEU:HD12	2.33	0.54
1:B:17:VAL:HG23	1:B:1421:CYS:SG	2.48	0.54
1:B:35:ILE:HD13	1:B:241:VAL:HG11	1.88	0.54
1:B:251:SER:HA	1:B:257:ARG:O	2.08	0.54
1:B:305:ASP:CG	1:B:326:ARG:HD2	2.33	0.54
1:B:443:LEU:HD12	2:C:1146:PHE:CE2	2.42	0.54
1:B:485:ASP:OD1	14:P:10:A:H4'	2.08	0.54
1:B:827:THR:O	1:B:831:THR:HB	2.08	0.54
1:B:1152:ILE:HD11	9:J:44:TYR:HD2	1.73	0.54
2:C:25:ILE:HD12	2:C:651:LEU:CD1	2.36	0.54
2:C:365:THR:HG21	2:C:370:PHE:CD1	2.43	0.54
2:C:642:ASP:CA	2:C:649:LYS:HG3	2.38	0.54
2:C:762:ASN:ND2	2:C:1024:ALA:HB3	2.18	0.54
5:F:14:ARG:HH21	5:F:141:VAL:CG1	2.21	0.54
7:H:44:TYR:CD2	7:H:105:PRO:HB2	2.43	0.54
11:L:67:PHE:C	11:L:68:PHE:HD2	2.16	0.54
1:B:115:LEU:HD12	1:B:142:CYS:HB3	1.89	0.54
1:B:490:HIS:HB3	2:C:1150:ARG:NH1	2.22	0.54
1:B:590:ARG:NH2	1:B:620:LYS:C	2.66	0.54
1:B:834:THR:HG21	1:B:1077:THR:OG1	2.08	0.54
1:B:1022:LEU:CD1	1:B:1026:LEU:HD12	2.38	0.54
1:B:1152:ILE:HG13	9:J:44:TYR:HB3	1.90	0.54
1:B:1308:THR:HG23	1:B:1309:ASP:N	2.21	0.54
1:B:1324:PRO:HB2	5:F:142:VAL:HG11	1.88	0.54
1:B:1343:ALA:HB2	5:F:150:VAL:CG2	2.35	0.54
2:C:1015:HIS:O	2:C:1018:PRO:HD2	2.08	0.54
2:C:1135:ARG:O	2:C:1136:ASP:C	2.50	0.54
2:C:1180:PHE:O	2:C:1181:GLU:O	2.26	0.54
3:D:246:ARG:HA	3:D:249:ASP:HB3	1.89	0.54
5:F:128:PRO:HA	5:F:129:PRO:C	2.32	0.54
8:I:82:PRO:C	8:I:84:ALA:H	2.16	0.54
11:L:48:ALA:O	11:L:51:LEU:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1001:ARG:NE	6:G:83:PRO:HD3	2.23	0.53
1:B:1254:ALA:O	1:B:1255:GLU:HB2	2.07	0.53
1:B:1329:THR:CG2	1:B:1331:SER:HB3	2.38	0.53
2:C:101:MET:HA	2:C:112:LEU:H	1.73	0.53
2:C:288:ALA:CB	2:C:331:LEU:HD12	2.38	0.53
2:C:653:VAL:HA	2:C:689:LEU:HD22	1.89	0.53
8:I:15:VAL:HA	8:I:26:ILE:HG12	1.90	0.53
1:B:152:VAL:CG1	1:B:153:PRO:HD2	2.38	0.53
1:B:453:MET:HB3	1:B:456:MET:HE2	1.89	0.53
1:B:709:THR:HB	1:B:712:GLU:H	1.73	0.53
1:B:1349:TYR:CE1	1:B:1368:MET:HE3	2.43	0.53
2:C:117:ALA:CB	2:C:122:LEU:HB2	2.38	0.53
2:C:274:PRO:O	2:C:275:TYR:HB2	2.07	0.53
2:C:642:ASP:CA	2:C:649:LYS:HA	2.29	0.53
3:D:52:GLU:HA	12:M:64:LEU:HD22	1.90	0.53
11:L:40:HIS:O	11:L:41:THR:C	2.51	0.53
11:L:40:HIS:O	11:L:43:GLY:N	2.41	0.53
11:L:58:PHE:CD1	11:L:59:ALA:N	2.76	0.53
1:B:92:HIS:CD2	1:B:304:MET:HE1	2.43	0.53
1:B:325:ILE:CG2	2:C:1210:MET:HE2	2.37	0.53
1:B:524:VAL:CG1	1:B:525:GLN:N	2.71	0.53
1:B:526:ASP:HB2	2:C:835:GLN:OE1	2.07	0.53
1:B:606:LEU:HB3	1:B:614:PHE:CD2	2.44	0.53
1:B:896:ARG:HD3	1:B:897:TYR:CE1	2.44	0.53
1:B:1118:VAL:CG2	1:B:1306:LEU:HB2	2.38	0.53
1:B:1264:GLU:HG3	1:B:1265:ASN:N	2.22	0.53
1:B:1380:GLY:C	1:B:1381:LEU:HD23	2.33	0.53
2:C:23:ALA:HB1	2:C:24:PRO:CD	2.29	0.53
2:C:100:PRO:HD3	2:C:172:ILE:CD1	2.38	0.53
2:C:112:LEU:HD12	2:C:113:TYR:H	1.72	0.53
2:C:365:THR:HG23	2:C:367:LEU:N	2.23	0.53
2:C:400:HIS:O	2:C:402:GLY:N	2.41	0.53
2:C:498:THR:CG2	2:C:537:LYS:HB2	2.38	0.53
2:C:653:VAL:HG22	2:C:689:LEU:HB3	1.90	0.53
2:C:707:PRO:HG2	2:C:708:GLU:H	1.72	0.53
3:D:16:ASP:C	3:D:240:VAL:HG11	2.33	0.53
3:D:26:ASP:O	3:D:27:LEU:C	2.50	0.53
3:D:69:LEU:HD12	3:D:69:LEU:H	1.73	0.53
4:E:154:PHE:CE2	4:E:163:VAL:HG21	2.43	0.53
5:F:156:LEU:HD12	5:F:195:VAL:CB	2.32	0.53
5:F:192:ARG:O	5:F:192:ARG:HG2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:117:GLN:C	7:H:119:LEU:N	2.66	0.53
8:I:32:THR:HG22	8:I:33:GLN:OE1	2.07	0.53
9:J:76:PRO:HD2	9:J:108:HIS:HD2	1.73	0.53
9:J:111:THR:CG2	9:J:112:SER:H	2.18	0.53
15:T:18:DT:OP2	15:T:18:DT:C7	2.57	0.53
15:T:24:DG:C2	15:T:25:DC:H1'	2.43	0.53
1:B:365:GLY:HA3	1:B:463:ILE:HD13	1.91	0.53
1:B:416:ARG:HG3	1:B:417:TYR:CE2	2.44	0.53
1:B:849:MET:HE3	1:B:1061:GLY:CA	2.39	0.53
2:C:46:GLN:HG3	2:C:47:GLN:N	2.14	0.53
2:C:53:GLN:HG2	2:C:547:VAL:HG21	1.90	0.53
2:C:165:VAL:HG11	2:C:448:ILE:HD13	1.91	0.53
2:C:233:PRO:HG2	2:C:234:ILE:HD13	1.90	0.53
2:C:273:LEU:O	2:C:276:ILE:HB	2.07	0.53
2:C:308:TRP:HZ3	9:J:45:ARG:HB3	1.72	0.53
2:C:483:LEU:CD1	2:C:491:THR:HG23	2.31	0.53
2:C:807:ARG:HG2	2:C:1045:SER:OG	2.08	0.53
2:C:1115:THR:HG22	2:C:1117:GLN:HG3	1.91	0.53
3:D:65:HIS:CE1	3:D:69:LEU:HD11	2.42	0.53
6:G:76:LYS:O	6:G:79:ARG:HD2	2.08	0.53
11:L:13:GLY:O	11:L:14:GLU:C	2.51	0.53
11:L:68:PHE:CD1	11:L:70:ARG:NH1	2.76	0.53
1:B:10:PRO:HD2	2:C:1191:ILE:O	2.09	0.53
1:B:32:VAL:O	1:B:57:ARG:HD3	2.09	0.53
1:B:332:LYS:H	1:B:337:ARG:HB3	1.74	0.53
1:B:547:LEU:HD13	11:L:58:PHE:HD1	1.74	0.53
1:B:760:GLN:HG2	1:B:765:VAL:HA	1.89	0.53
2:C:431:TYR:CG	2:C:447:ALA:HB2	2.42	0.53
2:C:516:ASN:N	2:C:516:ASN:ND2	2.30	0.53
2:C:1006:ILE:HD13	10:K:44:TYR:HE2	1.74	0.53
2:C:1110:PRO:HG3	2:C:1124:ARG:O	2.08	0.53
12:M:49:LYS:O	12:M:50:ASP:CB	2.47	0.53
1:B:53:LEU:CD2	1:B:54:ASN:N	2.68	0.53
1:B:62:ASP:HB3	1:B:64:ASN:ND2	2.23	0.53
1:B:137:ALA:O	1:B:138:ILE:C	2.51	0.53
1:B:399:HIS:CB	1:B:400:PRO:CD	2.86	0.53
1:B:1370:LEU:O	1:B:1373:ASP:HB2	2.09	0.53
3:D:183:TRP:CZ2	3:D:207:CYS:HB3	2.44	0.53
5:F:55:ARG:C	5:F:57:MET:N	2.63	0.53
7:H:49:LEU:HD21	7:H:77:VAL:HB	1.89	0.53
15:T:20:DT:C3'	15:T:21:DA:H5'	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ILE:HG23	2:C:1170:THR:HG23	1.91	0.53
1:B:382:PRO:CD	1:B:428:TYR:CE2	2.89	0.53
1:B:401:GLY:CA	1:B:435:HIS:HD2	2.22	0.53
1:B:814:PHE:O	1:B:817:ALA:HB3	2.09	0.53
1:B:947:PHE:N	1:B:947:PHE:CD1	2.76	0.53
1:B:1197:LEU:HD11	1:B:1238:ILE:HD11	1.90	0.53
2:C:224:GLN:O	2:C:238:ALA:HA	2.08	0.53
2:C:233:PRO:HG2	2:C:234:ILE:CD1	2.38	0.53
2:C:309:GLN:O	2:C:312:GLU:HB3	2.08	0.53
2:C:510:LYS:CB	2:C:511:PRO:HD3	2.39	0.53
3:D:98:VAL:HG23	3:D:122:SER:HB3	1.90	0.53
4:E:216:ASN:O	4:E:218:GLU:N	2.42	0.53
8:I:47:PHE:CD2	8:I:95:TYR:HD1	2.27	0.53
8:I:81:PRO:HB2	8:I:82:PRO:CD	2.36	0.53
8:I:106:GLU:HG2	8:I:112:ILE:HG12	1.91	0.53
11:L:19:LEU:HD21	11:L:35:PHE:CD2	2.42	0.53
12:M:34:CYS:O	12:M:36:SER:N	2.41	0.53
1:B:75:ASN:O	1:B:76:GLU:CB	2.57	0.53
1:B:711:ARG:O	1:B:714:PHE:HB3	2.08	0.53
1:B:783:THR:HG22	1:B:784:LEU:CD2	2.38	0.53
1:B:963:ILE:HD11	1:B:1048:ASN:HB2	1.89	0.53
1:B:1152:ILE:CG1	9:J:44:TYR:HB3	2.39	0.53
2:C:114:PRO:HD3	2:C:124:TYR:CE1	2.44	0.53
2:C:292:ILE:HG23	2:C:325:GLN:O	2.08	0.53
2:C:637:LEU:HD22	2:C:741:CYS:O	2.09	0.53
2:C:990:ILE:CG2	2:C:991:GLY:N	2.71	0.53
2:C:1147:LEU:HD23	2:C:1148:LYS:N	2.24	0.53
3:D:134:ILE:HG23	3:D:141:GLY:H	1.74	0.53
6:G:110:ASP:O	6:G:112:GLU:N	2.42	0.53
9:J:74:GLU:HB2	9:J:79:HIS:HA	1.89	0.53
10:K:3:VAL:CG2	10:K:18:TRP:HB2	2.34	0.53
1:B:504:LEU:HD11	6:G:91:ALA:CB	2.38	0.53
1:B:668:ASP:OD1	1:B:741:ASN:ND2	2.42	0.53
1:B:1106:ASN:O	1:B:1107:VAL:HB	2.09	0.53
1:B:1224:LEU:HD12	1:B:1241:ARG:O	2.08	0.53
1:B:1308:THR:HG23	1:B:1310:GLY:H	1.74	0.53
1:B:1316:VAL:O	1:B:1316:VAL:HG12	2.09	0.53
1:B:1438:THR:HB	2:C:1144:ALA:CB	2.36	0.53
1:B:1454:MET:HG3	1:B:1454:MET:O	2.09	0.53
2:C:96:TYR:N	2:C:129:PHE:O	2.30	0.53
2:C:203:PHE:HB3	2:C:205:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:370:PHE:HD2	2:C:373:ARG:CD	2.22	0.53
2:C:613:VAL:HG13	2:C:627:PHE:O	2.08	0.53
2:C:889:THR:HG22	2:C:891:ASP:H	1.74	0.53
2:C:1106:ARG:HD3	2:C:1126:GLY:O	2.09	0.53
2:C:1162:ILE:HD11	2:C:1194:ILE:HD13	1.90	0.53
4:E:66:ARG:O	4:E:70:PHE:HB2	2.08	0.53
6:G:93:ILE:HD13	6:G:148:VAL:HG12	1.91	0.53
8:I:25:ARG:HA	8:I:41:ASP:HA	1.90	0.53
1:B:34:LYS:CG	1:B:36:ARG:HH21	2.22	0.53
1:B:527:THR:CG2	1:B:650:GLN:HA	2.39	0.53
1:B:548:ASN:HA	11:L:60:ALA:HB1	1.91	0.53
1:B:826:ASP:O	1:B:827:THR:C	2.52	0.53
1:B:1152:ILE:HD11	9:J:44:TYR:HB3	1.90	0.53
1:B:1323:ASP:O	1:B:1325:THR:N	2.38	0.53
2:C:430:ARG:O	2:C:434:ARG:HD2	2.08	0.53
4:E:34:GLN:C	4:E:36:LYS:N	2.65	0.53
4:E:185:CYS:HB2	4:E:211:LEU:CD2	2.29	0.53
7:H:27:LYS:O	7:H:30:LEU:N	2.41	0.53
8:I:55:LEU:HD22	8:I:144:ILE:HG21	1.90	0.53
11:L:47:ARG:HD2	11:L:47:ARG:C	2.34	0.53
1:B:249:SER:O	1:B:250:ILE:HG13	2.09	0.52
1:B:416:ARG:HG3	1:B:417:TYR:CD2	2.44	0.52
1:B:470:LEU:H	1:B:470:LEU:CD2	2.17	0.52
1:B:551:TYR:CE2	11:L:62:LYS:HE2	2.44	0.52
1:B:596:THR:C	1:B:598:LEU:N	2.63	0.52
1:B:774:ARG:NH2	1:B:797:LYS:HB2	2.24	0.52
1:B:1443:VAL:O	1:B:1443:VAL:HG23	2.09	0.52
2:C:117:ALA:HA	2:C:122:LEU:HD12	1.90	0.52
2:C:999:MET:HG3	2:C:1000:PRO:CD	2.33	0.52
2:C:1005:GLY:O	2:C:1006:ILE:C	2.51	0.52
2:C:1177:HIS:CB	2:C:1179:GLN:HE21	2.21	0.52
3:D:18:VAL:O	3:D:19:ASP:C	2.52	0.52
4:E:217:LEU:O	4:E:219:THR:N	2.41	0.52
11:L:2:ASN:O	11:L:3:ALA:C	2.53	0.52
1:B:54:ASN:ND2	1:B:247:ARG:HH12	2.07	0.52
1:B:528:LEU:CD2	1:B:751:SER:HB3	2.38	0.52
1:B:608:ILE:C	1:B:610:GLY:N	2.65	0.52
1:B:860:LEU:CD1	1:B:1393:ASN:HD22	2.22	0.52
1:B:1239:ARG:HB3	1:B:1239:ARG:HH11	1.74	0.52
1:B:1348:LEU:O	1:B:1352:VAL:HG23	2.08	0.52
2:C:44:VAL:HG11	2:C:199:MET:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:212:LEU:HD21	2:C:461:LEU:HG	1.90	0.52
2:C:304:ASP:OD1	2:C:306:ASN:HB2	2.09	0.52
2:C:582:VAL:HG23	2:C:626:ILE:HB	1.91	0.52
2:C:732:SER:HB2	2:C:734:HIS:CD2	2.44	0.52
2:C:758:PHE:CZ	2:C:1044:ALA:HA	2.44	0.52
2:C:827:ILE:HG12	2:C:1012:ILE:HG13	1.91	0.52
2:C:844:SER:HB3	2:C:848:ARG:NH1	2.24	0.52
2:C:955:THR:HG22	2:C:956:THR:O	2.09	0.52
2:C:1215:ARG:C	2:C:1216:LEU:HD23	2.35	0.52
3:D:239:PRO:HB2	3:D:241:ASP:OD1	2.09	0.52
3:D:255:VAL:HG12	3:D:255:VAL:O	2.09	0.52
5:F:108:GLY:HA3	5:F:132:ILE:HG22	1.90	0.52
7:H:79:PHE:CE2	7:H:105:PRO:CG	2.93	0.52
1:B:116:ASP:C	1:B:118:HIS:N	2.68	0.52
1:B:384:ASN:C	1:B:386:ASP:N	2.66	0.52
1:B:388:LEU:CD2	1:B:432:VAL:HB	2.37	0.52
1:B:442:VAL:O	1:B:457:ALA:HA	2.10	0.52
1:B:883:LEU:CD2	1:B:1021:LEU:HB2	2.40	0.52
1:B:1313:LEU:HD23	1:B:1338:VAL:HG21	1.91	0.52
2:C:90:ILE:HG23	2:C:133:LYS:O	2.09	0.52
2:C:95:ILE:HG13	2:C:129:PHE:O	2.08	0.52
2:C:687:GLU:O	2:C:688:GLY:C	2.52	0.52
2:C:899:ILE:HG22	2:C:903:VAL:HG21	1.91	0.52
2:C:1010:LEU:C	2:C:1011:ILE:HG13	2.34	0.52
2:C:1174:LYS:O	2:C:1176:ASN:N	2.42	0.52
8:I:26:ILE:HG23	8:I:27:GLU:N	2.24	0.52
1:B:172:PRO:HG3	1:B:185:TRP:CZ2	2.45	0.52
1:B:399:HIS:O	1:B:401:GLY:N	2.43	0.52
1:B:418:SER:C	1:B:420:ARG:N	2.67	0.52
1:B:541:ILE:HG22	1:B:546:VAL:HG23	1.90	0.52
1:B:1193:LEU:CD2	1:B:1260:LEU:HD11	2.32	0.52
1:B:1427:ASN:O	1:B:1431:GLY:N	2.41	0.52
1:B:1428:VAL:HG22	2:C:1151:LEU:HD21	1.90	0.52
2:C:298:LEU:HD22	2:C:298:LEU:N	2.24	0.52
2:C:1001:PHE:CE1	2:C:1073:TYR:HB2	2.45	0.52
3:D:7:GLN:HG2	11:L:104:ASN:ND2	2.19	0.52
4:E:192:LYS:HD2	4:E:199:ASN:HA	1.91	0.52
6:G:79:ARG:HB3	6:G:144:GLU:OE1	2.09	0.52
1:B:332:LYS:CA	1:B:337:ARG:HD2	2.39	0.52
1:B:556:TRP:CE3	1:B:558:GLY:HA2	2.45	0.52
2:C:240:ILE:HG22	2:C:254:LEU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:825:VAL:HG13	2:C:826:ALA:H	1.73	0.52
2:C:995:ARG:NH1	3:D:165:LYS:HA	2.25	0.52
2:C:1106:ARG:HG3	2:C:1107:ALA:N	2.23	0.52
1:B:568:PRO:CG	8:I:46:LEU:HD22	2.37	0.52
1:B:747:VAL:HG21	1:B:758:ILE:HD11	1.91	0.52
1:B:796:SER:C	1:B:798:GLY:H	2.18	0.52
1:B:1289:ARG:NH1	1:B:1326:ARG:NH1	2.58	0.52
1:B:1364:ASN:O	1:B:1366:ARG:HG3	2.10	0.52
2:C:510:LYS:HG3	2:C:511:PRO:CD	2.38	0.52
2:C:525:ALA:O	2:C:768:THR:HG23	2.09	0.52
2:C:916:THR:HB	2:C:935:ARG:HD2	1.90	0.52
3:D:116:LYS:HG3	3:D:117:ASP:N	2.24	0.52
4:E:141:LEU:HD22	7:H:46:LEU:O	2.09	0.52
5:F:43:LYS:C	5:F:45:LYS:H	2.18	0.52
7:H:98:GLY:HA3	7:H:110:VAL:O	2.09	0.52
7:H:125:SER:OG	7:H:128:PRO:HA	2.09	0.52
11:L:55:LYS:HB3	11:L:81:TYR:CE1	2.45	0.52
1:B:532:ARG:NH2	1:B:748:MET:HE3	2.25	0.52
1:B:560:ILE:CG1	8:I:78:SER:HB2	2.39	0.52
1:B:798:GLY:HA2	1:B:815:PHE:CD1	2.45	0.52
1:B:947:PHE:CE2	1:B:954:TRP:CE2	2.98	0.52
1:B:1004:ASN:OD1	1:B:1005:GLU:N	2.42	0.52
1:B:1341:ILE:HD12	1:B:1379:GLY:O	2.10	0.52
2:C:245:GLU:O	2:C:246:LYS:HG3	2.09	0.52
8:I:40:LEU:CD1	8:I:123:MET:HB2	2.40	0.52
12:M:28:LYS:O	12:M:29:TYR:HD2	1.93	0.52
1:B:34:LYS:HB2	1:B:36:ARG:HH21	1.75	0.52
1:B:476:SER:N	1:B:477:PRO:CD	2.73	0.52
1:B:556:TRP:CZ3	1:B:558:GLY:HA2	2.45	0.52
1:B:1006:ILE:O	1:B:1009:ASN:HB2	2.09	0.52
1:B:1048:ASN:O	1:B:1049:ILE:C	2.52	0.52
1:B:1334:ASP:C	1:B:1336:MET:N	2.67	0.52
2:C:467:GLY:N	2:C:475:SER:CB	2.72	0.52
2:C:473:MET:C	2:C:475:SER:H	2.18	0.52
3:D:69:LEU:O	10:K:6:ARG:HD2	2.10	0.52
12:M:55:ILE:O	12:M:56:LEU:HB2	2.07	0.52
1:B:466:SER:CB	11:L:2:ASN:HD22	2.22	0.52
1:B:547:LEU:HD22	11:L:58:PHE:CD1	2.45	0.52
1:B:710:LEU:H	1:B:710:LEU:HD12	1.75	0.52
1:B:853:ASP:O	1:B:1000:LEU:HD21	2.10	0.52
1:B:863:VAL:HG11	1:B:866:PHE:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1018:PHE:O	1:B:1021:LEU:HB3	2.10	0.52
1:B:1107:VAL:O	1:B:1107:VAL:HG12	2.10	0.52
1:B:1381:LEU:HD23	1:B:1381:LEU:N	2.25	0.52
2:C:100:PRO:CG	2:C:172:ILE:HD12	2.39	0.52
2:C:115:GLN:HB2	2:C:194:GLU:HG2	1.92	0.52
2:C:248:SER:H	2:C:418:LYS:NZ	2.08	0.52
2:C:745:PRO:O	2:C:748:ILE:HG12	2.10	0.52
2:C:976:ILE:O	2:C:990:ILE:HB	2.10	0.52
3:D:18:VAL:O	3:D:18:VAL:HG12	2.09	0.52
4:E:130:LEU:O	4:E:132:GLN:N	2.32	0.52
5:F:26:ARG:HH22	5:F:133:GLU:CD	2.17	0.52
5:F:190:LEU:O	5:F:191:LYS:HG2	2.10	0.52
6:G:116:ASP:HB3	6:G:119:ARG:HB2	1.91	0.52
11:L:55:LYS:HB3	11:L:81:TYR:CD1	2.44	0.52
1:B:91:PHE:HB2	1:B:297:GLN:HE22	1.75	0.52
1:B:219:PHE:CE2	1:B:231:PRO:HD2	2.45	0.52
1:B:522:GLY:HA2	1:B:630:ILE:CD1	2.39	0.52
1:B:1332:PHE:CE1	1:B:1348:LEU:HD13	2.45	0.52
2:C:294:ASP:HB2	9:J:12:ASN:HA	1.91	0.52
2:C:637:LEU:HD11	2:C:703:ILE:HD13	1.91	0.52
2:C:642:ASP:O	2:C:644:GLU:N	2.40	0.52
2:C:755:ILE:HG23	2:C:809:MET:HE3	1.90	0.52
3:D:18:VAL:O	3:D:20:PHE:HD2	1.93	0.52
3:D:203:GLN:HG2	3:D:207:CYS:SG	2.50	0.52
4:E:16:LYS:HB3	4:E:16:LYS:HZ3	1.74	0.52
10:K:53:HIS:HE1	10:K:55:ASP:OD1	1.94	0.52
1:B:466:SER:O	1:B:467:THR:HG23	2.10	0.51
1:B:498:ARG:HG3	1:B:499:ALA:H	1.75	0.51
1:B:590:ARG:CD	1:B:604:GLY:HA2	2.39	0.51
1:B:606:LEU:HD11	1:B:608:ILE:HG13	1.92	0.51
1:B:1437:GLY:O	1:B:1439:GLY:N	2.43	0.51
2:C:1085:ILE:H	2:C:1085:ILE:CD1	2.22	0.51
3:D:112:ASN:CB	3:D:114:TYR:CE1	2.93	0.51
7:H:51:TYR:C	7:H:51:TYR:CD2	2.88	0.51
7:H:143:ILE:CG2	7:H:144:ARG:N	2.69	0.51
1:B:247:ARG:HH11	1:B:247:ARG:HG3	1.75	0.51
1:B:355:GLY:N	1:B:482:PHE:CZ	2.78	0.51
1:B:482:PHE:CE1	2:C:836:GLU:HB2	2.45	0.51
1:B:774:ARG:O	1:B:775:ILE:C	2.52	0.51
1:B:947:PHE:CD2	1:B:954:TRP:CE2	2.98	0.51
1:B:1152:ILE:HD11	9:J:44:TYR:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1446:ASP:O	1:B:1447:GLU:C	2.53	0.51
2:C:172:ILE:CD1	2:C:178:ASN:HD22	2.23	0.51
2:C:298:LEU:H	2:C:298:LEU:CD2	2.22	0.51
2:C:364:ILE:HG22	2:C:365:THR:N	2.25	0.51
2:C:579:ARG:CB	2:C:586:TRP:HE1	2.18	0.51
2:C:1010:LEU:O	2:C:1011:ILE:CG1	2.58	0.51
3:D:176:ILE:CG2	3:D:177:GLU:N	2.72	0.51
5:F:154:ILE:O	5:F:196:VAL:HA	2.11	0.51
7:H:153:GLN:O	7:H:154:VAL:C	2.53	0.51
1:B:6:TYR:CD1	1:B:7:SER:N	2.78	0.51
1:B:24:PRO:HD2	1:B:233:TRP:HE1	1.74	0.51
1:B:108:MET:HB3	1:B:210:ILE:HD13	1.91	0.51
1:B:458:HIS:CE1	1:B:507:VAL:HG21	2.45	0.51
1:B:951:GLU:HB3	1:B:954:TRP:HZ2	1.74	0.51
1:B:1006:ILE:CD1	5:F:163:GLU:HG3	2.31	0.51
1:B:1063:MET:SD	1:B:1436:ILE:HG12	2.50	0.51
1:B:1114:PRO:HB2	1:B:1311:VAL:CG2	2.39	0.51
1:B:1364:ASN:O	1:B:1365:TYR:C	2.53	0.51
2:C:425:THR:HA	2:C:428:ILE:HD12	1.91	0.51
2:C:654:ARG:HG3	2:C:654:ARG:HH11	1.76	0.51
2:C:810:GLU:HB2	2:C:815:ARG:HH22	1.76	0.51
4:E:16:LYS:CG	4:E:18:VAL:HG12	2.40	0.51
1:B:34:LYS:CB	1:B:36:ARG:HH21	2.23	0.51
1:B:821:ARG:NH1	1:B:821:ARG:HB2	2.25	0.51
1:B:1138:ILE:CG2	1:B:1316:VAL:HG13	2.40	0.51
2:C:203:PHE:N	2:C:203:PHE:CD1	2.79	0.51
2:C:324:ILE:CG2	2:C:325:GLN:N	2.73	0.51
2:C:549:THR:HG22	2:C:550:ASP:N	2.19	0.51
2:C:583:ASN:HD21	2:C:628:THR:HG22	1.74	0.51
2:C:1120:GLU:HG2	2:C:1121:GLY:N	2.23	0.51
4:E:214:LEU:C	4:E:216:ASN:H	2.18	0.51
8:I:143:LEU:N	8:I:143:LEU:HD12	2.26	0.51
9:J:13:MET:O	9:J:14:LEU:HD23	2.11	0.51
1:B:586:ILE:CG2	1:B:587:HIS:H	2.23	0.51
1:B:1019:CYS:O	1:B:1022:LEU:N	2.44	0.51
2:C:63:ILE:HA	2:C:421:PHE:HE2	1.76	0.51
2:C:603:LEU:CD1	2:C:609:ILE:HG13	2.27	0.51
3:D:56:THR:HG21	3:D:145:CYS:SG	2.50	0.51
9:J:101:PHE:HB2	9:J:110:PHE:CE2	2.45	0.51
11:L:10:PHE:N	11:L:10:PHE:HD2	2.09	0.51
1:B:208:LEU:HD23	1:B:208:LEU:C	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:526:ASP:OD1	2:C:1013:ASN:ND2	2.42	0.51
1:B:852:TYR:CE2	1:B:1060:PRO:HB2	2.45	0.51
1:B:1173:HIS:C	1:B:1174:PHE:HD1	2.17	0.51
2:C:547:VAL:HG12	2:C:612:GLU:OE2	2.11	0.51
2:C:614:SER:OG	2:C:627:PHE:HB2	2.10	0.51
2:C:806:THR:HG21	2:C:808:ALA:HB3	1.91	0.51
2:C:848:ARG:HD2	10:K:8:PHE:O	2.11	0.51
3:D:132:PRO:O	3:D:133:ILE:C	2.54	0.51
4:E:29:LEU:HD22	7:H:82:PHE:CE2	2.46	0.51
4:E:59:ILE:O	4:E:60:LYS:C	2.51	0.51
7:H:112:LYS:NZ	7:H:120:THR:HA	2.26	0.51
8:I:91:ASP:C	8:I:93:TYR:H	2.18	0.51
1:B:54:ASN:N	1:B:54:ASN:HD22	2.08	0.51
1:B:248:PRO:O	1:B:260:ASP:HB2	2.09	0.51
1:B:358:ASN:O	1:B:359:LEU:HD23	2.11	0.51
1:B:476:SER:N	1:B:477:PRO:HD3	2.26	0.51
1:B:848:ILE:HA	1:B:857:ARG:O	2.11	0.51
1:B:1121:GLU:CG	1:B:1122:PRO:HD2	2.40	0.51
2:C:708:GLU:HG3	2:C:709:ASP:H	1.75	0.51
2:C:752:ALA:O	2:C:755:ILE:HG13	2.11	0.51
3:D:232:VAL:HG11	3:D:244:VAL:HG22	1.92	0.51
4:E:172:LEU:HB3	4:E:176:GLU:OE1	2.11	0.51
5:F:23:VAL:HB	5:F:30:ILE:CD1	2.39	0.51
5:F:182:ASP:O	5:F:185:ALA:HB3	2.10	0.51
7:H:14:HIS:HD2	7:H:16:SER:HB2	1.70	0.51
10:K:8:PHE:H	10:K:49:MET:HE3	1.74	0.51
1:B:250:ILE:O	1:B:250:ILE:HG22	2.10	0.51
1:B:268:ASP:HB3	1:B:299:HIS:ND1	2.26	0.51
1:B:351:THR:HG22	2:C:1103:ILE:HA	1.92	0.51
1:B:709:THR:HG23	9:J:94:ASP:HA	1.91	0.51
1:B:868:TYR:CD1	1:B:868:TYR:C	2.85	0.51
2:C:244:LEU:HD21	2:C:366:GLN:HE21	1.71	0.51
2:C:284:ILE:HD13	2:C:333:PHE:HD2	1.76	0.51
2:C:582:VAL:HA	2:C:626:ILE:O	2.10	0.51
2:C:615:MET:C	2:C:616:ILE:HD12	2.36	0.51
2:C:840:ILE:CG2	2:C:994:TYR:HD1	2.24	0.51
2:C:1174:LYS:O	2:C:1175:LEU:C	2.54	0.51
4:E:220:LEU:O	4:E:221:TYR:HD1	1.93	0.51
5:F:96:PHE:CE1	5:F:100:ILE:HD11	2.46	0.51
7:H:132:SER:HB3	7:H:135:ASP:HB2	1.92	0.51
9:J:82:GLU:HB3	9:J:104:LEU:HG	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:18:LYS:HZ3	11:L:38:GLU:HG2	1.74	0.51
11:L:57:LEU:H	11:L:77:THR:HA	1.75	0.51
1:B:605:MET:HE2	1:B:607:ILE:HD11	1.91	0.51
1:B:882:SER:HA	1:B:952:ALA:O	2.11	0.51
1:B:1121:GLU:HB3	1:B:1124:HIS:HD2	1.75	0.51
2:C:165:VAL:O	2:C:167:ILE:HD12	2.11	0.51
2:C:388:CYS:C	2:C:390:LEU:H	2.19	0.51
2:C:498:THR:HG22	2:C:537:LYS:H	1.75	0.51
2:C:659:ALA:HA	2:C:662:MET:HE3	1.92	0.51
2:C:834:ASN:HA	2:C:838:SER:O	2.09	0.51
2:C:841:MET:HE3	2:C:1010:LEU:HD11	1.92	0.51
2:C:1032:SER:O	2:C:1036:ALA:HB2	2.11	0.51
9:J:55:THR:HG22	9:J:58:VAL:HG21	1.93	0.51
12:M:31:CYS:HA	12:M:56:LEU:HD23	1.92	0.51
1:B:78:PRO:CA	2:C:1201:LYS:HZ2	2.23	0.51
1:B:102:VAL:HG11	1:B:211:PHE:CE2	2.46	0.51
1:B:818:MET:HE1	2:C:516:ASN:ND2	2.26	0.51
1:B:958:VAL:HG12	1:B:960:ILE:HG13	1.92	0.51
1:B:1342:GLU:OE2	5:F:198:ILE:HD13	2.11	0.51
1:B:1350:LYS:O	1:B:1354:ASN:ND2	2.44	0.51
2:C:273:LEU:HB2	2:C:276:ILE:HG13	1.93	0.51
2:C:345:LYS:HG3	2:C:348:ARG:HH21	1.75	0.51
2:C:471:LYS:O	2:C:472:ALA:HB2	2.10	0.51
3:D:235:VAL:HG12	10:K:13:VAL:HG22	1.93	0.51
4:E:11:ARG:HD3	4:E:12:ARG:N	2.26	0.51
4:E:51:ASN:O	4:E:54:GLU:HB3	2.11	0.51
9:J:45:ARG:HE	9:J:47:GLU:HG3	1.75	0.51
1:B:639:PRO:CG	1:B:640:GLN:H	2.21	0.50
1:B:875:ALA:O	1:B:878:ILE:HG13	2.10	0.50
1:B:898:ARG:HB2	1:B:933:TYR:HE1	1.76	0.50
1:B:1299:VAL:HG12	1:B:1300:LYS:N	2.25	0.50
2:C:29:ASP:CB	2:C:658:ILE:HD13	2.39	0.50
2:C:167:ILE:HG22	2:C:453:ILE:HD12	1.91	0.50
2:C:758:PHE:CE1	2:C:1027:ILE:CG2	2.94	0.50
2:C:911:ILE:O	2:C:911:ILE:HG22	2.10	0.50
3:D:70:ILE:HG22	3:D:70:ILE:O	2.10	0.50
3:D:99:LEU:O	3:D:156:THR:HA	2.11	0.50
5:F:153:HIS:HB3	5:F:196:VAL:HG13	1.88	0.50
7:H:117:GLN:O	7:H:119:LEU:N	2.45	0.50
1:B:90:VAL:HG13	1:B:297:GLN:CD	2.36	0.50
1:B:157:ASP:C	1:B:159:THR:H	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:126:SER:O	2:C:169:ARG:HA	2.11	0.50
2:C:911:ILE:HD11	2:C:941:LEU:CD1	2.41	0.50
2:C:948:ILE:HG22	2:C:949:VAL:O	2.11	0.50
2:C:1160:VAL:HG12	2:C:1161:HIS:N	2.26	0.50
3:D:63:ILE:HA	3:D:66:ARG:HG3	1.94	0.50
3:D:77:ILE:HG23	3:D:161:LYS:HE3	1.93	0.50
8:I:42:ILE:O	8:I:44:VAL:HG23	2.11	0.50
12:M:55:ILE:O	12:M:56:LEU:CB	2.59	0.50
1:B:268:ASP:HB3	1:B:299:HIS:CE1	2.47	0.50
1:B:357:PRO:HD2	2:C:833:TYR:CE1	2.47	0.50
1:B:528:LEU:O	1:B:531:ILE:HG22	2.12	0.50
1:B:537:ARG:HH22	8:I:122:LEU:CD1	2.24	0.50
1:B:608:ILE:HG13	1:B:613:ILE:HD12	1.94	0.50
1:B:665:GLY:HA3	2:C:1086:PHE:CD1	2.46	0.50
1:B:1015:VAL:CG1	1:B:1019:CYS:SG	2.98	0.50
1:B:1094:VAL:HG13	1:B:1113:THR:CG2	2.36	0.50
2:C:29:ASP:O	2:C:30:SER:C	2.54	0.50
2:C:861:ASP:OD1	2:C:914:LYS:HD2	2.11	0.50
2:C:1212:ILE:O	2:C:1214:PRO:HD3	2.11	0.50
3:D:213:PRO:O	3:D:214:ASN:CB	2.59	0.50
3:D:243:VAL:O	3:D:243:VAL:HG12	2.11	0.50
5:F:182:ASP:HB3	5:F:185:ALA:CB	2.41	0.50
8:I:83:GLN:C	8:I:85:GLY:H	2.19	0.50
11:L:6:ARG:O	11:L:9:LEU:HG	2.11	0.50
11:L:73:LEU:CD2	11:L:75:ILE:HD11	2.40	0.50
12:M:30:ILE:O	12:M:56:LEU:HA	2.11	0.50
12:M:52:GLY:O	12:M:54:ARG:N	2.44	0.50
1:B:42:ASP:O	1:B:44:THR:N	2.41	0.50
1:B:362:ASP:OD2	1:B:459:ARG:HD3	2.11	0.50
1:B:598:LEU:HD22	8:I:25:ARG:NH1	2.27	0.50
1:B:635:ARG:HA	1:B:635:ARG:NH1	2.25	0.50
1:B:997:LEU:HD13	1:B:1018:PHE:CE2	2.46	0.50
1:B:1280:GLU:O	1:B:1281:ARG:C	2.54	0.50
1:B:1332:PHE:CD2	1:B:1332:PHE:N	2.80	0.50
1:B:1445:ILE:HD11	7:H:61:ILE:HG12	1.93	0.50
2:C:199:MET:HE2	2:C:492:LEU:HD23	1.93	0.50
2:C:409:ALA:O	2:C:413:LEU:HG	2.11	0.50
2:C:1034:VAL:HG12	2:C:1035:ALA:N	2.25	0.50
2:C:1069:PHE:HA	2:C:1085:ILE:O	2.11	0.50
3:D:22:LEU:HD11	11:L:101:LEU:HD11	1.94	0.50
3:D:213:PRO:HG2	3:D:214:ASN:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:10:THR:O	4:E:10:THR:HG22	2.12	0.50
6:G:88:TYR:N	6:G:88:TYR:CD1	2.79	0.50
7:H:49:LEU:N	7:H:49:LEU:HD23	2.25	0.50
7:H:63:PRO:O	7:H:64:THR:CB	2.59	0.50
8:I:130:ARG:HB3	8:I:133:ASN:HB2	1.93	0.50
11:L:6:ARG:O	11:L:8:GLU:N	2.45	0.50
11:L:68:PHE:N	11:L:68:PHE:CD2	2.76	0.50
1:B:568:PRO:HB2	3:D:221:TYR:CZ	2.46	0.50
1:B:622:VAL:O	1:B:622:VAL:HG13	2.11	0.50
1:B:1063:MET:HG3	2:C:1139:ILE:O	2.12	0.50
2:C:388:CYS:C	2:C:390:LEU:N	2.70	0.50
2:C:557:PHE:C	2:C:557:PHE:CD2	2.89	0.50
2:C:1095:LEU:H	2:C:1095:LEU:CD1	2.21	0.50
3:D:204:SER:O	3:D:207:CYS:SG	2.68	0.50
5:F:60:PHE:C	5:F:60:PHE:CD2	2.88	0.50
8:I:35:GLN:O	8:I:37:LYS:HG3	2.12	0.50
8:I:127:GLY:O	8:I:128:ASN:CB	2.58	0.50
10:K:1:MET:N	10:K:55:ASP:C	2.70	0.50
13:N:1:DC:H2''	13:N:2:DA:O5'	2.12	0.50
1:B:637:LYS:O	1:B:641:VAL:HG21	2.12	0.50
1:B:1153:TYR:HB2	1:B:1192:LEU:HD23	1.93	0.50
2:C:910:VAL:CG1	2:C:911:ILE:N	2.75	0.50
2:C:1010:LEU:O	2:C:1011:ILE:HG13	2.11	0.50
3:D:191:TYR:HD2	3:D:201:TRP:CD1	2.29	0.50
5:F:176:PRO:O	5:F:212:ARG:HA	2.12	0.50
6:G:143:PHE:CD1	6:G:143:PHE:C	2.86	0.50
7:H:95:SER:C	7:H:97:HIS:H	2.19	0.50
7:H:115:MET:HB2	7:H:116:PRO:CD	2.37	0.50
1:B:86:LEU:HD21	1:B:239:LEU:HB2	1.93	0.50
1:B:91:PHE:H	1:B:297:GLN:NE2	2.07	0.50
1:B:901:LEU:HB2	1:B:926:GLN:CG	2.28	0.50
1:B:1015:VAL:O	1:B:1017:LEU:N	2.45	0.50
1:B:1074:GLU:C	1:B:1076:ALA:N	2.68	0.50
1:B:1329:THR:HG22	1:B:1331:SER:HB3	1.93	0.50
2:C:58:THR:O	2:C:62:ILE:HG13	2.11	0.50
2:C:236:HIS:CE1	2:C:389:ALA:HA	2.47	0.50
2:C:265:SER:O	2:C:266:ALA:HB3	2.11	0.50
2:C:461:LEU:H	2:C:461:LEU:CD1	2.25	0.50
2:C:508:LEU:HG	2:C:509:ALA:N	2.27	0.50
2:C:945:GLU:O	2:C:946:ASN:HB3	2.10	0.50
2:C:1196:ILE:HB	2:C:1197:PRO:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:228:PHE:N	3:D:228:PHE:CD1	2.80	0.50
4:E:161:GLY:O	4:E:165:GLN:HG3	2.11	0.50
5:F:11:ARG:C	5:F:13:TRP:N	2.69	0.50
5:F:145:THR:HG21	5:F:187:TYR:CD2	2.46	0.50
6:G:103:MET:HE1	7:H:66:GLY:N	2.26	0.50
7:H:22:MET:O	7:H:23:LYS:C	2.54	0.50
8:I:95:TYR:CE2	8:I:97:MET:CG	2.92	0.50
12:M:38:LEU:O	12:M:39:SER:CB	2.58	0.50
1:B:498:ARG:HG3	1:B:499:ALA:N	2.26	0.50
1:B:1008:GLN:O	1:B:1011:GLN:HB3	2.11	0.50
1:B:1334:ASP:O	1:B:1336:MET:N	2.45	0.50
2:C:118:ARG:HD3	2:C:204:ILE:CD1	2.41	0.50
2:C:247:GLY:O	2:C:248:SER:HB3	2.11	0.50
2:C:846:ILE:HG23	2:C:974:PRO:HG2	1.93	0.50
2:C:1004:GLU:HB2	2:C:1006:ILE:HG12	1.94	0.50
2:C:1079:LYS:CG	2:C:1080:LYS:H	2.22	0.50
5:F:108:GLY:HA3	5:F:132:ILE:CG2	2.42	0.50
8:I:59:ILE:O	8:I:60:ALA:CB	2.59	0.50
9:J:82:GLU:HB3	9:J:104:LEU:HD12	1.94	0.50
9:J:82:GLU:OE2	9:J:104:LEU:HD12	2.11	0.50
1:B:260:ASP:OD1	1:B:261:ASP:N	2.45	0.50
1:B:482:PHE:C	1:B:484:GLY:H	2.20	0.50
1:B:1187:GLN:HG3	1:B:1188:GLN:HG3	1.94	0.50
1:B:1451:VAL:O	1:B:1454:MET:HG2	2.12	0.50
2:C:189:LEU:O	2:C:192:LEU:N	2.36	0.50
2:C:281:PRO:O	2:C:283:VAL:N	2.45	0.50
2:C:611:PRO:HG2	2:C:685:LEU:HD21	1.92	0.50
2:C:683:SER:C	2:C:685:LEU:H	2.20	0.50
2:C:873:THR:CG2	2:C:874:PHE:N	2.75	0.50
2:C:955:THR:HG23	2:C:956:THR:H	1.76	0.50
2:C:1008:PRO:HD3	2:C:1087:PHE:HE1	1.76	0.50
2:C:1072:MET:HE1	2:C:1087:PHE:HD1	1.76	0.50
4:E:51:ASN:O	4:E:51:ASN:OD1	2.30	0.50
4:E:176:GLU:HG2	4:E:197:SER:OG	2.11	0.50
5:F:48:ASP:CG	5:F:49:SER:N	2.70	0.50
6:G:75:PRO:HG3	6:G:78:GLN:OE1	2.12	0.50
6:G:77:ASP:OD1	6:G:78:GLN:N	2.45	0.50
14:P:8:U:H2'	14:P:9:A:C8	2.47	0.50
1:B:409:SER:O	1:B:411:ASP:N	2.45	0.49
1:B:546:VAL:HG21	1:B:572:TRP:CE3	2.46	0.49
1:B:852:TYR:CD1	6:G:136:ARG:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:886:ILE:CG2	1:B:887:GLY:H	2.25	0.49
1:B:1100:ARG:NH2	1:B:1351:GLU:HG2	2.27	0.49
1:B:1371:LEU:O	1:B:1375:MET:HG3	2.12	0.49
1:B:1397:LEU:O	1:B:1400:CYS:HB3	2.12	0.49
1:B:1418:LEU:HD12	1:B:1419:ASP:N	2.27	0.49
2:C:185:THR:N	2:C:188:ASP:HB2	2.26	0.49
2:C:601:ARG:HD3	2:C:605:ARG:HH21	1.77	0.49
4:E:144:THR:HG21	7:H:46:LEU:HD13	1.94	0.49
7:H:1:MET:SD	7:H:1:MET:C	2.95	0.49
11:L:7:PHE:HA	11:L:10:PHE:CE2	2.47	0.49
15:T:18:DT:H6	15:T:18:DT:O5'	1.94	0.49
1:B:50:ILE:HG22	1:B:52:GLY:H	1.77	0.49
1:B:344:ARG:HD2	2:C:1118:PRO:O	2.11	0.49
1:B:373:THR:HG21	2:C:1105:ALA:CB	2.42	0.49
1:B:500:GLU:OE1	2:C:1143:ALA:C	2.55	0.49
1:B:722:LEU:HD12	1:B:722:LEU:N	2.26	0.49
1:B:1254:ALA:O	1:B:1255:GLU:CB	2.60	0.49
1:B:1389:PHE:CD1	1:B:1390:ASN:N	2.80	0.49
2:C:234:ILE:HG21	2:C:237:VAL:HG23	1.94	0.49
2:C:386:LEU:C	2:C:388:CYS:N	2.68	0.49
2:C:401:PHE:HD2	2:C:521:LEU:HD12	1.77	0.49
2:C:704:ALA:HB2	2:C:738:PHE:CD2	2.47	0.49
2:C:981:ALA:HB2	2:C:987:LYS:HA	1.94	0.49
2:C:1099:VAL:C	2:C:1101:ASP:H	2.19	0.49
3:D:128:ASN:O	3:D:129:ILE:HG13	2.11	0.49
4:E:51:ASN:O	4:E:52:LEU:C	2.54	0.49
6:G:93:ILE:HD11	6:G:134:ILE:HD11	1.95	0.49
8:I:8:ASP:HB3	8:I:10:PHE:CE1	2.47	0.49
1:B:588:LEU:O	1:B:606:LEU:HA	2.12	0.49
1:B:896:ARG:HD3	1:B:897:TYR:HE1	1.77	0.49
1:B:896:ARG:HH22	1:B:1030:ARG:HH21	1.59	0.49
1:B:946:VAL:HB	1:B:947:PHE:HD1	1.76	0.49
1:B:1198:ASP:O	1:B:1202:MET:HG2	2.13	0.49
2:C:35:SER:O	2:C:39:ARG:HG3	2.12	0.49
2:C:570:VAL:CB	2:C:573:GLN:HB3	2.41	0.49
2:C:806:THR:CG2	2:C:808:ALA:HB3	2.42	0.49
4:E:216:ASN:O	4:E:217:LEU:C	2.54	0.49
8:I:5:LEU:HD12	8:I:60:ALA:HA	1.94	0.49
9:J:106:CYS:O	9:J:107:SER:HB2	2.11	0.49
1:B:12:ARG:CZ	2:C:1192:TYR:HE2	2.25	0.49
1:B:32:VAL:HG21	1:B:68:GLN:NE2	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ARG:O	1:B:138:ILE:HG13	2.12	0.49
1:B:347:PHE:CE2	1:B:493:GLN:OE1	2.64	0.49
1:B:396:PRO:HG3	1:B:416:ARG:HB3	1.95	0.49
1:B:577:ILE:C	1:B:579:SER:N	2.69	0.49
1:B:921:GLY:O	1:B:922:ASP:C	2.55	0.49
1:B:1377:THR:O	1:B:1379:GLY:N	2.45	0.49
1:B:1441:PHE:CE2	6:G:89:GLU:HG2	2.48	0.49
2:C:203:PHE:N	2:C:203:PHE:HD1	2.11	0.49
2:C:294:ASP:C	2:C:296:GLU:H	2.17	0.49
2:C:385:LEU:HD23	2:C:386:LEU:HD23	1.94	0.49
2:C:388:CYS:O	2:C:391:ASP:N	2.45	0.49
2:C:638:PHE:HB3	2:C:651:LEU:HD22	1.94	0.49
2:C:798:TYR:CD1	10:K:4:PRO:HB3	2.48	0.49
2:C:1110:PRO:O	2:C:1119:VAL:HG13	2.11	0.49
3:D:254:LYS:O	3:D:256:ALA:N	2.45	0.49
5:F:61:GLN:HB2	5:F:79:TRP:CE3	2.44	0.49
7:H:119:LEU:HD12	7:H:131:GLN:C	2.37	0.49
8:I:101:ALA:HB2	8:I:116:TYR:CE1	2.47	0.49
10:K:1:MET:HE2	10:K:56:LEU:HD12	1.94	0.49
11:L:61:TYR:O	11:L:62:LYS:HB3	2.12	0.49
11:L:90:ALA:O	11:L:94:ILE:HG13	2.12	0.49
1:B:77:CYS:C	1:B:78:PRO:O	2.51	0.49
1:B:225:ASN:HD22	1:B:228:PHE:N	1.97	0.49
1:B:446:ARG:HB2	1:B:487:MET:CG	2.42	0.49
1:B:544:ASP:CG	1:B:545:GLN:N	2.70	0.49
2:C:401:PHE:CD2	2:C:521:LEU:HD12	2.48	0.49
2:C:412:LEU:HB3	2:C:466:TRP:CZ2	2.47	0.49
2:C:785:TYR:CD1	2:C:786:ASN:N	2.80	0.49
2:C:859:TYR:CZ	2:C:941:LEU:HD12	2.47	0.49
2:C:861:ASP:OD1	2:C:862:GLN:N	2.45	0.49
4:E:40:HIS:C	4:E:42:GLY:H	2.20	0.49
4:E:51:ASN:O	4:E:52:LEU:O	2.31	0.49
5:F:16:PHE:O	5:F:19:VAL:N	2.45	0.49
5:F:46:TYR:CD2	5:F:58:MET:HG2	2.47	0.49
5:F:50:MET:HG3	5:F:50:MET:O	2.12	0.49
5:F:124:VAL:N	5:F:125:PRO:HD2	2.28	0.49
8:I:6:PHE:O	8:I:58:THR:HA	2.12	0.49
9:J:69:PRO:HG2	9:J:85:PHE:CE2	2.47	0.49
12:M:61:THR:HG22	12:M:62:LYS:N	2.27	0.49
1:B:1116:LEU:HB3	1:B:1308:THR:HG22	1.95	0.49
1:B:1161:THR:CG2	1:B:1163:ILE:HG13	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:45:SER:O	2:C:46:GLN:C	2.54	0.49
2:C:108:VAL:HG12	2:C:109:THR:N	2.25	0.49
2:C:526:GLU:HB2	2:C:771:SER:HB3	1.94	0.49
2:C:531:GLN:HG3	2:C:532:ALA:H	1.76	0.49
2:C:644:GLU:C	2:C:646:LEU:H	2.21	0.49
2:C:878:GLN:O	2:C:879:ARG:C	2.54	0.49
4:E:195:ILE:HG22	4:E:195:ILE:O	2.13	0.49
5:F:23:VAL:HG13	5:F:78:LEU:CD1	2.39	0.49
8:I:138:GLU:HG2	8:I:139:ASN:N	2.28	0.49
10:K:56:LEU:O	10:K:57:ILE:C	2.54	0.49
15:T:18:DT:C2'	15:T:19:DT:C5'	2.88	0.49
1:B:16:GLU:CD	2:C:1220:ARG:HA	2.38	0.49
1:B:244:PRO:CB	1:B:245:PRO:CD	2.91	0.49
1:B:408:ASP:O	1:B:410:GLY:N	2.38	0.49
1:B:963:ILE:HD11	1:B:1048:ASN:HB3	1.93	0.49
1:B:1423:GLY:O	1:B:1426:GLU:HB2	2.13	0.49
2:C:44:VAL:HG13	2:C:199:MET:HG2	1.94	0.49
2:C:60:GLN:NE2	2:C:94:LYS:HA	2.28	0.49
2:C:175:ARG:HG2	2:C:175:ARG:NH1	2.27	0.49
2:C:483:LEU:HD11	2:C:491:THR:CG2	2.33	0.49
2:C:798:TYR:HE2	3:D:62:PHE:CZ	2.30	0.49
2:C:975:GLN:HG2	2:C:976:ILE:N	2.28	0.49
2:C:1072:MET:CE	2:C:1087:PHE:HD1	2.25	0.49
2:C:1166:CYS:O	2:C:1168:LEU:N	2.45	0.49
2:C:1201:LYS:CG	2:C:1202:LEU:N	2.75	0.49
5:F:117:THR:HG22	5:F:119:SER:N	2.21	0.49
5:F:135:PHE:CB	5:F:140:LEU:HD11	2.40	0.49
11:L:12:LEU:HD12	11:L:12:LEU:N	2.20	0.49
12:M:44:ASP:O	12:M:45:ALA:HB3	2.11	0.49
1:B:44:THR:O	1:B:44:THR:HG22	2.12	0.49
1:B:356:ASP:OD1	1:B:358:ASN:HB2	2.13	0.49
1:B:567:LYS:CG	1:B:568:PRO:CD	2.80	0.49
1:B:586:ILE:HB	1:B:610:GLY:HA2	1.95	0.49
1:B:667:GLY:CA	3:D:192:TRP:CH2	2.95	0.49
1:B:901:LEU:N	1:B:926:GLN:NE2	2.55	0.49
1:B:1305:VAL:HG12	1:B:1306:LEU:N	2.27	0.49
2:C:683:SER:C	2:C:685:LEU:N	2.70	0.49
2:C:864:LYS:N	2:C:872:GLU:OE1	2.40	0.49
4:E:12:ARG:HH12	4:E:14:ARG:HG3	1.78	0.49
4:E:24:ALA:O	4:E:26:THR:N	2.36	0.49
5:F:106:GLN:HA	5:F:130:ALA:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:157:SER:C	5:F:159:ASP:N	2.69	0.49
1:B:162:VAL:HG12	1:B:163:SER:N	2.27	0.49
1:B:457:ALA:HB3	1:B:506:ALA:HA	1.94	0.49
1:B:598:LEU:HD23	8:I:122:LEU:HD12	1.95	0.49
1:B:738:LYS:HD2	1:B:740:LEU:HD21	1.95	0.49
1:B:852:TYR:CD2	1:B:1060:PRO:CB	2.96	0.49
1:B:1444:MET:HG3	7:H:60:ARG:HA	1.94	0.49
2:C:203:PHE:HB3	2:C:205:ILE:CD1	2.43	0.49
2:C:254:LEU:CD2	2:C:361:LEU:HD13	2.43	0.49
2:C:446:LEU:O	2:C:447:ALA:HB3	2.13	0.49
2:C:1017:ILE:N	2:C:1018:PRO:CD	2.76	0.49
3:D:99:LEU:HA	3:D:119:VAL:O	2.12	0.49
3:D:114:TYR:HB3	3:D:140:ASN:O	2.13	0.49
6:G:76:LYS:HE3	6:G:150:GLU:OE2	2.12	0.49
8:I:8:ASP:C	8:I:9:ILE:HG13	2.38	0.49
9:J:4:PHE:CD1	9:J:4:PHE:C	2.90	0.49
1:B:24:PRO:HG2	1:B:25:GLU:OE1	2.12	0.49
1:B:537:ARG:HH12	8:I:122:LEU:HG	1.77	0.49
1:B:613:ILE:O	1:B:614:PHE:HB3	2.12	0.49
1:B:648:ASN:O	1:B:649:ILE:C	2.54	0.49
1:B:954:TRP:HB3	1:B:955:PRO:HD2	1.95	0.49
1:B:1272:THR:C	1:B:1273:LEU:HD12	2.38	0.49
1:B:1323:ASP:OD1	1:B:1326:ARG:HG3	2.13	0.49
1:B:1335:ILE:CG2	1:B:1335:ILE:O	2.61	0.49
2:C:199:MET:N	2:C:199:MET:SD	2.86	0.49
2:C:1181:GLU:O	2:C:1182:CYS:CB	2.60	0.49
8:I:26:ILE:CG2	8:I:27:GLU:N	2.76	0.49
9:J:105:SER:O	9:J:106:CYS:HB2	2.12	0.49
1:B:34:LYS:N	1:B:34:LYS:CD	2.76	0.48
1:B:53:LEU:O	1:B:54:ASN:O	2.31	0.48
1:B:230:ARG:O	1:B:231:PRO:C	2.55	0.48
1:B:278:THR:HG22	1:B:278:THR:O	2.12	0.48
1:B:374:LEU:HB2	1:B:436:ILE:HD11	1.95	0.48
1:B:516:SER:O	1:B:517:ASN:C	2.55	0.48
1:B:1389:PHE:CG	1:B:1390:ASN:N	2.81	0.48
2:C:243:ALA:HB1	2:C:251:ILE:HG12	1.93	0.48
2:C:288:ALA:HA	2:C:331:LEU:HD12	1.94	0.48
2:C:378:LEU:HD12	2:C:378:LEU:C	2.38	0.48
3:D:10:ILE:HD12	11:L:108:GLU:O	2.13	0.48
3:D:20:PHE:CE1	3:D:230:MET:HE3	2.48	0.48
4:E:64:VAL:HA	4:E:129:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:9:LEU:HD12	7:H:10:ASN:H	1.76	0.48
8:I:56:THR:HB	8:I:145:ARG:HG2	1.95	0.48
10:K:5:VAL:O	10:K:6:ARG:O	2.31	0.48
1:B:40:THR:HG22	1:B:41:MET:CG	2.31	0.48
1:B:135:PHE:CD1	1:B:222:LEU:HD22	2.48	0.48
1:B:300:VAL:O	1:B:300:VAL:HG12	2.12	0.48
1:B:971:PHE:HE2	1:B:1040:GLN:HG2	1.78	0.48
1:B:1146:VAL:HG11	1:B:1202:MET:SD	2.53	0.48
2:C:30:SER:HB3	2:C:743:ILE:O	2.13	0.48
2:C:114:PRO:HG2	2:C:115:GLN:H	1.77	0.48
2:C:324:ILE:HG12	2:C:329:THR:HG22	1.95	0.48
2:C:351:TYR:CD2	2:C:355:ILE:HD11	2.49	0.48
2:C:1162:ILE:HD11	2:C:1194:ILE:CD1	2.43	0.48
3:D:100:THR:HG21	3:D:102:GLN:HE21	1.78	0.48
4:E:23:ASN:O	7:H:83:LYS:HB2	2.14	0.48
4:E:24:ALA:C	4:E:26:THR:N	2.69	0.48
5:F:157:SER:OG	5:F:159:ASP:HB2	2.14	0.48
9:J:85:PHE:CD2	9:J:85:PHE:N	2.72	0.48
9:J:99:LEU:O	9:J:111:THR:HG23	2.13	0.48
9:J:101:PHE:HB2	9:J:110:PHE:CZ	2.47	0.48
11:L:50:LEU:HD11	11:L:75:ILE:CD1	2.42	0.48
1:B:90:VAL:HG12	1:B:297:GLN:NE2	2.28	0.48
1:B:93:VAL:CG2	1:B:304:MET:HE3	2.43	0.48
1:B:1317:MET:HE2	1:B:1327:ILE:CG2	2.40	0.48
1:B:1333:ILE:O	1:B:1333:ILE:HD13	2.13	0.48
2:C:361:LEU:N	2:C:362:PRO:CD	2.76	0.48
2:C:363:HIS:O	2:C:365:THR:N	2.41	0.48
2:C:554:ILE:O	2:C:558:LEU:HG	2.13	0.48
2:C:847:ASP:O	2:C:849:GLY:N	2.46	0.48
3:D:44:LEU:CG	3:D:159:ALA:HB1	2.43	0.48
4:E:14:ARG:NH2	4:E:16:LYS:NZ	2.59	0.48
4:E:41:GLN:HB2	4:E:43:GLU:HG3	1.94	0.48
10:K:53:HIS:ND1	10:K:53:HIS:C	2.71	0.48
10:K:64:ASN:CB	10:K:65:PRO:CD	2.89	0.48
1:B:35:ILE:HG22	1:B:84:ILE:HD12	1.95	0.48
1:B:92:HIS:O	1:B:93:VAL:C	2.56	0.48
1:B:366:VAL:HG21	1:B:460:VAL:HG23	1.96	0.48
1:B:598:LEU:HA	8:I:122:LEU:CD1	2.38	0.48
1:B:1006:ILE:HD12	5:F:167:ARG:CG	2.44	0.48
1:B:1437:GLY:O	1:B:1438:THR:C	2.54	0.48
2:C:259:TYR:HB2	2:C:268:THR:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:288:ALA:CA	2:C:331:LEU:HD12	2.43	0.48
2:C:459:TYR:CD1	2:C:469:GLN:NE2	2.81	0.48
2:C:658:ILE:HG22	2:C:659:ALA:N	2.27	0.48
2:C:779:GLY:O	2:C:795:ILE:HA	2.13	0.48
2:C:802:PRO:HG2	2:C:805:THR:HG22	1.95	0.48
2:C:1183:LYS:HE3	2:C:1183:LYS:N	2.29	0.48
3:D:43:THR:O	3:D:77:ILE:HG13	2.12	0.48
4:E:31:GLN:C	4:E:33:PHE:H	2.22	0.48
4:E:189:ASP:HB3	7:H:167:TYR:OH	2.13	0.48
8:I:58:THR:HB	8:I:143:LEU:HD13	1.94	0.48
10:K:16:ASP:OD1	10:K:17:LYS:CD	2.62	0.48
11:L:60:ALA:O	11:L:73:LEU:HD12	2.14	0.48
15:T:18:DT:OP2	15:T:18:DT:H73	2.14	0.48
1:B:129:LYS:O	1:B:130:ASP:HB2	2.14	0.48
1:B:279:LEU:HB3	1:B:289:ILE:HD11	1.95	0.48
1:B:332:LYS:O	1:B:333:GLU:HB2	2.13	0.48
1:B:513:SER:HB2	1:B:520:CYS:HB3	1.95	0.48
1:B:650:GLN:HB3	1:B:654:ASN:ND2	2.28	0.48
1:B:698:GLN:NE2	9:J:99:LEU:HD21	2.28	0.48
1:B:942:PHE:HD2	1:B:942:PHE:O	1.96	0.48
1:B:1011:GLN:HE21	1:B:1015:VAL:HG21	1.77	0.48
2:C:180:TYR:N	2:C:180:TYR:CD1	2.81	0.48
2:C:797:TYR:HE1	2:C:854:LEU:HD23	1.78	0.48
2:C:890:TYR:O	2:C:893:LEU:HB2	2.13	0.48
2:C:1085:ILE:HG22	2:C:1086:PHE:N	2.28	0.48
2:C:1151:LEU:N	2:C:1151:LEU:HD12	2.28	0.48
3:D:73:GLN:HE21	3:D:75:MET:N	2.10	0.48
5:F:18:THR:O	5:F:19:VAL:C	2.57	0.48
7:H:139:ILE:CG2	7:H:140:LYS:H	2.16	0.48
1:B:218:ASP:O	1:B:219:PHE:C	2.55	0.48
1:B:302:THR:O	1:B:304:MET:N	2.47	0.48
1:B:390:GLN:HE21	1:B:394:ASN:HD21	1.62	0.48
1:B:414:ASP:C	1:B:414:ASP:OD1	2.57	0.48
1:B:718:VAL:O	1:B:722:LEU:HD12	2.13	0.48
1:B:1030:ARG:NH1	1:B:1035:TYR:OH	2.46	0.48
1:B:1152:ILE:CD1	9:J:44:TYR:HB3	2.44	0.48
1:B:1227:ILE:CG2	1:B:1228:TRP:N	2.77	0.48
2:C:390:LEU:O	2:C:391:ASP:C	2.56	0.48
2:C:744:HIS:ND1	2:C:745:PRO:HD2	2.29	0.48
2:C:773:MET:HA	2:C:776:GLN:HE21	1.78	0.48
2:C:843:GLN:N	2:C:994:TYR:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:136:ASN:HB3	5:F:139:ALA:HB3	1.95	0.48
6:G:75:PRO:HG2	6:G:78:GLN:HB2	1.96	0.48
9:J:69:PRO:HB2	9:J:85:PHE:CE2	2.49	0.48
11:L:7:PHE:C	11:L:7:PHE:CD1	2.91	0.48
1:B:491:VAL:HG12	1:B:492:PRO:O	2.14	0.48
1:B:836:TYR:CZ	1:B:840:ARG:HD2	2.48	0.48
1:B:912:LEU:O	1:B:978:PRO:HA	2.14	0.48
1:B:1142:THR:O	1:B:1143:LEU:C	2.56	0.48
1:B:1443:VAL:HG23	7:H:61:ILE:HB	1.96	0.48
2:C:31:TRP:O	2:C:32:ALA:C	2.57	0.48
2:C:486:TYR:CD2	2:C:486:TYR:N	2.80	0.48
2:C:508:LEU:O	2:C:509:ALA:CB	2.62	0.48
2:C:519:TRP:CD1	2:C:519:TRP:C	2.91	0.48
2:C:1079:LYS:CG	2:C:1080:LYS:N	2.75	0.48
3:D:101:LEU:C	3:D:102:GLN:HG3	2.38	0.48
4:E:71:LYS:HA	4:E:74:GLN:HG3	1.96	0.48
8:I:104:PHE:CE2	8:I:136:LYS:HG2	2.49	0.48
10:K:3:VAL:CG1	10:K:15:GLY:HA2	2.43	0.48
10:K:4:PRO:HD3	10:K:53:HIS:HD2	1.76	0.48
10:K:52:THR:O	10:K:53:HIS:C	2.57	0.48
1:B:88:LYS:HB3	1:B:89:PRO:HD2	1.95	0.48
1:B:298:PHE:O	1:B:301:ALA:HB3	2.12	0.48
1:B:1155:ASP:HB3	1:B:1241:ARG:HH21	1.79	0.48
1:B:1220:PHE:O	1:B:1221:LYS:HB2	2.14	0.48
1:B:1431:GLY:HA3	2:C:1152:MET:HE2	1.95	0.48
1:B:1450:LEU:O	1:B:1450:LEU:CG	2.60	0.48
2:C:834:ASN:ND2	2:C:1013:ASN:HA	2.29	0.48
2:C:908:GLU:O	2:C:909:ASP:C	2.56	0.48
2:C:1006:ILE:HG23	10:K:43:ARG:HG3	1.96	0.48
2:C:1044:ALA:O	2:C:1045:SER:O	2.31	0.48
3:D:236:GLY:O	3:D:237:SER:C	2.57	0.48
6:G:96:THR:O	6:G:100:GLN:HG3	2.14	0.48
8:I:102:TYR:H	8:I:102:TYR:HD2	1.57	0.48
8:I:130:ARG:HB3	8:I:133:ASN:CB	2.44	0.48
1:B:114:LEU:O	1:B:115:LEU:HG	2.13	0.48
1:B:341:MET:CE	1:B:843:LYS:HZ3	2.26	0.48
1:B:351:THR:HG21	2:C:1103:ILE:HG13	1.95	0.48
1:B:567:LYS:CB	1:B:568:PRO:HD2	2.41	0.48
1:B:826:ASP:O	1:B:830:LYS:N	2.32	0.48
1:B:858:ASN:ND2	1:B:860:LEU:H	2.12	0.48
1:B:923:LEU:O	1:B:927:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1276:VAL:HB	1:B:1279:ILE:CD1	2.43	0.48
2:C:479:VAL:HG12	2:C:480:SER:N	2.29	0.48
2:C:637:LEU:O	2:C:690:VAL:HG13	2.14	0.48
2:C:893:LEU:HD22	2:C:897:GLY:C	2.39	0.48
2:C:1102:LYS:C	2:C:1122:ARG:NH1	2.72	0.48
3:D:35:ARG:NH1	11:L:40:HIS:HB2	2.28	0.48
3:D:75:MET:HE2	3:D:239:PRO:CD	2.43	0.48
3:D:133:ILE:CD1	3:D:237:SER:N	2.77	0.48
3:D:148:ARG:CD	3:D:149:LYS:H	2.27	0.48
3:D:235:VAL:HG12	10:K:13:VAL:HG23	1.96	0.48
5:F:173:SER:O	5:F:175:LEU:N	2.46	0.48
7:H:10:ASN:OD1	7:H:71:ASN:HA	2.12	0.48
7:H:13:LEU:HD23	7:H:14:HIS:N	2.28	0.48
8:I:10:PHE:N	8:I:10:PHE:CD1	2.82	0.48
8:I:93:TYR:HB3	8:I:144:ILE:C	2.39	0.48
9:J:58:VAL:HG13	9:J:62:ILE:CD1	2.41	0.48
9:J:78:CYS:SG	9:J:106:CYS:HB2	2.54	0.48
1:B:490:HIS:ND1	2:C:1150:ARG:NH1	2.62	0.48
1:B:504:LEU:HD12	1:B:504:LEU:N	2.29	0.48
1:B:512:VAL:HA	1:B:519:PRO:HA	1.95	0.48
1:B:774:ARG:NH1	1:B:797:LYS:HG3	2.28	0.48
1:B:870:GLU:HB2	5:F:204:THR:HG21	1.96	0.48
1:B:1120:LEU:CD1	1:B:1304:TRP:O	2.61	0.48
1:B:1140:HIS:HA	1:B:1274:ARG:O	2.14	0.48
1:B:1332:PHE:H	1:B:1332:PHE:HD2	1.62	0.48
2:C:368:GLU:O	2:C:370:PHE:N	2.42	0.48
2:C:852:ARG:NH2	12:M:70:ARG:OXT	2.26	0.48
2:C:1200:ALA:O	2:C:1201:LYS:C	2.57	0.48
3:D:161:LYS:O	3:D:170:TRP:NE1	2.47	0.48
3:D:232:VAL:HG11	3:D:244:VAL:CG2	2.44	0.48
7:H:140:LYS:H	7:H:140:LYS:HG2	1.38	0.48
11:L:30:ALA:HB2	11:L:76:GLN:HG3	1.95	0.48
12:M:52:GLY:O	12:M:53:HIS:C	2.56	0.48
1:B:12:ARG:NH2	2:C:1192:TYR:HE2	2.12	0.47
1:B:317:LYS:O	1:B:318:SER:CB	2.62	0.47
1:B:722:LEU:HD23	1:B:799:PHE:CD1	2.49	0.47
2:C:258:LEU:HG	2:C:258:LEU:O	2.14	0.47
2:C:291:ILE:HD13	2:C:300:HIS:CD2	2.49	0.47
2:C:562:GLY:HA3	2:C:590:HIS:CE1	2.49	0.47
2:C:604:ARG:HB2	2:C:609:ILE:HB	1.95	0.47
2:C:641:GLU:C	2:C:643:ASP:H	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:809:MET:HE2	2:C:814:PHE:CD2	2.49	0.47
3:D:221:TYR:CD2	8:I:46:LEU:HD23	2.48	0.47
5:F:77:SER:O	5:F:105:PHE:HB3	2.14	0.47
5:F:93:MET:SD	5:F:97:VAL:CG2	3.02	0.47
7:H:39:THR:O	7:H:43:GLY:N	2.43	0.47
7:H:43:GLY:HA2	7:H:157:ILE:HD11	1.96	0.47
8:I:116:TYR:HB2	8:I:123:MET:HB3	1.96	0.47
1:B:54:ASN:HD21	1:B:247:ARG:NH1	2.11	0.47
1:B:355:GLY:N	1:B:482:PHE:CE1	2.81	0.47
1:B:409:SER:O	1:B:410:GLY:C	2.56	0.47
1:B:548:ASN:OD1	11:L:60:ALA:HB1	2.13	0.47
1:B:784:LEU:HD11	1:B:815:PHE:CE2	2.48	0.47
2:C:45:SER:O	2:C:48:LEU:N	2.47	0.47
2:C:48:LEU:O	2:C:49:ASP:C	2.57	0.47
2:C:367:LEU:HD12	2:C:370:PHE:CZ	2.48	0.47
2:C:405:ARG:HD2	2:C:631:GLY:HA3	1.96	0.47
2:C:550:ASP:OD1	2:C:552:MET:HE3	2.14	0.47
2:C:591:ARG:O	2:C:593:PRO:HD3	2.14	0.47
2:C:1002:THR:HG23	2:C:1006:ILE:O	2.14	0.47
2:C:1034:VAL:O	2:C:1036:ALA:N	2.47	0.47
3:D:83:SER:OG	3:D:160:LYS:HD3	2.14	0.47
3:D:143:LEU:HD21	3:D:146:LYS:HE2	1.96	0.47
3:D:172:PRO:O	3:D:235:VAL:HG22	2.12	0.47
4:E:156:ASP:C	4:E:158:GLU:H	2.21	0.47
14:P:8:U:O2'	14:P:9:A:H5'	2.13	0.47
1:B:50:ILE:HG22	1:B:52:GLY:N	2.28	0.47
1:B:629:LEU:HD22	1:B:633:VAL:CG2	2.44	0.47
1:B:784:LEU:HD21	1:B:815:PHE:HE2	1.80	0.47
1:B:853:ASP:CG	1:B:855:THR:HG22	2.38	0.47
1:B:1242:VAL:O	1:B:1243:VAL:CB	2.60	0.47
2:C:1004:GLU:OE2	2:C:1064:TYR:CE2	2.67	0.47
2:C:1138:MET:HE2	2:C:1146:PHE:CD2	2.49	0.47
3:D:208:GLU:C	3:D:210:GLU:N	2.71	0.47
3:D:252:GLN:HG3	11:L:95:ILE:HG23	1.96	0.47
4:E:118:THR:HB	4:E:121:LYS:HB3	1.94	0.47
5:F:124:VAL:CG1	5:F:132:ILE:HG13	2.44	0.47
6:G:135:ARG:CZ	6:G:143:PHE:CE2	2.97	0.47
6:G:147:SER:O	6:G:148:VAL:C	2.57	0.47
7:H:145:VAL:CG1	7:H:146:LYS:N	2.76	0.47
8:I:40:LEU:HD12	8:I:122:LEU:O	2.14	0.47
10:K:19:GLU:O	10:K:23:ASN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:108:GLU:O	11:L:112:GLN:HG2	2.15	0.47
1:B:184:SER:CB	1:B:199:LEU:HD23	2.44	0.47
1:B:441:PRO:HD2	1:B:498:ARG:CZ	2.44	0.47
1:B:816:HIS:CD2	2:C:764:SER:H	2.32	0.47
1:B:1224:LEU:HD12	1:B:1225:PHE:N	2.29	0.47
2:C:273:LEU:HG	2:C:276:ILE:HD12	1.95	0.47
2:C:298:LEU:N	2:C:298:LEU:CD2	2.77	0.47
2:C:600:LEU:HD13	2:C:626:ILE:HD11	1.96	0.47
2:C:628:THR:HG23	2:C:628:THR:O	2.13	0.47
2:C:811:TYR:HD1	2:C:811:TYR:H	1.61	0.47
2:C:882:THR:HB	2:C:934:LYS:C	2.39	0.47
2:C:908:GLU:O	2:C:909:ASP:O	2.33	0.47
2:C:1081:LEU:O	2:C:1083:ALA:N	2.48	0.47
4:E:30:GLY:O	4:E:31:GLN:C	2.57	0.47
4:E:206:GLU:C	4:E:208:GLU:N	2.70	0.47
7:H:15:PRO:O	7:H:16:SER:C	2.57	0.47
7:H:91:VAL:HG22	7:H:101:VAL:HG22	1.97	0.47
8:I:109:LYS:HB2	8:I:111:LEU:HD12	1.96	0.47
10:K:2:ILE:HG12	10:K:57:ILE:HD12	1.95	0.47
12:M:53:HIS:O	12:M:55:ILE:HG12	2.15	0.47
1:B:43:GLU:O	1:B:44:THR:HB	2.13	0.47
1:B:381:THR:O	1:B:383:TYR:N	2.48	0.47
1:B:455:MET:HE3	2:C:1134:GLU:HG3	1.97	0.47
1:B:535:THR:HG23	1:B:575:LYS:HG2	1.95	0.47
1:B:667:GLY:CA	3:D:192:TRP:HH2	2.27	0.47
1:B:789:LYS:HE3	9:J:67:THR:OG1	2.14	0.47
1:B:919:ILE:HG23	1:B:925:LEU:HD12	1.97	0.47
1:B:1315:GLU:C	1:B:1317:MET:N	2.67	0.47
2:C:284:ILE:HD13	2:C:333:PHE:CD2	2.49	0.47
2:C:792:MET:HA	2:C:856:PHE:O	2.14	0.47
2:C:996:ARG:NH1	3:D:38:ILE:HG23	2.30	0.47
2:C:1027:ILE:C	2:C:1029:CYS:N	2.72	0.47
2:C:1102:LYS:O	2:C:1103:ILE:C	2.58	0.47
3:D:69:LEU:N	3:D:69:LEU:CD1	2.77	0.47
3:D:77:ILE:HA	3:D:129:ILE:HD11	1.97	0.47
3:D:142:VAL:H	10:K:16:ASP:CB	2.27	0.47
3:D:148:ARG:CG	3:D:149:LYS:H	2.28	0.47
4:E:56:ARG:CD	4:E:149:THR:HA	2.36	0.47
8:I:118:PHE:C	8:I:120:GLY:N	2.73	0.47
9:J:4:PHE:HE1	9:J:6:PHE:HE2	1.63	0.47
10:K:56:LEU:O	10:K:59:LYS:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:LYS:HG3	2:C:1219:ASP:HA	1.97	0.47
1:B:295:LEU:O	1:B:298:PHE:HB3	2.15	0.47
1:B:335:ARG:NH1	2:C:1202:LEU:HD13	2.29	0.47
1:B:567:LYS:CB	8:I:96:VAL:H	2.20	0.47
1:B:753:GLY:HA2	1:B:757:ASN:ND2	2.30	0.47
1:B:884:ASP:C	1:B:886:ILE:H	2.22	0.47
1:B:898:ARG:HB2	1:B:933:TYR:CE1	2.49	0.47
1:B:959:ASN:OD1	1:B:961:ARG:HB3	2.14	0.47
1:B:1097:GLY:O	1:B:1100:ARG:HB3	2.14	0.47
1:B:1335:ILE:O	1:B:1335:ILE:HG22	2.14	0.47
2:C:861:ASP:CG	2:C:914:LYS:HD2	2.38	0.47
2:C:980:PHE:CA	2:C:1095:LEU:HD11	2.44	0.47
2:C:1079:LYS:N	3:D:27:LEU:HD21	2.30	0.47
3:D:44:LEU:HA	3:D:160:LYS:O	2.13	0.47
3:D:107:SER:C	3:D:109:SER:H	2.23	0.47
3:D:114:TYR:HE2	10:K:19:GLU:OE2	1.97	0.47
4:E:47:LEU:HD11	7:H:3:PHE:CE2	2.49	0.47
4:E:210:ILE:O	4:E:214:LEU:HD23	2.14	0.47
6:G:130:ILE:O	6:G:148:VAL:CG2	2.62	0.47
7:H:30:LEU:HD13	7:H:72:VAL:CG1	2.39	0.47
8:I:84:ALA:CA	8:I:87:ARG:HB2	2.40	0.47
8:I:102:TYR:N	8:I:102:TYR:HD2	2.09	0.47
8:I:128:ASN:OD1	8:I:128:ASN:O	2.32	0.47
10:K:1:MET:H2	10:K:55:ASP:HA	1.78	0.47
10:K:65:PRO:HG3	12:M:32:ALA:O	2.14	0.47
11:L:63:VAL:HG23	11:L:63:VAL:O	2.14	0.47
1:B:49:LYS:NZ	1:B:61:ILE:H	2.11	0.47
1:B:63:ARG:HG2	1:B:74:MET:SD	2.54	0.47
1:B:243:PRO:HB2	1:B:244:PRO:HD2	1.97	0.47
1:B:331:GLY:O	1:B:332:LYS:O	2.33	0.47
1:B:353:ILE:HG21	1:B:487:MET:CE	2.45	0.47
1:B:420:ARG:O	1:B:421:ALA:C	2.58	0.47
1:B:497:THR:O	1:B:498:ARG:C	2.57	0.47
1:B:537:ARG:NH1	8:I:120:GLY:O	2.48	0.47
1:B:543:LEU:O	1:B:544:ASP:C	2.57	0.47
1:B:781:ASP:O	1:B:789:LYS:HA	2.14	0.47
1:B:808:LEU:HD23	1:B:812:GLU:C	2.39	0.47
1:B:820:GLY:O	1:B:821:ARG:C	2.57	0.47
1:B:877:HIS:HD1	1:B:1056:SER:HA	1.80	0.47
1:B:951:GLU:HB3	1:B:954:TRP:CZ2	2.49	0.47
1:B:961:ARG:HG3	1:B:961:ARG:NH1	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1005:GLU:O	1:B:1006:ILE:C	2.58	0.47
1:B:1040:GLN:O	1:B:1041:ALA:C	2.58	0.47
1:B:1161:THR:HG22	1:B:1162:VAL:N	2.29	0.47
1:B:1329:THR:O	1:B:1331:SER:N	2.48	0.47
1:B:1345:ARG:HD2	1:B:1373:ASP:OD1	2.13	0.47
1:B:1402:PHE:O	1:B:1403:GLU:HB2	2.14	0.47
1:B:1410:PHE:HA	2:C:1212:ILE:CD1	2.45	0.47
2:C:230:ALA:N	2:C:231:PRO:HD2	2.29	0.47
2:C:284:ILE:HG23	2:C:324:ILE:CD1	2.44	0.47
2:C:373:ARG:HD2	2:C:567:GLU:OE2	2.14	0.47
2:C:461:LEU:N	2:C:461:LEU:CD1	2.77	0.47
2:C:483:LEU:HD21	2:C:491:THR:CG2	2.45	0.47
2:C:530:GLY:O	2:C:533:CYS:HB2	2.15	0.47
2:C:611:PRO:O	2:C:692:TYR:HB2	2.14	0.47
2:C:776:GLN:O	2:C:1095:LEU:HA	2.14	0.47
2:C:782:LEU:HB3	2:C:784:ASN:OD1	2.15	0.47
2:C:797:TYR:O	2:C:799:PRO:HD3	2.14	0.47
2:C:897:GLY:O	2:C:898:LEU:HD23	2.15	0.47
2:C:980:PHE:CD2	2:C:1094:ARG:HA	2.50	0.47
2:C:1034:VAL:C	2:C:1036:ALA:N	2.72	0.47
3:D:33:LEU:O	3:D:34:ARG:C	2.57	0.47
3:D:77:ILE:HA	3:D:77:ILE:HD13	1.68	0.47
3:D:89:GLU:O	3:D:90:ASP:HB3	2.15	0.47
3:D:186:LEU:HD12	3:D:186:LEU:N	2.30	0.47
4:E:27:LEU:CD1	4:E:173:HIS:HB2	2.43	0.47
5:F:11:ARG:HH21	5:F:141:VAL:HG21	1.79	0.47
5:F:111:VAL:CG1	5:F:137:GLU:HG2	2.45	0.47
7:H:1:MET:O	7:H:1:MET:HE2	2.15	0.47
8:I:40:LEU:HD23	8:I:42:ILE:HD11	1.97	0.47
8:I:113:ALA:HB2	8:I:126:GLU:HG3	1.97	0.47
12:M:30:ILE:HG22	12:M:31:CYS:H	1.79	0.47
12:M:36:SER:O	12:M:37:LYS:O	2.33	0.47
1:B:41:MET:N	1:B:41:MET:HE3	2.29	0.47
1:B:297:GLN:O	1:B:301:ALA:HB2	2.14	0.47
1:B:367:PRO:HB3	1:B:465:TYR:O	2.15	0.47
1:B:1340:GLY:HA2	5:F:183:PRO:HD2	1.96	0.47
2:C:581:PHE:HA	2:C:585:VAL:O	2.15	0.47
2:C:882:THR:HG21	2:C:935:ARG:CA	2.45	0.47
2:C:941:LEU:HD21	2:C:946:ASN:HA	1.97	0.47
2:C:1125:ASP:O	2:C:1126:GLY:O	2.33	0.47
2:C:1161:HIS:NE2	2:C:1175:LEU:HD21	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:181:ASP:OD1	3:D:185:LYS:HB2	2.15	0.47
6:G:92:ARG:O	6:G:93:ILE:C	2.56	0.47
6:G:109:VAL:HG11	6:G:127:GLU:OE2	2.14	0.47
7:H:59:GLY:HA3	7:H:70:PHE:CE2	2.50	0.47
11:L:73:LEU:HD21	11:L:75:ILE:HD11	1.96	0.47
1:B:115:LEU:CD1	1:B:142:CYS:HB3	2.45	0.47
1:B:492:PRO:O	1:B:493:GLN:NE2	2.47	0.47
1:B:714:PHE:CB	9:J:97:MET:HE1	2.45	0.47
1:B:780:VAL:HG23	2:C:699:GLU:OE1	2.14	0.47
1:B:1239:ARG:HB3	1:B:1239:ARG:NH1	2.30	0.47
1:B:1377:THR:O	1:B:1378:GLN:C	2.57	0.47
1:B:1377:THR:HA	5:F:212:ARG:HH21	1.79	0.47
2:C:370:PHE:HD2	2:C:373:ARG:HD2	1.79	0.47
3:D:113:VAL:O	3:D:144:ILE:N	2.48	0.47
7:H:27:LYS:HD3	7:H:51:TYR:CE2	2.50	0.47
7:H:88:ASP:OD2	7:H:88:ASP:N	2.40	0.47
10:K:36:LEU:CB	10:K:47:ARG:HH12	2.27	0.47
1:B:547:LEU:HD13	11:L:58:PHE:CD1	2.50	0.47
1:B:665:GLY:O	1:B:667:GLY:N	2.48	0.47
1:B:821:ARG:HB2	1:B:821:ARG:HH11	1.80	0.47
1:B:1265:ASN:C	1:B:1267:MET:N	2.71	0.47
2:C:129:PHE:HD2	2:C:166:PHE:HA	1.79	0.47
2:C:173:MET:HE3	2:C:203:PHE:HE1	1.80	0.47
2:C:205:ILE:O	2:C:206:ASN:C	2.57	0.47
2:C:376:PHE:CZ	2:C:569:TYR:HB3	2.50	0.47
2:C:430:ARG:HB3	2:C:434:ARG:CZ	2.45	0.47
2:C:582:VAL:CG2	2:C:626:ILE:HB	2.45	0.47
2:C:899:ILE:HG22	2:C:903:VAL:CG2	2.45	0.47
2:C:1115:THR:HG22	2:C:1115:THR:O	2.13	0.47
2:C:1182:CYS:O	2:C:1183:LYS:C	2.58	0.47
5:F:136:ASN:HB3	5:F:139:ALA:CB	2.45	0.47
7:H:34:VAL:HG11	7:H:74:TYR:OH	2.14	0.47
7:H:138:THR:HG23	7:H:139:ILE:HG13	1.97	0.47
9:J:100:PHE:N	9:J:100:PHE:CD1	2.83	0.47
15:T:18:DT:H2'	15:T:19:DT:H5'	1.95	0.47
1:B:255:SER:OG	2:C:918:ILE:HG21	2.15	0.46
1:B:264:PHE:O	1:B:267:ALA:HB3	2.14	0.46
1:B:965:GLN:HA	1:B:968:GLN:CG	2.44	0.46
1:B:1036:ARG:HG2	1:B:1036:ARG:HH11	1.80	0.46
1:B:1376:THR:HG23	1:B:1377:THR:N	2.29	0.46
2:C:324:ILE:HG22	2:C:325:GLN:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:578:THR:HG23	2:C:622:LYS:C	2.40	0.46
2:C:596:LEU:O	2:C:599:THR:HB	2.15	0.46
2:C:882:THR:O	2:C:884:ARG:N	2.48	0.46
3:D:186:LEU:HD21	3:D:224:GLN:C	2.40	0.46
4:E:6:SER:OG	4:E:7:THR:N	2.47	0.46
5:F:39:LEU:O	5:F:43:LYS:HG3	2.14	0.46
5:F:177:ARG:HD3	5:F:215:MET:CG	2.44	0.46
8:I:127:GLY:CA	8:I:130:ARG:HH22	2.28	0.46
11:L:77:THR:HG23	11:L:83:PRO:HB3	1.97	0.46
1:B:266:LEU:O	1:B:267:ALA:C	2.57	0.46
1:B:346:ASP:HB3	2:C:1108:ARG:N	2.30	0.46
2:C:308:TRP:CZ3	9:J:45:ARG:HB3	2.49	0.46
2:C:467:GLY:CA	2:C:475:SER:HB3	2.44	0.46
2:C:753:ALA:HA	2:C:756:ILE:HD12	1.97	0.46
2:C:903:VAL:HG12	2:C:904:ARG:N	2.29	0.46
2:C:1183:LYS:HA	2:C:1186:ASP:HA	1.97	0.46
3:D:124:LEU:O	3:D:127:ARG:HG2	2.16	0.46
3:D:191:TYR:HB3	3:D:201:TRP:CD1	2.50	0.46
4:E:51:ASN:HB3	4:E:178:ALA:HA	1.98	0.46
7:H:21:ARG:HD3	7:H:21:ARG:HA	1.68	0.46
15:T:14:DC:C2'	15:T:15:DT:H71	2.43	0.46
1:B:23:SER:HA	1:B:233:TRP:CD1	2.51	0.46
1:B:61:ILE:O	1:B:63:ARG:N	2.49	0.46
1:B:65:LEU:O	1:B:66:LYS:C	2.59	0.46
1:B:399:HIS:CE1	1:B:462:VAL:HG11	2.49	0.46
1:B:509:LEU:C	1:B:511:ILE:H	2.22	0.46
1:B:591:PHE:HA	1:B:595:THR:OG1	2.15	0.46
1:B:793:SER:HB2	1:B:794:PRO:HD2	1.97	0.46
1:B:1385:THR:HG22	1:B:1386:ARG:H	1.79	0.46
2:C:401:PHE:C	2:C:403:LYS:H	2.23	0.46
2:C:493:SER:N	2:C:751:VAL:HG11	2.30	0.46
2:C:825:VAL:O	2:C:826:ALA:HB2	2.14	0.46
2:C:865:LYS:HE2	2:C:871:THR:OG1	2.15	0.46
2:C:1151:LEU:CD1	2:C:1151:LEU:H	2.28	0.46
2:C:1159:ARG:HD3	2:C:1193:GLN:HB2	1.96	0.46
3:D:45:ALA:CA	3:D:72:LEU:HD12	2.37	0.46
3:D:47:ASP:CA	12:M:69:ALA:CB	2.91	0.46
3:D:133:ILE:HD11	3:D:237:SER:CA	2.42	0.46
4:E:139:LYS:C	4:E:139:LYS:HD3	2.40	0.46
7:H:145:VAL:CG1	7:H:146:LYS:H	2.27	0.46
11:L:5:ASP:O	11:L:6:ARG:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:42:LEU:HD21	11:L:46:ILE:HD11	1.97	0.46
12:M:27:LEU:HD23	12:M:27:LEU:H	1.79	0.46
12:M:33:GLU:C	12:M:35:SER:H	2.24	0.46
1:B:22:PHE:CE2	1:B:30:ILE:HD12	2.50	0.46
1:B:51:GLY:HA2	1:B:56:PRO:HA	1.97	0.46
1:B:591:PHE:CD2	1:B:595:THR:HB	2.50	0.46
1:B:828:ALA:HB1	2:C:530:GLY:HA2	1.91	0.46
1:B:1385:THR:HG22	1:B:1386:ARG:N	2.30	0.46
1:B:1418:LEU:HD12	1:B:1419:ASP:H	1.79	0.46
2:C:171:PRO:HD2	2:C:457:LEU:CD1	2.46	0.46
2:C:1002:THR:O	2:C:1003:ALA:C	2.57	0.46
3:D:234:SER:OG	3:D:235:VAL:N	2.48	0.46
4:E:118:THR:O	4:E:118:THR:HG22	2.15	0.46
7:H:138:THR:HG22	7:H:139:ILE:HG13	1.96	0.46
10:K:36:LEU:HD22	10:K:41:LEU:HD12	1.96	0.46
10:K:48:ARG:CD	10:K:49:MET:N	2.75	0.46
11:L:19:LEU:HD22	11:L:33:ILE:HG21	1.98	0.46
1:B:106:VAL:HG13	1:B:112:LYS:C	2.40	0.46
1:B:445:ASN:HA	1:B:478:TYR:CE2	2.49	0.46
1:B:500:GLU:O	1:B:504:LEU:HD13	2.15	0.46
1:B:710:LEU:N	1:B:710:LEU:HD12	2.30	0.46
1:B:807:GLY:HA2	2:C:760:ASP:O	2.15	0.46
1:B:886:ILE:HB	1:B:943:LEU:HD12	1.98	0.46
1:B:1006:ILE:HD12	5:F:167:ARG:HG3	1.98	0.46
1:B:1164:PRO:HG2	1:B:1165:GLU:H	1.80	0.46
2:C:276:ILE:HG22	2:C:276:ILE:O	2.15	0.46
2:C:423:LYS:CE	2:C:470:LYS:HZ1	2.29	0.46
2:C:498:THR:HG22	2:C:537:LYS:HB2	1.96	0.46
2:C:579:ARG:NH1	2:C:622:LYS:O	2.49	0.46
2:C:755:ILE:HG13	2:C:755:ILE:H	1.50	0.46
2:C:1006:ILE:HD13	10:K:44:TYR:CE2	2.51	0.46
4:E:12:ARG:HH21	4:E:12:ARG:HG3	1.80	0.46
4:E:20:GLU:O	4:E:21:GLU:O	2.32	0.46
5:F:147:HIS:HD2	5:F:149:LEU:H	1.62	0.46
7:H:27:LYS:O	7:H:28:THR:C	2.58	0.46
8:I:145:ARG:HG3	8:I:146:ARG:HG3	1.97	0.46
10:K:1:MET:H1	10:K:57:ILE:HG22	1.80	0.46
10:K:9:SER:HB2	10:K:45:CYS:HB2	1.97	0.46
1:B:51:GLY:O	1:B:56:PRO:HB3	2.16	0.46
1:B:71:GLN:CG	1:B:72:GLU:N	2.77	0.46
1:B:442:VAL:HG12	1:B:490:HIS:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:PHE:CZ	1:B:487:MET:HE3	2.51	0.46
1:B:563:PRO:HG3	1:B:572:TRP:CE2	2.49	0.46
1:B:639:PRO:CG	1:B:640:GLN:N	2.79	0.46
1:B:867:ILE:HD12	1:B:867:ILE:N	2.31	0.46
1:B:1102:LYS:O	1:B:1106:ASN:ND2	2.49	0.46
1:B:1215:ARG:NH1	1:B:1272:THR:O	2.49	0.46
1:B:1330:ASN:O	1:B:1332:PHE:N	2.48	0.46
2:C:299:GLU:HB3	2:C:571:PRO:HG3	1.97	0.46
2:C:570:VAL:CG2	2:C:573:GLN:HB3	2.46	0.46
2:C:803:LEU:CD1	2:C:1032:SER:HB3	2.46	0.46
2:C:873:THR:HG22	2:C:874:PHE:N	2.31	0.46
2:C:910:VAL:CG1	2:C:911:ILE:H	2.27	0.46
2:C:1138:MET:CE	2:C:1143:ALA:HB3	2.45	0.46
2:C:1197:PRO:HG2	2:C:1200:ALA:CB	2.27	0.46
3:D:34:ARG:HA	3:D:37:MET:CE	2.46	0.46
6:G:109:VAL:CG1	6:G:110:ASP:N	2.74	0.46
8:I:98:TYR:C	8:I:118:PHE:HD2	2.24	0.46
10:K:57:ILE:HG12	10:K:61:LEU:HD11	1.96	0.46
11:L:89:ASN:O	11:L:90:ALA:C	2.59	0.46
12:M:70:ARG:HG2	12:M:70:ARG:HH11	1.80	0.46
1:B:23:SER:O	1:B:27:VAL:HG23	2.16	0.46
1:B:343:LYS:HZ3	2:C:1151:LEU:C	2.21	0.46
1:B:709:THR:CB	1:B:712:GLU:HG3	2.42	0.46
1:B:874:ASP:O	1:B:875:ALA:C	2.57	0.46
1:B:886:ILE:HD12	1:B:943:LEU:CB	2.42	0.46
1:B:933:TYR:O	1:B:937:VAL:HG23	2.15	0.46
1:B:947:PHE:N	1:B:947:PHE:HD1	2.13	0.46
1:B:1403:GLU:O	15:T:16:DG:OP1	2.33	0.46
1:B:1424:VAL:HG11	2:C:1139:ILE:HD13	1.97	0.46
2:C:449:ASN:C	2:C:451:LYS:N	2.73	0.46
2:C:758:PHE:CZ	2:C:1031:LEU:HD22	2.48	0.46
2:C:1002:THR:CG2	2:C:1006:ILE:HG13	2.37	0.46
3:D:6:PRO:HG2	11:L:101:LEU:HB2	1.98	0.46
3:D:115:SER:HB3	3:D:142:VAL:HB	1.98	0.46
3:D:229:TYR:CD1	3:D:229:TYR:N	2.84	0.46
5:F:116:ILE:HG22	5:F:120:ALA:HB3	1.97	0.46
5:F:129:PRO:O	5:F:130:ALA:C	2.58	0.46
5:F:190:LEU:C	5:F:191:LYS:HG2	2.40	0.46
6:G:94:LEU:HD21	6:G:122:MET:HA	1.98	0.46
7:H:106:MET:HE2	7:H:106:MET:HB3	1.74	0.46
8:I:58:THR:HG22	8:I:59:ILE:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:82:GLU:C	9:J:104:LEU:HG	2.40	0.46
1:B:72:GLU:O	1:B:73:GLY:O	2.34	0.46
1:B:84:ILE:HD11	1:B:270:LEU:HD22	1.97	0.46
1:B:203:SER:O	1:B:206:GLU:HB3	2.15	0.46
1:B:403:LYS:O	1:B:404:TYR:CD2	2.68	0.46
1:B:438:ASP:O	1:B:439:ASN:HB2	2.15	0.46
1:B:444:PHE:HZ	1:B:487:MET:HE3	1.80	0.46
1:B:572:TRP:HA	1:B:576:GLN:OE1	2.16	0.46
1:B:650:GLN:HB3	1:B:654:ASN:HD21	1.81	0.46
1:B:650:GLN:C	1:B:654:ASN:ND2	2.74	0.46
2:C:240:ILE:HD13	2:C:377:PHE:HE2	1.81	0.46
2:C:244:LEU:HD13	2:C:247:GLY:O	2.15	0.46
2:C:361:LEU:HD11	2:C:381:MET:CE	2.44	0.46
2:C:362:PRO:C	2:C:363:HIS:O	2.55	0.46
2:C:557:PHE:CD2	2:C:557:PHE:O	2.69	0.46
2:C:654:ARG:O	2:C:656:GLY:N	2.48	0.46
2:C:807:ARG:HB3	2:C:807:ARG:NH1	2.30	0.46
2:C:879:ARG:NH1	2:C:883:LEU:HD22	2.30	0.46
2:C:1034:VAL:C	2:C:1036:ALA:H	2.23	0.46
2:C:1099:VAL:O	2:C:1101:ASP:N	2.49	0.46
3:D:146:LYS:C	3:D:147:LEU:HD23	2.41	0.46
3:D:163:ILE:N	3:D:163:ILE:CD1	2.68	0.46
3:D:191:TYR:CD2	3:D:201:TRP:CD1	3.04	0.46
3:D:221:TYR:CE1	3:D:222:LYS:HG3	2.51	0.46
3:D:252:GLN:CG	11:L:95:ILE:HG23	2.46	0.46
3:D:252:GLN:O	3:D:253:LYS:C	2.59	0.46
4:E:40:HIS:CB	7:H:73:LYS:HZ2	2.05	0.46
4:E:64:VAL:CG2	4:E:129:LEU:HD22	2.46	0.46
5:F:144:ILE:HG13	5:F:145:THR:N	2.29	0.46
9:J:72:ASP:HA	9:J:81:ARG:O	2.15	0.46
14:P:3:C:H42	15:T:26:DA:N6	2.13	0.46
1:B:106:VAL:HG12	1:B:107:CYS:N	2.30	0.46
1:B:578:LEU:HD23	1:B:612:ILE:CD1	2.46	0.46
1:B:590:ARG:NH2	1:B:620:LYS:CB	2.65	0.46
1:B:591:PHE:HA	1:B:595:THR:CG2	2.45	0.46
1:B:877:HIS:ND1	1:B:1056:SER:HA	2.31	0.46
1:B:897:TYR:N	1:B:897:TYR:CD1	2.84	0.46
2:C:34:ILE:O	2:C:35:SER:C	2.57	0.46
2:C:56:ASP:CB	2:C:57:TYR:HD1	2.28	0.46
2:C:361:LEU:CD1	2:C:381:MET:HE1	2.45	0.46
2:C:566:LEU:O	2:C:567:GLU:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:583:ASN:ND2	2:C:628:THR:HG22	2.30	0.46
2:C:681:TRP:O	2:C:682:SER:C	2.59	0.46
2:C:1214:PRO:HG2	2:C:1214:PRO:O	2.16	0.46
7:H:80:LYS:HG2	7:H:80:LYS:O	2.15	0.46
12:M:28:LYS:C	12:M:29:TYR:HD2	2.23	0.46
1:B:172:PRO:HA	1:B:184:SER:O	2.16	0.46
1:B:403:LYS:C	1:B:415:LEU:HB2	2.41	0.46
1:B:843:LYS:HA	1:B:846:GLU:HG3	1.98	0.46
1:B:919:ILE:O	1:B:920:LEU:C	2.59	0.46
2:C:33:VAL:HG21	2:C:638:PHE:CZ	2.40	0.46
2:C:216:GLU:HA	2:C:406:LEU:HD23	1.97	0.46
2:C:276:ILE:HD13	2:C:280:ILE:HD11	1.98	0.46
2:C:329:THR:HG22	2:C:329:THR:O	2.16	0.46
2:C:637:LEU:HD22	2:C:742:GLU:HA	1.97	0.46
2:C:746:SER:CB	2:C:1046:PRO:HG2	2.45	0.46
2:C:752:ALA:O	2:C:753:ALA:C	2.59	0.46
2:C:840:ILE:HB	2:C:1011:ILE:HB	1.98	0.46
2:C:841:MET:O	2:C:993:THR:HA	2.16	0.46
2:C:882:THR:C	2:C:884:ARG:H	2.23	0.46
2:C:1064:TYR:O	2:C:1065:GLN:C	2.58	0.46
4:E:137:ASN:HD22	4:E:138:ASN:N	2.14	0.46
8:I:7:ASP:O	8:I:8:ASP:HB2	2.15	0.46
10:K:14:VAL:O	10:K:14:VAL:CG1	2.58	0.46
10:K:28:ASP:O	10:K:29:GLU:C	2.58	0.46
10:K:48:ARG:O	10:K:49:MET:C	2.59	0.46
11:L:86:ALA:HA	11:L:89:ASN:ND2	2.31	0.46
15:T:22:DT:C2'	15:T:23:DT:O5'	2.64	0.46
1:B:18:GLN:HB3	2:C:1215:ARG:HG3	1.97	0.45
1:B:445:ASN:CB	1:B:455:MET:HG2	2.46	0.45
1:B:546:VAL:O	1:B:550:LEU:HG	2.16	0.45
1:B:857:ARG:NH1	6:G:139:PRO:HB2	2.31	0.45
2:C:363:HIS:HD2	2:C:585:VAL:HG22	1.81	0.45
2:C:418:LYS:HE2	2:C:422:LYS:HZ1	1.80	0.45
2:C:847:ASP:CB	3:D:167:HIS:CD2	2.95	0.45
2:C:910:VAL:C	2:C:911:ILE:HG13	2.42	0.45
2:C:1166:CYS:O	2:C:1166:CYS:SG	2.73	0.45
3:D:147:LEU:N	3:D:147:LEU:CD2	2.79	0.45
3:D:238:ILE:HG21	3:D:242:GLN:HB2	1.95	0.45
4:E:8:PHE:O	4:E:9:GLN:HB2	2.14	0.45
6:G:81:THR:HG23	6:G:144:GLU:CD	2.42	0.45
6:G:103:MET:HE1	7:H:65:ASP:CA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:28:LYS:HB3	12:M:39:SER:HA	1.97	0.45
15:T:11:DT:H1'	15:T:12:DA:H5'	1.97	0.45
1:B:266:LEU:HD21	1:B:303:TYR:CZ	2.51	0.45
1:B:350:ARG:CB	2:C:1128:LEU:HD11	2.46	0.45
1:B:427:GLN:HB2	1:B:430:TRP:CD1	2.51	0.45
1:B:672:ASP:O	1:B:673:GLY:C	2.59	0.45
1:B:709:THR:HG21	9:J:93:LYS:O	2.16	0.45
1:B:1317:MET:C	1:B:1319:VAL:H	2.24	0.45
2:C:195:CYS:SG	2:C:196:PRO:HD2	2.56	0.45
2:C:367:LEU:HD12	2:C:370:PHE:CE1	2.51	0.45
2:C:544:CYS:HB3	2:C:634:TYR:CE1	2.51	0.45
2:C:885:MET:HA	2:C:936:ASP:CB	2.46	0.45
2:C:1000:PRO:O	2:C:1007:VAL:HG23	2.16	0.45
3:D:35:ARG:HH11	11:L:41:THR:N	2.14	0.45
3:D:69:LEU:H	3:D:69:LEU:CD1	2.30	0.45
4:E:59:ILE:O	4:E:63:LEU:HB2	2.16	0.45
6:G:75:PRO:O	6:G:77:ASP:O	2.34	0.45
6:G:138:LEU:HB2	6:G:142:SER:O	2.15	0.45
8:I:62:SER:OG	8:I:63:LEU:N	2.48	0.45
10:K:32:GLU:H	10:K:32:GLU:CD	2.23	0.45
1:B:343:LYS:HB3	2:C:1117:GLN:OE1	2.17	0.45
1:B:630:ILE:HD13	1:B:646:PHE:CZ	2.51	0.45
1:B:782:ARG:NH2	2:C:699:GLU:O	2.45	0.45
1:B:1147:THR:HA	1:B:1197:LEU:HD23	1.98	0.45
1:B:1313:LEU:HD11	1:B:1317:MET:HE3	1.98	0.45
2:C:755:ILE:HG22	2:C:809:MET:HE3	1.98	0.45
2:C:1034:VAL:HG21	2:C:1055:ILE:HG23	1.98	0.45
2:C:1106:ARG:NH2	2:C:1109:GLY:H	2.14	0.45
3:D:91:HIS:CD2	3:D:91:HIS:O	2.69	0.45
3:D:100:THR:HG22	3:D:101:LEU:H	1.80	0.45
3:D:101:LEU:HD13	3:D:118:LEU:CD2	2.23	0.45
3:D:133:ILE:HD13	3:D:237:SER:N	2.32	0.45
5:F:124:VAL:HG13	5:F:132:ILE:HG13	1.98	0.45
6:G:135:ARG:HD3	6:G:143:PHE:CE2	2.50	0.45
8:I:82:PRO:O	8:I:84:ALA:N	2.36	0.45
8:I:84:ALA:HA	8:I:87:ARG:HD2	1.98	0.45
10:K:13:VAL:C	10:K:14:VAL:HG23	2.41	0.45
13:N:6:DA:C2	15:T:12:DA:C2	3.04	0.45
1:B:353:ILE:HG21	1:B:487:MET:HE3	1.99	0.45
1:B:414:ASP:OD1	1:B:416:ARG:CG	2.65	0.45
1:B:434:ARG:HD2	1:B:435:HIS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1104:ILE:C	1:B:1106:ASN:N	2.71	0.45
1:B:1220:PHE:CE2	1:B:1263:ILE:HG23	2.51	0.45
1:B:1444:MET:HB2	1:B:1444:MET:HE3	1.66	0.45
2:C:33:VAL:O	2:C:36:ALA:HB3	2.15	0.45
2:C:542:MET:HG2	2:C:747:MET:HB3	1.98	0.45
2:C:560:GLU:O	2:C:561:TRP:CD1	2.70	0.45
2:C:731:VAL:CG1	2:C:732:SER:H	2.23	0.45
2:C:996:ARG:HH21	3:D:175:ALA:HA	1.81	0.45
3:D:11:ARG:HD3	3:D:209:TYR:CZ	2.51	0.45
4:E:176:GLU:O	4:E:179:GLN:N	2.49	0.45
5:F:13:TRP:CZ3	5:F:39:LEU:HB2	2.51	0.45
7:H:1:MET:HE3	7:H:85:GLU:OE1	2.17	0.45
8:I:63:LEU:C	8:I:90:ALA:CB	2.86	0.45
8:I:142:LEU:C	8:I:143:LEU:HD12	2.41	0.45
9:J:32:CYS:SG	9:J:33:SER:N	2.86	0.45
1:B:6:TYR:CD1	1:B:6:TYR:C	2.93	0.45
1:B:219:PHE:CD2	1:B:231:PRO:HD2	2.51	0.45
1:B:320:ARG:HA	1:B:321:PRO:HD3	1.87	0.45
1:B:522:GLY:HA2	1:B:630:ILE:HD13	1.98	0.45
1:B:578:LEU:HD23	1:B:612:ILE:HD11	1.99	0.45
1:B:696:GLU:OE2	1:B:702:LEU:HD21	2.17	0.45
1:B:1017:LEU:O	1:B:1018:PHE:C	2.57	0.45
1:B:1159:ARG:O	1:B:1160:SER:HB3	2.16	0.45
1:B:1349:TYR:O	1:B:1350:LYS:C	2.58	0.45
1:B:1389:PHE:CD1	1:B:1389:PHE:C	2.94	0.45
1:B:1403:GLU:OE2	15:T:16:DG:H4'	2.16	0.45
1:B:1411:GLU:O	1:B:1411:GLU:HG2	2.15	0.45
2:C:54:PHE:HE1	2:C:414:ALA:HA	1.81	0.45
2:C:859:TYR:OH	2:C:941:LEU:CD1	2.65	0.45
2:C:877:PRO:C	2:C:878:GLN:HG3	2.42	0.45
2:C:1107:ALA:O	2:C:1108:ARG:O	2.35	0.45
3:D:8:VAL:HG21	11:L:105:PHE:CA	2.46	0.45
5:F:34:GLU:HG2	5:F:34:GLU:O	2.16	0.45
5:F:156:LEU:HD12	5:F:195:VAL:CG1	2.46	0.45
5:F:207:ARG:CB	5:F:207:ARG:HH11	2.29	0.45
7:H:91:VAL:HA	7:H:101:VAL:HA	1.98	0.45
8:I:76:THR:HG22	8:I:76:THR:O	2.15	0.45
8:I:92:ASP:C	8:I:93:TYR:CD1	2.94	0.45
1:B:302:THR:HA	1:B:305:ASP:O	2.17	0.45
1:B:511:ILE:O	1:B:519:PRO:HA	2.17	0.45
1:B:699:ALA:O	1:B:700:ASN:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:858:ASN:C	1:B:858:ASN:ND2	2.71	0.45
1:B:878:ILE:HG22	1:B:956:LEU:N	2.32	0.45
1:B:1154:TYR:N	9:J:41:PRO:O	2.49	0.45
1:B:1170:ILE:H	1:B:1170:ILE:HG13	1.49	0.45
2:C:172:ILE:HG22	2:C:173:MET:N	2.31	0.45
2:C:472:ALA:C	2:C:474:SER:H	2.24	0.45
2:C:487:THR:O	2:C:488:TYR:C	2.59	0.45
2:C:872:GLU:CD	2:C:914:LYS:HE2	2.42	0.45
2:C:995:ARG:HH11	3:D:165:LYS:HA	1.82	0.45
2:C:1039:GLY:O	10:K:32:GLU:HB2	2.15	0.45
2:C:1111:MET:SD	2:C:1118:PRO:HA	2.56	0.45
3:D:116:LYS:C	3:D:118:LEU:H	2.24	0.45
4:E:140:ASP:O	4:E:143:ASN:N	2.49	0.45
9:J:8:ARG:HG3	9:J:34:TYR:CE1	2.52	0.45
9:J:55:THR:HG23	9:J:86:PHE:CZ	2.52	0.45
9:J:86:PHE:CE1	9:J:100:PHE:HB2	2.52	0.45
1:B:38:PRO:HG2	1:B:39:GLU:N	2.31	0.45
1:B:332:LYS:HB2	1:B:337:ARG:NH1	2.32	0.45
1:B:606:LEU:CB	1:B:614:PHE:CE2	3.00	0.45
1:B:697:ALA:HB2	1:B:702:LEU:HD12	1.99	0.45
1:B:1209:MET:SD	1:B:1236:LEU:HB3	2.57	0.45
1:B:1260:LEU:C	1:B:1260:LEU:HD12	2.42	0.45
2:C:110:HIS:CD2	12:M:54:ARG:HH22	2.35	0.45
2:C:247:GLY:N	2:C:418:LYS:HZ1	2.14	0.45
2:C:287:ARG:C	2:C:289:LEU:H	2.24	0.45
2:C:510:LYS:CB	2:C:511:PRO:CD	2.94	0.45
2:C:683:SER:O	2:C:685:LEU:N	2.50	0.45
2:C:763:GLN:NE2	2:C:1021:MET:HE2	2.32	0.45
3:D:183:TRP:O	3:D:185:LYS:N	2.50	0.45
3:D:226:ASP:O	3:D:227:THR:HB	2.17	0.45
4:E:52:LEU:HB2	4:E:182:SER:HB3	1.98	0.45
4:E:68:ARG:O	4:E:72:ARG:HG3	2.16	0.45
7:H:45:ILE:O	7:H:45:ILE:HG22	2.17	0.45
7:H:114:LEU:HD23	7:H:161:GLY:C	2.41	0.45
9:J:54:GLU:OE2	9:J:118:ARG:NH1	2.49	0.45
1:B:24:PRO:HD2	1:B:233:TRP:NE1	2.32	0.45
1:B:130:ASP:H	1:B:134:ARG:HH21	1.64	0.45
1:B:376:TYR:C	1:B:376:TYR:CD2	2.95	0.45
1:B:390:GLN:HE21	1:B:394:ASN:ND2	2.15	0.45
1:B:844:ALA:C	1:B:845:LEU:HD23	2.41	0.45
1:B:874:ASP:C	1:B:874:ASP:OD1	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:898:ARG:HD3	1:B:933:TYR:CD1	2.52	0.45
1:B:1411:GLU:HA	1:B:1414:ALA:CB	2.46	0.45
2:C:53:GLN:HG2	2:C:547:VAL:HG22	1.95	0.45
2:C:118:ARG:HD3	2:C:204:ILE:HD13	1.99	0.45
2:C:205:ILE:N	2:C:205:ILE:CD1	2.79	0.45
2:C:400:HIS:O	2:C:400:HIS:ND1	2.48	0.45
2:C:616:ILE:HG13	2:C:697:GLU:HG2	1.98	0.45
2:C:983:ARG:CD	2:C:1091:TYR:HB3	2.47	0.45
2:C:1146:PHE:CZ	2:C:1150:ARG:HD2	2.52	0.45
3:D:3:GLU:OE1	3:D:4:GLU:HB2	2.17	0.45
3:D:8:VAL:HG11	11:L:105:PHE:CD1	2.48	0.45
3:D:10:ILE:CG2	3:D:13:ALA:HB2	2.46	0.45
5:F:16:PHE:O	5:F:17:ARG:C	2.59	0.45
5:F:113:GLN:HA	5:F:137:GLU:HG3	1.99	0.45
6:G:120:ILE:O	6:G:123:LYS:HB3	2.17	0.45
9:J:34:TYR:C	9:J:35:VAL:HG23	2.42	0.45
9:J:101:PHE:N	9:J:101:PHE:CD1	2.84	0.45
11:L:42:LEU:HD21	11:L:46:ILE:CD1	2.46	0.45
12:M:38:LEU:HD11	12:M:49:LYS:HE2	1.98	0.45
1:B:113:LEU:C	1:B:114:LEU:HD23	2.42	0.45
1:B:344:ARG:HG2	1:B:344:ARG:HH11	1.81	0.45
1:B:836:TYR:CD2	1:B:840:ARG:HD2	2.50	0.45
1:B:873:MET:HG2	1:B:957:PRO:HB3	1.99	0.45
1:B:1120:LEU:HD21	1:B:1304:TRP:O	2.17	0.45
2:C:65:GLU:HG3	2:C:66:ASP:OD1	2.17	0.45
2:C:100:PRO:HD3	2:C:172:ILE:HD12	1.99	0.45
2:C:224:GLN:HA	2:C:396:ASP:OD2	2.17	0.45
2:C:467:GLY:H	2:C:475:SER:CB	2.30	0.45
2:C:487:THR:O	2:C:490:SER:HB3	2.17	0.45
2:C:635:ARG:NH2	2:C:742:GLU:OE2	2.48	0.45
2:C:952:VAL:HG13	2:C:966:VAL:HG22	1.97	0.45
2:C:1151:LEU:HD13	2:C:1151:LEU:H	1.81	0.45
3:D:67:LEU:CD1	3:D:155:LEU:HD13	2.42	0.45
3:D:169:LYS:NZ	12:M:69:ALA:HB3	2.32	0.45
4:E:35:LEU:CD2	4:E:173:HIS:HB3	2.46	0.45
5:F:117:THR:C	5:F:119:SER:H	2.23	0.45
5:F:154:ILE:HG22	5:F:155:ARG:N	2.30	0.45
5:F:161:LYS:HD2	5:F:195:VAL:CG2	2.46	0.45
5:F:197:LYS:HE2	5:F:199:ILE:HD11	1.98	0.45
6:G:125:LEU:O	6:G:125:LEU:HG	2.16	0.45
8:I:58:THR:HG22	8:I:59:ILE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:34:TYR:O	9:J:35:VAL:CG2	2.65	0.45
10:K:16:ASP:O	10:K:18:TRP:N	2.49	0.45
10:K:36:LEU:HD11	10:K:51:LEU:HB2	1.98	0.45
10:K:57:ILE:CA	10:K:60:PHE:HD2	2.22	0.45
1:B:207:ILE:O	1:B:211:PHE:HD1	2.00	0.45
1:B:366:VAL:CG2	1:B:460:VAL:HG23	2.47	0.45
1:B:605:MET:HE2	1:B:607:ILE:CG1	2.47	0.45
1:B:946:VAL:HB	1:B:947:PHE:CD1	2.52	0.45
1:B:1120:LEU:HD11	1:B:1304:TRP:O	2.17	0.45
1:B:1434:ALA:O	1:B:1436:ILE:N	2.50	0.45
2:C:199:MET:HE2	2:C:492:LEU:HD21	1.99	0.45
2:C:281:PRO:HD2	2:C:284:ILE:HD12	1.98	0.45
2:C:360:PHE:HD2	2:C:374:LYS:HD3	1.82	0.45
2:C:1163:CYS:HB3	2:C:1166:CYS:O	2.17	0.45
3:D:22:LEU:C	3:D:22:LEU:HD23	2.42	0.45
3:D:70:ILE:HD11	3:D:144:ILE:CG1	2.47	0.45
3:D:236:GLY:C	3:D:238:ILE:N	2.73	0.45
3:D:258:ILE:N	3:D:258:ILE:HD12	2.32	0.45
5:F:124:VAL:N	5:F:125:PRO:CD	2.80	0.45
1:B:24:PRO:HB3	1:B:237:THR:HB	1.99	0.44
1:B:44:THR:C	1:B:46:THR:H	2.25	0.44
1:B:71:GLN:HE22	2:C:1176:ASN:CG	2.25	0.44
1:B:108:MET:HE3	1:B:210:ILE:CD1	2.47	0.44
1:B:338:GLY:O	1:B:342:GLY:O	2.35	0.44
1:B:358:ASN:ND2	2:C:833:TYR:OH	2.50	0.44
1:B:497:THR:HG22	1:B:498:ARG:N	2.32	0.44
1:B:567:LYS:HE3	8:I:46:LEU:HB3	1.98	0.44
1:B:1120:LEU:CD2	1:B:1304:TRP:O	2.65	0.44
1:B:1155:ASP:OD2	1:B:1162:VAL:N	2.49	0.44
2:C:281:PRO:C	2:C:283:VAL:N	2.72	0.44
2:C:313:MET:HE2	2:C:390:LEU:CG	2.47	0.44
2:C:433:GLN:C	2:C:434:ARG:HG3	2.43	0.44
2:C:473:MET:C	2:C:475:SER:N	2.74	0.44
2:C:707:PRO:O	2:C:711:GLU:HG2	2.17	0.44
2:C:935:ARG:O	2:C:935:ARG:HG3	2.18	0.44
2:C:977:GLY:HA3	2:C:1099:VAL:HB	2.00	0.44
2:C:1096:ARG:O	2:C:1097:HIS:CB	2.62	0.44
7:H:15:PRO:HG2	7:H:66:GLY:HA3	1.99	0.44
8:I:98:TYR:CD1	8:I:99:GLY:N	2.85	0.44
9:J:7:CYS:C	9:J:8:ARG:O	2.57	0.44
9:J:61:ASP:C	9:J:63:GLY:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:PRO:C	1:B:233:TRP:H	2.25	0.44
1:B:497:THR:O	1:B:500:GLU:N	2.42	0.44
1:B:541:ILE:HD12	1:B:577:ILE:HD11	1.99	0.44
1:B:567:LYS:CG	8:I:95:TYR:HA	2.48	0.44
1:B:899:VAL:CB	1:B:929:LEU:HD12	2.45	0.44
1:B:1102:LYS:O	1:B:1103:GLU:C	2.60	0.44
2:C:34:ILE:O	2:C:37:PHE:N	2.51	0.44
2:C:35:SER:HA	2:C:811:TYR:HE2	1.81	0.44
2:C:253:THR:HG22	2:C:254:LEU:N	2.33	0.44
2:C:254:LEU:HD22	2:C:361:LEU:HD13	1.99	0.44
2:C:449:ASN:O	2:C:451:LYS:N	2.50	0.44
2:C:1182:CYS:C	2:C:1183:LYS:O	2.60	0.44
3:D:93:ASP:C	3:D:95:CYS:H	2.24	0.44
4:E:138:ASN:ND2	7:H:35:GLU:HB3	2.32	0.44
5:F:23:VAL:HG12	5:F:28:TYR:HB2	1.99	0.44
7:H:27:LYS:O	7:H:30:LEU:HB3	2.18	0.44
9:J:15:TYR:N	9:J:15:TYR:HD1	2.13	0.44
10:K:57:ILE:HG12	10:K:61:LEU:CD1	2.48	0.44
1:B:372:LYS:HA	1:B:435:HIS:HD1	1.82	0.44
1:B:375:THR:OG1	1:B:376:TYR:N	2.49	0.44
1:B:380:VAL:HG23	1:B:430:TRP:O	2.17	0.44
1:B:709:THR:CG2	1:B:711:ARG:HB2	2.46	0.44
1:B:940:ARG:HG2	1:B:940:ARG:HH11	1.82	0.44
1:B:1189:SER:OG	1:B:1256:GLU:OE1	2.22	0.44
1:B:1340:GLY:O	1:B:1341:ILE:C	2.59	0.44
1:B:1343:ALA:O	1:B:1346:ALA:HB3	2.18	0.44
1:B:1373:ASP:C	1:B:1376:THR:HG22	2.43	0.44
1:B:1441:PHE:HZ	6:G:89:GLU:HA	1.79	0.44
2:C:25:ILE:HG23	2:C:658:ILE:HD12	2.00	0.44
2:C:51:PHE:CZ	2:C:172:ILE:HA	2.53	0.44
2:C:102:VAL:O	2:C:104:GLU:HG2	2.17	0.44
2:C:129:PHE:CD2	2:C:166:PHE:HA	2.52	0.44
2:C:361:LEU:HG	2:C:363:HIS:CE1	2.52	0.44
2:C:529:GLU:OE1	2:C:769:TYR:CE2	2.71	0.44
2:C:841:MET:SD	2:C:846:ILE:HD11	2.57	0.44
2:C:842:ASN:ND2	2:C:845:SER:CB	2.80	0.44
2:C:843:GLN:HB3	2:C:994:TYR:O	2.18	0.44
11:L:68:PHE:HD2	11:L:68:PHE:N	2.15	0.44
15:T:24:DG:H2'	15:T:25:DC:O4'	2.17	0.44
1:B:49:LYS:NZ	1:B:61:ILE:N	2.63	0.44
1:B:108:MET:HA	1:B:210:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:VAL:HA	1:B:242:PRO:HD2	1.88	0.44
1:B:269:ILE:CG2	1:B:300:VAL:HG22	2.47	0.44
1:B:289:ILE:C	1:B:291:GLU:N	2.76	0.44
1:B:546:VAL:O	1:B:546:VAL:HG12	2.16	0.44
1:B:709:THR:HG21	1:B:711:ARG:HB2	1.99	0.44
1:B:808:LEU:HD23	1:B:813:PHE:N	2.33	0.44
1:B:1104:ILE:C	1:B:1106:ASN:H	2.25	0.44
1:B:1423:GLY:HA3	1:B:1426:GLU:HG2	1.98	0.44
2:C:31:TRP:CZ3	2:C:34:ILE:HD12	2.53	0.44
2:C:167:ILE:CG2	2:C:453:ILE:HD11	2.42	0.44
2:C:210:LYS:HE2	2:C:462:ALA:C	2.41	0.44
2:C:570:VAL:HB	2:C:573:GLN:CB	2.47	0.44
2:C:906:SER:O	2:C:907:GLY:O	2.35	0.44
2:C:1065:GLN:HB2	3:D:201:TRP:CZ3	2.53	0.44
2:C:1076:HIS:CD2	11:L:40:HIS:CE1	3.05	0.44
3:D:193:TYR:CD1	3:D:193:TYR:C	2.95	0.44
5:F:182:ASP:OD1	5:F:183:PRO:HD2	2.17	0.44
9:J:16:PRO:HB3	9:J:27:PHE:CE2	2.52	0.44
9:J:65:ASP:CG	9:J:68:LEU:HD12	2.42	0.44
10:K:57:ILE:HG23	10:K:58:GLU:N	2.33	0.44
12:M:34:CYS:O	12:M:34:CYS:SG	2.74	0.44
14:P:6:A:C4	14:P:7:A:C8	3.06	0.44
14:P:8:U:H2'	14:P:9:A:H8	1.83	0.44
1:B:123:ARG:NH2	1:B:155:GLU:HG2	2.33	0.44
1:B:241:VAL:HG13	1:B:266:LEU:HD13	1.98	0.44
1:B:284:ALA:C	1:B:286:HIS:H	2.23	0.44
1:B:601:LYS:HB2	1:B:603:ASN:ND2	2.33	0.44
1:B:626:ASN:O	1:B:631:HIS:CD2	2.71	0.44
1:B:829:VAL:C	1:B:831:THR:N	2.74	0.44
1:B:1126:ALA:O	1:B:1128:GLN:N	2.47	0.44
2:C:458:LYS:O	2:C:459:TYR:C	2.60	0.44
2:C:838:SER:CA	2:C:989:THR:O	2.66	0.44
2:C:899:ILE:HD11	2:C:911:ILE:HG12	2.00	0.44
3:D:66:ARG:CZ	10:K:2:ILE:HG21	2.47	0.44
8:I:93:TYR:CD1	8:I:93:TYR:N	2.85	0.44
15:T:21:DA:H2'	15:T:22:DT:C6	2.53	0.44
1:B:227:VAL:HG12	4:E:15:LEU:HD23	1.98	0.44
1:B:738:LYS:HZ1	3:D:194:GLU:C	2.24	0.44
1:B:886:ILE:HG23	1:B:887:GLY:H	1.78	0.44
1:B:1118:VAL:HG12	1:B:1327:ILE:HG13	1.98	0.44
1:B:1444:MET:CE	6:G:135:ARG:HB2	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1447:GLU:OE2	7:H:23:LYS:HB2	2.17	0.44
2:C:429:PHE:C	2:C:431:TYR:H	2.25	0.44
2:C:636:PRO:O	2:C:743:ILE:HD11	2.17	0.44
2:C:684:LEU:O	2:C:689:LEU:HB2	2.17	0.44
2:C:753:ALA:HA	2:C:756:ILE:CD1	2.48	0.44
2:C:1004:GLU:OE2	2:C:1064:TYR:HE2	2.01	0.44
2:C:1162:ILE:HG23	2:C:1168:LEU:O	2.18	0.44
3:D:67:LEU:HD13	3:D:157:CYS:SG	2.57	0.44
5:F:12:LEU:HD22	5:F:55:ARG:CZ	2.48	0.44
9:J:83:ASN:OD1	9:J:103:CYS:HA	2.16	0.44
10:K:2:ILE:C	10:K:53:HIS:NE2	2.76	0.44
10:K:7:CYS:HA	10:K:49:MET:HE3	2.00	0.44
10:K:30:LEU:HD11	10:K:38:ARG:HH12	1.82	0.44
11:L:33:ILE:HD13	11:L:87:LEU:HD22	1.99	0.44
14:P:6:A:H2'	14:P:7:A:O4'	2.17	0.44
1:B:22:PHE:HD2	1:B:27:VAL:HG22	1.83	0.44
1:B:71:GLN:C	1:B:73:GLY:H	2.25	0.44
1:B:148:CYS:C	1:B:168:GLY:HA2	2.42	0.44
1:B:316:GLN:O	1:B:317:LYS:C	2.61	0.44
1:B:600:PRO:C	1:B:602:ASP:H	2.25	0.44
1:B:740:LEU:C	1:B:740:LEU:HD12	2.43	0.44
1:B:765:VAL:HG12	1:B:766:GLY:H	1.81	0.44
1:B:1224:LEU:HG	1:B:1226:VAL:HG23	2.00	0.44
1:B:1287:TYR:O	1:B:1302:PRO:HA	2.18	0.44
2:C:604:ARG:C	2:C:606:LYS:H	2.25	0.44
2:C:681:TRP:O	2:C:684:LEU:N	2.51	0.44
2:C:984:HIS:CD2	2:C:1025:HIS:HA	2.52	0.44
3:D:155:LEU:HB3	3:D:156:THR:H	1.46	0.44
5:F:78:LEU:CD2	5:F:80:VAL:HG23	2.43	0.44
10:K:48:ARG:HH21	10:K:49:MET:HE1	1.82	0.44
11:L:85:ASP:O	11:L:88:LYS:HB2	2.17	0.44
11:L:87:LEU:O	11:L:90:ALA:HB3	2.18	0.44
1:B:22:PHE:CD2	1:B:27:VAL:HG22	2.53	0.44
1:B:840:ARG:C	1:B:842:VAL:N	2.74	0.44
1:B:845:LEU:O	1:B:846:GLU:C	2.61	0.44
1:B:867:ILE:HG22	1:B:872:GLY:N	2.33	0.44
1:B:1051:ALA:O	1:B:1055:ARG:HG3	2.18	0.44
1:B:1118:VAL:HG23	1:B:1118:VAL:O	2.17	0.44
1:B:1157:ASP:C	1:B:1159:ARG:H	2.26	0.44
2:C:116:GLU:C	2:C:118:ARG:N	2.76	0.44
2:C:185:THR:H	2:C:188:ASP:CB	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:282:ILE:CD1	2:C:382:ILE:HG21	2.48	0.44
2:C:425:THR:O	2:C:428:ILE:HB	2.18	0.44
2:C:880:THR:CB	2:C:934:LYS:HD2	2.46	0.44
2:C:882:THR:HB	2:C:934:LYS:O	2.17	0.44
2:C:1178:ASN:O	2:C:1179:GLN:C	2.60	0.44
4:E:131:GLU:C	4:E:132:GLN:HG2	2.42	0.44
7:H:88:ASP:HB3	7:H:144:ARG:CA	2.42	0.44
11:L:68:PHE:HB3	11:L:70:ARG:NH1	2.32	0.44
1:B:18:GLN:O	2:C:1215:ARG:HG2	2.18	0.44
1:B:243:PRO:CB	1:B:244:PRO:HD2	2.46	0.44
1:B:507:VAL:N	1:B:508:PRO:CD	2.81	0.44
1:B:1015:VAL:O	1:B:1016:THR:C	2.60	0.44
1:B:1019:CYS:O	1:B:1020:CYS:C	2.59	0.44
1:B:1063:MET:O	1:B:1064:VAL:C	2.60	0.44
1:B:1215:ARG:HD2	1:B:1215:ARG:HA	1.86	0.44
1:B:1239:ARG:HH22	1:B:1241:ARG:HH22	1.65	0.44
1:B:1349:TYR:HB2	1:B:1372:VAL:HG21	1.98	0.44
2:C:303:TYR:O	2:C:304:ASP:HB2	2.18	0.44
2:C:361:LEU:HG	2:C:363:HIS:HE1	1.82	0.44
2:C:881:ASN:O	2:C:883:LEU:HG	2.18	0.44
2:C:913:GLY:HA2	2:C:938:SER:OG	2.18	0.44
2:C:1165:ILE:O	2:C:1217:TYR:CE1	2.71	0.44
4:E:40:HIS:CE1	4:E:41:GLN:HG3	2.53	0.44
4:E:176:GLU:O	4:E:177:VAL:C	2.61	0.44
4:E:208:GLU:O	4:E:212:LYS:HG3	2.18	0.44
5:F:175:LEU:HD23	5:F:175:LEU:HA	1.78	0.44
7:H:3:PHE:CD1	7:H:3:PHE:N	2.85	0.44
1:B:108:MET:N	1:B:108:MET:SD	2.91	0.43
1:B:239:LEU:HA	1:B:240:PRO:HD2	1.90	0.43
1:B:466:SER:O	2:C:1103:ILE:HD11	2.18	0.43
1:B:718:VAL:O	1:B:719:VAL:C	2.61	0.43
1:B:1346:ALA:CB	5:F:149:LEU:HD12	2.48	0.43
2:C:39:ARG:NH2	2:C:665:GLU:CG	2.77	0.43
2:C:255:GLN:O	2:C:271:ALA:CB	2.66	0.43
2:C:293:PRO:HD2	2:C:296:GLU:OE1	2.18	0.43
2:C:332:ASP:C	2:C:334:ILE:N	2.77	0.43
2:C:465:ASN:HD22	2:C:465:ASN:N	2.15	0.43
2:C:597:MET:HE1	2:C:615:MET:HE3	2.00	0.43
3:D:83:SER:OG	3:D:160:LYS:HB3	2.17	0.43
3:D:170:TRP:O	3:D:171:GLY:C	2.61	0.43
4:E:29:LEU:N	4:E:29:LEU:HD23	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:173:SER:C	5:F:175:LEU:N	2.77	0.43
6:G:99:LEU:O	6:G:102:SER:OG	2.29	0.43
6:G:106:PRO:HG2	7:H:18:PHE:C	2.43	0.43
7:H:91:VAL:HG12	7:H:92:VAL:N	2.32	0.43
8:I:55:LEU:HD22	8:I:144:ILE:HG23	1.96	0.43
8:I:82:PRO:C	8:I:84:ALA:N	2.76	0.43
8:I:130:ARG:CB	8:I:134:ASN:H	2.25	0.43
10:K:1:MET:N	10:K:57:ILE:HG22	2.33	0.43
10:K:38:ARG:C	10:K:40:GLY:H	2.26	0.43
10:K:64:ASN:HD22	10:K:65:PRO:HD3	1.83	0.43
11:L:6:ARG:C	11:L:8:GLU:H	2.26	0.43
11:L:53:ASP:C	11:L:55:LYS:H	2.26	0.43
1:B:2:VAL:HG13	2:C:1157:ALA:HB1	2.00	0.43
1:B:81:PHE:CE1	2:C:1208:MET:HE2	2.52	0.43
1:B:351:THR:HG22	2:C:1103:ILE:HG13	2.00	0.43
1:B:367:PRO:CB	1:B:466:SER:HA	2.48	0.43
1:B:552:TRP:HE1	11:L:62:LYS:HB2	1.83	0.43
1:B:668:ASP:HB3	1:B:741:ASN:ND2	2.27	0.43
1:B:1138:ILE:O	1:B:1275:GLY:HA3	2.19	0.43
1:B:1156:PRO:O	1:B:1158:PRO:HD3	2.18	0.43
2:C:234:ILE:N	2:C:234:ILE:HD12	2.34	0.43
2:C:289:LEU:HD22	2:C:371:GLU:O	2.17	0.43
2:C:383:ASN:CG	2:C:387:LEU:HD13	2.44	0.43
2:C:582:VAL:HB	2:C:587:HIS:HD2	1.82	0.43
2:C:616:ILE:N	2:C:616:ILE:CD1	2.70	0.43
2:C:1072:MET:HE3	2:C:1085:ILE:CB	2.21	0.43
2:C:1142:GLY:O	2:C:1144:ALA:N	2.51	0.43
2:C:1202:LEU:HD22	2:C:1206:GLU:CD	2.43	0.43
3:D:44:LEU:HD23	3:D:72:LEU:HD12	2.00	0.43
4:E:156:ASP:HB2	4:E:159:THR:HG23	2.01	0.43
8:I:56:THR:O	8:I:144:ILE:HA	2.18	0.43
8:I:128:ASN:O	8:I:128:ASN:CG	2.59	0.43
10:K:3:VAL:HA	10:K:53:HIS:CD2	2.53	0.43
1:B:43:GLU:HG3	1:B:46:THR:O	2.18	0.43
1:B:1114:PRO:HG2	1:B:1115:SER:N	2.33	0.43
2:C:329:THR:CA	2:C:332:ASP:HB3	2.44	0.43
2:C:488:TYR:CG	2:C:817:LEU:HD12	2.53	0.43
2:C:653:VAL:CG2	2:C:689:LEU:HB3	2.48	0.43
2:C:757:PRO:HD3	2:C:983:ARG:NH2	2.33	0.43
2:C:860:MET:HG2	2:C:861:ASP:N	2.32	0.43
2:C:1007:VAL:HG22	2:C:1008:PRO:CD	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1065:GLN:NE2	2:C:1066:SER:H	2.16	0.43
2:C:1165:ILE:O	2:C:1217:TYR:HE1	2.00	0.43
5:F:20:LYS:HZ3	5:F:60:PHE:HE1	1.63	0.43
5:F:124:VAL:HB	5:F:125:PRO:HD3	2.00	0.43
6:G:76:LYS:NZ	7:H:58:ARG:HH22	2.16	0.43
6:G:138:LEU:O	6:G:140:ASP:N	2.50	0.43
7:H:39:THR:HG22	7:H:40:GLY:N	2.33	0.43
9:J:82:GLU:HB3	9:J:104:LEU:CG	2.47	0.43
1:B:38:PRO:HG2	1:B:39:GLU:H	1.83	0.43
1:B:297:GLN:O	1:B:297:GLN:HG3	2.18	0.43
1:B:353:ILE:HG21	1:B:487:MET:CG	2.48	0.43
1:B:574:GLY:O	1:B:575:LYS:C	2.62	0.43
1:B:577:ILE:O	1:B:578:LEU:C	2.60	0.43
1:B:642:CYS:O	1:B:643:ALA:C	2.61	0.43
1:B:808:LEU:CD2	1:B:813:PHE:HA	2.47	0.43
2:C:234:ILE:HG21	2:C:237:VAL:CG2	2.48	0.43
2:C:637:LEU:CD2	2:C:742:GLU:HA	2.48	0.43
2:C:1076:HIS:CD2	11:L:40:HIS:NE2	2.85	0.43
2:C:1159:ARG:HD2	2:C:1159:ARG:C	2.43	0.43
4:E:64:VAL:C	4:E:66:ARG:N	2.74	0.43
5:F:113:GLN:HG2	5:F:137:GLU:OE1	2.18	0.43
5:F:153:HIS:ND1	5:F:184:VAL:HG11	2.33	0.43
8:I:84:ALA:O	8:I:89:LEU:HD21	2.18	0.43
8:I:95:TYR:HB3	8:I:144:ILE:HB	1.99	0.43
10:K:3:VAL:HG11	10:K:14:VAL:O	2.18	0.43
15:T:24:DG:H3'	15:T:25:DC:C5'	2.43	0.43
1:B:41:MET:HE3	1:B:41:MET:H	1.83	0.43
1:B:54:ASN:H	1:B:54:ASN:HD22	1.66	0.43
1:B:196:GLU:HG3	1:B:197:PRO:CD	2.41	0.43
1:B:443:LEU:HD12	2:C:1146:PHE:CZ	2.54	0.43
1:B:567:LYS:HZ3	8:I:47:PHE:HB3	1.82	0.43
1:B:786:HIS:HE1	2:C:519:TRP:CZ2	2.36	0.43
1:B:982:THR:O	1:B:985:ASP:HB2	2.19	0.43
1:B:1007:ILE:O	1:B:1008:GLN:C	2.61	0.43
1:B:1039:LYS:HE3	1:B:1043:ASP:OD2	2.18	0.43
1:B:1226:VAL:HG13	1:B:1239:ARG:O	2.18	0.43
1:B:1332:PHE:O	1:B:1333:ILE:C	2.61	0.43
2:C:229:ALA:HB1	2:C:231:PRO:HD2	2.01	0.43
2:C:435:THR:C	2:C:437:GLU:H	2.25	0.43
2:C:496:ARG:HB3	2:C:496:ARG:HH11	1.81	0.43
2:C:1035:ALA:HB1	2:C:1040:ASN:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:65:HIS:O	3:D:66:ARG:C	2.62	0.43
3:D:80:LEU:O	3:D:81:GLU:C	2.61	0.43
3:D:97:VAL:HB	3:D:159:ALA:HB3	2.00	0.43
3:D:142:VAL:O	3:D:142:VAL:HG12	2.19	0.43
3:D:193:TYR:C	3:D:193:TYR:HD1	2.27	0.43
4:E:175:PHE:CZ	7:H:85:GLU:HG3	2.48	0.43
9:J:74:GLU:HB2	9:J:79:HIS:CA	2.48	0.43
1:B:83:HIS:HA	1:B:239:LEU:O	2.18	0.43
1:B:113:LEU:HG	1:B:218:ASP:OD1	2.19	0.43
1:B:244:PRO:CB	1:B:245:PRO:HD3	2.37	0.43
1:B:269:ILE:HG23	1:B:300:VAL:CG2	2.48	0.43
1:B:463:ILE:HD12	1:B:469:ARG:CD	2.48	0.43
1:B:511:ILE:HA	1:B:521:MET:HE3	1.99	0.43
1:B:593:GLU:C	1:B:595:THR:N	2.76	0.43
1:B:719:VAL:O	1:B:720:ARG:C	2.62	0.43
1:B:962:ARG:O	1:B:963:ILE:C	2.60	0.43
1:B:1026:LEU:HD23	1:B:1026:LEU:HA	1.76	0.43
1:B:1127:ASP:HB3	1:B:1130:GLN:HB3	2.01	0.43
1:B:1127:ASP:O	1:B:1128:GLN:C	2.61	0.43
1:B:1211:GLN:O	1:B:1212:VAL:C	2.62	0.43
1:B:1227:ILE:CG2	1:B:1228:TRP:H	2.30	0.43
1:B:1293:SER:O	1:B:1294:PRO:C	2.59	0.43
1:B:1377:THR:OG1	1:B:1378:GLN:N	2.47	0.43
2:C:31:TRP:CE3	2:C:34:ILE:HD12	2.54	0.43
2:C:273:LEU:CG	2:C:276:ILE:HD12	2.48	0.43
2:C:383:ASN:ND2	2:C:387:LEU:HD22	2.34	0.43
2:C:806:THR:CG2	2:C:808:ALA:H	2.20	0.43
3:D:174:ALA:O	3:D:175:ALA:CB	2.67	0.43
4:E:187:THR:HG22	4:E:188:ALA:H	1.84	0.43
7:H:1:MET:O	7:H:3:PHE:HE1	2.00	0.43
7:H:35:GLU:CG	7:H:48:VAL:HG23	2.48	0.43
7:H:99:PHE:HZ	7:H:163:ILE:HD13	1.83	0.43
10:K:43:ARG:HG2	10:K:45:CYS:SG	2.59	0.43
11:L:59:ALA:HA	11:L:74:ARG:O	2.18	0.43
1:B:16:GLU:HB3	1:B:1418:LEU:HD11	1.99	0.43
1:B:207:ILE:HG23	1:B:211:PHE:CE1	2.53	0.43
1:B:345:VAL:CG1	2:C:1130:PHE:HB2	2.49	0.43
1:B:722:LEU:H	1:B:722:LEU:CD1	2.28	0.43
1:B:947:PHE:O	1:B:948:VAL:C	2.61	0.43
1:B:971:PHE:CE2	1:B:1040:GLN:HG2	2.54	0.43
1:B:1055:ARG:NE	6:G:154:ASP:OD1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1329:THR:C	1:B:1331:SER:N	2.74	0.43
2:C:55:VAL:HG13	2:C:97:VAL:HG21	2.00	0.43
2:C:314:LEU:HD12	2:C:314:LEU:N	2.31	0.43
2:C:459:TYR:HE2	2:C:465:ASN:HB2	1.83	0.43
2:C:866:TYR:N	2:C:866:TYR:CD1	2.87	0.43
2:C:956:THR:HG22	2:C:957:ASN:N	2.34	0.43
2:C:1183:LYS:N	2:C:1183:LYS:CE	2.82	0.43
3:D:29:MET:CE	11:L:98:LEU:HG	2.48	0.43
3:D:53:THR:HG22	3:D:54:ASN:N	2.34	0.43
4:E:63:LEU:HB3	4:E:129:LEU:HD21	2.00	0.43
4:E:153:ARG:HB3	4:E:154:PHE:CD1	2.53	0.43
5:F:46:TYR:CD1	5:F:46:TYR:N	2.87	0.43
5:F:124:VAL:HG13	5:F:132:ILE:CG1	2.48	0.43
7:H:20:PRO:CD	7:H:21:ARG:H	2.32	0.43
10:K:58:GLU:HA	10:K:61:LEU:HD12	1.99	0.43
11:L:52:ASN:O	11:L:53:ASP:C	2.61	0.43
12:M:27:LEU:HD23	12:M:27:LEU:N	2.34	0.43
1:B:122:MET:O	1:B:125:ALA:HB3	2.19	0.43
1:B:230:ARG:HB3	1:B:232:GLU:HG2	1.99	0.43
1:B:1021:LEU:O	1:B:1024:SER:HB3	2.19	0.43
1:B:1210:GLY:O	1:B:1211:GLN:C	2.60	0.43
2:C:247:GLY:H	2:C:418:LYS:NZ	2.17	0.43
2:C:281:PRO:HB2	2:C:283:VAL:HG23	2.00	0.43
2:C:345:LYS:C	2:C:347:LYS:H	2.27	0.43
2:C:510:LYS:HB2	2:C:511:PRO:HD3	2.01	0.43
2:C:778:MET:HE1	2:C:853:SER:CB	2.49	0.43
2:C:798:TYR:CE1	10:K:4:PRO:HB3	2.54	0.43
2:C:957:ASN:C	2:C:959:ASP:N	2.75	0.43
2:C:1034:VAL:O	2:C:1037:LEU:N	2.51	0.43
2:C:1215:ARG:O	2:C:1216:LEU:HD23	2.18	0.43
2:C:1219:ASP:O	2:C:1219:ASP:OD1	2.36	0.43
3:D:31:ASN:O	3:D:35:ARG:HG3	2.17	0.43
3:D:91:HIS:O	3:D:91:HIS:HD2	2.01	0.43
4:E:214:LEU:C	4:E:216:ASN:N	2.76	0.43
6:G:118:LEU:O	6:G:122:MET:HG3	2.17	0.43
8:I:30:SER:HB3	8:I:36:CYS:HB3	2.00	0.43
1:B:9:ALA:HB1	1:B:10:PRO:HD2	2.00	0.43
1:B:146:MET:HB3	1:B:171:GLN:O	2.18	0.43
1:B:229:SER:HB3	1:B:1413:GLY:O	2.18	0.43
1:B:249:SER:C	1:B:250:ILE:HG13	2.43	0.43
1:B:386:ASP:O	1:B:387:ARG:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:LEU:CD1	2:C:830:TYR:CD1	3.02	0.43
1:B:997:LEU:HD23	1:B:997:LEU:N	2.34	0.43
1:B:1230:GLU:C	1:B:1232:ASN:N	2.77	0.43
1:B:1291:VAL:HG13	1:B:1292:PRO:N	2.33	0.43
2:C:125:SER:CB	2:C:171:PRO:HA	2.49	0.43
2:C:490:SER:O	2:C:491:THR:C	2.61	0.43
2:C:531:GLN:HG3	2:C:532:ALA:N	2.34	0.43
3:D:10:ILE:CD1	11:L:109:TRP:HA	2.49	0.43
3:D:76:ASP:O	3:D:77:ILE:C	2.62	0.43
5:F:79:TRP:CD1	5:F:96:PHE:HE1	2.37	0.43
5:F:94:LYS:O	5:F:98:ILE:HG13	2.19	0.43
6:G:125:LEU:HD23	6:G:125:LEU:C	2.44	0.43
9:J:7:CYS:HB2	9:J:34:TYR:CG	2.54	0.43
9:J:58:VAL:HG12	9:J:58:VAL:O	2.19	0.43
9:J:75:CYS:C	9:J:77:LYS:H	2.27	0.43
1:B:80:HIS:N	1:B:243:PRO:HG3	2.33	0.43
1:B:265:LYS:HD3	1:B:302:THR:CG2	2.48	0.43
1:B:289:ILE:C	1:B:291:GLU:H	2.27	0.43
1:B:384:ASN:C	1:B:386:ASP:H	2.26	0.43
1:B:850:VAL:HG12	1:B:1060:PRO:HA	2.01	0.43
1:B:946:VAL:HG22	5:F:201:LYS:HD2	2.00	0.43
1:B:1167:GLU:O	1:B:1170:ILE:HG13	2.19	0.43
1:B:1313:LEU:O	1:B:1315:GLU:N	2.52	0.43
2:C:347:LYS:O	2:C:350:GLN:HB3	2.18	0.43
2:C:348:ARG:C	2:C:350:GLN:N	2.77	0.43
2:C:531:GLN:CG	2:C:532:ALA:H	2.31	0.43
2:C:948:ILE:O	2:C:968:VAL:HG13	2.19	0.43
2:C:1202:LEU:O	2:C:1203:LEU:C	2.60	0.43
3:D:100:THR:HG21	3:D:102:GLN:NE2	2.34	0.43
3:D:100:THR:CG2	3:D:102:GLN:HE21	2.32	0.43
4:E:34:GLN:O	4:E:47:LEU:HD23	2.18	0.43
5:F:82:PHE:N	5:F:82:PHE:CD1	2.87	0.43
7:H:1:MET:O	7:H:1:MET:CE	2.67	0.43
7:H:80:LYS:HE2	7:H:82:PHE:CE1	2.54	0.43
7:H:123:ALA:C	7:H:125:SER:H	2.26	0.43
8:I:15:VAL:CG2	8:I:26:ILE:HD11	2.37	0.43
8:I:113:ALA:HA	8:I:125:LEU:O	2.19	0.43
9:J:26:LEU:HD22	9:J:35:VAL:HG12	2.01	0.43
9:J:54:GLU:OE2	9:J:118:ARG:CZ	2.67	0.43
9:J:105:SER:O	9:J:106:CYS:CB	2.66	0.43
1:B:133:LYS:O	1:B:136:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:THR:C	1:B:304:MET:N	2.76	0.42
1:B:345:VAL:HG11	2:C:1130:PHE:HB2	2.00	0.42
1:B:465:TYR:CZ	11:L:4:PRO:HD2	2.54	0.42
1:B:494:SER:O	1:B:495:GLU:C	2.62	0.42
1:B:774:ARG:HB2	1:B:797:LYS:HB3	2.01	0.42
1:B:853:ASP:OD1	1:B:855:THR:CB	2.67	0.42
1:B:1368:MET:O	1:B:1372:VAL:HB	2.18	0.42
2:C:308:TRP:CD1	2:C:308:TRP:N	2.86	0.42
2:C:383:ASN:O	2:C:384:ARG:C	2.62	0.42
2:C:460:ALA:C	2:C:462:ALA:H	2.27	0.42
2:C:498:THR:HG22	2:C:537:LYS:O	2.18	0.42
2:C:654:ARG:C	2:C:656:GLY:N	2.76	0.42
2:C:657:HIS:O	2:C:660:LYS:HB3	2.19	0.42
2:C:680:THR:HB	2:C:681:TRP:H	1.55	0.42
2:C:792:MET:HG3	2:C:855:PHE:CE1	2.54	0.42
2:C:1003:ALA:HA	3:D:178:PHE:O	2.18	0.42
3:D:44:LEU:HD21	3:D:159:ALA:HB1	2.01	0.42
6:G:88:TYR:HD1	6:G:88:TYR:H	1.66	0.42
6:G:116:ASP:HB3	6:G:119:ARG:CB	2.49	0.42
8:I:116:TYR:HE2	8:I:140:ALA:HB3	1.84	0.42
9:J:90:GLN:HE21	9:J:92:ARG:HD2	1.82	0.42
1:B:30:ILE:HD11	2:C:1168:LEU:CD1	2.49	0.42
1:B:208:LEU:HD23	1:B:209:ASN:N	2.34	0.42
1:B:247:ARG:HG3	1:B:247:ARG:NH1	2.35	0.42
1:B:380:VAL:CG1	1:B:385:ILE:HG12	2.49	0.42
1:B:796:SER:C	1:B:798:GLY:N	2.77	0.42
1:B:1007:ILE:O	1:B:1010:ALA:N	2.52	0.42
1:B:1345:ARG:O	1:B:1346:ALA:C	2.62	0.42
1:B:1409:LEU:HD13	2:C:1207:LEU:HD21	2.01	0.42
2:C:37:PHE:CD1	2:C:41:LYS:HG3	2.53	0.42
2:C:95:ILE:HG13	2:C:130:VAL:HG22	2.01	0.42
2:C:487:THR:CG2	2:C:488:TYR:N	2.82	0.42
2:C:553:PRO:O	2:C:557:PHE:HB2	2.18	0.42
2:C:599:THR:O	2:C:603:LEU:HB2	2.19	0.42
2:C:801:LYS:O	10:K:52:THR:HG21	2.17	0.42
2:C:1160:VAL:CG1	2:C:1161:HIS:N	2.82	0.42
2:C:1177:HIS:HB2	2:C:1179:GLN:HE21	1.84	0.42
3:D:101:LEU:HD12	3:D:101:LEU:HA	1.88	0.42
3:D:166:GLU:C	11:L:6:ARG:NH1	2.77	0.42
11:L:31:VAL:CG1	11:L:32:VAL:N	2.81	0.42
1:B:269:ILE:HG12	1:B:299:HIS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ILE:HD11	1:B:300:VAL:HA	2.00	0.42
1:B:544:ASP:CG	1:B:545:GLN:H	2.27	0.42
1:B:590:ARG:HH11	1:B:590:ARG:CB	2.30	0.42
1:B:658:LEU:HD11	2:C:830:TYR:CE1	2.55	0.42
1:B:715:GLU:O	1:B:718:VAL:HB	2.19	0.42
1:B:787:PHE:HE1	1:B:796:SER:HA	1.82	0.42
1:B:898:ARG:HA	1:B:933:TYR:CD1	2.55	0.42
1:B:1064:VAL:HG12	1:B:1370:LEU:HD22	2.01	0.42
1:B:1215:ARG:HG2	1:B:1215:ARG:HH11	1.82	0.42
1:B:1437:GLY:HA3	6:G:88:TYR:CD2	2.53	0.42
2:C:424:LEU:O	2:C:428:ILE:HG13	2.19	0.42
2:C:510:LYS:O	2:C:511:PRO:C	2.63	0.42
2:C:528:PRO:HG3	2:C:536:VAL:HB	2.01	0.42
2:C:662:MET:HA	2:C:665:GLU:HB2	2.01	0.42
2:C:882:THR:C	2:C:884:ARG:N	2.77	0.42
2:C:1003:ALA:C	2:C:1005:GLY:H	2.28	0.42
2:C:1039:GLY:HA2	10:K:51:LEU:HD21	2.01	0.42
2:C:1084:GLN:HE21	2:C:1084:GLN:N	2.09	0.42
2:C:1170:THR:O	2:C:1171:VAL:C	2.62	0.42
3:D:35:ARG:HH11	11:L:41:THR:H	1.62	0.42
3:D:99:LEU:HD23	3:D:120:ILE:HA	2.00	0.42
3:D:242:GLN:O	3:D:244:VAL:N	2.53	0.42
4:E:160:VAL:O	4:E:160:VAL:HG12	2.20	0.42
7:H:44:TYR:HD2	7:H:105:PRO:HB2	1.85	0.42
8:I:117:SER:HA	8:I:121:LEU:O	2.19	0.42
12:M:59:ALA:O	12:M:60:ARG:O	2.38	0.42
15:T:18:DT:OP2	15:T:18:DT:H72	2.19	0.42
1:B:364:VAL:O	1:B:364:VAL:CG1	2.68	0.42
1:B:567:LYS:NZ	8:I:47:PHE:HB3	2.34	0.42
1:B:761:MET:HA	1:B:804:TYR:HB2	2.00	0.42
1:B:864:ILE:O	1:B:865:GLN:HG2	2.20	0.42
1:B:1011:GLN:NE2	1:B:1015:VAL:HG21	2.34	0.42
1:B:1063:MET:HG3	1:B:1436:ILE:HG23	2.01	0.42
1:B:1283:VAL:HG12	1:B:1284:MET:N	2.32	0.42
2:C:119:LEU:HD23	2:C:789:MET:HB2	2.02	0.42
2:C:185:THR:O	2:C:188:ASP:N	2.52	0.42
2:C:698:GLU:O	2:C:701:ILE:HG12	2.20	0.42
2:C:808:ALA:O	2:C:809:MET:C	2.62	0.42
2:C:948:ILE:HD12	2:C:969:ARG:NH1	2.34	0.42
2:C:1017:ILE:H	2:C:1018:PRO:HD2	1.84	0.42
2:C:1111:MET:HE1	2:C:1118:PRO:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1221:SER:C	2:C:1223:ASP:N	2.76	0.42
3:D:44:LEU:CD2	3:D:159:ALA:HB1	2.49	0.42
5:F:160:GLU:O	5:F:163:GLU:HB3	2.19	0.42
8:I:15:VAL:HG13	8:I:26:ILE:HG13	2.01	0.42
9:J:61:ASP:C	9:J:63:GLY:N	2.78	0.42
9:J:70:ARG:NH1	9:J:84:VAL:HB	2.35	0.42
1:B:44:THR:O	1:B:45:GLN:HB2	2.18	0.42
1:B:341:MET:HE1	2:C:1135:ARG:CZ	2.48	0.42
1:B:404:TYR:HB2	1:B:433:GLU:HB2	2.00	0.42
1:B:427:GLN:HB2	1:B:430:TRP:CG	2.54	0.42
1:B:546:VAL:HG21	1:B:572:TRP:HB2	2.01	0.42
1:B:557:ASP:OD1	1:B:557:ASP:N	2.52	0.42
1:B:565:ILE:O	1:B:570:PRO:HA	2.19	0.42
1:B:606:LEU:HG	1:B:613:ILE:HB	2.00	0.42
1:B:786:HIS:O	1:B:787:PHE:HD2	2.01	0.42
1:B:858:ASN:HD22	1:B:858:ASN:H	1.68	0.42
1:B:1155:ASP:CG	1:B:1162:VAL:HG23	2.45	0.42
1:B:1214:GLU:O	1:B:1218:GLN:HG2	2.19	0.42
1:B:1279:ILE:HG23	1:B:1308:THR:OG1	2.20	0.42
2:C:286:PHE:HE1	2:C:301:ILE:HD11	1.84	0.42
2:C:487:THR:HG22	2:C:488:TYR:N	2.34	0.42
2:C:496:ARG:HD3	2:C:751:VAL:HG22	2.01	0.42
2:C:566:LEU:HD22	2:C:586:TRP:HB3	2.01	0.42
2:C:638:PHE:HB2	2:C:741:CYS:HB3	2.01	0.42
2:C:799:PRO:HB3	2:C:818:PRO:HG2	2.00	0.42
2:C:1099:VAL:C	2:C:1101:ASP:N	2.76	0.42
3:D:27:LEU:O	3:D:28:ALA:C	2.62	0.42
3:D:180:TYR:CD1	3:D:180:TYR:C	2.97	0.42
3:D:239:PRO:O	3:D:240:VAL:C	2.63	0.42
4:E:17:LYS:O	4:E:17:LYS:HD3	2.19	0.42
4:E:66:ARG:HG3	7:H:51:TYR:CD1	2.55	0.42
4:E:137:ASN:HD22	4:E:137:ASN:C	2.26	0.42
8:I:130:ARG:CA	8:I:133:ASN:HB2	2.50	0.42
9:J:19:ASP:OD1	9:J:22:ASN:HB2	2.19	0.42
10:K:51:LEU:HD12	10:K:51:LEU:O	2.18	0.42
10:K:53:HIS:CE1	10:K:55:ASP:OD1	2.72	0.42
11:L:29:ASN:O	11:L:30:ALA:HB2	2.20	0.42
1:B:302:THR:O	1:B:303:TYR:C	2.62	0.42
1:B:399:HIS:CG	1:B:400:PRO:N	2.85	0.42
1:B:666:ILE:HD11	2:C:1086:PHE:HE1	1.85	0.42
1:B:773:LYS:H	1:B:773:LYS:HG3	1.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:858:ASN:ND2	1:B:858:ASN:H	2.17	0.42
1:B:885:THR:O	1:B:885:THR:CG2	2.66	0.42
1:B:1116:LEU:HB2	1:B:1329:THR:OG1	2.20	0.42
1:B:1259:MET:O	1:B:1261:LYS:N	2.49	0.42
1:B:1293:SER:OG	1:B:1295:THR:CG2	2.67	0.42
2:C:120:ARG:HB2	2:C:122:LEU:HG	2.00	0.42
2:C:287:ARG:C	2:C:289:LEU:N	2.74	0.42
2:C:583:ASN:CG	2:C:628:THR:HG22	2.44	0.42
2:C:612:GLU:O	2:C:613:VAL:C	2.62	0.42
2:C:806:THR:C	2:C:808:ALA:N	2.71	0.42
2:C:997:GLU:HB3	3:D:35:ARG:NH2	2.34	0.42
3:D:59:ALA:O	3:D:60:ASP:C	2.61	0.42
3:D:167:HIS:CD2	3:D:168:ALA:H	2.37	0.42
3:D:189:THR:HG22	3:D:190:ASP:N	2.34	0.42
5:F:61:GLN:HG2	5:F:62:ALA:N	2.35	0.42
5:F:177:ARG:HD3	5:F:215:MET:HG2	2.02	0.42
7:H:29:LYS:O	7:H:30:LEU:C	2.63	0.42
8:I:96:VAL:HG13	8:I:143:LEU:HG	2.01	0.42
9:J:69:PRO:HB2	9:J:85:PHE:HE2	1.84	0.42
12:M:46:VAL:O	12:M:46:VAL:HG12	2.19	0.42
13:N:5:DT:H2"	13:N:6:DA:C8	2.54	0.42
1:B:241:VAL:O	1:B:241:VAL:HG12	2.19	0.42
1:B:382:PRO:CD	1:B:428:TYR:HE2	2.32	0.42
1:B:471:ASN:O	1:B:474:VAL:HG12	2.19	0.42
1:B:658:LEU:CD1	2:C:831:SER:H	2.19	0.42
1:B:784:LEU:C	1:B:786:HIS:H	2.28	0.42
1:B:873:MET:HG3	1:B:1056:SER:O	2.20	0.42
1:B:1111:MET:HG3	1:B:1113:THR:O	2.19	0.42
1:B:1239:ARG:HH22	1:B:1241:ARG:NH2	2.16	0.42
1:B:1398:MET:C	1:B:1400:CYS:N	2.73	0.42
2:C:1130:PHE:O	2:C:1130:PHE:CD2	2.73	0.42
3:D:6:PRO:CG	11:L:101:LEU:HB2	2.49	0.42
4:E:18:VAL:O	4:E:18:VAL:HG13	2.19	0.42
4:E:206:GLU:C	4:E:208:GLU:H	2.28	0.42
5:F:117:THR:C	5:F:119:SER:N	2.77	0.42
8:I:100:THR:HA	8:I:138:GLU:O	2.20	0.42
11:L:42:LEU:CD2	11:L:46:ILE:CD1	2.98	0.42
1:B:56:PRO:O	1:B:57:ARG:CG	2.68	0.42
1:B:244:PRO:C	1:B:246:VAL:H	2.28	0.42
1:B:288:ALA:HA	1:B:291:GLU:CD	2.44	0.42
1:B:681:GLU:HA	1:B:684:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:925:LEU:C	1:B:927:VAL:N	2.77	0.42
1:B:1277:GLU:O	1:B:1278:ASN:HB2	2.20	0.42
2:C:30:SER:O	2:C:33:VAL:HG23	2.20	0.42
2:C:272:THR:OG1	2:C:279:ASP:OD1	2.37	0.42
2:C:401:PHE:O	2:C:404:LYS:N	2.45	0.42
2:C:653:VAL:CA	2:C:689:LEU:HD22	2.49	0.42
2:C:880:THR:O	2:C:880:THR:HG22	2.20	0.42
2:C:899:ILE:HD11	2:C:911:ILE:CA	2.42	0.42
2:C:997:GLU:OE2	2:C:997:GLU:N	2.51	0.42
2:C:1066:SER:O	2:C:1067:ARG:HD3	2.18	0.42
2:C:1159:ARG:HH11	2:C:1159:ARG:CB	2.21	0.42
3:D:49:VAL:CG1	3:D:155:LEU:HD22	2.50	0.42
8:I:116:TYR:O	8:I:122:LEU:HA	2.19	0.42
10:K:31:ASP:O	10:K:32:GLU:C	2.63	0.42
10:K:57:ILE:O	10:K:60:PHE:HB2	2.20	0.42
1:B:17:VAL:HA	2:C:1215:ARG:O	2.20	0.42
1:B:108:MET:HA	1:B:210:ILE:CG2	2.50	0.42
1:B:310:GLY:C	1:B:312:PRO:HD2	2.45	0.42
1:B:350:ARG:HH11	1:B:350:ARG:HG3	1.84	0.42
1:B:373:THR:HG21	2:C:1105:ALA:HB3	2.01	0.42
1:B:525:GLN:O	1:B:526:ASP:C	2.62	0.42
1:B:578:LEU:O	1:B:578:LEU:HG	2.19	0.42
1:B:618:GLU:O	1:B:619:LYS:C	2.62	0.42
1:B:808:LEU:HG	1:B:812:GLU:HB3	2.02	0.42
1:B:818:MET:HG3	1:B:818:MET:H	1.70	0.42
1:B:898:ARG:HA	1:B:933:TYR:HD1	1.85	0.42
1:B:1010:ALA:O	1:B:1011:GLN:C	2.63	0.42
1:B:1194:ARG:HG2	1:B:1194:ARG:HH11	1.83	0.42
1:B:1266:THR:HA	1:B:1270:ASN:HD22	1.84	0.42
1:B:1323:ASP:C	1:B:1325:THR:N	2.78	0.42
1:B:1329:THR:O	1:B:1330:ASN:C	2.63	0.42
1:B:1346:ALA:HB3	5:F:149:LEU:HD12	2.02	0.42
2:C:175:ARG:HH11	2:C:175:ARG:CG	2.28	0.42
2:C:405:ARG:HD2	2:C:631:GLY:CA	2.50	0.42
2:C:693:ILE:HD13	2:C:701:ILE:HD13	2.02	0.42
2:C:1039:GLY:HA2	10:K:51:LEU:CD2	2.49	0.42
4:E:130:LEU:C	4:E:132:GLN:H	2.24	0.42
7:H:45:ILE:HA	7:H:45:ILE:HD13	1.89	0.42
7:H:148:GLU:HB2	7:H:160:ILE:O	2.20	0.42
10:K:3:VAL:HG12	10:K:15:GLY:HA2	2.00	0.42
11:L:31:VAL:HG12	11:L:32:VAL:H	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ARG:NH2	1:B:839:ARG:HH12	2.18	0.42
1:B:600:PRO:CG	1:B:601:LYS:H	2.30	0.42
1:B:644:LYS:O	1:B:647:GLY:N	2.53	0.42
1:B:786:HIS:CD2	1:B:786:HIS:N	2.86	0.42
1:B:1163:ILE:HG22	1:B:1164:PRO:HD2	2.02	0.42
1:B:1173:HIS:O	1:B:1174:PHE:HD1	2.03	0.42
1:B:1341:ILE:HG22	5:F:182:ASP:OD2	2.20	0.42
1:B:1446:ASP:HB2	6:G:133:VAL:HG23	2.01	0.42
2:C:308:TRP:O	2:C:309:GLN:C	2.63	0.42
2:C:364:ILE:CG1	2:C:585:VAL:HG13	2.49	0.42
2:C:843:GLN:CB	2:C:994:TYR:O	2.68	0.42
2:C:910:VAL:HG12	2:C:912:ILE:N	2.29	0.42
2:C:970:THR:HG22	2:C:971:THR:N	2.34	0.42
2:C:1060:ARG:C	2:C:1062:HIS:H	2.28	0.42
2:C:1203:LEU:O	2:C:1207:LEU:HG	2.20	0.42
3:D:73:GLN:HE22	3:D:75:MET:HE3	1.85	0.42
4:E:119:ARG:HD3	4:E:221:TYR:CD2	2.55	0.42
4:E:187:THR:HG22	4:E:188:ALA:N	2.35	0.42
6:G:109:VAL:CG1	6:G:110:ASP:H	2.26	0.42
8:I:83:GLN:O	8:I:85:GLY:N	2.53	0.42
8:I:93:TYR:HA	8:I:145:ARG:HB3	2.02	0.42
9:J:100:PHE:N	9:J:100:PHE:HD1	2.18	0.42
1:B:382:PRO:CB	1:B:428:TYR:CE2	2.96	0.41
1:B:526:ASP:HB2	2:C:835:GLN:CD	2.45	0.41
1:B:552:TRP:HE1	11:L:62:LYS:CB	2.33	0.41
1:B:709:THR:CG2	9:J:93:LYS:O	2.68	0.41
1:B:853:ASP:OD1	1:B:855:THR:HB	2.20	0.41
2:C:345:LYS:O	2:C:346:GLU:HB2	2.20	0.41
2:C:519:TRP:NE1	2:C:635:ARG:NH2	2.67	0.41
2:C:1135:ARG:NH2	2:C:1136:ASP:OD1	2.52	0.41
3:D:66:ARG:NH1	10:K:2:ILE:CG2	2.78	0.41
3:D:116:LYS:HG3	3:D:117:ASP:H	1.84	0.41
3:D:148:ARG:HD3	3:D:149:LYS:H	1.85	0.41
3:D:174:ALA:O	10:K:10:CYS:O	2.38	0.41
4:E:13:ARG:HG2	4:E:13:ARG:HH11	1.85	0.41
4:E:118:THR:HB	4:E:121:LYS:HB2	2.01	0.41
4:E:185:CYS:O	4:E:211:LEU:HD22	2.19	0.41
8:I:16:ASP:HA	8:I:17:PRO:HD3	1.91	0.41
8:I:97:MET:HE2	8:I:142:LEU:HD23	2.02	0.41
10:K:44:TYR:O	10:K:47:ARG:HB2	2.19	0.41
1:B:174:ILE:H	1:B:174:ILE:HG13	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:ASP:OD1	1:B:416:ARG:HG2	2.21	0.41
1:B:471:ASN:OD1	1:B:473:SER:N	2.54	0.41
1:B:860:LEU:HA	1:B:1422:ARG:NH1	2.34	0.41
1:B:1313:LEU:HD23	1:B:1338:VAL:CG2	2.50	0.41
1:B:1370:LEU:O	1:B:1374:VAL:HG23	2.20	0.41
1:B:1405:THR:HB	1:B:1406:VAL:H	1.54	0.41
1:B:1437:GLY:CA	6:G:88:TYR:CD2	3.03	0.41
2:C:763:GLN:O	2:C:764:SER:C	2.63	0.41
2:C:1132:GLU:O	2:C:1133:MET:C	2.63	0.41
3:D:104:PHE:HD2	3:D:105:GLY:N	2.17	0.41
4:E:137:ASN:ND2	4:E:137:ASN:N	2.67	0.41
4:E:220:LEU:HB3	4:E:221:TYR:H	1.57	0.41
5:F:167:ARG:HA	5:F:167:ARG:HD3	1.72	0.41
6:G:130:ILE:HB	6:G:148:VAL:HG21	2.01	0.41
7:H:81:PRO:C	7:H:82:PHE:CD1	2.98	0.41
8:I:91:ASP:O	8:I:93:TYR:N	2.49	0.41
1:B:345:VAL:HG23	1:B:346:ASP:O	2.20	0.41
1:B:405:VAL:HG23	1:B:415:LEU:HD11	2.03	0.41
1:B:836:TYR:HE1	15:T:17:DC:OP1	2.03	0.41
1:B:855:THR:HG23	1:B:857:ARG:HG3	2.01	0.41
1:B:1332:PHE:N	1:B:1332:PHE:HD2	2.17	0.41
2:C:24:PRO:O	2:C:655:LYS:HB2	2.21	0.41
2:C:210:LYS:HG3	2:C:461:LEU:O	2.20	0.41
2:C:562:GLY:C	2:C:590:HIS:HD1	2.26	0.41
2:C:593:PRO:HG2	2:C:617:ARG:CZ	2.51	0.41
2:C:992:ILE:CD1	11:L:66:PRO:HB2	2.49	0.41
3:D:247:GLY:O	3:D:248:ILE:C	2.62	0.41
4:E:180:LEU:CD2	4:E:195:ILE:HD12	2.48	0.41
7:H:7:LEU:HD12	7:H:74:TYR:CZ	2.55	0.41
7:H:15:PRO:HD3	7:H:67:SER:N	2.36	0.41
9:J:13:MET:HG3	9:J:14:LEU:N	2.35	0.41
9:J:84:VAL:O	9:J:84:VAL:HG13	2.20	0.41
11:L:49:GLU:OE2	11:L:97:LYS:HE3	2.20	0.41
12:M:55:ILE:HG12	12:M:55:ILE:H	1.60	0.41
1:B:168:GLY:O	1:B:169:ASN:C	2.63	0.41
1:B:344:ARG:HG2	1:B:344:ARG:NH1	2.35	0.41
1:B:384:ASN:HB2	1:B:388:LEU:HD12	2.02	0.41
1:B:613:ILE:HG22	1:B:614:PHE:HD2	1.85	0.41
1:B:710:LEU:H	1:B:710:LEU:CD1	2.33	0.41
1:B:758:ILE:H	1:B:758:ILE:HG13	1.73	0.41
1:B:1134:ILE:O	1:B:1137:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1148:ILE:HD11	1:B:1198:ASP:CA	2.43	0.41
1:B:1215:ARG:NH1	1:B:1215:ARG:HG2	2.35	0.41
1:B:1277:GLU:C	1:B:1279:ILE:H	2.27	0.41
1:B:1425:SER:O	1:B:1429:ILE:HG13	2.20	0.41
2:C:54:PHE:O	2:C:58:THR:HB	2.21	0.41
2:C:446:LEU:HD23	2:C:446:LEU:N	2.36	0.41
2:C:613:VAL:CG1	2:C:627:PHE:O	2.68	0.41
2:C:711:GLU:H	2:C:712:PRO:HD2	1.86	0.41
2:C:1066:SER:C	2:C:1067:ARG:HD3	2.46	0.41
3:D:190:ASP:O	3:D:191:TYR:C	2.64	0.41
4:E:7:THR:O	4:E:9:GLN:N	2.53	0.41
4:E:173:HIS:HA	4:E:174:PRO:HD2	1.64	0.41
5:F:76:GLY:HA3	5:F:106:GLN:HB3	2.02	0.41
5:F:142:VAL:HG12	5:F:143:ASN:N	2.36	0.41
6:G:89:GLU:HB3	6:G:134:ILE:HD11	2.00	0.41
11:L:15:GLY:O	11:L:16:GLU:HG3	2.20	0.41
11:L:35:PHE:HE1	11:L:73:LEU:HB3	1.85	0.41
1:B:61:ILE:CG2	1:B:62:ASP:H	2.23	0.41
1:B:83:HIS:CD2	1:B:83:HIS:C	2.99	0.41
1:B:382:PRO:HB3	1:B:428:TYR:OH	2.20	0.41
1:B:568:PRO:HB2	3:D:221:TYR:CE1	2.55	0.41
1:B:577:ILE:O	1:B:579:SER:N	2.53	0.41
1:B:867:ILE:O	1:B:868:TYR:C	2.63	0.41
1:B:925:LEU:C	1:B:927:VAL:H	2.28	0.41
1:B:947:PHE:C	1:B:949:ASP:N	2.78	0.41
1:B:1303:GLU:O	1:B:1303:GLU:HG3	2.19	0.41
1:B:1446:ASP:HB2	6:G:133:VAL:CG2	2.50	0.41
2:C:280:ILE:CG2	2:C:285:ILE:HG13	2.50	0.41
2:C:401:PHE:C	2:C:403:LYS:N	2.78	0.41
2:C:594:ALA:HA	2:C:617:ARG:NH1	2.36	0.41
2:C:661:LEU:HD11	2:C:684:LEU:HD11	2.03	0.41
2:C:780:VAL:HG21	10:K:56:LEU:CD1	2.46	0.41
2:C:781:PHE:HE1	2:C:788:ARG:HD3	1.84	0.41
2:C:873:THR:O	2:C:914:LYS:HA	2.20	0.41
5:F:16:PHE:O	5:F:19:VAL:HG23	2.21	0.41
5:F:49:SER:C	5:F:51:GLY:H	2.29	0.41
5:F:144:ILE:HD13	5:F:183:PRO:HB3	2.02	0.41
6:G:128:LYS:HD3	6:G:149:GLU:O	2.20	0.41
7:H:23:LYS:HE2	7:H:27:LYS:HE3	2.03	0.41
7:H:77:VAL:O	7:H:77:VAL:CG1	2.68	0.41
7:H:139:ILE:CG2	7:H:140:LYS:N	2.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:100:THR:CG2	8:I:101:ALA:N	2.84	0.41
12:M:38:LEU:CD1	12:M:49:LYS:HE2	2.51	0.41
1:B:49:LYS:HZ3	1:B:61:ILE:HG13	1.84	0.41
1:B:50:ILE:C	1:B:52:GLY:N	2.64	0.41
1:B:320:ARG:NH2	14:P:3:C:O2'	2.54	0.41
1:B:513:SER:C	1:B:515:GLN:H	2.28	0.41
1:B:779:PHE:HD2	1:B:779:PHE:HA	1.79	0.41
1:B:817:ALA:O	1:B:818:MET:C	2.64	0.41
1:B:932:GLU:O	1:B:935:GLN:N	2.52	0.41
1:B:944:ARG:NE	1:B:1298:TYR:HE1	2.18	0.41
1:B:1029:ARG:HD2	1:B:1033:GLN:HE22	1.81	0.41
1:B:1104:ILE:O	1:B:1106:ASN:N	2.53	0.41
1:B:1129:GLU:O	1:B:1130:GLN:C	2.64	0.41
1:B:1202:MET:HE1	1:B:1212:VAL:CG2	2.50	0.41
1:B:1213:GLY:C	1:B:1215:ARG:N	2.77	0.41
1:B:1268:LEU:O	1:B:1269:GLU:HG2	2.21	0.41
2:C:181:LEU:HD21	2:C:194:GLU:HG3	2.03	0.41
2:C:376:PHE:HB3	2:C:586:TRP:CZ3	2.55	0.41
2:C:486:TYR:CE1	2:C:1096:ARG:NH2	2.85	0.41
2:C:527:THR:OG1	2:C:528:PRO:HD2	2.19	0.41
2:C:593:PRO:O	2:C:594:ALA:C	2.63	0.41
3:D:22:LEU:HD13	3:D:230:MET:CE	2.50	0.41
4:E:32:GLU:HG3	7:H:5:LYS:HE2	2.03	0.41
5:F:173:SER:C	5:F:175:LEU:H	2.29	0.41
5:F:190:LEU:N	5:F:190:LEU:HD23	2.36	0.41
7:H:95:SER:C	7:H:97:HIS:N	2.78	0.41
9:J:59:VAL:O	9:J:62:ILE:HG22	2.20	0.41
1:B:63:ARG:HA	1:B:74:MET:CE	2.51	0.41
1:B:474:VAL:C	1:B:477:PRO:HD2	2.45	0.41
1:B:730:GLY:O	1:B:731:ARG:C	2.63	0.41
1:B:994:GLN:O	1:B:995:GLU:C	2.63	0.41
2:C:186:GLU:HB3	2:C:187:SER:H	1.67	0.41
2:C:202:TYR:CD1	2:C:202:TYR:C	2.99	0.41
2:C:282:ILE:HG21	2:C:382:ILE:CD1	2.51	0.41
2:C:512:ARG:HH11	2:C:512:ARG:HG2	1.86	0.41
2:C:526:GLU:CB	2:C:771:SER:HB3	2.51	0.41
2:C:797:TYR:CE1	2:C:854:LEU:HD23	2.56	0.41
2:C:911:ILE:O	2:C:912:ILE:HG13	2.20	0.41
3:D:11:ARG:HB3	3:D:12:GLU:H	1.67	0.41
3:D:113:VAL:O	3:D:143:LEU:HD12	2.20	0.41
3:D:205:LYS:C	3:D:207:CYS:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:241:ASP:O	3:D:244:VAL:HB	2.21	0.41
3:D:260:LEU:O	3:D:263:THR:HB	2.21	0.41
4:E:159:THR:C	4:E:161:GLY:N	2.79	0.41
4:E:191:ALA:C	4:E:193:THR:N	2.78	0.41
5:F:13:TRP:HB2	5:F:42:PHE:CE2	2.56	0.41
5:F:91:LYS:C	5:F:93:MET:H	2.28	0.41
6:G:123:LYS:O	6:G:124:GLU:C	2.64	0.41
14:P:7:A:N3	14:P:7:A:H2'	2.35	0.41
15:T:20:DT:H2''	15:T:21:DA:C5'	2.47	0.41
1:B:12:ARG:NE	2:C:1192:TYR:HE2	2.18	0.41
1:B:337:ARG:O	1:B:337:ARG:HG2	2.19	0.41
1:B:447:GLN:NE2	15:T:20:DT:H4'	2.29	0.41
1:B:498:ARG:O	1:B:501:LEU:N	2.54	0.41
1:B:600:PRO:HG2	1:B:601:LYS:N	2.31	0.41
1:B:652:VAL:O	1:B:653:VAL:C	2.64	0.41
1:B:1068:ALA:HB1	1:B:1367:HIS:HA	2.02	0.41
2:C:51:PHE:HZ	2:C:172:ILE:HA	1.86	0.41
2:C:95:ILE:CG1	2:C:130:VAL:HG22	2.50	0.41
2:C:244:LEU:C	2:C:246:LYS:N	2.78	0.41
2:C:308:TRP:HA	2:C:311:LEU:HD12	2.02	0.41
2:C:310:MET:O	2:C:311:LEU:C	2.62	0.41
2:C:324:ILE:HD13	2:C:330:ALA:HA	2.02	0.41
2:C:370:PHE:HD2	2:C:373:ARG:HD3	1.86	0.41
2:C:488:TYR:O	2:C:489:SER:C	2.64	0.41
2:C:519:TRP:CZ3	2:C:748:ILE:HD13	2.56	0.41
2:C:706:GLN:H	2:C:710:LEU:HD12	1.85	0.41
2:C:802:PRO:HG2	2:C:805:THR:CG2	2.51	0.41
2:C:890:TYR:CE2	2:C:910:VAL:HG21	2.56	0.41
2:C:1074:ASN:N	2:C:1081:LEU:CD2	2.84	0.41
3:D:258:ILE:N	3:D:258:ILE:CD1	2.84	0.41
3:D:264:GLN:H	3:D:264:GLN:HG3	1.51	0.41
4:E:67:ARG:O	4:E:67:ARG:HG2	2.21	0.41
4:E:156:ASP:HB3	4:E:158:GLU:H	1.86	0.41
4:E:214:LEU:O	4:E:218:GLU:HB2	2.21	0.41
8:I:61:SER:O	8:I:62:SER:HB2	2.21	0.41
8:I:101:ALA:HA	8:I:116:TYR:HA	2.03	0.41
9:J:36:GLU:O	9:J:37:GLU:O	2.38	0.41
10:K:8:PHE:H	10:K:49:MET:HE1	1.84	0.41
11:L:58:PHE:HB3	11:L:76:GLN:HE21	1.86	0.41
12:M:54:ARG:H	12:M:54:ARG:HG3	1.55	0.41
13:N:2:DA:H4'	13:N:2:DA:OP1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:PHE:HE2	1:B:30:ILE:HD12	1.84	0.41
1:B:72:GLU:OE2	2:C:1175:LEU:HD12	2.20	0.41
1:B:265:LYS:HG3	1:B:303:TYR:HB2	2.02	0.41
1:B:316:GLN:O	1:B:318:SER:N	2.54	0.41
1:B:332:LYS:NZ	15:T:19:DT:OP2	2.51	0.41
1:B:384:ASN:O	1:B:386:ASP:N	2.53	0.41
1:B:464:PRO:O	1:B:465:TYR:HB2	2.21	0.41
1:B:503:GLN:HE21	6:G:90:ARG:NH2	2.17	0.41
1:B:850:VAL:HG21	1:B:1058:VAL:HG11	2.03	0.41
1:B:974:ASP:C	1:B:976:THR:H	2.27	0.41
1:B:1068:ALA:HA	1:B:1367:HIS:ND1	2.36	0.41
1:B:1101:LEU:HD11	1:B:1105:LEU:CD1	2.49	0.41
1:B:1111:MET:O	1:B:1112:LYS:C	2.64	0.41
1:B:1114:PRO:CG	1:B:1115:SER:H	2.34	0.41
1:B:1151:GLU:HB3	1:B:1153:TYR:HE1	1.86	0.41
1:B:1373:ASP:O	1:B:1374:VAL:C	2.63	0.41
2:C:38:PHE:CD2	2:C:43:LEU:HD23	2.56	0.41
2:C:281:PRO:HB3	2:C:320:ASP:OD2	2.21	0.41
2:C:303:TYR:N	2:C:303:TYR:CD2	2.88	0.41
2:C:466:TRP:CE3	2:C:466:TRP:HA	2.55	0.41
2:C:469:GLN:HB2	2:C:470:LYS:H	1.60	0.41
2:C:516:ASN:C	2:C:518:HIS:H	2.29	0.41
2:C:523:CYS:SG	2:C:524:PRO:HD2	2.61	0.41
2:C:589:VAL:CG1	2:C:590:HIS:H	2.28	0.41
2:C:601:ARG:C	2:C:603:LEU:H	2.28	0.41
2:C:604:ARG:C	2:C:606:LYS:N	2.79	0.41
2:C:784:ASN:O	2:C:788:ARG:HG3	2.21	0.41
2:C:882:THR:HG21	2:C:935:ARG:HA	2.02	0.41
2:C:995:ARG:O	2:C:996:ARG:C	2.64	0.41
2:C:1069:PHE:HD1	2:C:1069:PHE:N	2.04	0.41
2:C:1104:HIS:CG	2:C:1122:ARG:HB2	2.56	0.41
3:D:98:VAL:O	3:D:99:LEU:HD23	2.20	0.41
4:E:137:ASN:HD22	4:E:137:ASN:N	2.19	0.41
4:E:189:ASP:O	4:E:190:GLU:C	2.61	0.41
4:E:203:SER:O	4:E:204:ASP:C	2.64	0.41
5:F:84:ASP:O	5:F:86:PRO:HD3	2.21	0.41
5:F:116:ILE:O	5:F:121:MET:HE2	2.20	0.41
5:F:205:SER:O	5:F:206:GLY:C	2.64	0.41
6:G:81:THR:HG23	6:G:144:GLU:OE2	2.21	0.41
6:G:86:THR:HG23	6:G:89:GLU:CD	2.46	0.41
6:G:138:LEU:C	6:G:140:ASP:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:140:ASP:OD1	6:G:140:ASP:C	2.63	0.41
6:G:143:PHE:C	6:G:143:PHE:HD1	2.29	0.41
7:H:13:LEU:HD22	7:H:14:HIS:O	2.20	0.41
7:H:59:GLY:CA	7:H:70:PHE:CD2	3.00	0.41
7:H:79:PHE:CE2	7:H:105:PRO:HD2	2.55	0.41
10:K:10:CYS:SG	10:K:11:GLY:N	2.94	0.41
10:K:44:TYR:CA	10:K:47:ARG:HB2	2.39	0.41
11:L:102:LYS:O	11:L:106:GLU:HG3	2.21	0.41
12:M:30:ILE:CG2	12:M:31:CYS:N	2.84	0.41
15:T:14:DC:H2"	15:T:15:DT:C7	2.46	0.41
1:B:196:GLU:CG	1:B:197:PRO:HD2	2.40	0.41
1:B:209:ASN:O	1:B:210:ILE:C	2.64	0.41
1:B:289:ILE:HG22	1:B:290:GLU:N	2.36	0.41
1:B:560:ILE:HG13	8:I:79:TRP:H	1.85	0.41
1:B:1147:THR:HB	9:J:48:LEU:HD12	2.03	0.41
1:B:1306:LEU:HD23	1:B:1306:LEU:HA	1.83	0.41
1:B:1367:HIS:O	1:B:1368:MET:C	2.64	0.41
1:B:1392:SER:O	1:B:1394:THR:N	2.53	0.41
1:B:1409:LEU:CD1	2:C:1207:LEU:HD11	2.50	0.41
2:C:273:LEU:HB2	2:C:276:ILE:CG1	2.51	0.41
2:C:815:ARG:O	10:K:54:VAL:HG21	2.20	0.41
2:C:899:ILE:CG1	2:C:911:ILE:HA	2.51	0.41
2:C:1081:LEU:O	2:C:1082:MET:C	2.64	0.41
3:D:52:GLU:HA	12:M:64:LEU:CD2	2.50	0.41
4:E:75:LYS:O	4:E:76:LYS:HB2	2.21	0.41
4:E:137:ASN:H	4:E:137:ASN:HD22	1.69	0.41
5:F:121:MET:C	5:F:123:LEU:H	2.29	0.41
6:G:88:TYR:O	6:G:89:GLU:C	2.65	0.41
10:K:41:LEU:HD11	10:K:50:ILE:HG13	2.03	0.41
10:K:47:ARG:NH1	10:K:47:ARG:HG2	2.36	0.41
12:M:70:ARG:HG2	12:M:70:ARG:NH1	2.36	0.41
1:B:304:MET:C	1:B:324:SER:HB2	2.46	0.40
1:B:506:ALA:O	1:B:509:LEU:HB2	2.21	0.40
1:B:719:VAL:O	1:B:721:PHE:N	2.54	0.40
1:B:767:GLN:NE2	1:B:798:GLY:O	2.54	0.40
1:B:808:LEU:HD23	1:B:813:PHE:CA	2.51	0.40
1:B:870:GLU:HG2	5:F:208:TYR:CD1	2.56	0.40
1:B:973:ILE:HD11	1:B:1038:THR:H	1.86	0.40
1:B:1127:ASP:O	1:B:1130:GLN:N	2.54	0.40
2:C:69:LEU:HD13	2:C:429:PHE:CD1	2.57	0.40
2:C:498:THR:HG22	2:C:537:LYS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:592:ASN:OD1	2:C:595:ARG:HG3	2.20	0.40
2:C:1096:ARG:CA	2:C:1098:MET:HE2	2.51	0.40
3:D:44:LEU:HD23	3:D:44:LEU:C	2.46	0.40
3:D:100:THR:HB	3:D:119:VAL:HB	2.03	0.40
4:E:63:LEU:O	4:E:129:LEU:HD11	2.21	0.40
5:F:91:LYS:C	5:F:93:MET:N	2.79	0.40
6:G:99:LEU:HG	6:G:103:MET:HE2	2.02	0.40
9:J:10:CYS:SG	9:J:31:THR:HB	2.62	0.40
9:J:35:VAL:CG1	9:J:36:GLU:N	2.83	0.40
10:K:13:VAL:C	10:K:14:VAL:CG2	2.94	0.40
11:L:44:ASN:N	11:L:61:TYR:CE1	2.89	0.40
11:L:58:PHE:CE2	11:L:74:ARG:NE	2.77	0.40
1:B:218:ASP:O	1:B:219:PHE:O	2.39	0.40
1:B:220:THR:O	1:B:221:SER:C	2.65	0.40
1:B:282:ASN:O	1:B:284:ALA:N	2.55	0.40
1:B:426:LEU:HD13	1:B:432:VAL:HG21	2.03	0.40
1:B:466:SER:CB	11:L:2:ASN:ND2	2.82	0.40
1:B:481:ASP:C	1:B:482:PHE:CD2	2.99	0.40
1:B:608:ILE:O	1:B:610:GLY:N	2.55	0.40
1:B:853:ASP:OD1	1:B:855:THR:CG2	2.70	0.40
1:B:956:LEU:HA	1:B:956:LEU:HD23	1.79	0.40
1:B:964:ILE:HG22	1:B:965:GLN:N	2.36	0.40
1:B:998:LEU:HD22	1:B:1001:ARG:HG3	2.04	0.40
1:B:1226:VAL:HG12	1:B:1227:ILE:N	2.36	0.40
1:B:1368:MET:HE3	1:B:1368:MET:HB2	1.90	0.40
1:B:1376:THR:CG2	1:B:1377:THR:N	2.84	0.40
1:B:1442:ASP:HB2	6:G:135:ARG:HB3	2.04	0.40
2:C:118:ARG:CG	2:C:204:ILE:HD13	2.49	0.40
2:C:165:VAL:HG11	2:C:448:ILE:CD1	2.50	0.40
2:C:244:LEU:C	2:C:246:LYS:H	2.29	0.40
2:C:515:HIS:CD2	2:C:516:ASN:N	2.90	0.40
2:C:578:THR:C	2:C:589:VAL:HG13	2.46	0.40
2:C:899:ILE:CG2	2:C:903:VAL:HG21	2.52	0.40
2:C:1223:ASP:O	2:C:1224:PHE:HB2	2.21	0.40
4:E:51:ASN:ND2	4:E:54:GLU:OE2	2.53	0.40
5:F:83:CYS:C	5:F:85:GLU:H	2.27	0.40
7:H:22:MET:C	7:H:24:GLN:N	2.77	0.40
9:J:98:VAL:HG12	9:J:111:THR:HG22	2.03	0.40
1:B:112:LYS:HG2	1:B:113:LEU:N	2.36	0.40
1:B:269:ILE:HG23	1:B:300:VAL:HG22	2.03	0.40
1:B:534:LEU:HD13	1:B:656:TRP:CG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:GLY:HA3	2:C:1081:LEU:HD12	2.03	0.40
1:B:685:GLU:HG3	1:B:686:ALA:N	2.35	0.40
1:B:698:GLN:CD	9:J:99:LEU:HD21	2.46	0.40
1:B:784:LEU:HB3	1:B:785:PRO:HD2	2.02	0.40
1:B:848:ILE:HB	1:B:1065:GLY:HA3	2.03	0.40
1:B:894:GLU:O	1:B:895:LYS:C	2.64	0.40
1:B:1341:ILE:O	1:B:1344:GLY:N	2.54	0.40
2:C:31:TRP:CE3	2:C:31:TRP:HA	2.55	0.40
2:C:899:ILE:HD11	2:C:910:VAL:O	2.21	0.40
2:C:975:GLN:HG2	2:C:976:ILE:H	1.86	0.40
2:C:1081:LEU:C	2:C:1083:ALA:N	2.79	0.40
3:D:66:ARG:NH2	10:K:5:VAL:HG23	2.36	0.40
3:D:91:HIS:CD2	3:D:91:HIS:C	2.98	0.40
4:E:151:PHE:CD1	4:E:151:PHE:N	2.89	0.40
4:E:191:ALA:O	4:E:193:THR:N	2.55	0.40
4:E:218:GLU:O	4:E:219:THR:C	2.65	0.40
6:G:103:MET:O	6:G:104:ASN:HB2	2.22	0.40
6:G:143:PHE:CD1	6:G:143:PHE:N	2.88	0.40
8:I:104:PHE:CZ	8:I:136:LYS:HG2	2.56	0.40
14:P:5:C:H2'	14:P:6:A:H8	1.85	0.40
1:B:341:MET:HE3	1:B:341:MET:HB3	1.91	0.40
1:B:523:ILE:CD1	1:B:649:ILE:HG21	2.51	0.40
1:B:1230:GLU:C	1:B:1232:ASN:H	2.29	0.40
1:B:1441:PHE:CD1	1:B:1441:PHE:C	2.99	0.40
2:C:308:TRP:O	2:C:312:GLU:N	2.46	0.40
2:C:313:MET:HE2	2:C:390:LEU:HD21	2.03	0.40
2:C:460:ALA:O	2:C:462:ALA:N	2.47	0.40
2:C:540:SER:HB3	2:C:747:MET:O	2.21	0.40
2:C:611:PRO:HB3	2:C:685:LEU:HD11	2.03	0.40
2:C:789:MET:HE2	2:C:953:LEU:HD22	2.02	0.40
2:C:830:TYR:O	2:C:831:SER:C	2.62	0.40
2:C:849:GLY:O	2:C:850:LEU:C	2.63	0.40
2:C:999:MET:HG2	2:C:1007:VAL:CG2	2.52	0.40
2:C:1029:CYS:O	2:C:1030:LEU:C	2.64	0.40
2:C:1115:THR:HG22	2:C:1117:GLN:CG	2.51	0.40
2:C:1221:SER:O	2:C:1223:ASP:N	2.55	0.40
3:D:131:HIS:HA	3:D:132:PRO:HD3	1.78	0.40
4:E:40:HIS:CE1	4:E:41:GLN:CG	3.04	0.40
4:E:141:LEU:HD12	4:E:145:MET:HG2	2.03	0.40
5:F:11:ARG:O	5:F:13:TRP:N	2.54	0.40
5:F:147:HIS:CD2	5:F:149:LEU:HB2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:82:THR:HA	6:G:83:PRO:HD3	1.79	0.40
11:L:76:GLN:HG2	11:L:77:THR:N	2.35	0.40
1:B:350:ARG:C	1:B:351:THR:HG23	2.47	0.40
1:B:666:ILE:HG12	2:C:1030:LEU:HD22	2.04	0.40
1:B:735:VAL:HG12	1:B:735:VAL:O	2.21	0.40
1:B:754:SER:N	1:B:757:ASN:HD22	2.00	0.40
1:B:767:GLN:HE21	1:B:774:ARG:HB3	1.79	0.40
1:B:1010:ALA:O	1:B:1013:ASP:HB2	2.20	0.40
1:B:1140:HIS:CE1	1:B:1272:THR:HG23	2.56	0.40
1:B:1376:THR:O	1:B:1377:THR:C	2.64	0.40
2:C:193:LYS:HD3	2:C:787:VAL:HG11	2.03	0.40
2:C:237:VAL:HG12	2:C:238:ALA:N	2.36	0.40
2:C:293:PRO:HG2	2:C:296:GLU:CB	2.51	0.40
2:C:416:LEU:HD11	2:C:466:TRP:CZ2	2.57	0.40
2:C:865:LYS:C	2:C:866:TYR:HD1	2.29	0.40
2:C:882:THR:HG22	2:C:884:ARG:CB	2.50	0.40
3:D:160:LYS:C	3:D:161:LYS:O	2.64	0.40
4:E:12:ARG:NH1	4:E:14:ARG:HG3	2.36	0.40
6:G:89:GLU:HB3	6:G:134:ILE:HD13	2.03	0.40
7:H:88:ASP:CB	7:H:144:ARG:HA	2.44	0.40
8:I:24:CYS:CB	8:I:44:VAL:HG21	2.48	0.40
10:K:16:ASP:C	10:K:18:TRP:N	2.79	0.40
11:L:65:HIS:HD2	11:L:65:HIS:C	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1406/1733 (81%)	965 (69%)	284 (20%)	157 (11%)	0	6
2	C	1090/1224 (89%)	719 (66%)	243 (22%)	128 (12%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	264/318 (83%)	163 (62%)	70 (26%)	31 (12%)	0	5
4	E	173/221 (78%)	107 (62%)	43 (25%)	23 (13%)	0	3
5	F	212/215 (99%)	154 (73%)	36 (17%)	22 (10%)	0	7
6	G	82/155 (53%)	62 (76%)	13 (16%)	7 (8%)	0	11
7	H	169/171 (99%)	129 (76%)	26 (15%)	14 (8%)	0	11
8	I	129/146 (88%)	79 (61%)	30 (23%)	20 (16%)	0	3
9	J	117/122 (96%)	80 (68%)	24 (20%)	13 (11%)	0	6
10	K	63/70 (90%)	38 (60%)	12 (19%)	13 (21%)	0	1
11	L	112/120 (93%)	81 (72%)	24 (21%)	7 (6%)	1	15
12	M	44/70 (63%)	22 (50%)	8 (18%)	14 (32%)	0	0
All	All	3861/4565 (85%)	2599 (67%)	813 (21%)	449 (12%)	0	5

All (449) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	GLN
1	B	41	MET
1	B	48	ALA
1	B	54	ASN
1	B	57	ARG
1	B	62	ASP
1	B	67	CYS
1	B	93	VAL
1	B	130	ASP
1	B	149	GLU
1	B	154	SER
1	B	223	GLY
1	B	245	PRO
1	B	250	ILE
1	B	286	HIS
1	B	311	GLN
1	B	312	PRO
1	B	318	SER
1	B	322	VAL
1	B	331	GLY
1	B	332	LYS
1	B	335	ARG
1	B	336	ILE

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Mol	Chain	Res	Type
1	B	409	SER
1	B	419	LYS
1	B	536	LEU
1	B	543	LEU
1	B	567	LYS
1	B	752	LYS
1	B	755	PHE
1	B	765	VAL
1	B	780	VAL
1	B	789	LYS
1	B	980	ASP
1	B	986	ILE
1	B	995	GLU
1	B	1002	GLY
1	B	1016	THR
1	B	1114	PRO
1	B	1115	SER
1	B	1120	LEU
1	B	1124	HIS
1	B	1212	VAL
1	B	1223	ASP
1	B	1231	ASP
1	B	1242	VAL
1	B	1255	GLU
1	B	1261	LYS
1	B	1341	ILE
1	B	1365	TYR
1	B	1377	THR
1	B	1378	GLN
1	B	1393	ASN
2	C	21	GLU
2	C	45	SER
2	C	46	GLN
2	C	108	VAL
2	C	186	GLU
2	C	367	LEU
2	C	401	PHE
2	C	448	ILE
2	C	470	LYS
2	C	472	ALA
2	C	509	ALA
2	C	510	LYS

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Mol	Chain	Res	Type
2	C	591	ARG
2	C	708	GLU
2	C	709	ASP
2	C	731	VAL
2	C	751	VAL
2	C	826	ALA
2	C	907	GLY
2	C	909	ASP
2	C	943	SER
2	C	1003	ALA
2	C	1006	ILE
2	C	1011	ILE
2	C	1045	SER
2	C	1046	PRO
2	C	1156	ASP
2	C	1171	VAL
2	C	1175	LEU
2	C	1181	GLU
2	C	1182	CYS
2	C	1183	LYS
3	D	81	GLU
3	D	117	ASP
3	D	149	LYS
3	D	156	THR
3	D	175	ALA
3	D	184	ASN
3	D	209	TYR
4	E	9	GLN
4	E	19	GLU
4	E	21	GLU
4	E	31	GLN
4	E	169	SER
4	E	173	HIS
4	E	174	PRO
4	E	199	ASN
4	E	218	GLU
4	E	220	LEU
5	F	43	LYS
5	F	44	ALA
5	F	48	ASP
5	F	59	SER
5	F	73	PRO

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Mol	Chain	Res	Type
5	F	129	PRO
5	F	192	ARG
5	F	206	GLY
6	G	73	ALA
7	H	66	GLY
7	H	154	VAL
8	I	17	PRO
8	I	77	ARG
8	I	78	SER
8	I	81	PRO
8	I	84	ALA
8	I	108	SER
8	I	128	ASN
8	I	140	ALA
9	J	11	ASN
9	J	37	GLU
9	J	106	CYS
10	K	6	ARG
10	K	32	GLU
10	K	64	ASN
11	L	29	ASN
12	M	35	SER
12	M	37	LYS
12	M	50	ASP
12	M	53	HIS
12	M	55	ILE
12	M	59	ALA
12	M	60	ARG
1	B	42	ASP
1	B	44	THR
1	B	51	GLY
1	B	58	LEU
1	B	66	LYS
1	B	70	CYS
1	B	73	GLY
1	B	76	GLU
1	B	167	CYS
1	B	257	ARG
1	B	283	GLY
1	B	303	TYR
1	B	317	LYS
1	B	410	GLY

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Mol	Chain	Res	Type
1	B	415	LEU
1	B	666	ILE
1	B	718	VAL
1	B	719	VAL
1	B	829	VAL
1	B	846	GLU
1	B	847	ASP
1	B	871	ASP
1	B	968	GLN
1	B	979	SER
1	B	1050	GLU
1	B	1064	VAL
1	B	1116	LEU
1	B	1221	LYS
1	B	1314	SER
1	B	1335	ILE
1	B	1366	ARG
1	B	1405	THR
1	B	1438	THR
2	C	184	ALA
2	C	206	ASN
2	C	229	ALA
2	C	260	GLY
2	C	304	ASP
2	C	305	VAL
2	C	365	THR
2	C	368	GLU
2	C	369	GLY
2	C	389	ALA
2	C	450	ALA
2	C	460	ALA
2	C	466	TRP
2	C	467	GLY
2	C	471	LYS
2	C	480	SER
2	C	511	PRO
2	C	543	SER
2	C	643	ASP
2	C	655	LYS
2	C	688	GLY
2	C	728	ARG
2	C	734	HIS

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Mol	Chain	Res	Type
2	C	746	SER
2	C	825	VAL
2	C	827	ILE
2	C	883	LEU
2	C	1041	GLU
2	C	1082	MET
2	C	1096	ARG
2	C	1108	ARG
2	C	1112	GLN
2	C	1126	GLY
2	C	1155	SER
2	C	1167	GLY
2	C	1186	ASP
2	C	1188	LYS
3	D	94	LYS
3	D	110	THR
3	D	133	ILE
3	D	161	LYS
3	D	214	ASN
4	E	20	GLU
4	E	52	LEU
5	F	74	ASP
5	F	76	GLY
5	F	106	GLN
5	F	121	MET
5	F	174	GLN
7	H	17	PHE
7	H	64	THR
7	H	118	ASP
7	H	140	LYS
8	I	12	VAL
8	I	60	ALA
8	I	82	PRO
8	I	90	ALA
8	I	134	ASN
8	I	139	ASN
9	J	3	THR
9	J	8	ARG
9	J	33	SER
9	J	47	GLU
9	J	58	VAL
9	J	79	HIS

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Mol	Chain	Res	Type
10	K	2	ILE
10	K	17	LYS
10	K	24	LEU
10	K	27	GLU
10	K	28	ASP
10	K	29	GLU
10	K	39	LEU
11	L	7	PHE
11	L	14	GLU
11	L	15	GLY
1	B	3	GLY
1	B	43	GLU
1	B	59	GLY
1	B	69	THR
1	B	131	SER
1	B	219	PHE
1	B	232	GLU
1	B	244	PRO
1	B	253	ASN
1	B	361	LEU
1	B	399	HIS
1	B	526	ASP
1	B	591	PHE
1	B	639	PRO
1	B	706	HIS
1	B	720	ARG
1	B	922	ASP
1	B	997	LEU
1	B	1139	GLU
1	B	1402	PHE
1	B	1448	GLU
2	C	219	ALA
2	C	266	ALA
2	C	295	GLY
2	C	427	ASP
2	C	430	ARG
2	C	613	VAL
2	C	711	GLU
2	C	712	PRO
2	C	792	MET
2	C	836	GLU
2	C	848	ARG

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Mol	Chain	Res	Type
2	C	881	ASN
2	C	888	GLY
2	C	894	ASP
2	C	1018	PRO
2	C	1035	ALA
2	C	1074	ASN
2	C	1075	GLY
2	C	1100	ASP
2	C	1157	ALA
2	C	1176	ASN
3	D	60	ASP
3	D	95	CYS
3	D	138	GLU
3	D	148	ARG
3	D	240	VAL
4	E	8	PHE
4	E	131	GLU
4	E	139	LYS
4	E	198	LEU
5	F	3	GLN
5	F	50	MET
5	F	130	ALA
5	F	205	SER
7	H	20	PRO
7	H	67	SER
7	H	96	GLN
8	I	120	GLY
9	J	34	TYR
9	J	78	CYS
12	M	54	ARG
1	B	128	ILE
1	B	220	THR
1	B	424	ILE
1	B	428	TYR
1	B	465	TYR
1	B	510	GLN
1	B	587	HIS
1	B	636	GLU
1	B	825	ILE
1	B	958	VAL
1	B	1013	ASP
1	B	1051	ALA

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Mol	Chain	Res	Type
1	B	1054	LEU
1	B	1105	LEU
1	B	1109	LYS
1	B	1229	SER
1	B	1330	ASN
1	B	1390	ASN
2	C	56	ASP
2	C	94	LYS
2	C	115	GLN
2	C	198	ASP
2	C	282	ILE
2	C	394	ASP
2	C	402	GLY
2	C	436	VAL
2	C	461	LEU
2	C	465	ASN
2	C	605	ARG
2	C	879	ARG
2	C	978	ASP
2	C	1143	ALA
3	D	87	PHE
3	D	90	ASP
3	D	206	ASN
3	D	213	PRO
4	E	25	ALA
4	E	192	LYS
4	E	217	LEU
5	F	115	ASN
5	F	120	ALA
5	F	122	LYS
6	G	112	GLU
6	G	150	GLU
7	H	16	SER
7	H	50	ASP
7	H	139	ILE
8	I	52	GLN
9	J	9	ASP
12	M	26	THR
12	M	39	SER
12	M	45	ALA
12	M	56	LEU
1	B	61	ILE

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Mol	Chain	Res	Type
1	B	71	GLN
1	B	196	GLU
1	B	382	PRO
1	B	497	THR
1	B	661	GLY
1	B	775	ILE
1	B	821	ARG
1	B	972	HIS
1	B	1067	LEU
1	B	1324	PRO
1	B	1379	GLY
1	B	1394	THR
2	C	261	ARG
2	C	283	VAL
2	C	577	ALA
2	C	684	LEU
2	C	764	SER
2	C	800	GLN
2	C	832	GLY
2	C	946	ASN
2	C	982	SER
2	C	1097	HIS
3	D	9	LYS
3	D	132	PRO
3	D	173	ALA
3	D	208	GLU
4	E	32	GLU
4	E	155	ARG
4	E	168	LYS
5	F	40	GLU
6	G	111	LEU
6	G	139	PRO
7	H	128	PRO
8	I	32	THR
8	I	62	SER
8	I	92	ASP
8	I	119	GLY
9	J	57	GLY
10	K	33	GLY
11	L	41	THR
12	M	40	LEU
1	B	321	PRO

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Mol	Chain	Res	Type
1	B	400	PRO
1	B	759	ALA
1	B	975	HIS
1	B	1128	GLN
2	C	259	TYR
2	C	325	GLN
2	C	763	GLN
2	C	1131	GLY
2	C	1165	ILE
2	C	1170	THR
3	D	142	VAL
3	D	217	ASP
5	F	104	ASN
10	K	14	VAL
10	K	57	ILE
11	L	53	ASP
1	B	492	PRO
1	B	546	VAL
1	B	673	GLY
1	B	916	GLY
2	C	524	PRO
2	C	1017	ILE
3	D	139	GLY
3	D	243	VAL
6	G	74	ILE
6	G	117	PRO
7	H	34	VAL
11	L	66	PRO
1	B	35	ILE
1	B	78	PRO
1	B	138	ILE
1	B	380	VAL
1	B	1006	ILE
2	C	562	GLY
3	D	255	VAL
4	E	202	ILE
12	M	46	VAL
1	B	38	PRO
1	B	396	PRO
1	B	948	VAL
2	C	911	ILE
2	C	1214	PRO

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Mol	Chain	Res	Type
3	D	70	ILE
1	B	1435	PRO
2	C	571	PRO
2	C	636	PRO
2	C	867	GLY
1	B	1107	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1239/1520 (82%)	1117 (90%)	122 (10%)	7	27
2	C	962/1061 (91%)	860 (89%)	102 (11%)	6	24
3	D	234/274 (85%)	212 (91%)	22 (9%)	8	29
4	E	159/200 (80%)	132 (83%)	27 (17%)	2	13
5	F	196/197 (100%)	181 (92%)	15 (8%)	12	35
6	G	74/137 (54%)	67 (90%)	7 (10%)	8	28
7	H	152/152 (100%)	134 (88%)	18 (12%)	5	21
8	I	117/128 (91%)	106 (91%)	11 (9%)	8	29
9	J	113/116 (97%)	103 (91%)	10 (9%)	9	32
10	K	60/65 (92%)	53 (88%)	7 (12%)	5	21
11	L	99/102 (97%)	86 (87%)	13 (13%)	4	19
12	M	40/57 (70%)	36 (90%)	4 (10%)	7	26
All	All	3445/4009 (86%)	3087 (90%)	358 (10%)	7	25

All (358) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	18	GLN
1	B	32	VAL
1	B	34	LYS
1	B	37	PHE

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Mol	Chain	Res	Type
1	B	41	MET
1	B	43	GLU
1	B	57	ARG
1	B	62	ASP
1	B	67	CYS
1	B	68	GLN
1	B	93	VAL
1	B	108	MET
1	B	174	ILE
1	B	200	ARG
1	B	205	GLU
1	B	221	SER
1	B	245	PRO
1	B	261	ASP
1	B	265	LYS
1	B	270	LEU
1	B	276	LEU
1	B	289	ILE
1	B	312	PRO
1	B	320	ARG
1	B	322	VAL
1	B	326	ARG
1	B	335	ARG
1	B	345	VAL
1	B	360	GLU
1	B	375	THR
1	B	379	VAL
1	B	381	THR
1	B	385	ILE
1	B	394	ASN
1	B	396	PRO
1	B	406	ILE
1	B	408	ASP
1	B	417	TYR
1	B	434	ARG
1	B	436	ILE
1	B	442	VAL
1	B	443	LEU
1	B	445	ASN
1	B	450	LEU
1	B	451	HIS
1	B	461	LYS

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Mol	Chain	Res	Type
1	B	462	VAL
1	B	466	SER
1	B	493	GLN
1	B	503	GLN
1	B	504	LEU
1	B	512	VAL
1	B	518	LYS
1	B	560	ILE
1	B	562	THR
1	B	590	ARG
1	B	616	VAL
1	B	618	GLU
1	B	629	LEU
1	B	635	ARG
1	B	642	CYS
1	B	657	LEU
1	B	664	THR
1	B	666	ILE
1	B	690	VAL
1	B	741	ASN
1	B	768	GLN
1	B	774	ARG
1	B	779	PHE
1	B	821	ARG
1	B	827	THR
1	B	837	ILE
1	B	858	ASN
1	B	904	THR
1	B	907	THR
1	B	941	LYS
1	B	947	PHE
1	B	964	ILE
1	B	998	LEU
1	B	1035	TYR
1	B	1037	LEU
1	B	1067	LEU
1	B	1095	THR
1	B	1116	LEU
1	B	1120	LEU
1	B	1122	PRO
1	B	1138	ILE
1	B	1146	VAL

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Mol	Chain	Res	Type
1	B	1147	THR
1	B	1152	ILE
1	B	1163	ILE
1	B	1170	ILE
1	B	1173	HIS
1	B	1222	ASN
1	B	1240	CYS
1	B	1264	GLU
1	B	1271	ILE
1	B	1291	VAL
1	B	1295	THR
1	B	1297	GLU
1	B	1299	VAL
1	B	1332	PHE
1	B	1333	ILE
1	B	1337	GLU
1	B	1351	GLU
1	B	1359	ASP
1	B	1363	VAL
1	B	1371	LEU
1	B	1372	VAL
1	B	1381	LEU
1	B	1385	THR
1	B	1386	ARG
1	B	1391	ARG
1	B	1393	ASN
1	B	1400	CYS
1	B	1405	THR
1	B	1425	SER
1	B	1428	VAL
1	B	1432	GLN
1	B	1442	ASP
1	B	1444	MET
1	B	1445	ILE
2	C	20	ASP
2	C	25	ILE
2	C	44	VAL
2	C	57	TYR
2	C	63	ILE
2	C	98	THR
2	C	104	GLU
2	C	175	ARG

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Mol	Chain	Res	Type
2	C	180	TYR
2	C	203	PHE
2	C	205	ILE
2	C	250	PHE
2	C	258	LEU
2	C	276	ILE
2	C	283	VAL
2	C	286	PHE
2	C	289	LEU
2	C	298	LEU
2	C	323	VAL
2	C	365	THR
2	C	371	GLU
2	C	378	LEU
2	C	385	LEU
2	C	387	LEU
2	C	393	LYS
2	C	396	ASP
2	C	427	ASP
2	C	429	PHE
2	C	466	TRP
2	C	482	VAL
2	C	485	ARG
2	C	498	THR
2	C	502	ILE
2	C	511	PRO
2	C	513	GLN
2	C	516	ASN
2	C	539	LEU
2	C	544	CYS
2	C	582	VAL
2	C	602	THR
2	C	603	LEU
2	C	615	MET
2	C	616	ILE
2	C	619	ILE
2	C	629	ASP
2	C	635	ARG
2	C	644	GLU
2	C	683	SER
2	C	723	VAL
2	C	737	THR

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Mol	Chain	Res	Type
2	C	742	GLU
2	C	743	ILE
2	C	748	ILE
2	C	751	VAL
2	C	755	ILE
2	C	787	VAL
2	C	790	ASP
2	C	811	TYR
2	C	835	GLN
2	C	837	ASP
2	C	839	MET
2	C	862	GLN
2	C	865	LYS
2	C	866	TYR
2	C	878	GLN
2	C	883	LEU
2	C	901	PRO
2	C	909	ASP
2	C	944	THR
2	C	953	LEU
2	C	999	MET
2	C	1002	THR
2	C	1006	ILE
2	C	1010	LEU
2	C	1012	ILE
2	C	1045	SER
2	C	1046	PRO
2	C	1047	PHE
2	C	1060	ARG
2	C	1069	PHE
2	C	1077	THR
2	C	1084	GLN
2	C	1085	ILE
2	C	1092	TYR
2	C	1095	LEU
2	C	1098	MET
2	C	1103	ILE
2	C	1108	ARG
2	C	1122	ARG
2	C	1151	LEU
2	C	1159	ARG
2	C	1162	ILE

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Mol	Chain	Res	Type
2	C	1170	THR
2	C	1172	ILE
2	C	1175	LEU
2	C	1182	CYS
2	C	1183	LYS
2	C	1185	CYS
2	C	1192	TYR
2	C	1202	LEU
2	C	1212	ILE
2	C	1222	ARG
3	D	3	GLU
3	D	8	VAL
3	D	58	LEU
3	D	74	SER
3	D	77	ILE
3	D	83	SER
3	D	129	ILE
3	D	138	GLU
3	D	144	ILE
3	D	147	LEU
3	D	163	ILE
3	D	166	GLU
3	D	190	ASP
3	D	193	TYR
3	D	209	TYR
3	D	212	PRO
3	D	226	ASP
3	D	228	PHE
3	D	235	VAL
3	D	238	ILE
3	D	240	VAL
3	D	266	ASP
4	E	5	THR
4	E	8	PHE
4	E	9	GLN
4	E	11	ARG
4	E	14	ARG
4	E	16	LYS
4	E	20	GLU
4	E	22	GLU
4	E	29	LEU
4	E	40	HIS

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Mol	Chain	Res	Type
4	E	47	LEU
4	E	50	LEU
4	E	63	LEU
4	E	70	PHE
4	E	126	ILE
4	E	137	ASN
4	E	139	LYS
4	E	141	LEU
4	E	148	LEU
4	E	170	THR
4	E	174	PRO
4	E	182	SER
4	E	202	ILE
4	E	204	ASP
4	E	211	LEU
4	E	214	LEU
4	E	221	TYR
5	F	46	TYR
5	F	60	PHE
5	F	74	ASP
5	F	77	SER
5	F	78	LEU
5	F	92	THR
5	F	93	MET
5	F	94	LYS
5	F	104	ASN
5	F	132	ILE
5	F	169	ARG
5	F	190	LEU
5	F	198	ILE
5	F	207	ARG
5	F	213	ILE
6	G	74	ILE
6	G	90	ARG
6	G	107	VAL
6	G	111	LEU
6	G	118	LEU
6	G	123	LYS
6	G	143	PHE
7	H	1	MET
7	H	7	LEU
7	H	9	LEU

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Mol	Chain	Res	Type
7	H	11	ILE
7	H	13	LEU
7	H	45	ILE
7	H	49	LEU
7	H	56	ILE
7	H	74	TYR
7	H	77	VAL
7	H	79	PHE
7	H	87	VAL
7	H	88	ASP
7	H	114	LEU
7	H	140	LYS
7	H	152	SER
7	H	165	GLU
7	H	171	ILE
8	I	7	ASP
8	I	10	PHE
8	I	17	PRO
8	I	26	ILE
8	I	57	VAL
8	I	93	TYR
8	I	96	VAL
8	I	102	TYR
8	I	106	GLU
8	I	110	ASP
8	I	130	ARG
9	J	8	ARG
9	J	15	TYR
9	J	31	THR
9	J	51	ASN
9	J	52	ILE
9	J	59	VAL
9	J	85	PHE
9	J	86	PHE
9	J	99	LEU
9	J	100	PHE
10	K	3	VAL
10	K	13	VAL
10	K	16	ASP
10	K	19	GLU
10	K	24	LEU
10	K	43	ARG

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Mol	Chain	Res	Type
10	K	44	TYR
11	L	10	PHE
11	L	12	LEU
11	L	47	ARG
11	L	50	LEU
11	L	61	TYR
11	L	65	HIS
11	L	68	PHE
11	L	78	THR
11	L	89	ASN
11	L	102	LYS
11	L	111	LEU
11	L	113	THR
11	L	114	LEU
12	M	35	SER
12	M	44	ASP
12	M	54	ARG
12	M	55	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	54	ASN
1	B	68	GLN
1	B	71	GLN
1	B	160	GLN
1	B	169	ASN
1	B	171	GLN
1	B	213	HIS
1	B	225	ASN
1	B	256	GLN
1	B	297	GLN
1	B	339	ASN
1	B	358	ASN
1	B	390	GLN
1	B	394	ASN
1	B	435	HIS
1	B	493	GLN
1	B	603	ASN
1	B	654	ASN
1	B	698	GLN
1	B	706	HIS

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Mol	Chain	Res	Type
1	B	723	ASN
1	B	741	ASN
1	B	757	ASN
1	B	760	GLN
1	B	768	GLN
1	B	786	HIS
1	B	858	ASN
1	B	881	GLN
1	B	903	ASN
1	B	926	GLN
1	B	1033	GLN
1	B	1106	ASN
1	B	1124	HIS
1	B	1130	GLN
1	B	1140	HIS
1	B	1173	HIS
1	B	1203	ASN
1	B	1232	ASN
1	B	1258	HIS
1	B	1270	ASN
1	B	1354	ASN
1	B	1393	ASN
2	C	53	GLN
2	C	60	GLN
2	C	110	HIS
2	C	115	GLN
2	C	121	ASN
2	C	178	ASN
2	C	236	HIS
2	C	363	HIS
2	C	366	GLN
2	C	383	ASN
2	C	433	GLN
2	C	465	ASN
2	C	515	HIS
2	C	516	ASN
2	C	518	HIS
2	C	538	ASN
2	C	573	GLN
2	C	734	HIS
2	C	744	HIS
2	C	763	GLN

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Mol	Chain	Res	Type
2	C	770	GLN
2	C	821	GLN
2	C	842	ASN
2	C	862	GLN
2	C	957	ASN
2	C	958	GLN
2	C	975	GLN
2	C	1015	HIS
2	C	1062	HIS
2	C	1065	GLN
2	C	1074	ASN
2	C	1084	GLN
2	C	1093	GLN
2	C	1117	GLN
2	C	1141	HIS
2	C	1161	HIS
2	C	1176	ASN
2	C	1179	GLN
3	D	7	GLN
3	D	65	HIS
3	D	73	GLN
3	D	102	GLN
3	D	112	ASN
3	D	167	HIS
4	E	9	GLN
4	E	39	ASN
4	E	74	GLN
4	E	132	GLN
4	E	137	ASN
4	E	143	ASN
4	E	173	HIS
4	E	179	GLN
4	E	216	ASN
5	F	101	GLN
5	F	104	ASN
5	F	106	GLN
5	F	115	ASN
5	F	147	HIS
6	G	104	ASN
7	H	14	HIS
7	H	53	ASN
7	H	97	HIS

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Mol	Chain	Res	Type
7	H	122	ASN
7	H	126	ASN
7	H	158	HIS
8	I	83	GLN
8	I	137	GLN
9	J	12	ASN
9	J	90	GLN
9	J	108	HIS
9	J	114	GLN
11	L	44	ASN
11	L	65	HIS
11	L	76	GLN
11	L	110	ASN
12	M	53	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	7/16 (43%)	1 (14%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	7	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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, 95th 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 ²)	Q < 0.9
1	B	1416/1733 (81%)	-0.10	17 (1%) 76 59	76, 129, 175, 200	0
2	C	1108/1224 (90%)	0.07	18 (1%) 70 52	79, 140, 185, 200	0
3	D	266/318 (83%)	-0.11	0 100 100	93, 126, 168, 188	0
4	E	177/221 (80%)	0.05	3 (1%) 69 51	106, 142, 182, 190	0
5	F	214/215 (99%)	0.02	1 (0%) 87 73	99, 160, 187, 200	0
6	G	84/155 (54%)	-0.23	1 (1%) 76 59	73, 107, 138, 147	0
7	H	171/171 (100%)	0.03	1 (0%) 85 71	98, 127, 164, 174	0
8	I	133/146 (91%)	0.35	5 (3%) 44 34	134, 165, 186, 196	0
9	J	119/122 (97%)	0.18	1 (0%) 82 65	122, 165, 189, 200	0
10	K	65/70 (92%)	-0.14	1 (1%) 72 54	92, 121, 158, 169	0
11	L	114/120 (95%)	-0.11	1 (0%) 81 64	94, 128, 156, 170	0
12	M	46/70 (65%)	0.36	2 (4%) 40 31	120, 172, 195, 198	0
13	N	7/14 (50%)	0.98	0 100 100	84, 199, 200, 200	1 (14%)
14	P	8/16 (50%)	0.29	0 100 100	198, 199, 200, 200	0
15	T	18/26 (69%)	0.87	0 100 100	116, 198, 200, 200	1 (5%)
All	All	3946/4621 (85%)	-0.00	51 (1%) 75 57	73, 136, 184, 200	2 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1081	LEU	4.8
2	C	335	GLY	4.5
2	C	882	THR	3.5
10	K	65	PRO	3.4
8	I	63	LEU	3.3
4	E	25	ALA	3.0
1	B	251	SER	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	879	ARG	2.9
5	F	32	GLN	2.8
9	J	2	THR	2.8
2	C	963	PHE	2.8
1	B	2	VAL	2.8
1	B	292	ALA	2.7
2	C	508	LEU	2.7
8	I	140	ALA	2.7
2	C	507	LYS	2.7
4	E	10	THR	2.7
1	B	69	THR	2.6
1	B	142	CYS	2.6
1	B	310	GLY	2.5
1	B	1257	ASP	2.5
1	B	34	LYS	2.5
1	B	1176	LEU	2.5
8	I	13	SER	2.5
1	B	3	GLY	2.4
2	C	883	LEU	2.4
4	E	8	PHE	2.4
1	B	481	ASP	2.4
6	G	72	LYS	2.4
12	M	27	LEU	2.3
1	B	250	ILE	2.3
2	C	870	ILE	2.3
2	C	510	LYS	2.2
2	C	1096	ARG	2.2
2	C	70	ILE	2.2
2	C	250	PHE	2.2
2	C	471	LYS	2.2
2	C	436	VAL	2.2
2	C	486	TYR	2.1
8	I	76	THR	2.1
2	C	246	LYS	2.1
2	C	831	SER	2.1
1	B	480	ALA	2.1
7	H	96	GLN	2.1
1	B	105	CYS	2.1
11	L	114	LEU	2.1
8	I	119	GLY	2.1
12	M	25	ALA	2.0
1	B	483	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	995	GLU	2.0
2	C	245	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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	B	1736	1/1	0.83	0.12	153,153,153,153	0
16	ZN	J	124	1/1	0.97	0.06	200,200,200,200	0
16	ZN	M	71	1/1	0.99	0.04	174,174,174,174	0
16	ZN	D	319	1/1	1.00	0.06	98,98,98,98	0
16	ZN	J	123	1/1	1.00	0.08	136,136,136,136	0
16	ZN	B	1734	1/1	1.00	0.04	149,149,149,149	0
16	ZN	K	71	1/1	1.00	0.03	113,113,113,113	0
16	ZN	B	1735	1/1	1.00	0.05	110,110,110,110	0
16	ZN	C	1225	1/1	1.00	0.08	104,104,104,104	0

6.5 Other polymers [i](#)

There are no such residues in this entry.