



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:39 AM UTC

PDB ID : 3HOZ / pdb_00003hoz
Title : Complete RNA polymerase II elongation complex IV with a T-U mismatch and a frayed RNA 3'-guanine
Authors : Sydow, J.F.; Brueckner, F.; Cheung, A.C.M.; Damsma, G.E.; Dengl, S.; Lehmann, E.; Vassylyev, D.; Cramer, P.
Deposited on : 2009-06-03
Resolution : 3.65 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

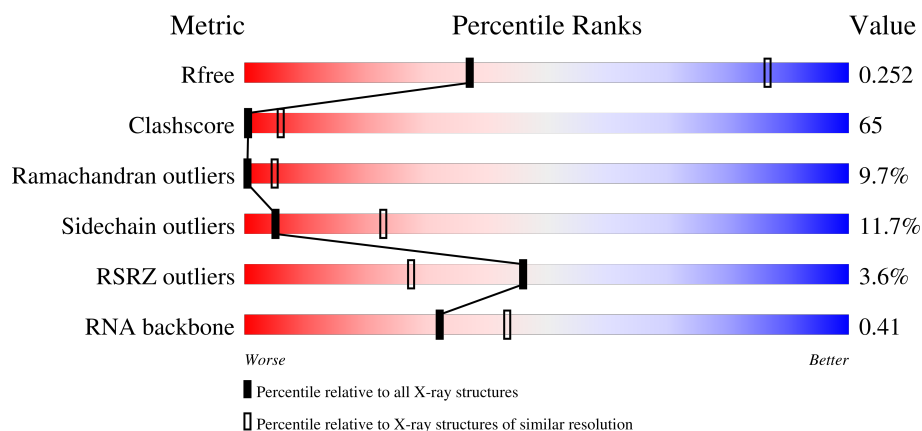
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)
RNA backbone	3983	1027 (4.26-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	2% 21% 46% 13% • 18%
2	B	1224	4% 21% 49% 18% • 9%
3	C	347	16% 47% 13% • 23%
4	D	221	5% 18% 45% 14% • 19%

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	12	
14	T	26	
15	P	18	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 31961 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1418	Total	C	N	O	S	0	0	0
			11158	7030	1951	2115	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1109	Total	C	N	O	S	0	0	0
			8821	5584	1546	1636	55			

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

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

There are 30 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	179	Total	C	N	O	S	0	0	0
			1443	892	258	291	2			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	136	Total	C	N	O	S	0	0	0
			1092	688	184	215	5			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	0
			924	593	157	172	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
14	T	19	Total	Br	C	N	O	P	0	0	0
			387	1	185	69	114	18			

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

*AP*GP*GP*CP*UP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	11	Total	C	N	O	P	0	0	0
			232	105	44	73	10			

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

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

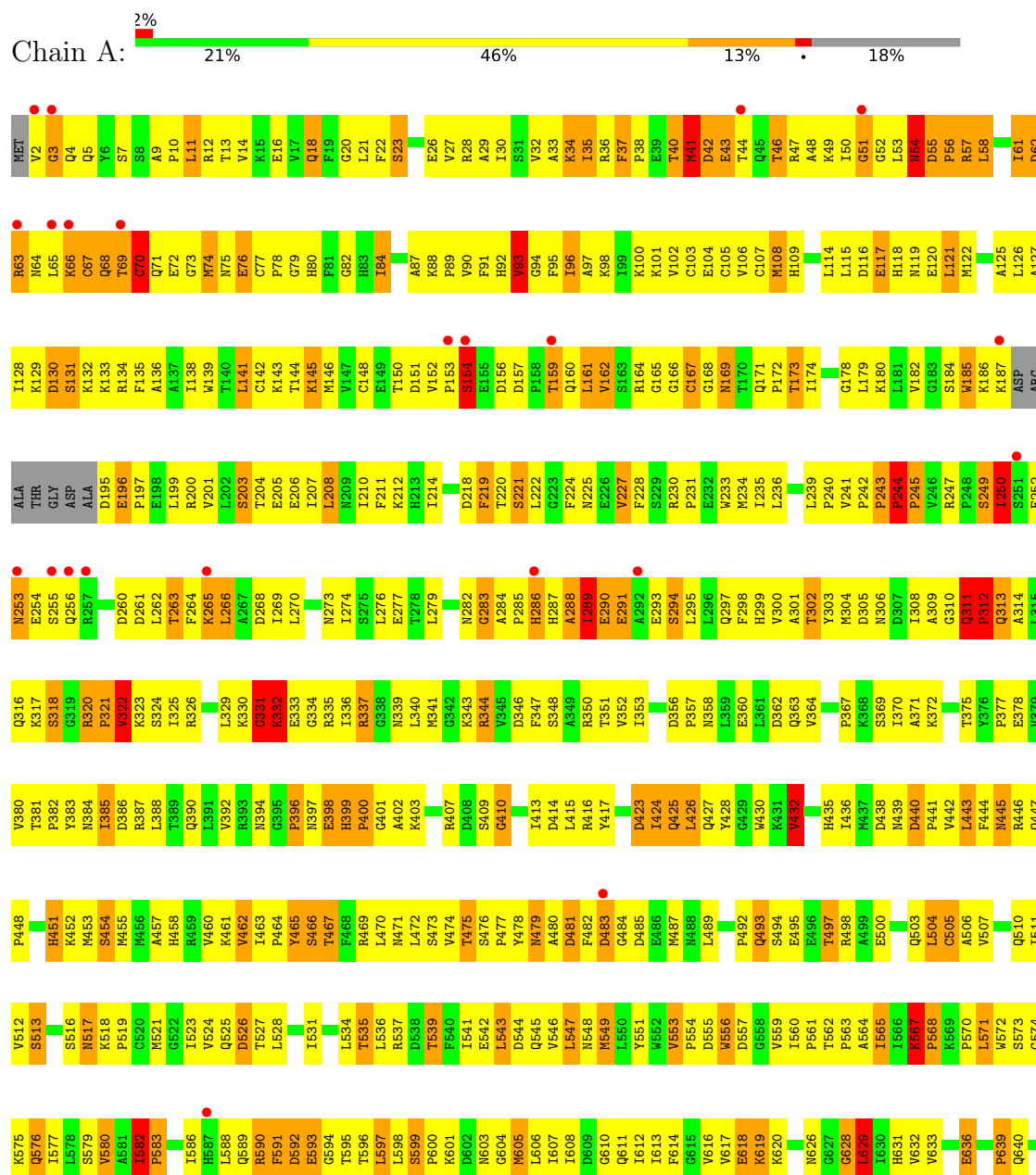
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

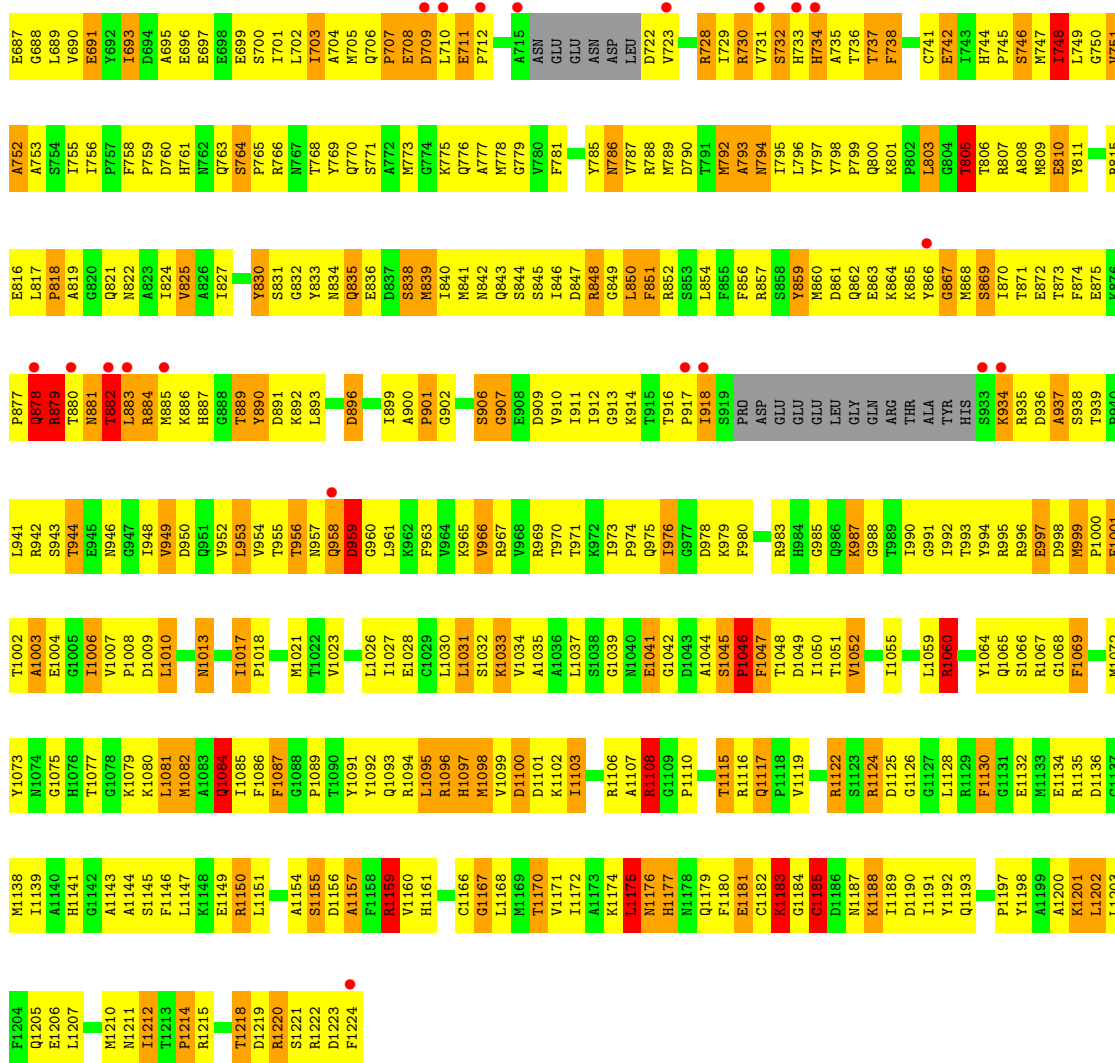
3 Residue-property plots

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

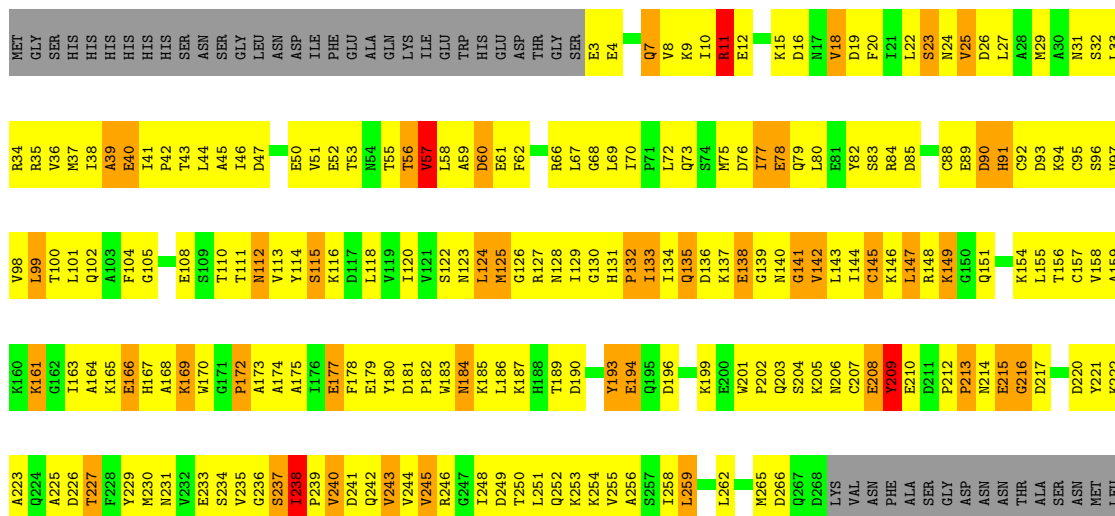






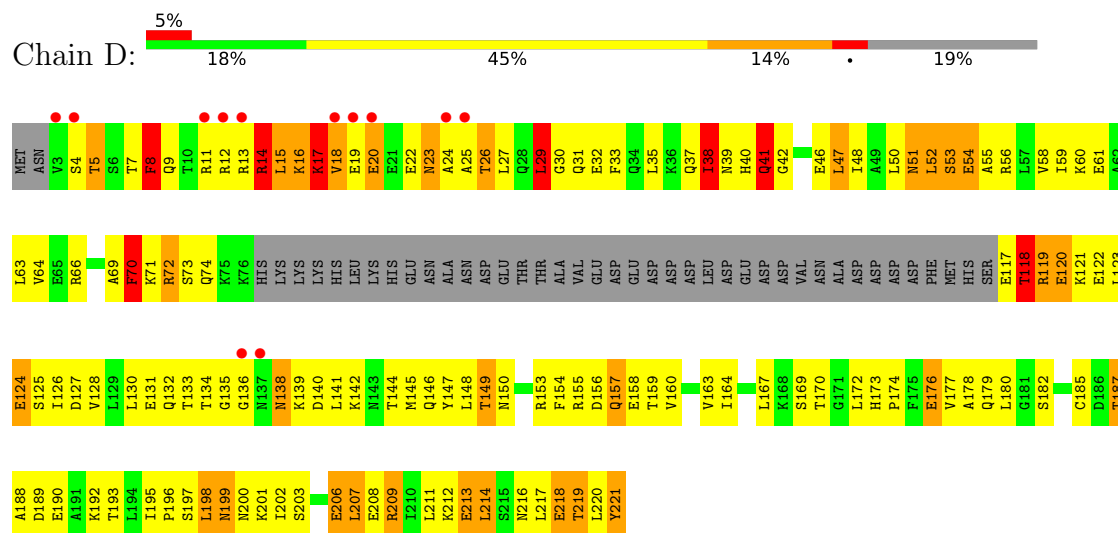
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 16% 47% 13% 23%

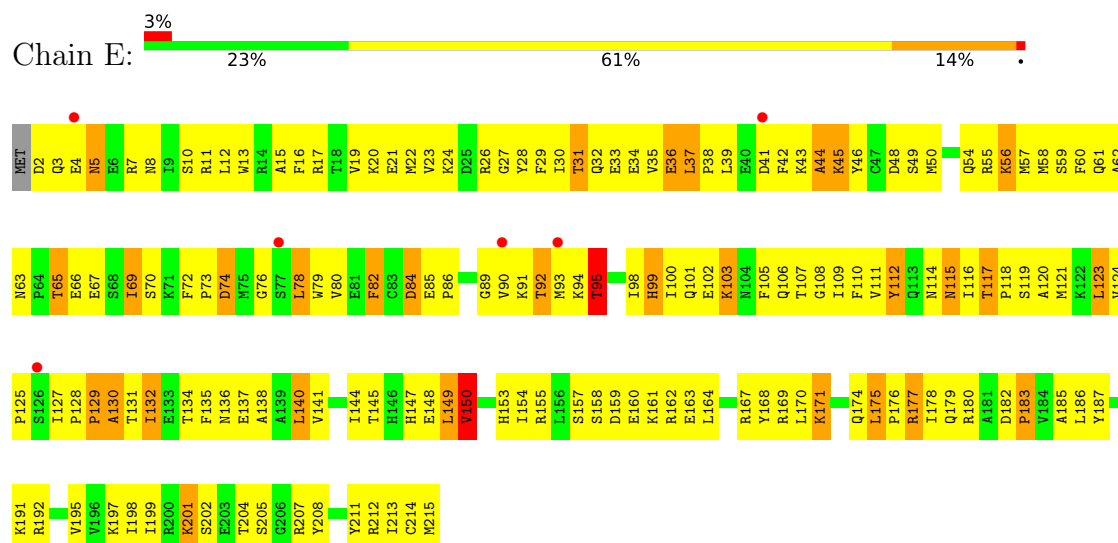


GLY
SER
ASN
GLU
ASP
VAL
MET
MET
THR
GLY
ALA
GLY
GLN
ASP
PRO
THR
SER
ASN
ALA
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GLY
SER
GLY
GLY
TVR
ASP
ASN
ALA
TRP

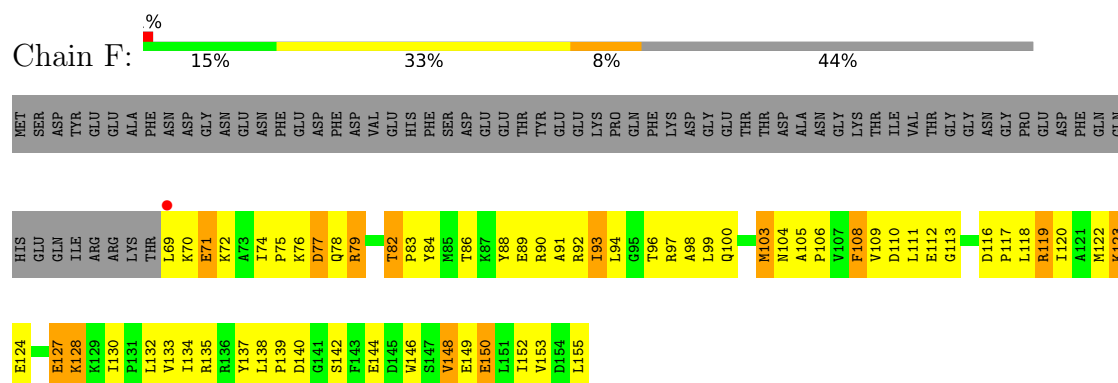
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



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



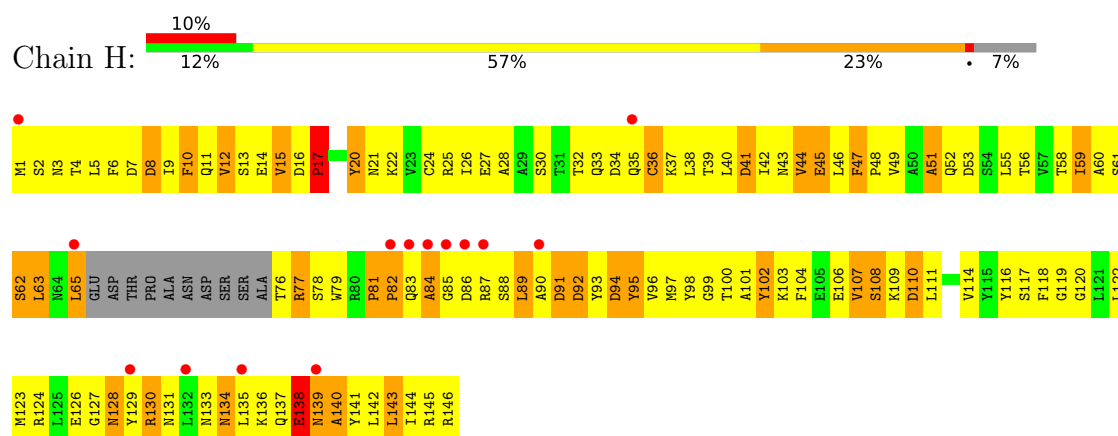
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



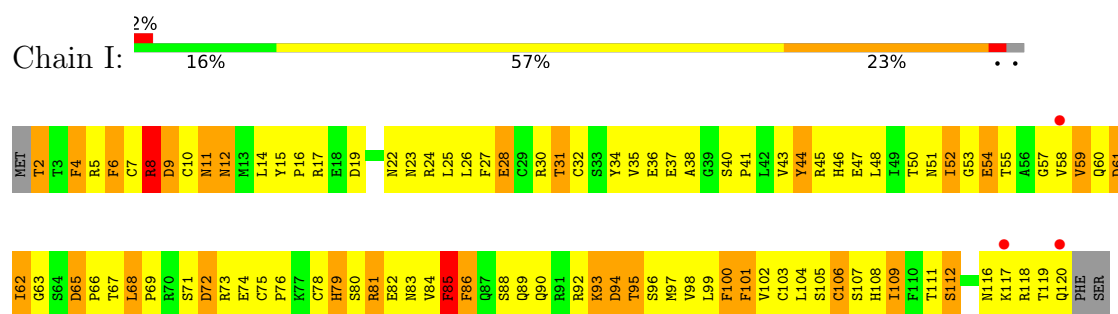
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7



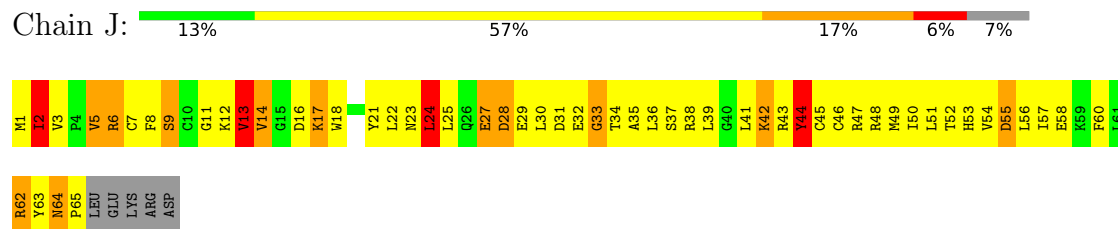
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



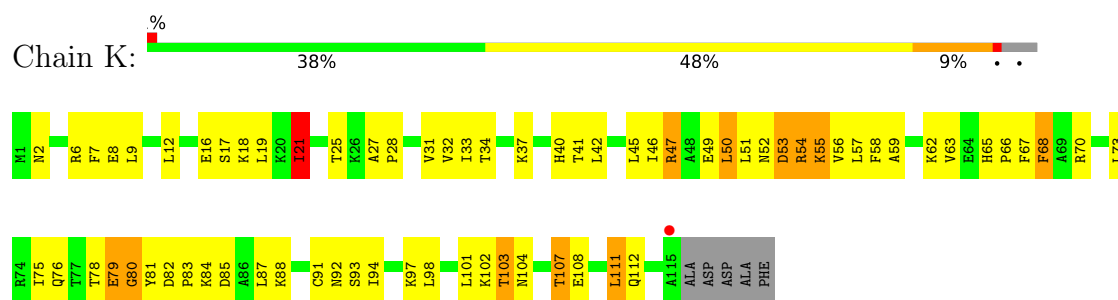
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9



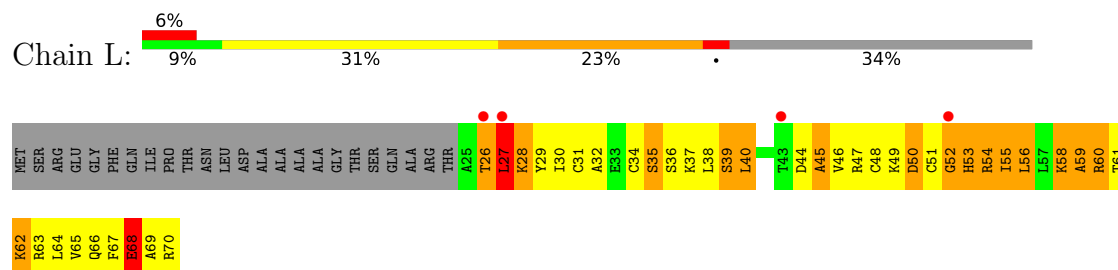
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



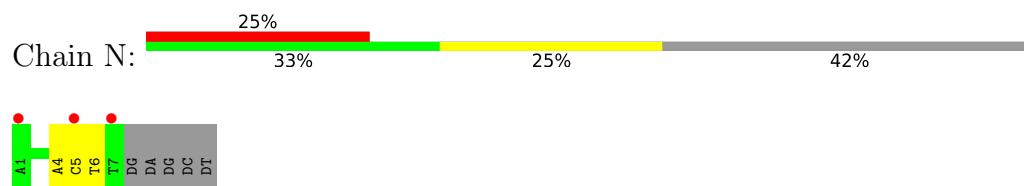
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11



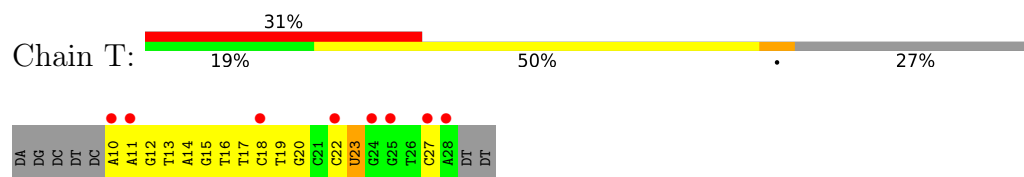
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



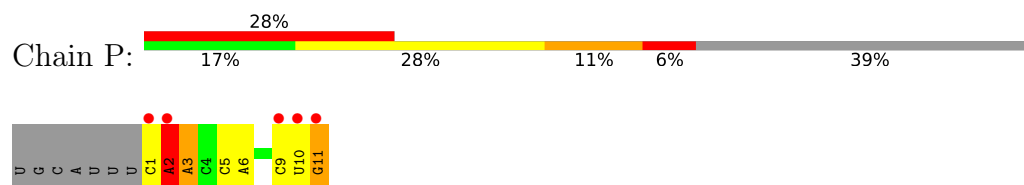
- Molecule 13: 5'-D(*AP*CP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3'



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	221.43Å 393.75Å 281.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.65 50.00 – 3.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.65) 99.9 (50.00-3.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 3.67Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.210 , 0.253 0.210 , 0.252	Depositor DCC
R_{free} test set	2674 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	88.8	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 119.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.025 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	31961	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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, BRU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.65	0/11358	1.17	94/15360 (0.6%)
2	B	0.60	0/8991	1.11	68/12121 (0.6%)
3	C	0.60	0/2133	1.12	14/2891 (0.5%)
4	D	0.60	0/1453	1.24	17/1947 (0.9%)
5	E	0.56	0/1788	1.13	21/2406 (0.9%)
6	F	0.70	0/717	1.31	9/967 (0.9%)
7	G	0.65	0/1368	1.27	17/1844 (0.9%)
8	H	0.51	0/1110	1.07	11/1502 (0.7%)
9	I	0.51	0/989	1.11	12/1331 (0.9%)
10	J	0.59	0/541	1.17	3/727 (0.4%)
11	K	0.58	0/942	1.02	3/1272 (0.2%)
12	L	0.63	0/365	1.21	4/485 (0.8%)
13	N	0.40	0/152	0.84	0/232
14	T	0.38	0/410	0.78	0/629
15	P	0.48	0/259	0.87	1/402 (0.2%)
All	All	0.61	0/32576	1.14	274/44116 (0.6%)

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	J	0	1

There are no bond length outliers.

All (274) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	26	THR	N-CA-C	-13.78	93.51	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	71	GLU	N-CA-C	-12.61	96.62	112.88
2	B	1185	CYS	N-CA-C	-12.28	97.06	114.12
1	A	629	LEU	N-CA-C	-11.73	98.22	111.71
3	C	39	ALA	N-CA-C	11.57	128.07	112.68
5	E	5	ASN	N-CA-C	-11.30	99.04	113.72
7	G	62	LEU	CA-C-N	-11.29	105.73	119.84
7	G	62	LEU	C-N-CA	-11.29	105.73	119.84
5	E	171	LYS	N-CA-C	-11.09	96.22	110.53
2	B	296	GLU	N-CA-C	-10.57	100.51	113.41
7	G	65	ASP	N-CA-C	-10.37	95.02	109.95
2	B	681	TRP	N-CA-C	-10.30	98.83	111.40
1	A	289	ILE	N-CA-C	-10.18	101.98	111.45
2	B	363	HIS	N-CA-C	-10.14	97.45	110.53
4	D	38	ILE	N-CA-C	9.98	121.77	109.30
2	B	882	THR	N-CA-C	9.76	122.93	111.02
4	D	188	ALA	N-CA-C	-9.63	100.63	112.38
2	B	976	ILE	N-CA-C	9.37	120.18	110.72
1	A	511	ILE	N-CA-C	9.27	119.87	110.23
1	A	117	GLU	N-CA-C	-9.08	101.47	112.54
2	B	1177	HIS	N-CA-C	-8.98	101.87	112.92
10	J	44	TYR	N-CA-C	8.93	123.18	111.75
4	D	25	ALA	N-CA-C	-8.82	99.54	110.65
1	A	513	SER	N-CA-C	8.75	120.78	109.93
4	D	72	ARG	N-CA-C	-8.69	101.94	112.54
2	B	1130	PHE	N-CA-C	-8.65	96.82	109.11
1	A	710	LEU	N-CA-C	-8.65	101.06	111.69
9	I	85	PHE	N-CA-C	8.50	120.87	110.41
10	J	9	SER	N-CA-C	8.41	120.14	110.97
12	L	62	LYS	N-CA-C	-8.41	102.06	111.14
1	A	864	ILE	N-CA-C	-8.35	105.11	112.12
1	A	266	LEU	N-CA-C	-8.17	102.31	111.14
1	A	243	PRO	CA-C-N	8.16	128.79	120.38
1	A	243	PRO	C-N-CA	8.16	128.79	120.38
1	A	535	THR	N-CA-C	8.14	121.70	111.69
1	A	440	ASP	N-CA-C	-8.06	99.19	110.31
12	L	68	GLU	N-CA-C	-8.00	99.97	110.53
1	A	861	GLY	N-CA-C	-7.99	104.29	115.32
8	H	34	ASP	N-CA-C	-7.97	104.52	112.97
4	D	31	GLN	N-CA-C	-7.83	102.99	112.54
2	B	428	ILE	N-CA-C	-7.76	102.71	110.62
10	J	5	VAL	N-CA-C	-7.72	97.13	108.87
1	A	636	GLU	N-CA-C	7.71	119.76	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1310	GLY	N-CA-C	-7.65	101.50	111.37
2	B	1115	THR	N-CA-C	7.63	121.07	111.69
1	A	1256	GLU	N-CA-C	7.51	119.25	111.14
3	C	112	ASN	N-CA-C	7.51	121.15	109.07
6	F	82	THR	CA-C-N	7.48	128.12	120.04
6	F	82	THR	C-N-CA	7.48	128.12	120.04
2	B	628	THR	N-CA-C	-7.43	103.34	113.30
12	L	58	LYS	N-CA-C	7.43	123.42	112.94
2	B	606	LYS	N-CA-C	-7.39	104.11	113.43
1	A	143	LYS	N-CA-C	-7.29	103.85	112.89
3	C	40	GLU	N-CA-C	7.27	121.01	112.72
2	B	1201	LYS	N-CA-C	-7.27	103.35	111.28
2	B	825	VAL	N-CA-C	7.25	118.72	108.36
1	A	279	LEU	N-CA-C	-7.17	104.79	113.97
2	B	760	ASP	N-CA-C	-7.17	104.91	112.93
1	A	56	PRO	N-CA-C	-7.15	97.74	112.47
4	D	209	ARG	N-CA-C	-7.14	103.19	110.97
1	A	1207	LEU	N-CA-C	7.12	120.17	108.99
6	F	74	ILE	CA-C-N	7.07	127.11	119.90
6	F	74	ILE	C-N-CA	7.07	127.11	119.90
2	B	208	SER	N-CA-C	7.06	120.46	110.50
1	A	1174	PHE	N-CA-C	-7.04	103.82	113.18
1	A	1311	VAL	N-CA-C	7.00	118.21	108.12
1	A	646	PHE	N-CA-C	-6.98	102.73	111.11
1	A	931	GLU	N-CA-C	-6.97	103.76	111.36
7	G	64	THR	N-CA-C	-6.96	103.92	113.18
1	A	311	GLN	N-CA-C	6.95	125.17	109.81
2	B	297	ILE	N-CA-C	-6.91	103.74	110.72
1	A	40	THR	N-CA-C	-6.87	102.38	111.24
2	B	1184	GLY	N-CA-C	-6.86	105.76	113.79
3	C	238	ILE	CA-C-N	6.86	127.94	119.98
3	C	238	ILE	C-N-CA	6.86	127.94	119.98
1	A	1241	ARG	N-CA-C	6.85	121.49	112.72
1	A	1451	VAL	N-CA-C	-6.83	106.13	112.96
2	B	851	PHE	N-CA-C	6.79	123.00	113.56
1	A	553	VAL	CA-C-N	6.77	126.45	119.82
1	A	553	VAL	C-N-CA	6.77	126.45	119.82
1	A	847	ASP	N-CA-C	6.71	121.18	113.19
2	B	434	ARG	N-CA-C	-6.64	106.39	114.75
2	B	526	GLU	N-CA-C	6.62	119.07	108.41
2	B	1009	ASP	N-CA-C	-6.56	105.57	113.97
5	E	177	ARG	N-CA-C	6.54	120.72	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	436	ILE	N-CA-C	-6.54	101.13	109.30
2	B	934	LYS	N-CA-C	6.47	119.94	108.24
2	B	703	ILE	N-CA-C	6.45	118.69	108.89
2	B	66	ASP	N-CA-C	-6.45	104.99	112.92
1	A	513	SER	CA-C-N	6.42	126.54	119.87
1	A	513	SER	C-N-CA	6.42	126.54	119.87
4	D	8	PHE	N-CA-C	6.42	124.46	110.80
4	D	41	GLN	N-CA-C	-6.41	105.75	112.93
1	A	1155	ASP	CA-C-N	6.39	125.96	119.19
1	A	1155	ASP	C-N-CA	6.39	125.96	119.19
1	A	998	LEU	N-CA-C	6.39	119.54	109.96
2	B	1033	LYS	N-CA-C	-6.35	104.28	111.07
1	A	590	ARG	N-CA-C	6.35	118.95	108.48
4	D	169	SER	N-CA-C	-6.33	105.87	113.97
7	G	129	SER	N-CA-C	6.33	116.42	108.45
9	I	28	GLU	N-CA-C	6.32	116.79	107.88
1	A	505	CYS	N-CA-C	6.30	120.31	111.30
1	A	467	THR	N-CA-C	6.29	119.44	109.50
9	I	61	ASP	N-CA-C	-6.28	105.28	114.39
1	A	108	MET	N-CA-C	-6.27	102.41	110.19
2	B	805	THR	N-CA-C	6.26	118.46	109.14
1	A	331	GLY	N-CA-C	6.25	128.00	113.18
5	E	63	ASN	N-CA-C	6.25	119.38	108.82
1	A	1258	HIS	N-CA-C	-6.22	104.39	112.23
7	G	40	GLY	N-CA-C	-6.22	105.04	113.37
1	A	564	ALA	N-CA-C	-6.21	104.62	111.82
2	B	112	LEU	N-CA-C	6.18	118.28	110.24
6	F	127	GLU	N-CA-C	-6.18	103.16	111.87
4	D	54	GLU	N-CA-C	-6.16	104.33	112.34
2	B	1170	THR	N-CA-C	6.16	118.50	111.11
5	E	150	VAL	CA-C-N	6.14	126.60	120.52
5	E	150	VAL	C-N-CA	6.14	126.60	120.52
11	K	68	PHE	N-CA-C	6.14	118.53	108.52
5	E	149	LEU	CA-C-N	-6.13	116.64	123.02
5	E	149	LEU	C-N-CA	-6.13	116.64	123.02
1	A	3	GLY	N-CA-C	-6.13	98.65	113.18
1	A	398	GLU	N-CA-C	-6.13	102.27	110.55
8	H	45	GLU	N-CA-C	-6.12	105.72	113.43
2	B	901	PRO	N-CA-C	6.12	121.55	114.03
6	F	148	VAL	N-CA-C	-6.10	103.43	111.05
8	H	16	ASP	N-CA-C	6.08	119.13	109.40
1	A	466	SER	N-CA-C	6.08	123.75	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	117	THR	N-CA-C	6.08	117.05	109.57
4	D	70	PHE	N-CA-C	-6.08	105.73	113.02
9	I	31	THR	N-CA-C	-6.07	104.86	112.93
1	A	580	VAL	N-CA-C	-6.07	105.11	113.00
1	A	964	ILE	N-CA-C	-6.05	106.61	111.81
2	B	307	ASP	N-CA-C	-6.05	101.25	109.54
1	A	291	GLU	N-CA-C	-6.04	105.40	112.89
2	B	1045	SER	CA-C-N	6.00	127.34	119.84
2	B	1045	SER	C-N-CA	6.00	127.34	119.84
2	B	649	LYS	N-CA-C	-5.97	101.64	110.48
1	A	244	PRO	N-CA-C	5.97	117.98	110.70
9	I	112	SER	N-CA-C	-5.94	104.57	112.94
3	C	57	VAL	N-CA-C	-5.92	104.68	113.39
1	A	480	ALA	N-CA-C	5.92	118.84	109.96
1	A	425	GLN	N-CA-C	-5.90	97.60	107.80
1	A	174	ILE	N-CA-C	5.89	117.49	108.71
1	A	82	GLY	N-CA-C	-5.88	103.07	111.42
1	A	242	PRO	CA-C-N	5.88	126.43	120.38
1	A	242	PRO	C-N-CA	5.88	126.43	120.38
3	C	194	GLU	N-CA-C	-5.87	104.87	112.68
2	B	803	LEU	N-CA-C	-5.87	104.24	111.40
12	L	52	GLY	N-CA-C	-5.84	105.73	112.73
1	A	1389	PHE	N-CA-C	5.83	118.39	111.33
2	B	603	LEU	N-CA-C	-5.82	104.53	111.69
1	A	1403	GLU	N-CA-C	5.80	123.15	110.80
2	B	1001	PHE	N-CA-C	5.77	117.96	109.24
2	B	1159	ARG	N-CA-C	5.77	118.12	108.02
2	B	896	ASP	N-CA-C	-5.77	106.20	113.18
8	H	36	CYS	N-CA-C	5.76	117.84	108.63
2	B	658	ILE	N-CA-C	5.74	115.92	110.53
1	A	1345	ARG	N-CA-C	-5.71	104.42	111.33
1	A	23	SER	N-CA-C	-5.71	102.88	110.07
1	A	1404	GLU	N-CA-C	5.69	119.53	112.59
7	G	138	THR	N-CA-C	5.69	115.90	107.88
1	A	950	GLY	N-CA-C	-5.67	107.22	114.37
5	E	84	ASP	N-CA-C	-5.65	106.37	113.20
8	H	110	ASP	N-CA-C	-5.65	104.63	112.03
1	A	30	ILE	CB-CA-C	-5.64	104.65	112.04
2	B	732	SER	N-CA-C	5.64	116.71	108.14
2	B	663	ALA	N-CA-C	-5.64	104.83	110.97
15	P	2	A	C2'-C3'-O3'	5.61	122.11	113.70
4	D	176	GLU	N-CA-C	-5.60	104.81	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	ALA	N-CA-C	-5.59	98.89	110.80
1	A	1076	ALA	N-CA-C	-5.59	105.96	112.89
5	E	103	LYS	N-CA-C	-5.59	106.30	113.01
7	G	133	SER	N-CA-C	-5.57	104.59	111.33
6	F	108	PHE	N-CA-C	5.57	118.87	112.97
1	A	55	ASP	CA-C-N	-5.56	112.89	119.84
1	A	55	ASP	C-N-CA	-5.56	112.89	119.84
1	A	362	ASP	N-CA-C	5.55	119.80	113.19
6	F	77	ASP	N-CA-C	-5.55	101.49	110.32
3	C	96	SER	N-CA-C	5.55	117.28	108.79
1	A	1312	ASN	N-CA-C	-5.54	97.96	107.61
2	B	748	ILE	N-CA-C	-5.54	104.16	111.09
2	B	1060	ARG	N-CA-C	-5.53	105.26	112.23
9	I	109	ILE	N-CA-C	5.52	115.60	107.15
1	A	682	THR	N-CA-C	-5.52	105.42	111.82
7	G	76	ALA	N-CA-C	5.51	115.81	108.38
1	A	539	THR	N-CA-C	5.49	118.58	109.46
2	B	1052	VAL	N-CA-C	-5.48	105.03	110.62
1	A	432	VAL	CB-CA-C	-5.48	104.69	111.32
8	H	138	GLU	N-CA-C	-5.47	105.23	111.14
1	A	1444	MET	N-CA-C	5.46	118.64	109.95
3	C	259	LEU	N-CA-C	-5.46	104.97	111.03
9	I	65	ASP	CA-C-N	5.45	125.28	119.28
9	I	65	ASP	C-N-CA	5.45	125.28	119.28
11	K	21	ILE	N-CA-C	5.41	115.65	107.80
7	G	104	GLY	CA-C-N	5.41	125.02	119.56
7	G	104	GLY	C-N-CA	5.41	125.02	119.56
1	A	504	LEU	N-CA-C	5.40	119.82	112.04
1	A	970	THR	N-CA-C	-5.40	105.55	111.82
5	E	118	PRO	N-CA-C	-5.40	106.82	113.84
2	B	1096	ARG	N-CA-C	-5.40	103.22	110.24
7	G	145	VAL	N-CA-C	5.40	116.25	108.48
4	D	18	VAL	N-CA-C	5.40	115.86	107.28
9	I	81	ARG	N-CA-C	-5.38	106.90	112.93
8	H	103	LYS	N-CA-C	5.38	118.33	109.72
1	A	815	PHE	N-CA-C	-5.37	105.50	111.36
2	B	1189	ILE	CB-CA-C	-5.37	106.27	111.05
2	B	99	LYS	CA-C-N	5.37	126.55	119.84
2	B	99	LYS	C-N-CA	5.37	126.55	119.84
2	B	464	GLY	N-CA-C	-5.33	107.43	114.95
7	G	63	PRO	N-CA-C	5.33	123.45	112.47
3	C	91	HIS	N-CA-C	5.33	117.18	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	201	LYS	N-CA-C	-5.32	103.51	110.53
2	B	650	GLU	N-CA-C	5.32	116.61	108.52
2	B	1101	ASP	N-CA-C	-5.31	106.18	113.30
5	E	175	LEU	CA-C-N	5.31	126.14	119.98
5	E	175	LEU	C-N-CA	5.31	126.14	119.98
1	A	1275	GLY	N-CA-C	5.30	122.53	112.62
2	B	1084	GLN	N-CA-C	-5.30	101.47	109.85
7	G	139	ILE	N-CA-C	5.30	120.36	109.34
2	B	1013	ASN	N-CA-C	5.28	116.31	109.65
7	G	135	ASP	N-CA-C	5.28	117.35	110.53
9	I	68	LEU	CA-C-N	5.28	125.48	120.31
9	I	68	LEU	C-N-CA	5.28	125.48	120.31
2	B	52	ASN	N-CA-C	-5.28	105.22	110.97
5	E	95	THR	CA-C-N	5.26	127.59	120.38
5	E	95	THR	C-N-CA	5.26	127.59	120.38
7	G	22	MET	N-CA-C	-5.26	105.68	112.68
2	B	498	THR	N-CA-C	5.26	117.47	108.90
2	B	665	GLU	N-CA-C	-5.25	105.45	111.07
2	B	832	GLY	N-CA-C	-5.25	107.40	116.01
3	C	51	VAL	N-CA-C	5.24	115.64	107.99
1	A	173	THR	N-CA-C	-5.23	101.90	109.59
1	A	1101	LEU	N-CA-C	-5.23	105.58	111.28
8	H	20	TYR	N-CA-C	5.22	117.11	108.49
1	A	734	GLU	N-CA-C	5.21	117.70	111.71
1	A	567	LYS	CA-C-N	-5.20	113.34	119.84
1	A	567	LYS	C-N-CA	-5.20	113.34	119.84
4	D	201	LYS	N-CA-C	5.20	117.62	111.33
1	A	639	PRO	N-CA-C	-5.19	106.64	113.65
2	B	233	PRO	N-CA-C	-5.18	107.27	114.27
2	B	335	GLY	N-CA-C	-5.18	100.91	113.18
2	B	890	TYR	N-CA-C	-5.18	106.12	112.90
1	A	698	GLN	N-CA-C	-5.18	106.47	112.89
1	A	1102	LYS	N-CA-C	-5.17	105.53	111.07
5	E	99	HIS	N-CA-C	-5.17	105.54	111.07
8	H	41	ASP	N-CA-C	-5.17	102.83	110.48
11	K	55	LYS	N-CA-C	-5.16	106.58	112.92
1	A	1445	ILE	CB-CA-C	-5.16	103.92	110.98
3	C	135	GLN	N-CA-C	-5.15	105.76	113.89
4	D	51	ASN	N-CA-C	-5.14	102.14	110.32
2	B	366	GLN	N-CA-C	-5.14	106.41	113.30
1	A	55	ASP	N-CA-CB	5.12	119.48	110.37
5	E	63	ASN	CA-C-N	5.12	126.24	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	63	ASN	C-N-CA	5.12	126.24	119.84
1	A	1169	ILE	N-CA-C	5.12	119.61	112.50
1	A	263	THR	N-CA-C	-5.11	106.31	112.54
1	A	227	VAL	N-CA-C	5.09	116.19	111.81
2	B	1117	GLN	N-CA-C	-5.09	104.28	110.13
2	B	127	GLY	N-CA-C	5.08	118.70	112.14
8	H	16	ASP	CA-C-N	5.08	126.19	119.84
8	H	16	ASP	C-N-CA	5.08	126.19	119.84
3	C	11	ARG	N-CA-C	-5.08	99.98	110.80
1	A	582	ILE	CA-C-N	5.08	126.19	119.84
1	A	582	ILE	C-N-CA	5.08	126.19	119.84
2	B	949	VAL	N-CA-C	-5.07	102.34	109.63
5	E	56	LYS	N-CA-C	-5.06	106.20	112.38
1	A	227	VAL	CB-CA-C	-5.05	105.74	111.55
2	B	371	GLU	N-CA-C	-5.04	105.30	111.75
3	C	19	ASP	N-CA-C	-5.04	103.14	110.24
9	I	8	ARG	N-CA-C	-5.04	100.07	110.80
4	D	29	LEU	N-CA-C	-5.03	103.29	110.59
7	G	53	ASN	N-CA-C	5.03	118.25	112.57
2	B	838	SER	N-CA-C	-5.02	101.57	109.50
2	B	749	LEU	N-CA-C	5.01	116.40	110.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	44	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11158	0	11228	1487	0
2	B	8821	0	8850	1289	0
3	C	2095	0	2051	324	0
4	D	1443	0	1466	222	0
5	E	1752	0	1776	230	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	705	0	731	94	0
7	G	1340	0	1357	177	0
8	H	1092	0	1069	185	0
9	I	971	0	929	146	0
10	J	532	0	542	121	0
11	K	924	0	934	116	0
12	L	363	0	388	86	0
13	N	137	0	82	4	0
14	T	387	0	214	25	0
15	P	232	0	122	14	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	P	1	0	0	0	0
All	All	31961	0	31739	4157	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 65.

All (4157) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:508:LEU:HD13	2:B:510:LYS:HE2	1.26	1.16
1:A:53:LEU:HD23	1:A:54:ASN:N	1.61	1.16
2:B:744:HIS:HD2	2:B:745:PRO:HD2	1.07	1.14
1:A:1208:THR:HB	1:A:1211:GLN:HG3	1.24	1.13
2:B:559:SER:HA	2:B:563:MET:HB3	1.15	1.13
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.85	1.11
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.25	1.11
2:B:806:THR:HG22	2:B:808:ALA:H	1.12	1.10
1:A:53:LEU:HD23	1:A:54:ASN:H	0.96	1.09
3:C:112:ASN:HB3	3:C:114:TYR:HE1	1.10	1.09
8:H:4:THR:HA	8:H:60:ALA:HB2	1.32	1.08
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.17	1.08
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.33	1.08
2:B:744:HIS:CD2	2:B:745:PRO:HD2	1.89	1.07
3:C:112:ASN:HB3	3:C:114:TYR:CE1	1.89	1.07
1:A:1242:VAL:HG12	1:A:1243:VAL:N	1.68	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:40:LEU:HD13	8:H:123:MET:HE3	1.36	1.05
2:B:261:ARG:HH11	2:B:261:ARG:HB3	1.19	1.05
2:B:345:LYS:HG2	2:B:346:GLU:H	1.17	1.05
1:A:567:LYS:HE3	1:A:568:PRO:HD2	1.38	1.05
5:E:117:THR:HG22	5:E:119:SER:H	1.21	1.05
6:F:90:ARG:HD3	6:F:155:LEU:HD13	1.38	1.05
1:A:567:LYS:HB3	8:H:96:VAL:H	1.21	1.04
1:A:1206:ASP:HB3	1:A:1274:ARG:HH22	1.19	1.04
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.40	1.03
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.39	1.02
10:J:64:ASN:HB3	10:J:65:PRO:CD	1.90	1.01
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.08	1.01
1:A:265:LYS:N	1:A:265:LYS:HE3	1.74	1.01
1:A:1242:VAL:HG12	1:A:1243:VAL:H	0.85	1.01
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.41	1.00
7:G:26:LEU:HD12	7:G:56:ILE:HD11	1.37	1.00
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.43	1.00
1:A:1244:ARG:HE	1:A:1245:PRO:HD2	1.21	1.00
5:E:56:LYS:HE2	5:E:84:ASP:HB2	1.40	1.00
1:A:1242:VAL:CG1	1:A:1243:VAL:H	1.71	1.00
2:B:510:LYS:CG	2:B:511:PRO:HD3	1.92	0.99
1:A:1445:ILE:H	1:A:1445:ILE:HD12	1.28	0.99
1:A:323:LYS:H	1:A:323:LYS:HD2	1.21	0.99
2:B:510:LYS:HG3	2:B:511:PRO:HD3	1.00	0.99
1:A:12:ARG:HB3	2:B:1218:THR:HG22	1.40	0.98
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.43	0.98
1:A:1202:MET:HE1	1:A:1212:VAL:HG21	1.41	0.98
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.43	0.98
1:A:381:THR:HG22	1:A:383:TYR:H	1.23	0.98
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.94	0.97
1:A:41:MET:HB3	1:A:49:LYS:HA	1.44	0.97
7:G:34:VAL:HG11	7:G:74:TYR:HE1	1.30	0.97
7:G:139:ILE:HG23	7:G:140:LYS:HG3	1.46	0.97
2:B:882:THR:HG23	2:B:884:ARG:H	1.22	0.97
7:G:112:LYS:HA	7:G:115:MET:HE3	1.41	0.97
1:A:783:THR:HG21	1:A:796:SER:O	1.65	0.97
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.64	0.96
1:A:1364:ASN:OD1	1:A:1366:ARG:HG2	1.65	0.96
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.47	0.96
2:B:289:LEU:HD13	2:B:375:ALA:HB2	1.46	0.95
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.31	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.49	0.95
2:B:243:ALA:HB2	2:B:251:ILE:HD13	1.45	0.95
2:B:1187:ASN:O	2:B:1188:LYS:HB2	1.64	0.95
10:J:53:HIS:HD2	10:J:54:VAL:N	1.63	0.95
1:A:63:ARG:HA	1:A:74:MET:HE2	1.46	0.95
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.49	0.95
2:B:999:MET:HA	2:B:999:MET:HE3	1.46	0.95
7:G:138:THR:HG22	7:G:139:ILE:N	1.80	0.94
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.48	0.94
1:A:672:ASP:HB3	1:A:736:ASN:OD1	1.68	0.94
4:D:220:LEU:CD2	4:D:221:TYR:H	1.80	0.94
1:A:344:ARG:HB3	1:A:344:ARG:HH11	1.30	0.94
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.47	0.93
2:B:429:PHE:HA	2:B:432:MET:HE3	1.48	0.93
2:B:510:LYS:HG3	2:B:511:PRO:CD	1.96	0.93
2:B:806:THR:N	2:B:809:MET:HE3	1.83	0.93
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.48	0.93
1:A:41:MET:CB	1:A:49:LYS:HA	1.98	0.93
1:A:1187:GLN:HB2	1:A:1244:ARG:HG2	1.48	0.93
1:A:1329:THR:HG22	1:A:1331:SER:H	1.30	0.93
1:A:629:LEU:O	1:A:633:VAL:HG23	1.69	0.93
3:C:177:GLU:HG3	3:C:231:ASN:HB3	1.51	0.93
6:F:103:MET:HE2	7:G:66:GLY:H	1.33	0.93
1:A:98:LYS:O	1:A:102:VAL:HG23	1.69	0.93
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.04	0.93
2:B:865:LYS:HB2	2:B:961:LEU:HD11	1.52	0.92
6:F:77:ASP:O	6:F:78:GLN:HB2	1.66	0.92
8:H:89:LEU:C	8:H:91:ASP:H	1.74	0.92
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.48	0.92
1:A:913:LEU:HD12	1:A:914:GLU:H	1.32	0.92
7:G:138:THR:HG22	7:G:139:ILE:H	1.31	0.92
1:A:66:LYS:NZ	1:A:68:GLN:H	1.68	0.92
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.02	0.92
2:B:737:THR:HG21	9:I:66:PRO:HA	1.52	0.92
4:D:60:LYS:HE3	4:D:126:ILE:HD11	1.52	0.92
4:D:14:ARG:HB3	4:D:14:ARG:HH11	1.34	0.92
1:A:182:VAL:HG22	1:A:201:VAL:HA	1.52	0.91
1:A:1094:VAL:HG22	1:A:1113:THR:HG21	1.51	0.91
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.52	0.91
1:A:66:LYS:HZ3	1:A:68:GLN:H	0.96	0.91
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.10	0.91
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.00	0.91
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.53	0.91
2:B:773:MET:SD	2:B:987:LYS:HD2	2.11	0.91
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.53	0.91
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.51	0.90
12:L:40:LEU:HD13	12:L:44:ASP:HB3	1.53	0.90
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.53	0.90
2:B:241:ARG:HA	2:B:253:THR:HG22	1.53	0.90
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.50	0.90
1:A:55:ASP:C	1:A:57:ARG:H	1.75	0.90
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.53	0.90
1:A:107:CYS:HA	1:A:171:GLN:NE2	1.85	0.90
15:P:10:U:H5'	15:P:11:G:O3'	1.71	0.90
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.54	0.90
2:B:597:MET:HA	2:B:597:MET:HE3	1.53	0.90
4:D:24:ALA:HB3	4:D:26:THR:HG23	1.53	0.90
8:H:59:ILE:HG22	8:H:60:ALA:H	1.37	0.90
8:H:84:ALA:HB2	8:H:87:ARG:HD2	1.54	0.89
3:C:112:ASN:CB	3:C:114:TYR:HE1	1.83	0.89
6:F:82:THR:HG22	6:F:84:TYR:H	1.34	0.89
2:B:615:MET:HB3	2:B:626:ILE:HG12	1.50	0.89
3:C:102:GLN:HG2	3:C:154:LYS:HG3	1.52	0.89
5:E:180:ARG:HB2	5:E:215:MET:OXT	1.70	0.89
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.12	0.89
1:A:1170:ILE:H	1:A:1170:ILE:HD12	1.35	0.89
1:A:567:LYS:HE3	1:A:568:PRO:CD	2.01	0.89
1:A:107:CYS:HA	1:A:171:GLN:HE22	1.37	0.89
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.38	0.89
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.54	0.88
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.08	0.88
4:D:220:LEU:HD23	4:D:221:TYR:H	1.36	0.88
2:B:364:ILE:HG13	2:B:585:VAL:HG22	1.54	0.88
6:F:69:LEU:HB3	6:F:71:GLU:CD	1.97	0.88
8:H:95:TYR:HE2	8:H:97:MET:HG3	1.37	0.88
1:A:185:TRP:HE3	1:A:185:TRP:H	1.18	0.88
5:E:23:VAL:O	5:E:28:TYR:HB2	1.73	0.88
6:F:103:MET:CE	7:G:66:GLY:H	1.86	0.88
11:K:21:ILE:HG23	11:K:33:ILE:HG12	1.56	0.88
7:G:88:ASP:HB3	7:G:144:ARG:HA	1.54	0.88
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.57	0.87
1:A:1076:ALA:HA	1:A:1079:MET:HE2	1.57	0.87
2:B:707:PRO:HG2	2:B:708:GLU:H	1.39	0.87
2:B:882:THR:HG23	2:B:884:ARG:N	1.90	0.87
12:L:55:ILE:HG12	12:L:56:LEU:H	1.40	0.87
1:A:225:ASN:HD22	1:A:228:PHE:H	1.16	0.87
4:D:138:ASN:HD21	7:G:35:GLU:HB3	1.37	0.87
5:E:78:LEU:HA	5:E:107:THR:HB	1.56	0.87
2:B:603:LEU:HD13	2:B:608:ASP:HB2	1.55	0.87
3:C:33:LEU:HG	3:C:37:MET:HE2	1.56	0.87
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.10	0.87
1:A:34:LYS:NZ	1:A:57:ARG:NH2	2.23	0.86
9:I:105:SER:O	9:I:106:CYS:HB3	1.75	0.86
4:D:126:ILE:HD13	4:D:145:MET:HE2	1.57	0.86
1:A:341:MET:HE2	1:A:843:LYS:HZ1	1.41	0.86
1:A:671:ALA:HB3	1:A:676:MET:HG3	1.57	0.86
3:C:73:GLN:HE21	3:C:75:MET:H	1.21	0.86
2:B:168:GLY:H	2:B:450:ALA:HB1	1.38	0.86
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.40	0.86
1:A:1308:THR:HG23	1:A:1309:ASP:N	1.90	0.86
5:E:22:MET:HE3	5:E:26:ARG:HE	1.37	0.86
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.58	0.86
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.11	0.85
1:A:1116:LEU:HB3	1:A:1308:THR:HG21	1.58	0.85
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.12	0.85
1:A:1107:VAL:HG12	1:A:1107:VAL:O	1.76	0.85
7:G:26:LEU:CD1	7:G:56:ILE:HD11	2.05	0.85
2:B:278:GLN:HG2	2:B:279:ASP:H	1.40	0.85
4:D:154:PHE:CD1	4:D:163:VAL:HG21	2.10	0.85
1:A:901:LEU:H	1:A:926:GLN:NE2	1.74	0.85
2:B:705:MET:HA	2:B:705:MET:HE3	1.58	0.85
14:T:10:DA:H2"	14:T:11:DA:N7	1.90	0.85
2:B:597:MET:SD	2:B:624:LEU:HD11	2.16	0.85
1:A:332:LYS:C	1:A:334:GLY:H	1.85	0.85
1:A:668:ASP:HB3	1:A:741:ASN:HD21	1.41	0.85
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.59	0.85
6:F:99:LEU:O	6:F:103:MET:HG2	1.77	0.85
1:A:549:MET:HE1	1:A:656:TRP:CD1	2.11	0.85
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	1.92	0.85
5:E:120:ALA:O	5:E:123:LEU:HG	1.77	0.84
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:GLU:HG3	2:B:66:ASP:H	1.41	0.84
5:E:114:ASN:O	5:E:115:ASN:HB3	1.74	0.84
1:A:567:LYS:HB3	8:H:96:VAL:N	1.92	0.84
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.59	0.84
2:B:806:THR:HG22	2:B:808:ALA:N	1.92	0.84
2:B:664:THR:HA	2:B:667:GLN:HE21	1.41	0.84
3:C:22:LEU:HD22	3:C:230:MET:HE1	1.60	0.84
2:B:345:LYS:HE2	2:B:349:ILE:HD11	1.60	0.83
2:B:579:ARG:HB2	2:B:586:TRP:NE1	1.93	0.83
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.59	0.83
1:A:225:ASN:ND2	1:A:228:PHE:H	1.73	0.83
2:B:841:MET:HG2	2:B:846:ILE:HD11	1.60	0.83
1:A:698:GLN:HA	9:I:97:MET:O	1.78	0.83
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.60	0.83
2:B:882:THR:HG23	2:B:884:ARG:HB2	1.59	0.83
8:H:130:ARG:NH1	8:H:130:ARG:HB2	1.93	0.83
4:D:23:ASN:H	4:D:23:ASN:HD22	1.24	0.83
1:A:18:GLN:HG2	1:A:1418:LEU:HD13	1.58	0.83
1:A:503:GLN:HE21	6:F:90:ARG:NH2	1.76	0.83
1:A:1116:LEU:N	1:A:1308:THR:HG22	1.92	0.83
1:A:341:MET:HE2	1:A:843:LYS:NZ	1.93	0.83
1:A:534:LEU:O	1:A:574:GLY:HA3	1.77	0.83
2:B:805:THR:HG22	2:B:806:THR:H	1.43	0.83
7:G:138:THR:CG2	7:G:139:ILE:H	1.91	0.83
1:A:167:CYS:HB2	1:A:169:ASN:HD21	1.43	0.83
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.60	0.83
2:B:425:THR:HA	2:B:428:ILE:HD12	1.59	0.82
1:A:1293:SER:OG	1:A:1295:THR:HG23	1.79	0.82
2:B:882:THR:HG21	2:B:935:ARG:HA	1.62	0.82
2:B:110:HIS:CB	12:L:54:ARG:HH22	1.92	0.82
7:G:122:ASN:ND2	7:G:125:SER:HB3	1.93	0.82
1:A:40:THR:HG22	1:A:41:MET:HG3	1.62	0.82
2:B:559:SER:HA	2:B:563:MET:CB	2.07	0.82
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.77	0.82
1:A:1348:LEU:O	1:A:1352:VAL:HG23	1.78	0.82
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.13	0.82
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.76	0.82
5:E:56:LYS:NZ	5:E:85:GLU:HG3	1.94	0.82
1:A:230:ARG:HG3	1:A:233:TRP:CZ3	2.13	0.82
1:A:591:PHE:HA	1:A:595:THR:HG21	1.59	0.82
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1312:ASN:HD21	1:A:1315:GLU:HG3	1.45	0.82
3:C:120:ILE:HD13	3:C:124:LEU:HD11	1.61	0.82
3:C:128:ASN:O	3:C:129:ILE:HG13	1.77	0.82
8:H:65:LEU:N	8:H:65:LEU:HD23	1.95	0.82
2:B:583:ASN:ND2	2:B:628:THR:HG22	1.95	0.82
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.15	0.82
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.60	0.82
1:A:66:LYS:HZ3	1:A:68:GLN:N	1.78	0.81
2:B:1095:LEU:H	2:B:1095:LEU:HD12	1.45	0.81
1:A:831:THR:HG23	1:A:832:ALA:H	1.44	0.81
2:B:798:TYR:HE2	3:C:62:PHE:CE2	1.97	0.81
1:A:390:GLN:HE21	1:A:394:ASN:HD22	1.27	0.81
1:A:646:PHE:O	1:A:650:GLN:HG3	1.80	0.81
1:A:1420:ASP:HB2	1:A:1422:ARG:HG3	1.61	0.81
2:B:815:ARG:HD3	2:B:1041:GLU:OE2	1.79	0.81
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.46	0.81
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.15	0.81
1:A:332:LYS:HA	1:A:337:ARG:HB3	1.62	0.81
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.44	0.81
1:A:42:ASP:O	1:A:44:THR:N	2.13	0.81
1:A:341:MET:HE1	2:B:1135:ARG:NH1	1.96	0.81
10:J:53:HIS:CD2	10:J:54:VAL:N	2.47	0.81
1:A:56:PRO:O	1:A:57:ARG:HG3	1.81	0.81
5:E:207:ARG:HB3	5:E:207:ARG:HH11	1.45	0.81
1:A:903:ASN:HD22	1:A:904:THR:N	1.78	0.81
2:B:642:ASP:HA	2:B:649:LYS:HA	1.62	0.81
5:E:124:VAL:HG13	5:E:132:ILE:HG13	1.62	0.81
7:G:119:LEU:HD11	7:G:130:TYR:HB3	1.63	0.81
1:A:11:LEU:O	1:A:11:LEU:HD23	1.81	0.81
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.43	0.81
1:A:666:ILE:HD12	1:A:667:GLY:H	1.45	0.81
1:A:1387:HIS:HA	1:A:1391:ARG:HH11	1.45	0.81
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.62	0.81
8:H:130:ARG:HB2	8:H:130:ARG:HH11	1.45	0.81
1:A:666:ILE:H	2:B:1026:LEU:HD13	1.44	0.80
2:B:577:ALA:CB	2:B:589:VAL:HG11	2.10	0.80
1:A:49:LYS:NZ	1:A:61:ILE:HG13	1.96	0.80
2:B:842:ASN:HD22	2:B:845:SER:H	1.27	0.80
2:B:975:GLN:HG2	2:B:976:ILE:H	1.45	0.80
9:I:93:LYS:H	9:I:93:LYS:HD3	1.46	0.80
1:A:754:SER:H	1:A:757:ASN:HD22	1.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.45	0.80
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.63	0.80
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.64	0.80
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.16	0.80
3:C:177:GLU:HG3	3:C:231:ASN:HD22	1.45	0.80
1:A:1186:ASP:O	1:A:1187:GLN:HB3	1.81	0.80
2:B:613:VAL:HG13	2:B:627:PHE:O	1.82	0.80
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.78	0.80
9:I:6:PHE:HB3	9:I:12:ASN:O	1.82	0.80
14:T:15:DG:H2'	14:T:16:DT:H71	1.63	0.80
14:T:16:DT:H2''	14:T:17:DT:H5'	1.62	0.80
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.64	0.80
2:B:278:GLN:CG	2:B:279:ASP:H	1.93	0.80
3:C:66:ARG:NH1	10:J:2:ILE:HG21	1.97	0.80
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.79	0.80
1:A:831:THR:HG23	1:A:832:ALA:N	1.96	0.80
1:A:1202:MET:HE1	1:A:1212:VAL:CG2	2.11	0.80
2:B:1182:CYS:O	2:B:1182:CYS:SG	2.39	0.80
2:B:803:LEU:HD12	2:B:1032:SER:HB3	1.61	0.80
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.63	0.79
3:C:98:VAL:C	3:C:99:LEU:HD23	2.07	0.79
7:G:30:LEU:HD22	7:G:72:VAL:HG11	1.63	0.79
5:E:22:MET:CE	5:E:26:ARG:HH21	1.94	0.79
1:A:697:ALA:HB2	1:A:702:LEU:HD12	1.64	0.79
2:B:172:ILE:HD13	2:B:178:ASN:HD22	1.46	0.79
5:E:44:ALA:O	5:E:45:LYS:HB2	1.81	0.79
1:A:571:LEU:HD22	8:H:46:LEU:HD11	1.65	0.79
2:B:165:VAL:HG11	2:B:448:ILE:HD13	1.64	0.79
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.46	0.79
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.18	0.79
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.17	0.79
1:A:567:LYS:CE	1:A:568:PRO:HD2	2.12	0.79
2:B:661:LEU:HD11	2:B:684:LEU:HD21	1.64	0.79
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.62	0.79
12:L:32:ALA:CB	12:L:55:ILE:HG13	2.12	0.79
12:L:60:ARG:HG2	12:L:61:THR:H	1.46	0.79
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.18	0.79
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.65	0.79
4:D:29:LEU:HD12	7:G:82:PHE:CZ	2.18	0.79
1:A:69:THR:O	1:A:71:GLN:N	2.16	0.79
1:A:1241:ARG:O	1:A:1242:VAL:HG23	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.63	0.79
2:B:221:ASN:OD1	2:B:242:SER:HA	1.83	0.79
5:E:117:THR:HG22	5:E:119:SER:N	1.96	0.78
7:G:9:LEU:HD12	7:G:10:ASN:H	1.48	0.78
2:B:942:ARG:HH22	14:T:23:BRU:H5"	1.47	0.78
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.65	0.78
1:A:535:THR:HG21	1:A:616:VAL:HA	1.66	0.78
5:E:117:THR:HB	5:E:120:ALA:HB2	1.65	0.78
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.18	0.78
7:G:14:HIS:CD2	7:G:16:SER:H	2.01	0.78
2:B:613:VAL:HG22	2:B:628:THR:HA	1.66	0.78
7:G:128:PRO:O	7:G:138:THR:HG23	1.84	0.78
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.65	0.78
1:A:710:LEU:H	1:A:710:LEU:HD12	1.47	0.78
2:B:126:SER:OG	2:B:172:ILE:HD11	1.84	0.78
2:B:294:ASP:H	9:I:12:ASN:ND2	1.81	0.78
4:D:203:SER:OG	4:D:206:GLU:HB2	1.83	0.78
7:G:106:MET:HG2	7:G:107:LYS:N	1.97	0.78
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.14	0.78
1:A:665:GLY:O	1:A:667:GLY:N	2.16	0.78
2:B:583:ASN:HD21	2:B:628:THR:CG2	1.95	0.78
1:A:53:LEU:CD2	1:A:54:ASN:H	1.89	0.78
1:A:265:LYS:HE3	1:A:265:LYS:CA	2.13	0.78
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.66	0.78
2:B:773:MET:HE2	2:B:985:GLY:HA2	1.66	0.78
4:D:159:THR:O	4:D:163:VAL:HG23	1.83	0.78
4:D:130:LEU:HD13	4:D:142:LYS:HD3	1.65	0.77
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.18	0.77
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.65	0.77
7:G:129:SER:HB3	7:G:138:THR:OG1	1.84	0.77
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.67	0.77
2:B:516:ASN:HD22	2:B:516:ASN:N	1.81	0.77
2:B:465:ASN:HD22	2:B:465:ASN:N	1.81	0.77
2:B:955:THR:HG22	2:B:956:THR:O	1.83	0.77
4:D:14:ARG:HB3	4:D:14:ARG:NH1	1.98	0.77
4:D:71:LYS:HA	4:D:74:GLN:CG	2.14	0.77
10:J:23:ASN:C	10:J:25:LEU:H	1.93	0.77
2:B:547:VAL:HG12	2:B:612:GLU:OE2	1.85	0.77
5:E:117:THR:HB	5:E:120:ALA:CB	2.15	0.77
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.65	0.77
2:B:25:ILE:HD11	2:B:653:VAL:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:253:LYS:O	3:C:256:ALA:HB3	1.84	0.77
1:A:1135:ARG:HG2	1:A:1136:SER:N	2.00	0.77
4:D:202:ILE:HD13	4:D:207:LEU:HB2	1.65	0.77
5:E:124:VAL:HG13	5:E:132:ILE:CG1	2.14	0.77
8:H:59:ILE:HG22	8:H:60:ALA:N	1.97	0.77
10:J:1:MET:N	10:J:57:ILE:H	1.82	0.77
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.49	0.77
2:B:745:PRO:O	2:B:748:ILE:HG12	1.85	0.77
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.66	0.77
8:H:127:GLY:O	8:H:128:ASN:HB2	1.83	0.77
1:A:1261:LYS:O	1:A:1264:GLU:HB3	1.85	0.76
7:G:115:MET:HB3	7:G:116:PRO:HD2	1.65	0.76
1:A:1030:ARG:HG2	1:A:1034:GLU:OE2	1.86	0.76
2:B:589:VAL:HG12	2:B:590:HIS:H	1.50	0.76
2:B:987:LYS:HE3	15:P:11:G:O2'	1.85	0.76
1:A:666:ILE:N	2:B:1026:LEU:HD13	2.00	0.76
2:B:193:LYS:NZ	12:L:32:ALA:HB1	1.99	0.76
2:B:435:THR:C	2:B:437:GLU:H	1.93	0.76
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.01	0.76
5:E:198:ILE:HD11	5:E:212:ARG:HG3	1.65	0.76
14:T:27:DC:H42	15:P:2:A:H61	1.30	0.76
2:B:327:ARG:NH2	2:B:371:GLU:HG2	2.00	0.76
2:B:796:LEU:HD21	2:B:821:GLN:HE21	1.50	0.76
8:H:100:THR:HG23	8:H:138:GLU:HA	1.68	0.76
13:N:5:DC:H2''	13:N:6:DT:OP2	1.84	0.76
1:A:427:GLN:HG3	1:A:430:TRP:CE2	2.21	0.76
1:A:675:THR:O	1:A:679:ILE:HG13	1.85	0.76
1:A:1214:GLU:O	1:A:1218:GLN:HG2	1.85	0.76
1:A:1409:LEU:HD13	2:B:1207:LEU:HD11	1.66	0.76
2:B:254:LEU:HD12	2:B:272:THR:O	1.85	0.76
2:B:261:ARG:HB3	2:B:261:ARG:NH1	1.98	0.76
2:B:975:GLN:HG2	2:B:976:ILE:N	2.00	0.76
1:A:913:LEU:HD12	1:A:914:GLU:N	1.99	0.76
1:A:388:LEU:O	1:A:392:VAL:HG23	1.87	0.75
2:B:603:LEU:HD12	2:B:609:ILE:HG23	1.67	0.75
12:L:49:LYS:O	12:L:50:ASP:HB2	1.85	0.75
1:A:1206:ASP:HB3	1:A:1274:ARG:NH2	1.99	0.75
2:B:565:PRO:HB2	2:B:567:GLU:HG2	1.67	0.75
2:B:654:ARG:H	2:B:657:HIS:HD2	1.31	0.75
2:B:882:THR:CG2	2:B:884:ARG:H	2.00	0.75
4:D:167:LEU:HD21	4:D:214:LEU:HD21	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1158:PRO:HG2	1:A:1159:ARG:HE	1.49	0.75
2:B:278:GLN:HG2	2:B:279:ASP:N	2.00	0.75
3:C:220:ASP:CG	3:C:223:ALA:HB2	2.11	0.75
8:H:84:ALA:HB1	8:H:87:ARG:HB2	1.69	0.75
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.00	0.75
7:G:21:ARG:NH1	7:G:24:GLN:HB2	2.01	0.75
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.20	0.75
1:A:264:PHE:HB3	1:A:265:LYS:HZ1	1.52	0.75
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.01	0.75
2:B:351:TYR:O	2:B:355:ILE:HG13	1.86	0.75
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.68	0.75
1:A:524:VAL:HG12	1:A:525:GLN:H	1.49	0.75
2:B:272:THR:HG23	2:B:279:ASP:OD1	1.87	0.75
2:B:112:LEU:HD12	2:B:113:TYR:H	1.52	0.74
2:B:235:SER:C	2:B:236:HIS:HD2	1.95	0.74
2:B:345:LYS:HG2	2:B:346:GLU:N	1.99	0.74
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.01	0.74
3:C:259:LEU:HD21	11:K:91:CYS:HB3	1.69	0.74
1:A:1033:GLN:HA	1:A:1036:ARG:HH12	1.52	0.74
2:B:408:LEU:O	2:B:412:LEU:HD12	1.87	0.74
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.02	0.74
1:A:605:MET:HE2	1:A:607:ILE:CG1	2.16	0.74
8:H:130:ARG:HD3	8:H:130:ARG:N	2.02	0.74
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.23	0.74
1:A:1436:ILE:O	1:A:1437:GLY:C	2.30	0.74
2:B:710:LEU:CA	2:B:733:HIS:HB3	2.18	0.74
5:E:144:ILE:HG13	5:E:145:THR:N	2.03	0.74
1:A:886:ILE:HG23	1:A:887:GLY:N	2.03	0.74
2:B:955:THR:HG22	2:B:956:THR:N	2.02	0.74
3:C:115:SER:HB3	3:C:141:GLY:O	1.86	0.74
1:A:709:THR:HG22	1:A:710:LEU:H	1.53	0.74
2:B:549:THR:HB	2:B:628:THR:OG1	1.87	0.74
1:A:399:HIS:O	1:A:401:GLY:N	2.20	0.74
3:C:99:LEU:HD23	3:C:99:LEU:N	2.02	0.74
9:I:85:PHE:H	9:I:85:PHE:HD2	1.35	0.74
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.68	0.74
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.53	0.74
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.50	0.74
2:B:848:ARG:HH22	2:B:996:ARG:HD3	1.53	0.74
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.69	0.74
8:H:130:ARG:HH11	8:H:130:ARG:H	1.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:46:ILE:O	11:K:50:LEU:HB2	1.88	0.74
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.51	0.74
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.18	0.74
2:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.66	0.74
3:C:16:ASP:C	3:C:240:VAL:HG11	2.12	0.74
7:G:18:PHE:HA	7:G:22:MET:HE3	1.67	0.74
15:P:5:C:O2'	15:P:6:A:H5'	1.88	0.74
2:B:68:THR:HG22	2:B:91:SER:HA	1.70	0.74
4:D:71:LYS:HA	4:D:74:GLN:HG3	1.70	0.74
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.18	0.73
7:G:125:SER:OG	7:G:128:PRO:HA	1.88	0.73
1:A:288:ALA:HA	1:A:291:GLU:OE1	1.89	0.73
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.69	0.73
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.23	0.73
2:B:114:PRO:HG2	2:B:115:GLN:H	1.54	0.73
2:B:637:LEU:HD12	2:B:693:ILE:HD11	1.69	0.73
5:E:22:MET:HE3	5:E:26:ARG:NE	2.02	0.73
1:A:12:ARG:HB3	2:B:1218:THR:CG2	2.18	0.73
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.69	0.73
2:B:508:LEU:HD13	2:B:510:LYS:CE	2.14	0.73
8:H:89:LEU:O	8:H:91:ASP:N	2.22	0.73
1:A:308:ILE:HG22	1:A:309:ALA:H	1.51	0.73
3:C:3:GLU:HG2	3:C:4:GLU:HG3	1.70	0.73
8:H:139:ASN:O	8:H:140:ALA:HB2	1.89	0.73
11:K:65:HIS:HD2	11:K:67:PHE:H	1.36	0.73
12:L:55:ILE:O	12:L:56:LEU:HB2	1.88	0.73
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.17	0.73
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.18	0.73
2:B:110:HIS:HB3	12:L:54:ARG:HH22	1.51	0.73
2:B:622:LYS:HE2	9:I:59:VAL:CG2	2.19	0.73
2:B:918:ILE:HG21	2:B:935:ARG:NH2	2.03	0.73
3:C:183:TRP:O	3:C:185:LYS:N	2.21	0.73
3:C:189:THR:HG22	3:C:190:ASP:N	2.01	0.73
8:H:123:MET:HE1	8:H:142:LEU:HD21	1.69	0.73
12:L:53:HIS:HB3	12:L:55:ILE:CD1	2.18	0.73
1:A:898:ARG:HD2	1:A:899:VAL:N	2.04	0.73
2:B:219:ALA:HB2	2:B:405:ARG:NH1	2.03	0.73
2:B:557:PHE:HD2	2:B:557:PHE:O	1.72	0.73
2:B:999:MET:HA	2:B:999:MET:CE	2.18	0.73
4:D:7:THR:O	4:D:9:GLN:N	2.21	0.73
4:D:193:THR:HG21	7:G:167:TYR:CD1	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:30:ILE:O	12:L:56:LEU:HD23	1.88	0.73
1:A:157:ASP:OD2	1:A:159:THR:HB	1.88	0.73
1:A:1329:THR:HG22	1:A:1331:SER:N	2.03	0.73
3:C:22:LEU:HG	3:C:25:VAL:HG21	1.71	0.73
4:D:4:SER:O	4:D:5:THR:HB	1.88	0.73
4:D:23:ASN:N	4:D:23:ASN:ND2	2.33	0.73
1:A:35:ILE:HA	1:A:52:GLY:O	1.89	0.73
1:A:62:ASP:O	1:A:63:ARG:C	2.30	0.73
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.71	0.73
5:E:207:ARG:HB3	5:E:207:ARG:NH1	2.03	0.73
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.68	0.73
1:A:55:ASP:CG	1:A:55:ASP:O	2.29	0.72
2:B:800:GLN:HB3	10:J:52:THR:HG22	1.71	0.72
2:B:186:GLU:HG3	10:J:62:ARG:HH22	1.52	0.72
2:B:842:ASN:ND2	2:B:845:SER:H	1.86	0.72
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	1.89	0.72
11:K:12:LEU:HD12	11:K:37:LYS:HG2	1.71	0.72
14:T:16:DT:H2''	14:T:17:DT:C5'	2.20	0.72
1:A:117:GLU:H	1:A:117:GLU:CD	1.96	0.72
1:A:1127:ASP:CG	1:A:1130:GLN:HB2	2.13	0.72
2:B:134:LYS:HE2	2:B:164:LYS:NZ	2.04	0.72
2:B:865:LYS:NZ	2:B:869:SER:HA	2.04	0.72
5:E:164:LEU:HD13	5:E:211:TYR:CE2	2.25	0.72
1:A:66:LYS:HD3	1:A:67:CYS:N	2.05	0.72
2:B:653:VAL:HG23	2:B:689:LEU:HB3	1.70	0.72
3:C:189:THR:HG22	3:C:190:ASP:H	1.53	0.72
7:G:1:MET:SD	7:G:2:PHE:N	2.62	0.72
1:A:858:ASN:C	1:A:858:ASN:HD22	1.98	0.72
3:C:167:HIS:CD2	12:L:70:ARG:HB3	2.24	0.72
3:C:209:TYR:HD1	3:C:209:TYR:H	1.35	0.72
1:A:102:VAL:CG1	1:A:211:PHE:HE1	2.02	0.72
1:A:310:GLY:O	1:A:312:PRO:HD2	1.88	0.72
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.72	0.72
2:B:515:HIS:CD2	2:B:517:THR:HG23	2.25	0.72
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.69	0.72
4:D:23:ASN:H	4:D:23:ASN:ND2	1.88	0.72
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.71	0.72
1:A:70:CYS:O	1:A:72:GLU:HG2	1.89	0.72
1:A:425:GLN:OE1	1:A:425:GLN:N	2.22	0.72
1:A:767:GLN:NE2	1:A:774:ARG:HB3	2.05	0.72
2:B:705:MET:H	2:B:710:LEU:HD12	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:160:VAL:O	4:D:164:ILE:HG13	1.89	0.72
8:H:11:GLN:HA	8:H:53:ASP:O	1.89	0.72
1:A:103:CYS:SG	1:A:108:MET:HE1	2.29	0.72
1:A:666:ILE:CD1	1:A:667:GLY:H	2.02	0.72
1:A:858:ASN:ND2	1:A:860:LEU:H	1.88	0.72
2:B:248:SER:H	2:B:418:LYS:HZ1	1.35	0.72
2:B:806:THR:H	2:B:809:MET:HE3	1.54	0.72
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.72	0.72
7:G:21:ARG:HD2	7:G:24:GLN:HB3	1.72	0.72
1:A:34:LYS:HZ1	1:A:57:ARG:NH2	1.87	0.72
1:A:1205:LYS:O	1:A:1207:LEU:HG	1.89	0.72
1:A:1387:HIS:O	1:A:1391:ARG:HD3	1.90	0.72
2:B:824:ILE:HG12	10:J:48:ARG:HH12	1.53	0.72
3:C:7:GLN:HG3	11:K:104:ASN:HD22	1.53	0.72
12:L:55:ILE:HD13	12:L:55:ILE:H	1.55	0.72
2:B:44:VAL:HG21	2:B:199:MET:O	1.90	0.71
2:B:644:GLU:OE2	2:B:646:LEU:HB2	1.90	0.71
2:B:428:ILE:HG22	2:B:432:MET:HE2	1.71	0.71
2:B:549:THR:HG22	2:B:550:ASP:N	2.05	0.71
2:B:891:ASP:C	2:B:893:LEU:H	1.97	0.71
3:C:79:GLN:HE21	3:C:127:ARG:HD3	1.55	0.71
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.71	0.71
8:H:62:SER:O	8:H:63:LEU:HG	1.89	0.71
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.71	0.71
7:G:111:THR:CG2	7:G:114:LEU:HD13	2.20	0.71
8:H:102:TYR:OH	8:H:122:LEU:HD22	1.89	0.71
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.72	0.71
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.25	0.71
9:I:116:ASN:C	9:I:117:LYS:HD2	2.15	0.71
12:L:32:ALA:HB2	12:L:55:ILE:HG13	1.73	0.71
1:A:135:PHE:CD1	1:A:222:LEU:HD22	2.24	0.71
1:A:305:ASP:OD2	1:A:326:ARG:HD3	1.90	0.71
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.20	0.71
1:A:960:ILE:O	1:A:963:ILE:HG22	1.90	0.71
2:B:542:MET:HE2	2:B:747:MET:HG3	1.72	0.71
3:C:76:ASP:OD2	3:C:128:ASN:N	2.24	0.71
10:J:64:ASN:HB3	10:J:65:PRO:HD2	1.73	0.71
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.91	0.71
1:A:381:THR:HG22	1:A:383:TYR:N	2.03	0.71
1:A:503:GLN:HE21	6:F:90:ARG:HH22	1.34	0.71
2:B:345:LYS:CG	2:B:346:GLU:H	1.99	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:THR:HG22	3:C:57:VAL:H	1.54	0.71
1:A:344:ARG:HB3	1:A:344:ARG:NH1	2.06	0.71
2:B:248:SER:H	2:B:418:LYS:NZ	1.88	0.71
2:B:1031:LEU:HD11	2:B:1042:GLY:HA3	1.73	0.71
1:A:821:ARG:HB2	1:A:821:ARG:NH1	2.06	0.71
1:A:866:PHE:C	1:A:867:ILE:HD12	2.15	0.71
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.73	0.71
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.72	0.71
1:A:50:ILE:C	1:A:52:GLY:H	1.98	0.70
1:A:335:ARG:NH1	2:B:1202:LEU:HD13	2.05	0.70
2:B:860:MET:HG3	2:B:965:LYS:HG2	1.72	0.70
1:A:670:ILE:HG23	1:A:805:LEU:HD21	1.73	0.70
2:B:424:LEU:O	2:B:428:ILE:HG13	1.90	0.70
2:B:879:ARG:NH2	2:B:885:MET:HE2	2.06	0.70
3:C:66:ARG:NH2	10:J:3:VAL:O	2.24	0.70
4:D:24:ALA:CB	4:D:26:THR:HG23	2.21	0.70
5:E:197:LYS:HE2	5:E:199:ILE:HD11	1.73	0.70
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.72	0.70
9:I:71:SER:OG	9:I:83:ASN:HB2	1.92	0.70
11:K:68:PHE:HD1	11:K:70:ARG:HH12	1.39	0.70
1:A:1424:VAL:HG11	2:B:1139:ILE:CD1	2.20	0.70
9:I:34:TYR:CD2	9:I:35:VAL:N	2.60	0.70
1:A:268:ASP:HB3	1:A:299:HIS:ND1	2.05	0.70
2:B:243:ALA:HA	2:B:250:PHE:O	1.91	0.70
2:B:890:TYR:O	2:B:893:LEU:HB2	1.91	0.70
2:B:983:ARG:NH1	2:B:1028:GLU:OE1	2.24	0.70
7:G:34:VAL:HG11	7:G:74:TYR:CE1	2.21	0.70
1:A:444:PHE:HB3	1:A:458:HIS:HD2	1.56	0.70
1:A:1148:ILE:HD11	1:A:1198:ASP:HA	1.74	0.70
1:A:1244:ARG:HB2	1:A:1245:PRO:CD	2.22	0.70
2:B:842:ASN:ND2	2:B:845:SER:OG	2.24	0.70
8:H:82:PRO:C	8:H:84:ALA:H	1.98	0.70
1:A:763:ALA:O	1:A:803:SER:HB3	1.91	0.70
2:B:705:MET:N	2:B:710:LEU:HD12	2.05	0.70
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.56	0.70
3:C:11:ARG:HH12	3:C:205:LYS:NZ	1.90	0.70
9:I:55:THR:HG23	9:I:86:PHE:HZ	1.55	0.70
1:A:1081:LEU:HD11	1:A:1098:VAL:H	1.55	0.70
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.22	0.70
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.27	0.70
2:B:600:LEU:O	2:B:609:ILE:HD11	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.72	0.70
2:B:805:THR:HA	2:B:809:MET:HE1	1.73	0.70
3:C:93:ASP:OD1	3:C:122:SER:HB2	1.92	0.70
12:L:27:LEU:HD13	12:L:37:LYS:HD2	1.74	0.70
1:A:244:PRO:HB2	1:A:245:PRO:CD	2.18	0.70
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.21	0.70
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.07	0.70
2:B:681:TRP:HA	2:B:684:LEU:HD12	1.74	0.70
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.26	0.70
4:D:71:LYS:HG2	4:D:74:GLN:HG3	1.74	0.70
12:L:38:LEU:HD11	12:L:49:LYS:HE2	1.74	0.70
2:B:1122:ARG:HB3	14:T:22:DC:OP1	1.92	0.70
3:C:143:LEU:HD21	3:C:146:LYS:HE2	1.73	0.70
5:E:202:SER:OG	5:E:204:THR:HG22	1.90	0.70
9:I:55:THR:HG21	9:I:109:ILE:HD13	1.73	0.70
1:A:63:ARG:CA	1:A:74:MET:HE2	2.21	0.70
1:A:866:PHE:O	1:A:867:ILE:HD12	1.91	0.70
4:D:190:GLU:O	4:D:193:THR:HG22	1.92	0.70
4:D:208:GLU:O	4:D:212:LYS:HG3	1.92	0.70
9:I:50:THR:HG23	9:I:52:ILE:HG12	1.73	0.70
1:A:567:LYS:HE3	1:A:568:PRO:CG	2.21	0.69
1:A:883:LEU:HD11	1:A:1017:LEU:HD11	1.73	0.69
2:B:345:LYS:O	2:B:347:LYS:HG2	1.92	0.69
3:C:186:LEU:CD2	3:C:225:ALA:HB2	2.22	0.69
4:D:124:GLU:CD	4:D:124:GLU:H	2.00	0.69
8:H:4:THR:HA	8:H:60:ALA:CB	2.17	0.69
11:K:107:THR:O	11:K:111:LEU:HG	1.92	0.69
1:A:500:GLU:O	1:A:504:LEU:HB2	1.93	0.69
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.22	0.69
1:A:982:THR:HB	1:A:985:ASP:H	1.56	0.69
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.57	0.69
1:A:53:LEU:CD2	1:A:54:ASN:N	2.50	0.69
1:A:1155:ASP:OD2	1:A:1161:THR:HA	1.93	0.69
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.57	0.69
3:C:89:GLU:O	3:C:90:ASP:HB3	1.93	0.69
5:E:23:VAL:HG13	5:E:78:LEU:HD13	1.74	0.69
5:E:90:VAL:HB	5:E:117:THR:HG21	1.73	0.69
7:G:51:TYR:O	7:G:54:ILE:HG13	1.91	0.69
2:B:882:THR:CG2	2:B:934:LYS:O	2.41	0.69
5:E:164:LEU:HD22	5:E:211:TYR:CD2	2.27	0.69
4:D:156:ASP:C	4:D:158:GLU:H	2.01	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:86:THR:HG23	6:F:89:GLU:OE1	1.92	0.69
8:H:130:ARG:HH11	8:H:130:ARG:CB	2.05	0.69
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.57	0.69
9:I:102:VAL:HG22	9:I:109:ILE:HG12	1.73	0.69
1:A:351:THR:HG22	2:B:1103:ILE:CA	2.23	0.69
1:A:443:LEU:HD12	2:B:1146:PHE:CE2	2.28	0.69
1:A:898:ARG:HD2	1:A:899:VAL:H	1.57	0.69
1:A:1291:VAL:HG22	1:A:1292:PRO:CD	2.23	0.69
8:H:58:THR:HB	8:H:143:LEU:HD13	1.73	0.69
1:A:67:CYS:C	1:A:68:GLN:HG3	2.17	0.69
1:A:105:CYS:SG	1:A:139:TRP:HA	2.32	0.69
1:A:916:GLY:O	1:A:919:ILE:HG22	1.93	0.69
1:A:1317:MET:HE1	1:A:1339:LEU:HD21	1.75	0.69
2:B:789:MET:HE2	2:B:953:LEU:HD22	1.72	0.69
3:C:186:LEU:HD21	3:C:225:ALA:HB2	1.74	0.69
4:D:23:ASN:HD22	4:D:23:ASN:N	1.91	0.69
12:L:30:ILE:HG22	12:L:31:CYS:N	2.07	0.69
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.75	0.69
1:A:249:SER:O	1:A:250:ILE:HG13	1.91	0.69
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.75	0.69
1:A:1420:ASP:O	1:A:1421:CYS:HB2	1.93	0.69
2:B:60:GLN:O	2:B:63:ILE:HG22	1.93	0.69
2:B:957:ASN:HD21	2:B:961:LEU:HB2	1.58	0.69
2:B:1002:THR:OG1	2:B:1006:ILE:HG13	1.93	0.69
3:C:133:ILE:HD12	3:C:237:SER:N	2.08	0.69
5:E:128:PRO:HA	5:E:129:PRO:C	2.18	0.69
1:A:512:VAL:HA	1:A:519:PRO:HA	1.75	0.68
1:A:1095:THR:HG21	1:A:1112:LYS:CB	2.23	0.68
2:B:134:LYS:HE2	2:B:164:LYS:HZ3	1.58	0.68
2:B:405:ARG:NE	2:B:629:ASP:OD2	2.26	0.68
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.28	0.68
5:E:32:GLN:HG3	5:E:36:GLU:OE2	1.93	0.68
8:H:76:THR:O	8:H:77:ARG:HB2	1.92	0.68
1:A:444:PHE:HB3	1:A:458:HIS:CD2	2.27	0.68
1:A:853:ASP:O	1:A:854:ASN:HB2	1.92	0.68
1:A:1312:ASN:ND2	1:A:1315:GLU:HG3	2.08	0.68
2:B:805:THR:HG22	2:B:806:THR:N	2.07	0.68
6:F:109:VAL:HG12	6:F:110:ASP:N	2.05	0.68
7:G:21:ARG:HD2	7:G:24:GLN:CB	2.23	0.68
1:A:323:LYS:HD2	1:A:323:LYS:N	2.04	0.68
1:A:741:ASN:HD22	1:A:742:ASN:N	1.90	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:115:MET:HG2	7:G:163:ILE:HD11	1.74	0.68
10:J:12:LYS:O	10:J:14:VAL:HG23	1.93	0.68
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.74	0.68
1:A:567:LYS:CB	1:A:568:PRO:CD	2.69	0.68
1:A:1254:ALA:O	1:A:1255:GLU:HB2	1.92	0.68
1:A:1255:GLU:HG2	1:A:1258:HIS:HD2	1.58	0.68
4:D:50:LEU:HD11	7:G:4:ILE:HD11	1.74	0.68
1:A:167:CYS:HB2	1:A:169:ASN:ND2	2.08	0.68
2:B:737:THR:CG2	9:I:66:PRO:HA	2.23	0.68
2:B:987:LYS:H	2:B:987:LYS:HD3	1.57	0.68
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.74	0.68
5:E:28:TYR:C	5:E:65:THR:HG22	2.19	0.68
2:B:873:THR:O	2:B:914:LYS:HA	1.93	0.68
5:E:124:VAL:N	5:E:125:PRO:HD2	2.09	0.68
14:T:11:DA:H2''	14:T:12:DG:H5'	1.75	0.68
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.22	0.68
2:B:597:MET:HE1	2:B:624:LEU:HD21	1.76	0.68
14:T:10:DA:H2''	14:T:11:DA:C8	2.29	0.68
1:A:335:ARG:HH12	2:B:1206:GLU:CD	2.02	0.68
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.75	0.68
1:A:605:MET:HE2	1:A:607:ILE:HG12	1.75	0.68
1:A:1029:ARG:HH11	1:A:1029:ARG:HG3	1.59	0.68
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.06	0.68
1:A:1188:GLN:OE1	1:A:1241:ARG:HD2	1.93	0.68
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.76	0.68
4:D:13:ARG:C	4:D:15:LEU:H	2.02	0.68
5:E:31:THR:HG23	5:E:34:GLU:HB2	1.74	0.68
6:F:96:THR:O	6:F:100:GLN:HG3	1.93	0.68
7:G:116:PRO:HG2	7:G:119:LEU:CB	2.24	0.68
11:K:65:HIS:CD2	11:K:67:PHE:H	2.11	0.68
1:A:154:SER:HB3	1:A:162:VAL:CG2	2.24	0.68
1:A:709:THR:HG23	9:I:94:ASP:HA	1.75	0.68
2:B:237:VAL:HG22	2:B:257:LYS:HA	1.75	0.68
4:D:24:ALA:HB3	4:D:26:THR:CG2	2.24	0.68
12:L:48:CYS:HB3	12:L:51:CYS:O	1.93	0.68
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.34	0.68
2:B:464:GLY:O	2:B:477:ALA:HA	1.94	0.68
2:B:43:LEU:HD11	2:B:811:TYR:O	1.94	0.67
2:B:232:SER:HA	14:T:11:DA:OP1	1.93	0.67
4:D:190:GLU:C	4:D:193:THR:HG22	2.19	0.67
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:THR:HB	1:A:712:GLU:H	1.59	0.67
1:A:1158:PRO:HG2	1:A:1159:ARG:NE	2.09	0.67
2:B:473:MET:HE3	2:B:474:SER:N	2.09	0.67
2:B:847:ASP:C	2:B:849:GLY:H	2.02	0.67
10:J:27:GLU:O	10:J:29:GLU:N	2.28	0.67
2:B:705:MET:H	2:B:710:LEU:CD1	2.07	0.67
1:A:284:ALA:O	1:A:286:HIS:N	2.28	0.67
2:B:34:ILE:HG12	2:B:542:MET:HE1	1.77	0.67
4:D:59:ILE:HG21	4:D:145:MET:SD	2.35	0.67
1:A:34:LYS:HZ2	1:A:57:ARG:NH2	1.90	0.67
1:A:369:SER:HB3	11:K:2:ASN:OD1	1.93	0.67
2:B:589:VAL:HG12	2:B:590:HIS:N	2.10	0.67
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.22	0.67
1:A:596:THR:C	1:A:598:LEU:H	2.03	0.67
1:A:683:ILE:HD13	1:A:801:GLU:CG	2.24	0.67
1:A:886:ILE:HG23	1:A:887:GLY:H	1.58	0.67
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	1.94	0.67
2:B:863:GLU:O	2:B:961:LEU:HD13	1.94	0.67
3:C:254:LYS:O	3:C:258:ILE:HD13	1.94	0.67
6:F:103:MET:HE2	7:G:66:GLY:N	2.09	0.67
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.24	0.67
1:A:743:VAL:O	1:A:747:VAL:HG23	1.94	0.67
1:A:1187:GLN:HA	1:A:1244:ARG:HB3	1.76	0.67
2:B:846:ILE:CG2	2:B:974:PRO:HG2	2.23	0.67
5:E:69:ILE:N	5:E:69:ILE:HD12	2.09	0.67
1:A:524:VAL:HG12	1:A:525:GLN:N	2.10	0.67
1:A:946:VAL:HG12	1:A:947:PHE:CD2	2.30	0.67
5:E:48:ASP:CG	5:E:49:SER:H	2.01	0.67
6:F:89:GLU:O	6:F:93:ILE:HD12	1.94	0.67
1:A:567:LYS:HZ3	8:H:46:LEU:HB2	1.59	0.67
1:A:718:VAL:O	1:A:722:LEU:HD12	1.95	0.67
2:B:399:ASP:OD2	2:B:510:LYS:HB2	1.95	0.67
4:D:32:GLU:OE1	7:G:41:LYS:HE2	1.94	0.67
1:A:341:MET:HE1	2:B:1135:ARG:HH11	1.60	0.67
1:A:809:THR:OG1	1:A:812:GLU:HG3	1.94	0.67
1:A:1313:LEU:C	1:A:1315:GLU:H	2.02	0.67
2:B:68:THR:HG22	2:B:91:SER:HB3	1.77	0.67
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.30	0.67
2:B:778:MET:HE1	2:B:1094:ARG:HD3	1.77	0.67
2:B:863:GLU:OE2	2:B:873:THR:HA	1.94	0.67
2:B:899:ILE:HG22	2:B:900:ALA:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:30:SER:HB2	8:H:36:CYS:HB3	1.77	0.67
9:I:55:THR:HG23	9:I:86:PHE:CZ	2.30	0.67
2:B:515:HIS:H	2:B:518:HIS:HD2	1.43	0.66
4:D:119:ARG:HH11	4:D:119:ARG:HG3	1.60	0.66
5:E:94:LYS:O	5:E:98:ILE:HG13	1.95	0.66
9:I:50:THR:HG22	9:I:51:ASN:N	2.10	0.66
9:I:80:SER:OG	9:I:105:SER:HB2	1.95	0.66
1:A:332:LYS:O	1:A:333:GLU:HB2	1.94	0.66
1:A:382:PRO:CA	1:A:428:TYR:HE2	2.07	0.66
1:A:567:LYS:CB	8:H:95:TYR:HA	2.24	0.66
1:A:925:LEU:HD13	1:A:983:ILE:CG2	2.24	0.66
2:B:882:THR:C	2:B:884:ARG:H	2.00	0.66
2:B:1187:ASN:O	2:B:1188:LYS:CB	2.42	0.66
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.78	0.66
9:I:55:THR:HG22	9:I:55:THR:O	1.94	0.66
8:H:95:TYR:HE2	8:H:97:MET:CG	2.06	0.66
9:I:58:VAL:HG13	9:I:62:ILE:HD13	1.78	0.66
1:A:122:MET:HA	1:A:141:LEU:CD1	2.25	0.66
1:A:684:ALA:O	1:A:687:LYS:HB2	1.94	0.66
1:A:688:LYS:HD2	1:A:691:LEU:HD23	1.77	0.66
1:A:873:MET:C	1:A:1058:VAL:HG23	2.19	0.66
1:A:1223:ASP:HA	1:A:1243:VAL:HG11	1.76	0.66
2:B:251:ILE:O	2:B:251:ILE:HG22	1.96	0.66
2:B:570:VAL:HG21	2:B:573:GLN:CD	2.20	0.66
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.24	0.66
2:B:917:PRO:O	2:B:918:ILE:HG13	1.95	0.66
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.30	0.66
1:A:55:ASP:N	1:A:56:PRO:HD3	2.10	0.66
3:C:124:LEU:HD21	3:C:129:ILE:O	1.95	0.66
3:C:161:LYS:O	3:C:170:TRP:NE1	2.27	0.66
4:D:185:CYS:O	4:D:211:LEU:HD22	1.94	0.66
9:I:76:PRO:HD2	9:I:108:HIS:CD2	2.29	0.66
1:A:446:ARG:HB3	1:A:478:TYR:HB3	1.77	0.66
1:A:547:LEU:HD13	11:K:58:PHE:CD1	2.31	0.66
3:C:184:ASN:OD1	3:C:187:LYS:HA	1.94	0.66
4:D:29:LEU:HD22	4:D:29:LEU:N	2.10	0.66
6:F:69:LEU:HD13	6:F:71:GLU:OE1	1.96	0.66
6:F:82:THR:CG2	6:F:84:TYR:H	2.09	0.66
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.77	0.66
1:A:7:SER:HB3	2:B:1193:GLN:HE22	1.60	0.66
1:A:49:LYS:HZ1	1:A:61:ILE:N	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.60	0.66
1:A:563:PRO:HD3	8:H:79:TRP:CD1	2.31	0.66
1:A:942:PHE:HE1	5:E:207:ARG:HD3	1.58	0.66
2:B:394:ASP:OD2	2:B:394:ASP:N	2.23	0.66
2:B:558:LEU:CD2	2:B:596:LEU:HD11	2.26	0.66
8:H:58:THR:HG22	8:H:59:ILE:H	1.60	0.66
2:B:69:LEU:HB3	2:B:429:PHE:HE1	1.61	0.66
2:B:110:HIS:HB2	12:L:54:ARG:NH2	2.10	0.66
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.78	0.66
2:B:1099:VAL:HG13	2:B:1100:ASP:N	2.11	0.66
5:E:19:VAL:O	5:E:23:VAL:HG23	1.95	0.66
5:E:48:ASP:HB3	5:E:54:GLN:NE2	2.10	0.66
1:A:1027:ALA:O	1:A:1031:VAL:HG23	1.96	0.66
1:A:23:SER:HA	1:A:233:TRP:CD1	2.31	0.66
1:A:503:GLN:NE2	6:F:90:ARG:HH22	1.93	0.66
2:B:1060:ARG:CZ	3:C:202:PRO:HG3	2.25	0.66
4:D:54:GLU:O	4:D:58:VAL:HG23	1.95	0.66
7:G:27:LYS:HD3	7:G:51:TYR:CE2	2.31	0.66
1:A:914:GLU:HB2	1:A:979:SER:O	1.96	0.65
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.75	0.65
2:B:882:THR:HG23	2:B:884:ARG:CB	2.24	0.65
2:B:1115:THR:O	2:B:1116:ARG:HB2	1.94	0.65
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.29	0.65
7:G:111:THR:HG23	7:G:114:LEU:HD13	1.77	0.65
9:I:4:PHE:HE2	9:I:14:LEU:O	1.79	0.65
1:A:471:ASN:OD1	1:A:472:LEU:N	2.30	0.65
1:A:1152:ILE:HD13	1:A:1260:LEU:HD23	1.78	0.65
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.31	0.65
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.77	0.65
2:B:309:GLN:CD	9:I:52:ILE:HD11	2.21	0.65
2:B:654:ARG:H	2:B:657:HIS:CD2	2.12	0.65
2:B:654:ARG:HH11	2:B:654:ARG:HG3	1.61	0.65
2:B:902:GLY:O	12:L:65:VAL:HG11	1.97	0.65
4:D:156:ASP:O	4:D:158:GLU:N	2.30	0.65
9:I:6:PHE:N	9:I:6:PHE:CD1	2.64	0.65
12:L:30:ILE:O	12:L:56:LEU:HA	1.95	0.65
1:A:122:MET:HA	1:A:141:LEU:HD11	1.79	0.65
1:A:1313:LEU:O	1:A:1315:GLU:N	2.30	0.65
2:B:1001:PHE:CE2	3:C:34:ARG:NE	2.65	0.65
2:B:1124:ARG:HB3	2:B:1124:ARG:HH11	1.60	0.65
3:C:166:GLU:C	11:K:6:ARG:NH1	2.54	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:116:ILE:O	5:E:121:MET:HE2	1.96	0.65
8:H:43:ASN:ND2	8:H:46:LEU:HD12	2.11	0.65
9:I:85:PHE:CD1	9:I:99:LEU:HD13	2.31	0.65
10:J:27:GLU:O	10:J:29:GLU:HG3	1.95	0.65
1:A:49:LYS:HZ1	1:A:61:ILE:CG1	2.07	0.65
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.26	0.65
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.27	0.65
1:A:1255:GLU:HG2	1:A:1258:HIS:CD2	2.31	0.65
2:B:65:GLU:OE1	2:B:418:LYS:HE3	1.97	0.65
2:B:882:THR:HG21	2:B:934:LYS:O	1.95	0.65
3:C:172:PRO:O	3:C:235:VAL:HG23	1.95	0.65
7:G:27:LYS:HG2	7:G:54:ILE:HD12	1.77	0.65
10:J:3:VAL:HA	10:J:53:HIS:CE1	2.32	0.65
12:L:32:ALA:HB3	12:L:55:ILE:HG13	1.77	0.65
1:A:709:THR:HG22	1:A:710:LEU:N	2.10	0.65
2:B:189:LEU:O	2:B:192:LEU:N	2.29	0.65
3:C:34:ARG:NH1	3:C:35:ARG:HG2	2.12	0.65
3:C:73:GLN:HE21	3:C:75:MET:N	1.93	0.65
5:E:56:LYS:HZ2	5:E:85:GLU:HG3	1.62	0.65
7:G:1:MET:SD	7:G:79:PHE:CD1	2.90	0.65
8:H:109:LYS:HG2	8:H:110:ASP:OD1	1.96	0.65
12:L:28:LYS:HB3	12:L:39:SER:HB2	1.79	0.65
1:A:66:LYS:O	1:A:67:CYS:HB2	1.96	0.65
1:A:90:VAL:HG11	1:A:297:GLN:HA	1.77	0.65
2:B:243:ALA:CB	2:B:251:ILE:HD13	2.21	0.65
2:B:516:ASN:N	2:B:516:ASN:ND2	2.44	0.65
2:B:978:ASP:OD2	2:B:1098:MET:HG2	1.96	0.65
4:D:12:ARG:HG2	4:D:12:ARG:HH11	1.61	0.65
5:E:17:ARG:O	5:E:20:LYS:HB2	1.97	0.65
7:G:123:ALA:C	7:G:125:SER:H	2.04	0.65
1:A:102:VAL:HB	1:A:211:PHE:CE1	2.32	0.65
1:A:1195:LEU:HD11	1:A:1267:MET:HE1	1.78	0.65
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.77	0.65
2:B:193:LYS:HZ2	12:L:32:ALA:HB1	1.60	0.65
4:D:66:ARG:HD2	4:D:133:THR:HB	1.78	0.65
5:E:176:PRO:O	5:E:212:ARG:HA	1.97	0.65
6:F:82:THR:HG22	6:F:84:TYR:N	2.09	0.65
11:K:63:VAL:HG23	11:K:63:VAL:O	1.95	0.65
1:A:37:PHE:N	1:A:37:PHE:CD1	2.64	0.65
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.31	0.65
1:A:903:ASN:HD22	1:A:904:THR:H	1.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:GLN:O	1:A:1134:ILE:HG13	1.97	0.65
2:B:944:THR:HG21	2:B:1122:ARG:NH2	2.12	0.65
2:B:955:THR:CG2	2:B:956:THR:N	2.60	0.65
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.21	0.65
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.78	0.65
7:G:126:ASN:C	7:G:126:ASN:HD22	2.05	0.65
1:A:7:SER:HB3	2:B:1193:GLN:NE2	2.11	0.65
2:B:378:LEU:HD12	2:B:378:LEU:O	1.97	0.65
2:B:879:ARG:NH2	2:B:885:MET:CE	2.60	0.65
2:B:879:ARG:H	2:B:879:ARG:CD	2.10	0.65
2:B:1037:LEU:HD21	2:B:1064:TYR:HE1	1.62	0.65
3:C:242:GLN:C	3:C:244:VAL:H	2.05	0.65
9:I:61:ASP:C	9:I:63:GLY:H	2.05	0.65
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.79	0.65
2:B:25:ILE:CG2	2:B:658:ILE:HD12	2.27	0.65
2:B:579:ARG:HA	2:B:589:VAL:HG13	1.78	0.65
6:F:118:LEU:O	6:F:122:MET:HG3	1.96	0.65
10:J:1:MET:H1	10:J:57:ILE:H	1.45	0.65
12:L:53:HIS:O	12:L:55:ILE:HD13	1.97	0.65
1:A:250:ILE:O	1:A:250:ILE:HG22	1.96	0.64
1:A:977:LYS:HB3	1:A:978:PRO:HD2	1.78	0.64
1:A:1352:VAL:O	1:A:1355:VAL:HG12	1.96	0.64
2:B:90:ILE:HD11	2:B:432:MET:SD	2.38	0.64
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.27	0.64
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.20	0.64
4:D:56:ARG:HA	4:D:148:LEU:HD13	1.78	0.64
5:E:98:ILE:HA	5:E:101:GLN:HB3	1.79	0.64
7:G:116:PRO:HD2	7:G:119:LEU:HD23	1.79	0.64
8:H:84:ALA:O	8:H:85:GLY:C	2.41	0.64
12:L:55:ILE:HG12	12:L:56:LEU:N	2.11	0.64
1:A:904:THR:O	1:A:904:THR:HG22	1.97	0.64
2:B:294:ASP:O	2:B:296:GLU:N	2.30	0.64
3:C:244:VAL:O	3:C:248:ILE:HG13	1.98	0.64
1:A:961:ARG:HG2	1:A:965:GLN:HE21	1.62	0.64
8:H:25:ARG:HA	8:H:41:ASP:HA	1.79	0.64
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.79	0.64
1:A:390:GLN:NE2	1:A:394:ASN:HD22	1.95	0.64
2:B:639:ILE:HG22	2:B:641:GLU:HG2	1.79	0.64
2:B:708:GLU:HG3	2:B:709:ASP:H	1.63	0.64
2:B:872:GLU:CD	2:B:914:LYS:HE3	2.23	0.64
3:C:31:ASN:OD1	3:C:34:ARG:HD3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:165:LYS:O	11:K:6:ARG:NH1	2.31	0.64
4:D:144:THR:O	4:D:148:LEU:HB2	1.97	0.64
7:G:59:GLY:HA3	7:G:70:PHE:CD2	2.33	0.64
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.81	0.64
2:B:56:ASP:HB3	2:B:57:TYR:CD1	2.32	0.64
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.79	0.64
4:D:119:ARG:HG3	4:D:119:ARG:NH1	2.12	0.64
7:G:9:LEU:HD12	7:G:10:ASN:N	2.13	0.64
8:H:84:ALA:CB	8:H:87:ARG:HD2	2.27	0.64
1:A:347:PHE:HE2	1:A:375:THR:HG23	1.61	0.64
1:A:573:SER:O	1:A:576:GLN:HB2	1.97	0.64
4:D:128:VAL:C	4:D:130:LEU:N	2.54	0.64
4:D:153:ARG:C	4:D:154:PHE:CD2	2.76	0.64
4:D:156:ASP:C	4:D:158:GLU:N	2.54	0.64
1:A:35:ILE:HG22	1:A:35:ILE:O	1.96	0.64
1:A:535:THR:CG2	1:A:616:VAL:HA	2.27	0.64
2:B:98:THR:HG23	2:B:127:GLY:O	1.98	0.64
2:B:885:MET:HA	2:B:936:ASP:CB	2.26	0.64
2:B:1159:ARG:HB3	2:B:1159:ARG:NH1	2.12	0.64
5:E:127:ILE:O	5:E:127:ILE:HG13	1.96	0.64
7:G:111:THR:O	7:G:114:LEU:N	2.28	0.64
14:T:18:DC:H2"	14:T:19:DT:OP2	1.97	0.64
1:A:153:PRO:HD3	1:A:161:LEU:HD13	1.77	0.64
1:A:596:THR:O	1:A:598:LEU:N	2.31	0.64
1:A:1444:MET:HG3	7:G:59:GLY:O	1.97	0.64
1:A:1445:ILE:HD11	7:G:68:ALA:HB1	1.80	0.64
2:B:597:MET:HA	2:B:597:MET:CE	2.27	0.64
2:B:916:THR:HB	2:B:935:ARG:HD2	1.80	0.64
2:B:1102:LYS:O	2:B:1103:ILE:C	2.41	0.64
2:B:1181:GLU:HB2	2:B:1188:LYS:HG3	1.79	0.64
4:D:66:ARG:O	4:D:70:PHE:HB2	1.98	0.64
4:D:145:MET:O	4:D:149:THR:HB	1.96	0.64
5:E:144:ILE:HG13	5:E:145:THR:H	1.61	0.64
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.63	0.64
2:B:515:HIS:H	2:B:518:HIS:CD2	2.16	0.64
3:C:196:ASP:OD2	3:C:199:LYS:HE3	1.98	0.64
7:G:116:PRO:HG2	7:G:119:LEU:HB3	1.78	0.64
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.78	0.64
10:J:1:MET:N	10:J:56:LEU:N	2.46	0.64
1:A:1258:HIS:O	1:A:1262:LYS:HE3	1.97	0.64
2:B:408:LEU:O	2:B:411:PRO:HD2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:LYS:HG3	2:B:426:LYS:O	1.97	0.64
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.79	0.64
5:E:78:LEU:HD21	5:E:80:VAL:HG23	1.80	0.64
1:A:478:TYR:O	1:A:479:ASN:HB2	1.97	0.63
1:A:794:PRO:HG2	1:A:795:GLU:OE2	1.98	0.63
3:C:120:ILE:CD1	3:C:124:LEU:HD11	2.27	0.63
1:A:590:ARG:O	1:A:591:PHE:HB2	1.98	0.63
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.81	0.63
1:A:1341:ILE:HD12	1:A:1379:GLY:O	1.97	0.63
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.79	0.63
3:C:100:THR:HG21	3:C:102:GLN:HE21	1.64	0.63
4:D:138:ASN:HB3	4:D:141:LEU:HB3	1.80	0.63
1:A:984:LYS:HG2	1:A:988:LEU:HD11	1.80	0.63
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.78	0.63
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.29	0.63
2:B:221:ASN:O	2:B:222:ILE:HG13	1.99	0.63
2:B:289:LEU:HD13	2:B:375:ALA:CB	2.25	0.63
2:B:996:ARG:HH12	3:C:175:ALA:H	1.46	0.63
3:C:236:GLY:O	3:C:238:ILE:N	2.31	0.63
4:D:35:LEU:HD11	4:D:173:HIS:CD2	2.33	0.63
4:D:179:GLN:OE1	4:D:179:GLN:HA	1.97	0.63
7:G:87:VAL:HG23	7:G:103:VAL:HG21	1.79	0.63
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.33	0.63
1:A:1107:VAL:O	1:A:1107:VAL:CG1	2.45	0.63
1:A:1387:HIS:CE1	13:N:4:DA:H5'	2.33	0.63
2:B:558:LEU:HD11	2:B:596:LEU:HD21	1.79	0.63
9:I:58:VAL:HG13	9:I:62:ILE:CD1	2.29	0.63
1:A:185:TRP:N	1:A:185:TRP:CE3	2.65	0.63
2:B:798:TYR:CE2	3:C:62:PHE:CE2	2.82	0.63
11:K:54:ARG:HG2	11:K:54:ARG:HH11	1.63	0.63
1:A:1094:VAL:HG13	1:A:1113:THR:CG2	2.28	0.63
1:A:1187:GLN:CB	1:A:1244:ARG:HG2	2.25	0.63
1:A:1223:ASP:HA	1:A:1243:VAL:CG1	2.28	0.63
3:C:11:ARG:HH12	3:C:205:LYS:CE	2.11	0.63
4:D:123:LEU:O	4:D:127:ASP:HB2	1.99	0.63
8:H:56:THR:HB	8:H:145:ARG:HG2	1.79	0.63
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.13	0.63
1:A:710:LEU:HD12	1:A:710:LEU:N	2.14	0.63
2:B:364:ILE:O	2:B:365:THR:HB	1.97	0.63
2:B:579:ARG:HG2	2:B:579:ARG:HH11	1.64	0.63
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:PHE:N	1:A:37:PHE:HD1	1.97	0.63
1:A:134:ARG:HD2	1:A:221:SER:O	1.98	0.63
1:A:288:ALA:HA	1:A:291:GLU:CD	2.24	0.63
2:B:56:ASP:HB3	2:B:57:TYR:HD1	1.63	0.63
2:B:235:SER:C	2:B:236:HIS:CD2	2.77	0.63
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.80	0.63
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.17	0.63
1:A:308:ILE:HG22	1:A:309:ALA:N	2.13	0.63
2:B:35:SER:HA	2:B:811:TYR:HE2	1.63	0.63
2:B:839:MET:CE	2:B:1010:LEU:HD21	2.28	0.63
5:E:84:ASP:O	5:E:86:PRO:HD3	1.97	0.63
7:G:91:VAL:HG23	7:G:141:SER:O	1.98	0.63
11:K:31:VAL:HG12	11:K:32:VAL:N	2.13	0.63
1:A:93:VAL:HG23	1:A:304:MET:HE3	1.81	0.62
1:A:347:PHE:H	2:B:1107:ALA:HA	1.63	0.62
1:A:390:GLN:O	1:A:394:ASN:HB2	1.99	0.62
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.81	0.62
2:B:995:ARG:NH1	3:C:165:LYS:HG2	2.14	0.62
3:C:163:ILE:HG13	3:C:165:LYS:H	1.64	0.62
3:C:179:GLU:HG2	3:C:180:TYR:N	2.14	0.62
12:L:53:HIS:HB3	12:L:55:ILE:HD11	1.80	0.62
2:B:756:ILE:O	2:B:759:PRO:HD3	1.98	0.62
2:B:891:ASP:O	2:B:893:LEU:N	2.32	0.62
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.34	0.62
3:C:20:PHE:CE1	3:C:230:MET:HE3	2.33	0.62
5:E:213:ILE:HG12	5:E:214:CYS:H	1.64	0.62
7:G:20:PRO:HD2	7:G:21:ARG:H	1.64	0.62
11:K:82:ASP:OD1	11:K:84:LYS:N	2.32	0.62
1:A:145:LYS:HA	1:A:145:LYS:HE3	1.81	0.62
1:A:714:PHE:O	1:A:718:VAL:HG23	2.00	0.62
1:A:754:SER:N	1:A:757:ASN:HD22	1.96	0.62
1:A:1018:PHE:O	1:A:1021:LEU:HB3	1.98	0.62
1:A:11:LEU:HB2	2:B:1193:GLN:HG2	1.81	0.62
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.34	0.62
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.34	0.62
1:A:1161:THR:C	1:A:1163:ILE:H	2.07	0.62
1:A:1353:TYR:C	1:A:1353:TYR:CD2	2.77	0.62
2:B:987:LYS:HG3	15:P:11:G:O2'	1.99	0.62
12:L:61:THR:HG22	12:L:62:LYS:N	2.15	0.62
1:A:266:LEU:HD21	1:A:303:TYR:CE1	2.34	0.62
1:A:367:PRO:HG2	1:A:370:ILE:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:THR:O	1:A:698:GLN:HG3	1.98	0.62
1:A:831:THR:CG2	1:A:832:ALA:H	2.13	0.62
1:A:1239:ARG:HH22	1:A:1241:ARG:HH22	1.45	0.62
1:A:1420:ASP:N	1:A:1420:ASP:OD2	2.31	0.62
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.00	0.62
2:B:293:PRO:HG2	2:B:296:GLU:HB3	1.81	0.62
2:B:637:LEU:CD2	2:B:742:GLU:HA	2.30	0.62
2:B:654:ARG:N	2:B:657:HIS:HD2	1.96	0.62
5:E:78:LEU:HD23	5:E:78:LEU:C	2.23	0.62
8:H:77:ARG:HG2	8:H:78:SER:H	1.63	0.62
9:I:44:TYR:CD1	9:I:45:ARG:N	2.68	0.62
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.82	0.62
2:B:616:ILE:HD12	2:B:616:ILE:N	2.14	0.62
2:B:844:SER:O	2:B:847:ASP:HB2	2.00	0.62
2:B:948:ILE:HG22	2:B:949:VAL:O	1.99	0.62
5:E:157:SER:O	5:E:159:ASP:N	2.33	0.62
8:H:11:GLN:O	8:H:28:ALA:HB1	2.00	0.62
10:J:3:VAL:HA	10:J:53:HIS:ND1	2.14	0.62
12:L:26:THR:CG2	12:L:27:LEU:N	2.63	0.62
1:A:41:MET:HB2	1:A:49:LYS:HA	1.81	0.62
1:A:1171:GLN:O	1:A:1174:PHE:HB2	2.00	0.62
2:B:345:LYS:N	2:B:347:LYS:HE2	2.15	0.62
2:B:954:VAL:O	12:L:55:ILE:O	2.16	0.62
2:B:957:ASN:O	2:B:959:ASP:N	2.33	0.62
3:C:34:ARG:HH11	3:C:35:ARG:HG2	1.64	0.62
3:C:92:CYS:SG	3:C:94:LYS:HB3	2.40	0.62
4:D:192:LYS:HD2	4:D:199:ASN:HA	1.81	0.62
9:I:93:LYS:HD3	9:I:93:LYS:N	2.15	0.62
1:A:106:VAL:HG12	1:A:107:CYS:N	2.15	0.62
1:A:590:ARG:HG2	1:A:604:GLY:HA2	1.80	0.62
1:A:718:VAL:HG12	1:A:722:LEU:HD11	1.81	0.62
1:A:984:LYS:HG2	1:A:988:LEU:CD1	2.30	0.62
2:B:217:ARG:HD2	2:B:217:ARG:C	2.24	0.62
2:B:466:TRP:O	2:B:468:GLU:N	2.33	0.62
2:B:582:VAL:HG23	2:B:626:ILE:HB	1.80	0.62
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.81	0.62
1:A:399:HIS:O	1:A:400:PRO:C	2.40	0.62
1:A:782:ARG:NH2	2:B:699:GLU:O	2.33	0.62
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.35	0.62
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.99	0.62
2:B:57:TYR:HD1	2:B:57:TYR:N	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.82	0.62
3:C:148:ARG:H	3:C:151:GLN:HG3	1.65	0.62
3:C:235:VAL:HG13	10:J:13:VAL:HG22	1.82	0.62
5:E:99:HIS:O	5:E:103:LYS:HG2	1.99	0.62
10:J:27:GLU:C	10:J:29:GLU:H	2.08	0.62
1:A:75:ASN:HD22	2:B:1116:ARG:NH1	1.97	0.62
1:A:1218:GLN:O	1:A:1221:LYS:HG3	2.00	0.62
2:B:642:ASP:CA	2:B:649:LYS:HA	2.30	0.62
1:A:1170:ILE:HD12	1:A:1170:ILE:N	2.13	0.61
2:B:615:MET:CB	2:B:626:ILE:HG12	2.29	0.61
2:B:707:PRO:HG2	2:B:708:GLU:N	2.13	0.61
7:G:132:SER:HB3	7:G:135:ASP:H	1.65	0.61
9:I:84:VAL:HG13	9:I:84:VAL:O	2.00	0.61
1:A:1336:MET:HE2	1:A:1381:LEU:HG	1.81	0.61
2:B:879:ARG:H	2:B:879:ARG:NE	1.97	0.61
2:B:996:ARG:NH2	3:C:38:ILE:HG23	2.15	0.61
2:B:1130:PHE:HZ	2:B:1138:MET:HG2	1.65	0.61
3:C:205:LYS:O	3:C:205:LYS:HG2	2.00	0.61
4:D:128:VAL:C	4:D:130:LEU:H	2.07	0.61
1:A:69:THR:O	1:A:71:GLN:HG3	2.01	0.61
1:A:69:THR:HG21	2:B:1174:LYS:HZ2	1.65	0.61
1:A:774:ARG:HB2	1:A:797:LYS:O	2.01	0.61
2:B:305:VAL:O	2:B:305:VAL:HG12	1.99	0.61
2:B:563:MET:HE1	2:B:580:VAL:HB	1.82	0.61
4:D:4:SER:O	4:D:5:THR:CB	2.47	0.61
10:J:44:TYR:H	10:J:44:TYR:HD2	1.48	0.61
1:A:2:VAL:HG22	1:A:3:GLY:H	1.66	0.61
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.35	0.61
1:A:150:THR:HG23	1:A:166:GLY:HA2	1.81	0.61
1:A:661:GLY:HA3	2:B:1081:LEU:HD22	1.81	0.61
2:B:465:ASN:N	2:B:465:ASN:ND2	2.45	0.61
2:B:617:ARG:HA	2:B:624:LEU:HD12	1.83	0.61
2:B:953:LEU:CD2	2:B:965:LYS:HB2	2.30	0.61
4:D:195:ILE:CG2	4:D:198:LEU:HG	2.31	0.61
8:H:5:LEU:HG	8:H:60:ALA:HA	1.83	0.61
9:I:44:TYR:HD1	9:I:45:ARG:N	1.98	0.61
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.30	0.61
1:A:288:ALA:HA	1:A:291:GLU:CG	2.30	0.61
1:A:768:GLN:CG	1:A:816:HIS:HA	2.28	0.61
1:A:1150:SER:HB3	1:A:1195:LEU:CD2	2.31	0.61
2:B:20:ASP:C	2:B:22:SER:H	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:12:ARG:NH1	4:D:14:ARG:HA	2.15	0.61
7:G:26:LEU:HD11	7:G:70:PHE:CD1	2.35	0.61
9:I:101:PHE:N	9:I:101:PHE:CD1	2.68	0.61
1:A:320:ARG:NE	1:A:323:LYS:HZ1	1.97	0.61
1:A:482:PHE:CE1	2:B:836:GLU:HB2	2.35	0.61
1:A:898:ARG:HD3	1:A:933:TYR:CD1	2.36	0.61
2:B:218:SER:CB	2:B:241:ARG:HH12	2.14	0.61
6:F:90:ARG:HD3	6:F:155:LEU:CD1	2.22	0.61
1:A:982:THR:C	1:A:984:LYS:H	2.07	0.61
2:B:290:GLY:O	2:B:292:ILE:HG13	2.01	0.61
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.83	0.61
2:B:906:SER:HA	2:B:946:ASN:HB2	1.82	0.61
3:C:11:ARG:HH12	3:C:205:LYS:HE2	1.66	0.61
3:C:50:GLU:OE1	12:L:64:LEU:HD13	2.00	0.61
4:D:207:LEU:HD12	4:D:207:LEU:O	2.00	0.61
6:F:109:VAL:HG11	6:F:123:LYS:HG2	1.81	0.61
2:B:39:ARG:CZ	2:B:665:GLU:HG2	2.30	0.61
2:B:283:VAL:HG21	2:B:317:CYS:O	2.00	0.61
2:B:637:LEU:HD11	2:B:703:ILE:HD13	1.81	0.61
2:B:797:TYR:HE1	2:B:854:LEU:CD2	2.13	0.61
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.83	0.61
8:H:38:LEU:HD12	8:H:124:ARG:O	2.01	0.61
1:A:16:GLU:OE1	4:D:13:ARG:NH2	2.32	0.61
1:A:517:ASN:HD22	1:A:1364:ASN:HD22	1.47	0.61
1:A:691:LEU:O	1:A:694:THR:HB	2.01	0.61
1:A:1141:THR:CG2	1:A:1205:LYS:HD3	2.31	0.61
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.15	0.61
1:A:1445:ILE:HD12	1:A:1445:ILE:N	2.08	0.61
2:B:123:THR:OG1	2:B:458:LYS:HE2	2.01	0.61
2:B:360:PHE:CD2	2:B:361:LEU:HB2	2.35	0.61
3:C:123:ASN:HD21	3:C:125:MET:HA	1.64	0.61
10:J:14:VAL:O	10:J:14:VAL:HG12	2.01	0.61
1:A:1241:ARG:O	1:A:1242:VAL:CG2	2.48	0.61
2:B:57:TYR:CD1	2:B:57:TYR:N	2.68	0.61
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.48	0.61
5:E:157:SER:C	5:E:159:ASP:H	2.09	0.61
9:I:86:PHE:CE1	9:I:100:PHE:HB2	2.36	0.61
10:J:53:HIS:CD2	10:J:53:HIS:C	2.77	0.61
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.81	0.60
1:A:537:ARG:NH1	8:H:120:GLY:O	2.34	0.60
3:C:66:ARG:NH1	10:J:2:ILE:CG2	2.63	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:LEU:N	3:C:147:LEU:HD23	2.16	0.60
6:F:111:LEU:C	6:F:113:GLY:H	2.08	0.60
1:A:714:PHE:HB2	9:I:97:MET:HE1	1.83	0.60
1:A:1244:ARG:HB2	1:A:1245:PRO:HD2	1.82	0.60
2:B:288:ALA:O	2:B:331:LEU:HD11	2.00	0.60
2:B:750:GLY:O	2:B:751:VAL:C	2.44	0.60
2:B:912:ILE:O	2:B:938:SER:HB3	2.01	0.60
6:F:90:ARG:NH1	6:F:94:LEU:HD11	2.15	0.60
1:A:733:ALA:O	1:A:737:LEU:HG	2.01	0.60
1:A:1308:THR:CG2	1:A:1309:ASP:N	2.62	0.60
2:B:204:ILE:C	2:B:205:ILE:HD12	2.26	0.60
2:B:1124:ARG:HB3	2:B:1124:ARG:NH1	2.16	0.60
3:C:31:ASN:O	3:C:35:ARG:HG3	2.01	0.60
8:H:58:THR:HG22	8:H:59:ILE:N	2.15	0.60
8:H:89:LEU:C	8:H:91:ASP:N	2.47	0.60
1:A:469:ARG:NH2	2:B:991:GLY:O	2.35	0.60
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.82	0.60
1:A:1385:THR:HG22	1:A:1386:ARG:H	1.67	0.60
7:G:55:ASP:OD1	7:G:57:GLN:HG3	2.02	0.60
8:H:143:LEU:HD12	8:H:143:LEU:N	2.17	0.60
9:I:73:ARG:HD2	9:I:101:PHE:CE2	2.35	0.60
1:A:54:ASN:HB3	1:A:247:ARG:HH22	1.67	0.60
1:A:219:PHE:HE1	1:A:230:ARG:HE	1.48	0.60
1:A:289:ILE:HG22	1:A:290:GLU:N	2.16	0.60
1:A:869:GLY:O	5:E:204:THR:HG21	2.01	0.60
2:B:37:PHE:HE1	2:B:41:LYS:HG3	1.64	0.60
2:B:235:SER:OG	2:B:236:HIS:CD2	2.54	0.60
3:C:97:VAL:HG12	3:C:99:LEU:CD2	2.32	0.60
4:D:155:ARG:HD3	4:D:221:TYR:CE1	2.37	0.60
6:F:75:PRO:O	6:F:77:ASP:O	2.19	0.60
1:A:1342:GLU:CG	5:E:198:ILE:HD13	2.32	0.60
2:B:205:ILE:HD12	2:B:205:ILE:N	2.17	0.60
2:B:284:ILE:HD13	2:B:324:ILE:HD12	1.84	0.60
5:E:171:LYS:HG2	5:E:174:GLN:CD	2.26	0.60
7:G:115:MET:HB3	7:G:116:PRO:CD	2.32	0.60
9:I:46:HIS:CE1	9:I:48:LEU:HD23	2.37	0.60
11:K:94:ILE:O	11:K:98:LEU:HG	2.00	0.60
1:A:40:THR:HB	1:A:41:MET:HE2	1.84	0.60
4:D:130:LEU:HD13	4:D:142:LYS:CD	2.32	0.60
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.83	0.60
12:L:38:LEU:O	12:L:39:SER:HB3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:THR:HA	1:A:305:ASP:O	2.02	0.60
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.36	0.60
2:B:309:GLN:HG3	9:I:52:ILE:HD12	1.84	0.60
2:B:558:LEU:HD21	2:B:596:LEU:HD11	1.84	0.60
2:B:781:PHE:HE2	2:B:795:ILE:HD11	1.65	0.60
2:B:847:ASP:C	2:B:849:GLY:N	2.59	0.60
3:C:177:GLU:CG	3:C:231:ASN:HB3	2.29	0.60
5:E:37:LEU:CD1	5:E:41:ASP:HB2	2.31	0.60
7:G:85:GLU:HG2	7:G:87:VAL:HG13	1.83	0.60
1:A:23:SER:HA	1:A:233:TRP:NE1	2.16	0.60
1:A:100:LYS:HE2	1:A:104:GLU:OE2	2.01	0.60
1:A:102:VAL:HG21	1:A:234:MET:HE1	1.82	0.60
1:A:351:THR:CG2	2:B:1103:ILE:HG13	2.32	0.60
1:A:718:VAL:O	1:A:721:PHE:HB2	2.01	0.60
1:A:1070:GLN:O	1:A:1074:GLU:HB2	2.02	0.60
2:B:891:ASP:C	2:B:893:LEU:N	2.55	0.60
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.32	0.60
3:C:33:LEU:O	3:C:33:LEU:HD12	2.01	0.60
5:E:192:ARG:HH11	5:E:192:ARG:HG3	1.67	0.60
8:H:65:LEU:HD23	8:H:65:LEU:H	1.66	0.60
10:J:5:VAL:HG12	10:J:6:ARG:CG	2.32	0.60
10:J:7:CYS:HA	10:J:49:MET:HE3	1.84	0.60
10:J:21:TYR:HB2	10:J:39:LEU:CD1	2.32	0.60
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.82	0.60
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.01	0.60
1:A:1161:THR:HG21	1:A:1163:ILE:HD12	1.83	0.60
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.17	0.60
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.01	0.60
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.83	0.60
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.37	0.60
2:B:126:SER:CB	2:B:172:ILE:HD11	2.32	0.60
2:B:557:PHE:O	2:B:557:PHE:CD2	2.53	0.60
3:C:182:PRO:HD2	3:C:210:GLU:OE1	2.01	0.60
5:E:99:HIS:CE1	5:E:103:LYS:HG3	2.37	0.60
10:J:1:MET:H1	10:J:56:LEU:N	2.00	0.60
1:A:754:SER:H	1:A:757:ASN:ND2	1.98	0.59
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.83	0.59
2:B:260:GLY:O	2:B:267:ARG:NH1	2.34	0.59
2:B:360:PHE:CD2	2:B:360:PHE:C	2.80	0.59
2:B:435:THR:C	2:B:437:GLU:N	2.60	0.59
2:B:559:SER:CA	2:B:563:MET:HB3	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1174:LYS:O	2:B:1175:LEU:C	2.44	0.59
4:D:29:LEU:HD12	7:G:82:PHE:CE2	2.37	0.59
5:E:212:ARG:HG3	5:E:212:ARG:HH11	1.67	0.59
6:F:103:MET:O	6:F:104:ASN:HB2	2.01	0.59
1:A:385:ILE:HD11	1:A:426:LEU:HB2	1.82	0.59
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.84	0.59
2:B:1177:HIS:HB3	2:B:1179:GLN:HE21	1.67	0.59
3:C:7:GLN:HG3	11:K:104:ASN:ND2	2.17	0.59
8:H:59:ILE:O	8:H:60:ALA:HB3	2.01	0.59
8:H:83:GLN:C	8:H:85:GLY:H	2.10	0.59
11:K:21:ILE:HG22	11:K:31:VAL:HG11	1.84	0.59
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.83	0.59
1:A:401:GLY:C	1:A:435:HIS:HD2	2.09	0.59
1:A:1148:ILE:HG12	1:A:1198:ASP:HB2	1.83	0.59
2:B:68:THR:HA	2:B:90:ILE:O	2.02	0.59
2:B:781:PHE:H	2:B:781:PHE:HD2	1.49	0.59
2:B:1031:LEU:HD11	2:B:1042:GLY:CA	2.32	0.59
3:C:35:ARG:NH1	11:K:41:THR:H	2.00	0.59
4:D:9:GLN:HG3	4:D:9:GLN:O	2.03	0.59
1:A:186:LYS:O	1:A:187:LYS:HB2	2.01	0.59
2:B:797:TYR:O	10:J:1:MET:HG2	2.02	0.59
4:D:56:ARG:HD3	4:D:149:THR:HA	1.84	0.59
5:E:136:ASN:OD1	5:E:138:ALA:N	2.35	0.59
1:A:353:ILE:HD12	1:A:470:LEU:HD21	1.85	0.59
2:B:347:LYS:HG3	2:B:348:ARG:H	1.67	0.59
2:B:852:ARG:HH22	12:L:70:ARG:C	2.10	0.59
2:B:868:MET:O	2:B:870:ILE:HG13	2.01	0.59
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.32	0.59
3:C:208:GLU:O	3:C:210:GLU:N	2.36	0.59
3:C:258:ILE:HD11	11:K:42:LEU:HD21	1.83	0.59
4:D:51:ASN:O	4:D:52:LEU:O	2.20	0.59
8:H:30:SER:CB	8:H:36:CYS:HB3	2.32	0.59
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.27	0.59
1:A:102:VAL:HG11	1:A:211:PHE:HE1	1.68	0.59
1:A:447:GLN:NE2	14:T:20:DG:H4'	2.17	0.59
1:A:464:PRO:HG2	1:A:465:TYR:HD1	1.68	0.59
1:A:567:LYS:HD2	8:H:95:TYR:CG	2.38	0.59
1:A:1094:VAL:HG13	1:A:1113:THR:HG21	1.84	0.59
2:B:120:ARG:NH1	12:L:54:ARG:HH11	2.01	0.59
2:B:745:PRO:O	2:B:747:MET:N	2.36	0.59
2:B:1031:LEU:HD12	2:B:1031:LEU:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:49:LEU:HG	7:G:76:ALA:HA	1.84	0.59
1:A:264:PHE:C	1:A:265:LYS:HE3	2.27	0.59
1:A:567:LYS:HD2	8:H:95:TYR:HA	1.84	0.59
1:A:666:ILE:HD11	2:B:1086:PHE:HE1	1.67	0.59
1:A:671:ALA:O	1:A:676:MET:HE3	2.03	0.59
2:B:248:SER:N	2:B:418:LYS:HZ1	2.00	0.59
2:B:297:ILE:HG22	2:B:298:LEU:HD22	1.85	0.59
2:B:549:THR:HG22	2:B:550:ASP:H	1.66	0.59
2:B:1084:GLN:N	2:B:1084:GLN:NE2	2.51	0.59
8:H:33:GLN:C	8:H:35:GLN:H	2.10	0.59
11:K:57:LEU:HB2	11:K:76:GLN:HG2	1.84	0.59
1:A:311:GLN:O	1:A:312:PRO:C	2.45	0.59
1:A:964:ILE:O	1:A:967:ALA:HB3	2.03	0.59
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.32	0.59
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.82	0.59
2:B:332:ASP:OD1	2:B:348:ARG:HD2	2.03	0.59
2:B:708:GLU:O	2:B:710:LEU:N	2.36	0.59
2:B:999:MET:HB3	2:B:1007:VAL:HG21	1.85	0.59
1:A:88:LYS:HG3	1:A:276:LEU:HD21	1.85	0.59
1:A:325:ILE:HG22	2:B:1210:MET:HE2	1.84	0.59
1:A:353:ILE:CD1	1:A:487:MET:HE2	2.32	0.59
1:A:444:PHE:CB	1:A:458:HIS:HD2	2.16	0.59
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.43	0.59
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.33	0.59
2:B:732:SER:HB2	2:B:734:HIS:NE2	2.18	0.59
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.31	0.59
6:F:69:LEU:HB3	6:F:71:GLU:OE2	2.02	0.59
15:P:10:U:H5'	15:P:11:G:C3'	2.33	0.59
1:A:416:ARG:HH11	1:A:417:TYR:HE1	1.51	0.59
1:A:476:SER:OG	1:A:477:PRO:HD3	2.03	0.59
1:A:1161:THR:C	1:A:1163:ILE:N	2.61	0.59
2:B:562:GLY:HA3	2:B:590:HIS:ND1	2.17	0.59
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.16	0.59
2:B:1084:GLN:N	2:B:1084:GLN:HE21	2.01	0.59
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.67	0.59
7:G:90:THR:HG22	7:G:91:VAL:O	2.03	0.59
1:A:925:LEU:HD13	1:A:983:ILE:HG21	1.83	0.58
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.27	0.58
2:B:975:GLN:O	2:B:990:ILE:HD12	2.02	0.58
3:C:69:LEU:N	3:C:69:LEU:HD12	2.17	0.58
6:F:109:VAL:HG21	6:F:124:GLU:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.66	0.58
11:K:18:LYS:NZ	11:K:37:LYS:O	2.35	0.58
2:B:360:PHE:HD2	2:B:361:LEU:HB2	1.68	0.58
3:C:40:GLU:HA	3:C:163:ILE:HD12	1.85	0.58
3:C:146:LYS:C	3:C:147:LEU:HD23	2.28	0.58
5:E:92:THR:O	5:E:95:THR:HB	2.03	0.58
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.32	0.58
7:G:126:ASN:C	7:G:126:ASN:ND2	2.60	0.58
9:I:19:ASP:HB3	9:I:24:ARG:HG2	1.85	0.58
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.85	0.58
1:A:1239:ARG:HH12	1:A:1241:ARG:HH12	1.50	0.58
1:A:1259:MET:HA	1:A:1262:LYS:CD	2.33	0.58
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.11	0.58
3:C:97:VAL:HG12	3:C:99:LEU:HD21	1.85	0.58
4:D:17:LYS:HD2	4:D:18:VAL:HG13	1.84	0.58
9:I:116:ASN:O	9:I:117:LYS:HD2	2.03	0.58
1:A:186:LYS:NZ	1:A:197:PRO:HD3	2.18	0.58
1:A:596:THR:C	1:A:598:LEU:N	2.58	0.58
1:A:1286:LYS:HB2	1:A:1304:TRP:CZ3	2.39	0.58
2:B:185:THR:O	2:B:186:GLU:C	2.46	0.58
2:B:246:LYS:HA	2:B:249:ARG:CZ	2.33	0.58
5:E:93:MET:CG	5:E:123:LEU:HD12	2.34	0.58
11:K:65:HIS:HD2	11:K:67:PHE:N	2.01	0.58
1:A:203:SER:O	1:A:206:GLU:HB3	2.03	0.58
1:A:1094:VAL:CG2	1:A:1113:THR:HG21	2.29	0.58
1:A:1308:THR:HG23	1:A:1310:GLY:H	1.69	0.58
2:B:65:GLU:HG3	2:B:66:ASP:N	2.14	0.58
2:B:353:LYS:O	2:B:357:GLN:HG2	2.03	0.58
2:B:557:PHE:CD2	2:B:557:PHE:C	2.81	0.58
2:B:801:LYS:O	10:J:52:THR:CG2	2.51	0.58
2:B:953:LEU:HD23	2:B:953:LEU:O	2.04	0.58
4:D:120:GLU:OE1	4:D:120:GLU:O	2.22	0.58
8:H:42:ILE:HG23	8:H:95:TYR:CE1	2.39	0.58
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.85	0.58
1:A:857:ARG:NH1	6:F:139:PRO:HB2	2.19	0.58
1:A:1076:ALA:CA	1:A:1079:MET:HE2	2.32	0.58
2:B:47:GLN:O	2:B:173:MET:HE1	2.04	0.58
2:B:295:GLY:H	2:B:298:LEU:HD23	1.69	0.58
3:C:32:SER:O	3:C:36:VAL:HG23	2.03	0.58
4:D:130:LEU:C	4:D:132:GLN:H	2.11	0.58
1:A:332:LYS:HD3	1:A:333:GLU:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ILE:HD11	2:B:1067:ARG:O	2.03	0.58
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.85	0.58
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.03	0.58
2:B:542:MET:HG2	2:B:747:MET:HE3	1.86	0.58
7:G:58:ARG:HH11	7:G:58:ARG:HG3	1.68	0.58
1:A:256:GLN:NE2	2:B:935:ARG:HH12	2.01	0.58
1:A:503:GLN:NE2	6:F:90:ARG:NH2	2.48	0.58
1:A:710:LEU:H	1:A:710:LEU:CD1	2.15	0.58
1:A:1066:VAL:O	1:A:1070:GLN:HG3	2.04	0.58
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.85	0.58
2:B:1187:ASN:HD21	2:B:1190:ASP:HB3	1.69	0.58
3:C:177:GLU:HG3	3:C:231:ASN:ND2	2.18	0.58
8:H:81:PRO:HB3	8:H:82:PRO:HD2	1.85	0.58
9:I:80:SER:HB2	9:I:103:CYS:SG	2.43	0.58
1:A:205:GLU:H	1:A:205:GLU:CD	2.11	0.58
2:B:468:GLU:OE1	2:B:470:LYS:HE3	2.04	0.58
2:B:871:THR:HG22	2:B:872:GLU:O	2.04	0.58
2:B:955:THR:CG2	2:B:956:THR:H	2.17	0.58
3:C:114:TYR:CD2	3:C:140:ASN:CB	2.86	0.58
6:F:111:LEU:C	6:F:113:GLY:N	2.62	0.58
9:I:78:CYS:SG	9:I:106:CYS:SG	3.01	0.58
1:A:119:ASN:O	1:A:122:MET:HB3	2.04	0.58
1:A:265:LYS:O	1:A:269:ILE:HG13	2.02	0.58
1:A:1241:ARG:O	1:A:1242:VAL:CB	2.52	0.58
1:A:1438:THR:O	6:F:92:ARG:NH1	2.37	0.58
2:B:398:ARG:NH1	2:B:398:ARG:HB2	2.19	0.58
2:B:770:GLN:CD	2:B:983:ARG:HA	2.27	0.58
2:B:906:SER:O	2:B:941:LEU:HD23	2.04	0.58
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.85	0.58
4:D:52:LEU:HD21	4:D:147:TYR:HE2	1.68	0.58
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.34	0.58
9:I:8:ARG:HG3	9:I:34:TYR:HE1	1.66	0.58
1:A:567:LYS:CB	8:H:96:VAL:H	2.05	0.57
1:A:665:GLY:C	1:A:666:ILE:HD12	2.28	0.57
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.86	0.57
2:B:758:PHE:HE1	2:B:1027:ILE:HG22	1.69	0.57
3:C:124:LEU:O	3:C:127:ARG:HG2	2.03	0.57
4:D:35:LEU:H	4:D:35:LEU:HD12	1.68	0.57
5:E:129:PRO:O	5:E:130:ALA:C	2.47	0.57
11:K:67:PHE:C	11:K:68:PHE:HD2	2.11	0.57
11:K:79:GLU:HG3	11:K:80:GLY:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LYS:O	1:A:130:ASP:HB2	2.04	0.57
1:A:1208:THR:HB	1:A:1211:GLN:CG	2.16	0.57
2:B:557:PHE:HD2	2:B:557:PHE:C	2.11	0.57
3:C:226:ASP:O	3:C:227:THR:HB	2.04	0.57
4:D:118:THR:O	4:D:121:LYS:N	2.29	0.57
4:D:163:VAL:O	4:D:167:LEU:HG	2.04	0.57
5:E:15:ALA:O	5:E:19:VAL:HG23	2.03	0.57
5:E:124:VAL:HA	5:E:132:ILE:CD1	2.33	0.57
5:E:213:ILE:HG12	5:E:214:CYS:N	2.18	0.57
10:J:57:ILE:O	10:J:60:PHE:HB2	2.04	0.57
1:A:628:GLY:O	1:A:632:VAL:HG23	2.03	0.57
2:B:254:LEU:HD11	2:B:273:LEU:HD23	1.85	0.57
3:C:123:ASN:C	3:C:125:MET:H	2.12	0.57
5:E:153:HIS:O	5:E:154:ILE:HG13	2.04	0.57
8:H:40:LEU:CD1	8:H:123:MET:HE3	2.22	0.57
1:A:102:VAL:HB	1:A:211:PHE:CZ	2.39	0.57
1:A:828:ALA:C	1:A:831:THR:HG22	2.30	0.57
1:A:833:GLU:O	1:A:837:ILE:HG13	2.04	0.57
1:A:851:HIS:O	1:A:853:ASP:N	2.37	0.57
1:A:855:THR:HG21	1:A:857:ARG:NE	2.20	0.57
2:B:758:PHE:CE1	2:B:1027:ILE:CG2	2.87	0.57
2:B:839:MET:HE3	2:B:1010:LEU:CD2	2.32	0.57
2:B:996:ARG:HH21	3:C:38:ILE:HG23	1.69	0.57
4:D:123:LEU:CD1	4:D:149:THR:HG21	2.33	0.57
5:E:147:HIS:CD2	5:E:149:LEU:H	2.21	0.57
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.85	0.57
1:A:196:GLU:HG2	1:A:197:PRO:HD2	1.87	0.57
1:A:265:LYS:HE3	1:A:265:LYS:HA	1.85	0.57
1:A:317:LYS:O	1:A:318:SER:CB	2.52	0.57
1:A:322:VAL:O	1:A:322:VAL:CG1	2.53	0.57
1:A:1009:ASN:CG	1:A:1012:ARG:HH12	2.13	0.57
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.40	0.57
2:B:25:ILE:HG21	2:B:658:ILE:HD12	1.86	0.57
2:B:121:ASN:HA	2:B:207:GLY:HA2	1.85	0.57
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.26	0.57
2:B:411:PRO:O	2:B:414:ALA:HB3	2.04	0.57
2:B:483:LEU:HD11	2:B:491:THR:CG2	2.33	0.57
2:B:1202:LEU:O	2:B:1206:GLU:HG3	2.04	0.57
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.86	0.57
12:L:30:ILE:HG22	12:L:31:CYS:H	1.69	0.57
14:T:16:DT:HI'	14:T:17:DT:H5''	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLY:O	1:A:169:ASN:C	2.47	0.57
1:A:1116:LEU:HB3	1:A:1308:THR:CG2	2.32	0.57
2:B:914:LYS:HG2	2:B:937:ALA:HB3	1.87	0.57
5:E:22:MET:CE	5:E:26:ARG:NH2	2.67	0.57
7:G:13:LEU:HD22	7:G:17:PHE:HB2	1.85	0.57
1:A:438:ASP:O	1:A:439:ASN:HB2	2.05	0.57
1:A:446:ARG:HB2	1:A:487:MET:SD	2.44	0.57
1:A:903:ASN:ND2	1:A:904:THR:N	2.52	0.57
1:A:1237:ILE:HG22	1:A:1238:ILE:N	2.19	0.57
2:B:168:GLY:N	2:B:450:ALA:HB1	2.16	0.57
2:B:294:ASP:C	2:B:296:GLU:H	2.12	0.57
2:B:707:PRO:CG	2:B:708:GLU:H	2.15	0.57
3:C:238:ILE:HG22	3:C:243:VAL:HG23	1.87	0.57
4:D:47:LEU:HD11	7:G:3:PHE:CD2	2.40	0.57
5:E:67:GLU:O	5:E:70:SER:N	2.37	0.57
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.34	0.57
1:A:853:ASP:OD1	1:A:855:THR:HB	2.04	0.57
2:B:129:PHE:HD2	2:B:166:PHE:HA	1.70	0.57
2:B:326:ASP:OD2	2:B:328:GLU:HB3	2.05	0.57
2:B:708:GLU:O	2:B:709:ASP:C	2.48	0.57
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.05	0.57
2:B:1202:LEU:HD22	2:B:1206:GLU:CD	2.30	0.57
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.85	0.57
7:G:21:ARG:CZ	7:G:24:GLN:HB2	2.35	0.57
10:J:2:ILE:HG12	10:J:57:ILE:HD12	1.86	0.57
15:P:2:A:H2'	15:P:3:A:H8	1.70	0.57
1:A:555:ASP:O	1:A:556:TRP:C	2.48	0.57
1:A:774:ARG:O	1:A:775:ILE:C	2.47	0.57
1:A:1037:LEU:HD22	1:A:1041:ALA:HB1	1.86	0.57
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.05	0.57
2:B:176:SER:O	2:B:182:SER:HB3	2.05	0.57
2:B:222:ILE:H	2:B:240:ILE:CD1	2.17	0.57
2:B:865:LYS:HZ3	2:B:869:SER:HA	1.69	0.57
2:B:992:ILE:HG12	2:B:993:THR:N	2.20	0.57
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.37	0.57
3:C:99:LEU:HD12	3:C:118:LEU:HD13	1.87	0.57
3:C:177:GLU:HG3	3:C:231:ASN:CB	2.32	0.57
8:H:130:ARG:HH11	8:H:130:ARG:N	2.00	0.57
1:A:332:LYS:C	1:A:334:GLY:N	2.52	0.57
1:A:372:LYS:HA	1:A:435:HIS:CE1	2.39	0.57
1:A:598:LEU:O	1:A:599:SER:C	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:ILE:HG12	1:A:732:LEU:HD12	1.86	0.57
2:B:110:HIS:CB	12:L:54:ARG:NH2	2.64	0.57
2:B:222:ILE:HD11	2:B:627:PHE:CZ	2.40	0.57
2:B:810:GLU:HA	2:B:815:ARG:NH2	2.20	0.57
2:B:865:LYS:C	2:B:866:TYR:HD1	2.13	0.57
3:C:56:THR:HG21	3:C:145:CYS:SG	2.45	0.57
4:D:7:THR:O	4:D:7:THR:HG23	2.03	0.57
5:E:56:LYS:NZ	5:E:84:ASP:H	2.03	0.57
6:F:103:MET:HE1	7:G:65:ASP:HB2	1.87	0.57
7:G:106:MET:HG3	7:G:157:ILE:O	2.04	0.57
8:H:130:ARG:NH1	8:H:130:ARG:H	2.01	0.57
1:A:325:ILE:CG2	2:B:1210:MET:HE2	2.35	0.56
1:A:1166:ASP:OD2	1:A:1239:ARG:HD2	2.05	0.56
2:B:431:TYR:CD1	2:B:447:ALA:HB2	2.40	0.56
2:B:865:LYS:O	2:B:866:TYR:HD1	1.88	0.56
3:C:259:LEU:CD2	11:K:91:CYS:HB3	2.35	0.56
4:D:47:LEU:HD13	4:D:48:ILE:N	2.19	0.56
4:D:52:LEU:O	4:D:54:GLU:N	2.35	0.56
5:E:30:ILE:HG22	5:E:31:THR:O	2.05	0.56
14:T:15:DG:H2"	14:T:16:DT:H6	1.70	0.56
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.86	0.56
1:A:897:TYR:HB3	1:A:936:LEU:CD1	2.35	0.56
1:A:1045:VAL:O	1:A:1049:ILE:HG13	2.05	0.56
2:B:68:THR:HG22	2:B:91:SER:CB	2.34	0.56
2:B:916:THR:HB	2:B:935:ARG:CG	2.35	0.56
9:I:10:CYS:SG	9:I:32:CYS:HB3	2.44	0.56
9:I:14:LEU:HA	9:I:28:GLU:O	2.06	0.56
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.40	0.56
1:A:54:ASN:HA	1:A:58:LEU:HD12	1.86	0.56
1:A:380:VAL:HG12	1:A:428:TYR:HA	1.86	0.56
1:A:477:PRO:HG2	1:A:521:MET:HG2	1.87	0.56
1:A:831:THR:CG2	1:A:832:ALA:N	2.65	0.56
1:A:963:ILE:HD13	1:A:1049:ILE:HG12	1.87	0.56
2:B:295:GLY:O	2:B:299:GLU:HG3	2.06	0.56
2:B:637:LEU:HB2	2:B:693:ILE:HD11	1.86	0.56
2:B:822:ASN:ND2	10:J:52:THR:HG21	2.20	0.56
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.05	0.56
3:C:124:LEU:O	3:C:126:GLY:N	2.38	0.56
3:C:254:LYS:HE2	11:K:42:LEU:HD13	1.86	0.56
4:D:134:THR:HG22	4:D:135:GLY:N	2.20	0.56
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:139:ILE:CG2	7:G:140:LYS:N	2.68	0.56
8:H:12:VAL:HG13	8:H:26:ILE:HD11	1.87	0.56
9:I:7:CYS:SG	9:I:8:ARG:O	2.64	0.56
9:I:118:ARG:NH1	9:I:120:GLN:HB2	2.20	0.56
11:K:93:SER:OG	11:K:97:LYS:HE3	2.06	0.56
12:L:52:GLY:O	12:L:53:HIS:C	2.48	0.56
1:A:57:ARG:O	1:A:68:GLN:HG2	2.06	0.56
1:A:64:ASN:O	1:A:65:LEU:C	2.48	0.56
1:A:69:THR:C	1:A:71:GLN:N	2.60	0.56
1:A:698:GLN:NE2	9:I:99:LEU:HD11	2.21	0.56
1:A:875:ALA:HA	1:A:878:ILE:CD1	2.36	0.56
2:B:186:GLU:HG3	10:J:62:ARG:NH2	2.18	0.56
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.36	0.56
2:B:300:HIS:O	2:B:303:TYR:HE2	1.87	0.56
2:B:308:TRP:CH2	9:I:45:ARG:HG2	2.41	0.56
2:B:519:TRP:C	2:B:519:TRP:CD1	2.83	0.56
2:B:850:LEU:HD12	2:B:851:PHE:N	2.20	0.56
2:B:885:MET:HA	2:B:936:ASP:HB3	1.87	0.56
5:E:22:MET:HE1	5:E:26:ARG:HH21	1.70	0.56
6:F:94:LEU:HD22	6:F:122:MET:HG2	1.87	0.56
7:G:20:PRO:CD	7:G:21:ARG:H	2.18	0.56
9:I:44:TYR:CD1	9:I:44:TYR:C	2.83	0.56
1:A:381:THR:HG23	1:A:382:PRO:CD	2.32	0.56
1:A:868:TYR:OH	1:A:1366:ARG:HD3	2.05	0.56
1:A:1317:MET:O	1:A:1322:ILE:HD11	2.04	0.56
2:B:276:ILE:CG2	2:B:336:ARG:HB2	2.36	0.56
2:B:459:TYR:CZ	2:B:469:GLN:HG2	2.41	0.56
2:B:553:PRO:HG2	2:B:554:ILE:HD12	1.87	0.56
2:B:805:THR:HA	2:B:809:MET:CE	2.35	0.56
2:B:918:ILE:HD12	2:B:935:ARG:NH1	2.21	0.56
2:B:1156:ASP:O	2:B:1157:ALA:O	2.23	0.56
3:C:33:LEU:O	3:C:37:MET:HG3	2.05	0.56
6:F:111:LEU:O	6:F:113:GLY:N	2.32	0.56
6:F:127:GLU:O	6:F:128:LYS:C	2.48	0.56
7:G:34:VAL:HG13	7:G:45:ILE:HG21	1.88	0.56
7:G:48:VAL:HG13	7:G:74:TYR:HD1	1.69	0.56
8:H:26:ILE:HG22	8:H:40:LEU:O	2.05	0.56
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.34	0.56
11:K:88:LYS:O	11:K:91:CYS:HB2	2.04	0.56
1:A:129:LYS:O	1:A:130:ASP:CB	2.53	0.56
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.86	0.56
1:A:591:PHE:HA	1:A:595:THR:CG2	2.35	0.56
1:A:714:PHE:CB	9:I:97:MET:HE1	2.36	0.56
1:A:1006:ILE:HD11	5:E:163:GLU:HG3	1.87	0.56
1:A:1159:ARG:N	1:A:1159:ARG:HD2	2.21	0.56
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.20	0.56
2:B:68:THR:HG22	2:B:91:SER:CA	2.35	0.56
2:B:189:LEU:HD13	2:B:196:PRO:HA	1.88	0.56
2:B:798:TYR:HE2	3:C:62:PHE:CZ	2.23	0.56
2:B:886:LYS:NZ	2:B:936:ASP:OD1	2.39	0.56
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.88	0.56
3:C:221:TYR:CE1	3:C:222:LYS:HG3	2.41	0.56
5:E:157:SER:C	5:E:159:ASP:N	2.62	0.56
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.88	0.56
1:A:973:ILE:HD13	1:A:1037:LEU:HA	1.88	0.56
1:A:974:ASP:C	1:A:976:THR:H	2.14	0.56
1:A:1316:VAL:O	1:A:1316:VAL:HG12	2.05	0.56
2:B:120:ARG:NH1	12:L:54:ARG:HD2	2.20	0.56
2:B:745:PRO:C	2:B:747:MET:H	2.13	0.56
2:B:865:LYS:HZ2	2:B:869:SER:HA	1.69	0.56
4:D:14:ARG:NH1	4:D:16:LYS:HD2	2.21	0.56
1:A:332:LYS:O	1:A:334:GLY:N	2.38	0.56
2:B:303:TYR:CD2	2:B:303:TYR:N	2.74	0.56
3:C:73:GLN:NE2	3:C:75:MET:H	2.00	0.56
1:A:1033:GLN:HA	1:A:1036:ARG:NH1	2.19	0.56
2:B:26:THR:HB	2:B:708:GLU:OE1	2.06	0.56
2:B:284:ILE:HD13	2:B:333:PHE:CD2	2.41	0.56
2:B:359:GLU:O	2:B:362:PRO:HD3	2.05	0.56
2:B:640:VAL:O	2:B:641:GLU:C	2.48	0.56
5:E:147:HIS:HB3	5:E:150:VAL:CG2	2.36	0.56
1:A:50:ILE:C	1:A:52:GLY:N	2.62	0.56
1:A:69:THR:C	1:A:71:GLN:H	2.13	0.56
1:A:787:PHE:HE1	1:A:796:SER:HA	1.70	0.56
2:B:615:MET:HB3	2:B:626:ILE:CG1	2.30	0.56
2:B:842:ASN:O	2:B:846:ILE:HG13	2.06	0.56
5:E:179:GLN:HA	5:E:179:GLN:OE1	2.06	0.56
7:G:87:VAL:HB	7:G:103:VAL:HG11	1.87	0.56
1:A:108:MET:HB3	1:A:210:ILE:CD1	2.36	0.55
1:A:125:ALA:C	1:A:127:ALA:H	2.14	0.55
2:B:129:PHE:CE2	2:B:166:PHE:CD1	2.94	0.55
2:B:1174:LYS:O	2:B:1176:ASN:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1182:CYS:O	2:B:1183:LYS:C	2.49	0.55
3:C:235:VAL:HG21	10:J:6:ARG:NH2	2.21	0.55
5:E:112:TYR:CE1	5:E:136:ASN:HA	2.41	0.55
5:E:164:LEU:CD2	5:E:211:TYR:CD2	2.88	0.55
8:H:95:TYR:CE2	8:H:97:MET:HE2	2.41	0.55
1:A:34:LYS:HZ1	1:A:57:ARG:HH21	1.55	0.55
1:A:56:PRO:O	1:A:57:ARG:CG	2.52	0.55
1:A:335:ARG:NH1	2:B:1206:GLU:OE1	2.38	0.55
1:A:427:GLN:HB2	1:A:430:TRP:CD1	2.41	0.55
1:A:1444:MET:CE	6:F:135:ARG:HB2	2.34	0.55
2:B:186:GLU:CG	10:J:62:ARG:HH22	2.19	0.55
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.88	0.55
2:B:430:ARG:HB3	2:B:434:ARG:NH2	2.21	0.55
3:C:226:ASP:O	3:C:227:THR:CB	2.53	0.55
3:C:243:VAL:O	3:C:243:VAL:HG12	2.06	0.55
8:H:12:VAL:CG1	8:H:26:ILE:HD11	2.36	0.55
1:A:341:MET:CE	2:B:1135:ARG:NH1	2.70	0.55
1:A:590:ARG:HB3	1:A:605:MET:N	2.22	0.55
1:A:1168:GLU:O	1:A:1171:GLN:OE1	2.24	0.55
2:B:810:GLU:HA	2:B:815:ARG:HH22	1.71	0.55
2:B:990:ILE:HG22	2:B:991:GLY:N	2.21	0.55
2:B:1115:THR:HG22	2:B:1117:GLN:H	1.70	0.55
3:C:100:THR:CG2	3:C:102:GLN:HE21	2.18	0.55
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.41	0.55
4:D:50:LEU:HD21	7:G:4:ILE:HD12	1.87	0.55
5:E:169:ARG:HB3	6:F:140:ASP:OD2	2.07	0.55
7:G:101:VAL:HG12	7:G:102:GLN:N	2.21	0.55
12:L:61:THR:HG22	12:L:63:ARG:H	1.71	0.55
1:A:66:LYS:NZ	1:A:68:GLN:N	2.46	0.55
1:A:88:LYS:HD3	1:A:293:GLU:CD	2.31	0.55
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.87	0.55
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.89	0.55
2:B:20:ASP:O	2:B:22:SER:N	2.35	0.55
2:B:39:ARG:HH21	2:B:665:GLU:CD	2.15	0.55
2:B:711:GLU:HB2	2:B:712:PRO:CD	2.36	0.55
2:B:830:TYR:O	2:B:831:SER:C	2.49	0.55
2:B:999:MET:HB3	2:B:1007:VAL:CG2	2.36	0.55
2:B:1050:ILE:HG22	2:B:1051:THR:N	2.21	0.55
7:G:51:TYR:C	7:G:51:TYR:CD2	2.84	0.55
8:H:12:VAL:CG1	8:H:51:ALA:HA	2.36	0.55
1:A:55:ASP:C	1:A:57:ARG:N	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:LEU:CD2	8:H:46:LEU:HD11	2.36	0.55
1:A:616:VAL:HG12	1:A:617:VAL:N	2.21	0.55
1:A:780:VAL:O	1:A:782:ARG:HG2	2.07	0.55
1:A:979:SER:OG	1:A:980:ASP:N	2.38	0.55
1:A:1308:THR:HG23	1:A:1309:ASP:H	1.69	0.55
2:B:315:LYS:N	2:B:316:PRO:HD2	2.22	0.55
2:B:842:ASN:HD21	2:B:844:SER:HB2	1.72	0.55
2:B:1161:HIS:NE2	2:B:1175:LEU:HD21	2.22	0.55
6:F:128:LYS:HD3	6:F:149:GLU:O	2.06	0.55
10:J:23:ASN:C	10:J:25:LEU:N	2.57	0.55
1:A:311:GLN:O	1:A:313:GLN:N	2.40	0.55
1:A:567:LYS:HB3	8:H:95:TYR:CA	2.36	0.55
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.87	0.55
5:E:56:LYS:HZ3	5:E:84:ASP:H	1.54	0.55
6:F:94:LEU:HD21	6:F:122:MET:HA	1.89	0.55
9:I:6:PHE:HA	9:I:14:LEU:HG	1.89	0.55
9:I:73:ARG:O	9:I:81:ARG:HA	2.07	0.55
1:A:605:MET:HE2	1:A:607:ILE:HG13	1.87	0.55
1:A:672:ASP:CG	1:A:674:PRO:HD2	2.32	0.55
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.07	0.55
1:A:870:GLU:HG2	5:E:208:TYR:CD2	2.41	0.55
2:B:281:PRO:HB3	2:B:320:ASP:OD2	2.06	0.55
2:B:704:ALA:HB2	2:B:738:PHE:CD2	2.42	0.55
3:C:10:ILE:HG13	11:K:108:GLU:HB3	1.87	0.55
3:C:189:THR:CG2	3:C:190:ASP:N	2.70	0.55
4:D:39:ASN:HD22	4:D:41:GLN:HB2	1.71	0.55
5:E:82:PHE:CD1	5:E:82:PHE:N	2.74	0.55
12:L:38:LEU:HG	12:L:39:SER:H	1.71	0.55
1:A:266:LEU:HD21	1:A:303:TYR:CZ	2.41	0.55
1:A:590:ARG:HG3	1:A:591:PHE:N	2.21	0.55
1:A:925:LEU:HD13	1:A:983:ILE:HG22	1.88	0.55
1:A:1029:ARG:HH11	1:A:1029:ARG:CG	2.20	0.55
1:A:1385:THR:CG2	1:A:1386:ARG:N	2.69	0.55
2:B:549:THR:CG2	2:B:550:ASP:N	2.70	0.55
2:B:916:THR:O	2:B:935:ARG:HG2	2.07	0.55
4:D:14:ARG:CZ	4:D:16:LYS:HD2	2.37	0.55
5:E:124:VAL:N	5:E:125:PRO:CD	2.70	0.55
7:G:74:TYR:H	7:G:74:TYR:HD2	1.55	0.55
7:G:129:SER:CB	7:G:138:THR:OG1	2.55	0.55
8:H:128:ASN:ND2	8:H:131:ASN:OD1	2.39	0.55
1:A:51:GLY:C	1:A:56:PRO:HB3	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASN:ND2	2:B:1116:ARG:NH1	2.54	0.55
1:A:399:HIS:CB	1:A:400:PRO:CD	2.78	0.55
1:A:443:LEU:O	1:A:489:LEU:HD12	2.06	0.55
1:A:899:VAL:CG1	1:A:929:LEU:HD12	2.37	0.55
1:A:940:ARG:O	1:A:944:ARG:HG3	2.06	0.55
1:A:1030:ARG:CG	1:A:1034:GLU:OE2	2.53	0.55
1:A:1120:LEU:HD23	1:A:1304:TRP:O	2.06	0.55
1:A:1244:ARG:NE	1:A:1245:PRO:HD2	2.05	0.55
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.42	0.55
2:B:745:PRO:C	2:B:747:MET:N	2.63	0.55
2:B:1045:SER:O	2:B:1048:THR:HG23	2.06	0.55
3:C:91:HIS:ND1	3:C:158:VAL:HG11	2.21	0.55
8:H:139:ASN:O	8:H:140:ALA:CB	2.54	0.55
10:J:16:ASP:OD1	10:J:16:ASP:N	2.34	0.55
1:A:65:LEU:O	1:A:66:LYS:C	2.50	0.55
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.36	0.55
1:A:579:SER:HA	1:A:582:ILE:HG13	1.87	0.55
1:A:1105:LEU:HD22	1:A:1384:VAL:HG21	1.89	0.55
2:B:857:ARG:HH21	2:B:942:ARG:CZ	2.20	0.55
5:E:48:ASP:CG	5:E:49:SER:N	2.64	0.55
8:H:63:LEU:HD11	8:H:141:TYR:CD2	2.42	0.55
10:J:31:ASP:OD1	10:J:34:THR:OG1	2.25	0.55
1:A:53:LEU:C	1:A:54:ASN:HD22	2.15	0.54
1:A:62:ASP:O	1:A:64:ASN:N	2.40	0.54
1:A:211:PHE:O	1:A:214:ILE:HG13	2.07	0.54
1:A:225:ASN:ND2	1:A:227:VAL:H	2.05	0.54
1:A:331:GLY:O	1:A:332:LYS:O	2.24	0.54
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.42	0.54
1:A:738:LYS:HG3	1:A:740:LEU:HG	1.88	0.54
1:A:982:THR:C	1:A:984:LYS:N	2.64	0.54
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.71	0.54
1:A:1287:TYR:CD1	1:A:1305:VAL:HG21	2.42	0.54
2:B:91:SER:OG	2:B:133:LYS:HB2	2.07	0.54
2:B:235:SER:O	2:B:236:HIS:HD2	1.88	0.54
3:C:91:HIS:HD2	3:C:91:HIS:O	1.90	0.54
4:D:71:LYS:HA	4:D:74:GLN:CB	2.36	0.54
4:D:220:LEU:HD22	4:D:221:TYR:H	1.66	0.54
1:A:288:ALA:HA	1:A:291:GLU:HG3	1.88	0.54
1:A:427:GLN:O	1:A:428:TYR:C	2.49	0.54
1:A:689:LYS:HE2	1:A:721:PHE:CE2	2.41	0.54
1:A:1110:ASN:HD22	1:A:1110:ASN:H	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1214:GLU:C	1:A:1218:GLN:HE21	2.16	0.54
2:B:345:LYS:C	2:B:346:GLU:HG3	2.31	0.54
2:B:1068:GLY:O	2:B:1069:PHE:O	2.25	0.54
3:C:138:GLU:OE1	3:C:138:GLU:N	2.40	0.54
4:D:155:ARG:HD3	4:D:221:TYR:CZ	2.43	0.54
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.37	0.54
1:A:133:LYS:O	1:A:136:ALA:HB3	2.06	0.54
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.90	0.54
1:A:962:ARG:O	1:A:964:ILE:N	2.41	0.54
2:B:90:ILE:CD1	2:B:432:MET:SD	2.94	0.54
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.90	0.54
5:E:21:GLU:O	5:E:24:LYS:HG2	2.08	0.54
7:G:51:TYR:C	7:G:51:TYR:HD2	2.16	0.54
10:J:14:VAL:CG1	10:J:50:ILE:HD11	2.37	0.54
11:K:52:ASN:O	11:K:54:ARG:N	2.40	0.54
11:K:108:GLU:O	11:K:112:GLN:HG2	2.07	0.54
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.88	0.54
1:A:868:TYR:CZ	1:A:1366:ARG:HD3	2.42	0.54
2:B:222:ILE:HD11	2:B:627:PHE:HZ	1.72	0.54
2:B:882:THR:C	2:B:884:ARG:N	2.66	0.54
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.47	0.54
3:C:43:THR:CG2	3:C:44:LEU:N	2.70	0.54
7:G:119:LEU:HD12	7:G:120:THR:H	1.72	0.54
1:A:472:LEU:O	1:A:475:THR:HB	2.07	0.54
1:A:668:ASP:HB3	1:A:741:ASN:ND2	2.17	0.54
2:B:288:ALA:HA	2:B:331:LEU:HD12	1.90	0.54
4:D:69:ALA:HB2	4:D:72:ARG:NH2	2.22	0.54
8:H:1:MET:O	8:H:1:MET:HG2	2.07	0.54
8:H:84:ALA:C	8:H:86:ASP:N	2.58	0.54
15:P:2:A:H2'	15:P:3:A:C8	2.43	0.54
1:A:1349:TYR:C	1:A:1349:TYR:CD2	2.86	0.54
2:B:332:ASP:O	2:B:334:ILE:N	2.33	0.54
2:B:427:ASP:HA	2:B:430:ARG:HD2	1.87	0.54
2:B:520:GLY:H	2:B:748:ILE:HG22	1.73	0.54
2:B:563:MET:SD	2:B:580:VAL:HG11	2.48	0.54
2:B:936:ASP:OD1	2:B:937:ALA:N	2.41	0.54
4:D:156:ASP:HB2	4:D:159:THR:OG1	2.08	0.54
7:G:1:MET:SD	7:G:79:PHE:CE1	3.01	0.54
8:H:82:PRO:C	8:H:84:ALA:N	2.64	0.54
9:I:22:ASN:O	9:I:23:ASN:HB2	2.07	0.54
1:A:75:ASN:O	1:A:76:GLU:CB	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PHE:CB	1:A:265:LYS:HZ1	2.18	0.54
1:A:320:ARG:NE	1:A:323:LYS:NZ	2.55	0.54
1:A:1313:LEU:C	1:A:1315:GLU:N	2.65	0.54
2:B:313:MET:CE	2:B:386:LEU:HD22	2.37	0.54
2:B:345:LYS:HA	2:B:348:ARG:HE	1.72	0.54
2:B:487:THR:HG22	2:B:490:SER:H	1.73	0.54
2:B:642:ASP:H	2:B:649:LYS:HE3	1.72	0.54
2:B:653:VAL:HA	2:B:657:HIS:CD2	2.43	0.54
3:C:8:VAL:HG12	3:C:9:LYS:N	2.22	0.54
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.42	0.54
4:D:20:GLU:CD	4:D:20:GLU:H	2.16	0.54
4:D:209:ARG:HG2	4:D:209:ARG:HH11	1.72	0.54
9:I:88:SER:C	9:I:90:GLN:H	2.15	0.54
10:J:1:MET:O	10:J:2:ILE:O	2.26	0.54
1:A:1444:MET:HE1	6:F:135:ARG:CB	2.35	0.54
2:B:580:VAL:HG22	2:B:624:LEU:HB3	1.89	0.54
2:B:616:ILE:HG23	2:B:700:SER:OG	2.08	0.54
3:C:8:VAL:HG12	3:C:9:LYS:H	1.72	0.54
7:G:115:MET:HE1	7:G:130:TYR:CE2	2.42	0.54
8:H:8:ASP:OD2	8:H:9:ILE:N	2.40	0.54
1:A:399:HIS:CG	1:A:400:PRO:N	2.74	0.54
1:A:541:ILE:HD11	1:A:656:TRP:CD1	2.42	0.54
1:A:833:GLU:HG3	1:A:1102:LYS:HE2	1.90	0.54
1:A:1244:ARG:HE	1:A:1245:PRO:CD	2.07	0.54
2:B:69:LEU:HB3	2:B:429:PHE:CE1	2.40	0.54
2:B:849:GLY:O	2:B:850:LEU:C	2.51	0.54
2:B:866:TYR:CB	2:B:870:ILE:HB	2.36	0.54
2:B:914:LYS:HE2	2:B:937:ALA:HB1	1.90	0.54
4:D:35:LEU:HD12	4:D:35:LEU:N	2.23	0.54
4:D:130:LEU:O	4:D:132:GLN:N	2.37	0.54
8:H:9:ILE:HD13	8:H:146:ARG:HH12	1.72	0.54
8:H:130:ARG:HB3	8:H:134:ASN:H	1.73	0.54
11:K:31:VAL:HG12	11:K:32:VAL:H	1.72	0.54
1:A:443:LEU:HD22	1:A:455:MET:HE2	1.90	0.54
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.38	0.54
1:A:1191:TRP:CZ3	9:I:43:VAL:HG21	2.43	0.54
2:B:327:ARG:HH21	2:B:371:GLU:HG2	1.70	0.54
2:B:398:ARG:NH1	2:B:398:ARG:CB	2.71	0.54
2:B:637:LEU:HD22	2:B:741:CYS:O	2.07	0.54
2:B:644:GLU:HB3	2:B:648:HIS:O	2.07	0.54
2:B:794:ASN:N	2:B:794:ASN:ND2	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:17:LYS:HD2	4:D:17:LYS:C	2.33	0.54
8:H:127:GLY:O	8:H:128:ASN:CB	2.53	0.54
9:I:7:CYS:HB2	9:I:34:TYR:CG	2.43	0.54
1:A:416:ARG:HG3	1:A:417:TYR:CD1	2.43	0.53
1:A:464:PRO:HG2	1:A:465:TYR:CD1	2.43	0.53
2:B:590:HIS:NE2	2:B:592:ASN:O	2.40	0.53
3:C:137:LYS:HB3	3:C:138:GLU:OE1	2.07	0.53
3:C:251:LEU:O	3:C:255:VAL:HG23	2.08	0.53
4:D:117:GLU:HG2	4:D:122:GLU:OE2	2.08	0.53
5:E:192:ARG:HG3	5:E:192:ARG:NH1	2.23	0.53
9:I:101:PHE:HD1	9:I:101:PHE:H	1.56	0.53
12:L:61:THR:CG2	12:L:63:ARG:HG3	2.37	0.53
1:A:853:ASP:OD1	1:A:853:ASP:C	2.51	0.53
1:A:942:PHE:CE1	5:E:207:ARG:HD3	2.40	0.53
1:A:962:ARG:O	1:A:965:GLN:N	2.41	0.53
2:B:209:GLU:OE2	2:B:485:ARG:NE	2.36	0.53
4:D:208:GLU:HA	4:D:211:LEU:HD12	1.90	0.53
10:J:53:HIS:NE2	10:J:55:ASP:HA	2.24	0.53
1:A:335:ARG:O	1:A:339:ASN:HB2	2.08	0.53
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.73	0.53
1:A:1121:GLU:HB2	1:A:1321:GLY:O	2.08	0.53
1:A:1147:THR:HB	9:I:48:LEU:CD1	2.38	0.53
2:B:801:LYS:O	10:J:52:THR:HG23	2.08	0.53
2:B:831:SER:HB3	2:B:994:TYR:OH	2.09	0.53
2:B:866:TYR:O	2:B:867:GLY:C	2.50	0.53
3:C:66:ARG:NH1	3:C:144:ILE:O	2.42	0.53
3:C:82:TYR:O	3:C:83:SER:C	2.50	0.53
3:C:114:TYR:CD2	3:C:140:ASN:HB2	2.43	0.53
3:C:143:LEU:O	3:C:143:LEU:HG	2.08	0.53
3:C:239:PRO:O	3:C:242:GLN:N	2.42	0.53
5:E:108:GLY:O	5:E:132:ILE:HG22	2.09	0.53
5:E:112:TYR:O	5:E:137:GLU:HG3	2.08	0.53
8:H:37:LYS:HD2	8:H:126:GLU:OE2	2.09	0.53
9:I:62:ILE:O	9:I:62:ILE:HG12	2.08	0.53
10:J:53:HIS:CD2	10:J:54:VAL:C	2.86	0.53
1:A:50:ILE:O	1:A:52:GLY:N	2.40	0.53
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.37	0.53
1:A:481:ASP:OD1	1:A:485:ASP:OD2	2.25	0.53
1:A:547:LEU:HD21	1:A:560:ILE:HD13	1.90	0.53
1:A:741:ASN:HD22	1:A:741:ASN:C	2.16	0.53
1:A:965:GLN:HA	1:A:968:GLN:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1280:GLU:O	1:A:1281:ARG:C	2.51	0.53
2:B:63:ILE:HD12	2:B:421:PHE:CE2	2.44	0.53
2:B:641:GLU:C	2:B:643:ASP:H	2.16	0.53
2:B:1138:MET:HE2	2:B:1146:PHE:CD2	2.44	0.53
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.89	0.53
3:C:100:THR:HG22	3:C:101:LEU:N	2.23	0.53
4:D:13:ARG:O	4:D:15:LEU:N	2.42	0.53
4:D:155:ARG:HD3	4:D:221:TYR:OH	2.07	0.53
5:E:90:VAL:HA	5:E:120:ALA:CB	2.36	0.53
10:J:53:HIS:HD2	10:J:54:VAL:C	2.17	0.53
11:K:12:LEU:HG	11:K:16:GLU:HB2	1.90	0.53
12:L:58:LYS:O	12:L:59:ALA:O	2.27	0.53
1:A:853:ASP:OD1	1:A:855:THR:N	2.42	0.53
1:A:1186:ASP:O	1:A:1187:GLN:CB	2.53	0.53
1:A:1343:ALA:O	1:A:1346:ALA:HB3	2.08	0.53
2:B:192:LEU:O	2:B:193:LYS:HB2	2.08	0.53
2:B:398:ARG:CB	2:B:398:ARG:HH11	2.21	0.53
2:B:637:LEU:HD21	2:B:742:GLU:OE2	2.09	0.53
2:B:872:GLU:OE1	2:B:914:LYS:HE3	2.07	0.53
2:B:1065:GLN:HB3	2:B:1069:PHE:O	2.09	0.53
3:C:166:GLU:C	11:K:6:ARG:HH11	2.16	0.53
3:C:189:THR:CG2	3:C:190:ASP:H	2.21	0.53
4:D:149:THR:CG2	4:D:150:ASN:N	2.72	0.53
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.91	0.53
12:L:34:CYS:O	12:L:34:CYS:SG	2.67	0.53
1:A:93:VAL:HG21	1:A:301:ALA:O	2.08	0.53
1:A:184:SER:CB	1:A:199:LEU:HD23	2.39	0.53
1:A:270:LEU:O	1:A:274:ILE:HG13	2.08	0.53
1:A:356:ASP:OD1	1:A:358:ASN:N	2.42	0.53
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.43	0.53
1:A:549:MET:SD	1:A:577:ILE:CD1	2.96	0.53
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.23	0.53
2:B:864:LYS:HG3	2:B:872:GLU:OE1	2.09	0.53
3:C:177:GLU:O	3:C:230:MET:HA	2.09	0.53
9:I:50:THR:CG2	9:I:51:ASN:N	2.71	0.53
12:L:36:SER:O	12:L:37:LYS:C	2.51	0.53
1:A:350:ARG:HB2	2:B:1128:LEU:CD1	2.39	0.53
1:A:590:ARG:NH2	1:A:620:LYS:HB2	2.23	0.53
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.91	0.53
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.23	0.53
2:B:222:ILE:N	2:B:240:ILE:CD1	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:728:ARG:HH12	2:B:1047:PHE:HB3	1.73	0.53
2:B:797:TYR:C	2:B:798:TYR:HD2	2.17	0.53
5:E:112:TYR:C	5:E:112:TYR:CD1	2.86	0.53
1:A:666:ILE:CD1	1:A:667:GLY:N	2.72	0.53
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.39	0.53
1:A:1325:THR:O	5:E:148:GLU:HB2	2.08	0.53
2:B:58:THR:O	2:B:62:ILE:HG13	2.08	0.53
2:B:644:GLU:C	2:B:646:LEU:H	2.17	0.53
2:B:658:ILE:HG22	2:B:662:MET:HE2	1.89	0.53
2:B:1059:LEU:HD23	2:B:1065:GLN:O	2.09	0.53
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.91	0.53
3:C:241:ASP:O	3:C:245:VAL:HG23	2.09	0.53
4:D:193:THR:HG21	7:G:167:TYR:HD1	1.73	0.53
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.91	0.53
8:H:13:SER:HB3	8:H:27:GLU:O	2.09	0.53
9:I:111:THR:OG1	9:I:112:SER:N	2.42	0.53
1:A:1315:GLU:C	1:A:1317:MET:H	2.17	0.53
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.89	0.53
2:B:254:LEU:HD23	2:B:381:MET:CE	2.36	0.53
2:B:292:ILE:HD11	2:B:327:ARG:H	1.74	0.53
2:B:331:LEU:CD2	2:B:353:LYS:HG2	2.38	0.53
2:B:363:HIS:O	2:B:364:ILE:HB	2.09	0.53
2:B:376:PHE:CZ	2:B:569:TYR:HB3	2.44	0.53
2:B:558:LEU:HD22	2:B:596:LEU:HD11	1.91	0.53
2:B:619:ILE:HG22	2:B:620:ARG:N	2.24	0.53
2:B:957:ASN:O	2:B:958:GLN:C	2.52	0.53
3:C:43:THR:HG22	3:C:44:LEU:N	2.24	0.53
4:D:47:LEU:HD13	4:D:48:ILE:H	1.74	0.53
7:G:119:LEU:HD12	7:G:120:THR:N	2.24	0.53
8:H:133:ASN:O	8:H:135:LEU:N	2.41	0.53
10:J:23:ASN:O	10:J:25:LEU:N	2.42	0.53
1:A:593:GLU:C	1:A:595:THR:H	2.15	0.53
1:A:659:HIS:O	2:B:1081:LEU:HD23	2.09	0.53
1:A:697:ALA:HB1	9:I:97:MET:HE3	1.91	0.53
1:A:719:VAL:HG13	1:A:723:ASN:ND2	2.24	0.53
1:A:786:HIS:N	1:A:786:HIS:CD2	2.74	0.53
2:B:185:THR:H	2:B:188:ASP:HB2	1.73	0.53
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.89	0.53
2:B:763:GLN:HG2	2:B:765:PRO:CD	2.35	0.53
3:C:120:ILE:HD11	3:C:130:GLY:O	2.08	0.53
3:C:148:ARG:N	3:C:151:GLN:HG3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:123:MET:HE1	8:H:142:LEU:CD2	2.36	0.53
1:A:9:ALA:O	1:A:10:PRO:C	2.52	0.52
1:A:102:VAL:CB	1:A:211:PHE:HE1	2.22	0.52
1:A:337:ARG:HD3	1:A:839:ARG:NH2	2.24	0.52
1:A:377:PRO:HD3	1:A:493:GLN:OE1	2.08	0.52
1:A:385:ILE:CD1	1:A:426:LEU:HB2	2.39	0.52
1:A:853:ASP:OD1	1:A:855:THR:CB	2.56	0.52
1:A:1191:TRP:HZ3	9:I:43:VAL:HG21	1.73	0.52
2:B:31:TRP:CZ2	2:B:807:ARG:HB2	2.44	0.52
2:B:244:LEU:O	2:B:249:ARG:HG3	2.08	0.52
2:B:619:ILE:O	2:B:622:LYS:N	2.34	0.52
2:B:806:THR:HA	2:B:1045:SER:OG	2.09	0.52
2:B:882:THR:HG22	2:B:883:LEU:N	2.24	0.52
2:B:1219:ASP:C	2:B:1219:ASP:OD1	2.51	0.52
3:C:18:VAL:O	3:C:20:PHE:HD2	1.92	0.52
3:C:258:ILE:HD12	3:C:258:ILE:N	2.24	0.52
5:E:178:ILE:HG22	5:E:213:ILE:O	2.08	0.52
8:H:9:ILE:HG23	8:H:55:LEU:C	2.34	0.52
12:L:26:THR:HG23	12:L:27:LEU:H	1.73	0.52
1:A:154:SER:CB	1:A:162:VAL:CG2	2.87	0.52
1:A:710:LEU:HD22	9:I:96:SER:HA	1.90	0.52
1:A:925:LEU:C	1:A:927:VAL:N	2.66	0.52
2:B:816:GLU:O	2:B:817:LEU:HD23	2.09	0.52
2:B:875:GLU:O	2:B:877:PRO:HD3	2.08	0.52
3:C:123:ASN:ND2	3:C:125:MET:HA	2.24	0.52
3:C:133:ILE:CD1	3:C:236:GLY:C	2.82	0.52
6:F:109:VAL:CG1	6:F:110:ASP:N	2.72	0.52
7:G:111:THR:O	7:G:112:LYS:C	2.52	0.52
7:G:115:MET:HA	7:G:163:ILE:HG13	1.91	0.52
11:K:53:ASP:C	11:K:55:LYS:H	2.18	0.52
1:A:7:SER:C	1:A:9:ALA:H	2.17	0.52
1:A:132:LYS:HE3	1:A:1411:GLU:HG3	1.90	0.52
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.90	0.52
1:A:306:ASN:ND2	1:A:322:VAL:HG12	2.25	0.52
1:A:595:THR:C	1:A:596:THR:HG23	2.34	0.52
1:A:692:ASP:O	1:A:694:THR:N	2.42	0.52
1:A:851:HIS:HB2	1:A:855:THR:HG22	1.92	0.52
1:A:897:TYR:HB3	1:A:936:LEU:HD12	1.92	0.52
1:A:1006:ILE:CD1	5:E:163:GLU:HG3	2.39	0.52
1:A:1215:ARG:NH1	1:A:1272:THR:O	2.43	0.52
1:A:1402:PHE:CG	1:A:1403:GLU:HG2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:PHE:C	2:B:360:PHE:HD2	2.16	0.52
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.44	0.52
2:B:874:PHE:HA	2:B:913:GLY:O	2.09	0.52
2:B:1175:LEU:O	2:B:1176:ASN:HB2	2.10	0.52
3:C:39:ALA:O	3:C:164:ALA:HB3	2.09	0.52
3:C:104:PHE:HD2	3:C:105:GLY:N	2.07	0.52
8:H:27:GLU:HG2	8:H:39:THR:HA	1.90	0.52
8:H:91:ASP:O	8:H:93:TYR:N	2.39	0.52
8:H:106:GLU:O	8:H:108:SER:N	2.32	0.52
1:A:12:ARG:NH1	2:B:1218:THR:HB	2.25	0.52
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.91	0.52
1:A:851:HIS:HB2	1:A:855:THR:CG2	2.39	0.52
1:A:886:ILE:CG2	1:A:887:GLY:N	2.71	0.52
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.74	0.52
5:E:61:GLN:NE2	5:E:105:PHE:CE2	2.78	0.52
12:L:60:ARG:HG2	12:L:61:THR:N	2.21	0.52
1:A:356:ASP:OD1	1:A:358:ASN:HB2	2.09	0.52
1:A:626:ASN:O	1:A:631:HIS:CD2	2.62	0.52
1:A:666:ILE:HD12	1:A:667:GLY:N	2.21	0.52
1:A:864:ILE:HG22	1:A:865:GLN:HG3	1.91	0.52
2:B:373:ARG:NH2	2:B:587:HIS:HA	2.24	0.52
2:B:642:ASP:C	2:B:644:GLU:H	2.18	0.52
2:B:1116:ARG:HD2	2:B:1198:TYR:CD1	2.44	0.52
3:C:148:ARG:NH1	10:J:64:ASN:HA	2.24	0.52
7:G:88:ASP:HB3	7:G:144:ARG:CA	2.32	0.52
7:G:106:MET:CG	7:G:107:LYS:N	2.72	0.52
1:A:13:THR:HB	1:A:1432:GLN:NE2	2.25	0.52
1:A:1161:THR:OG1	1:A:1239:ARG:NH2	2.43	0.52
1:A:1397:LEU:HB2	1:A:1426:GLU:OE1	2.10	0.52
2:B:193:LYS:HZ1	12:L:32:ALA:HB1	1.75	0.52
2:B:383:ASN:O	2:B:387:LEU:HD12	2.10	0.52
2:B:549:THR:CG2	2:B:550:ASP:H	2.23	0.52
2:B:866:TYR:HB3	2:B:870:ILE:HD12	1.90	0.52
2:B:901:PRO:HD2	12:L:59:ALA:O	2.10	0.52
4:D:47:LEU:HD11	7:G:3:PHE:HD2	1.74	0.52
4:D:71:LYS:CG	4:D:74:GLN:HG3	2.40	0.52
15:P:1:C:O2	15:P:1:C:H2'	2.10	0.52
1:A:54:ASN:N	1:A:54:ASN:HD22	2.07	0.52
1:A:1200:ALA:HA	1:A:1203:ASN:HD22	1.74	0.52
1:A:1218:GLN:O	1:A:1221:LYS:HE3	2.10	0.52
1:A:1385:THR:HG21	1:A:1387:HIS:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:GLU:HG2	2:B:246:LYS:HG3	1.90	0.52
2:B:313:MET:O	2:B:316:PRO:HD2	2.09	0.52
2:B:819:ALA:O	2:B:1093:GLN:HG2	2.09	0.52
2:B:878:GLN:O	2:B:879:ARG:C	2.53	0.52
2:B:1095:LEU:HD12	2:B:1095:LEU:N	2.15	0.52
2:B:1115:THR:HG22	2:B:1117:GLN:N	2.24	0.52
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.89	0.52
3:C:184:ASN:OD1	3:C:187:LYS:CA	2.58	0.52
8:H:9:ILE:HG12	8:H:56:THR:HA	1.92	0.52
1:A:92:HIS:O	1:A:94:GLY:N	2.42	0.52
1:A:252:PHE:O	1:A:256:GLN:NE2	2.42	0.52
1:A:316:GLN:O	1:A:317:LYS:C	2.51	0.52
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.91	0.52
2:B:282:ILE:CG2	2:B:382:ILE:HD11	2.40	0.52
7:G:87:VAL:HG23	7:G:87:VAL:O	2.08	0.52
12:L:53:HIS:C	12:L:55:ILE:HD13	2.34	0.52
14:T:15:DG:H2"	14:T:16:DT:C6	2.45	0.52
1:A:35:ILE:CD1	1:A:241:VAL:HG11	2.40	0.52
1:A:305:ASP:OD1	1:A:306:ASN:N	2.43	0.52
1:A:335:ARG:NH1	2:B:1206:GLU:CD	2.68	0.52
1:A:953:ASN:C	1:A:954:TRP:CD1	2.88	0.52
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.92	0.52
1:A:1166:ASP:O	1:A:1167:GLU:C	2.52	0.52
3:C:242:GLN:C	3:C:244:VAL:N	2.63	0.52
3:C:249:ASP:O	3:C:252:GLN:HB3	2.09	0.52
6:F:138:LEU:HB2	6:F:142:SER:HB2	1.90	0.52
8:H:98:TYR:C	8:H:118:PHE:HD2	2.16	0.52
1:A:34:LYS:HB2	1:A:36:ARG:NH2	2.25	0.52
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.91	0.52
1:A:233:TRP:C	1:A:235:ILE:H	2.16	0.52
1:A:440:ASP:O	1:A:460:VAL:HG23	2.11	0.52
1:A:795:GLU:CD	1:A:795:GLU:H	2.17	0.52
1:A:1353:TYR:C	1:A:1353:TYR:HD2	2.17	0.52
1:A:1445:ILE:HD12	7:G:59:GLY:O	2.10	0.52
2:B:498:THR:O	2:B:536:VAL:HA	2.09	0.52
2:B:787:VAL:O	2:B:787:VAL:HG12	2.10	0.52
3:C:168:ALA:O	3:C:170:TRP:N	2.42	0.52
3:C:233:GLU:CG	3:C:234:SER:H	2.23	0.52
3:C:236:GLY:C	3:C:238:ILE:N	2.66	0.52
4:D:5:THR:O	4:D:5:THR:HG23	2.10	0.52
4:D:147:TYR:OH	7:G:103:VAL:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:139:ILE:HG23	7:G:140:LYS:N	2.24	0.52
8:H:104:PHE:CD2	8:H:114:VAL:HG12	2.44	0.52
10:J:3:VAL:N	10:J:53:HIS:HE1	2.08	0.52
11:K:73:LEU:HD21	11:K:75:ILE:HD11	1.92	0.52
1:A:49:LYS:NZ	1:A:61:ILE:N	2.58	0.51
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.10	0.51
1:A:1230:GLU:O	1:A:1232:ASN:N	2.43	0.51
2:B:276:ILE:HG23	2:B:336:ARG:HB2	1.91	0.51
2:B:705:MET:HA	2:B:705:MET:CE	2.35	0.51
5:E:147:HIS:HD2	5:E:149:LEU:H	1.58	0.51
7:G:1:MET:HE3	7:G:80:LYS:O	2.09	0.51
7:G:116:PRO:HG2	7:G:119:LEU:HB2	1.92	0.51
9:I:53:GLY:O	9:I:89:GLN:HB2	2.10	0.51
1:A:71:GLN:C	1:A:73:GLY:H	2.17	0.51
1:A:528:LEU:O	1:A:531:ILE:HG22	2.11	0.51
1:A:697:ALA:HB2	1:A:702:LEU:CD1	2.39	0.51
1:A:988:LEU:O	1:A:992:ASP:HB2	2.10	0.51
1:A:1412:ALA:HA	1:A:1417:GLU:OE2	2.10	0.51
2:B:638:PHE:HB3	2:B:651:LEU:HD22	1.92	0.51
2:B:806:THR:HB	2:B:809:MET:HG3	1.92	0.51
2:B:1007:VAL:HG22	2:B:1008:PRO:CD	2.37	0.51
2:B:1166:CYS:SG	2:B:1166:CYS:O	2.69	0.51
5:E:207:ARG:NH1	5:E:207:ARG:CB	2.71	0.51
11:K:107:THR:HG22	11:K:108:GLU:N	2.24	0.51
1:A:68:GLN:OE1	1:A:68:GLN:O	2.27	0.51
1:A:722:LEU:HD12	1:A:722:LEU:H	1.75	0.51
1:A:999:VAL:HG12	1:A:1000:LEU:HD12	1.92	0.51
1:A:1268:LEU:O	1:A:1269:GLU:HG3	2.10	0.51
2:B:360:PHE:HE2	2:B:361:LEU:HD13	1.75	0.51
2:B:360:PHE:O	2:B:361:LEU:C	2.53	0.51
2:B:640:VAL:O	2:B:640:VAL:HG12	2.10	0.51
2:B:707:PRO:O	2:B:708:GLU:O	2.28	0.51
2:B:755:ILE:O	2:B:755:ILE:HG22	2.09	0.51
2:B:871:THR:HG22	2:B:872:GLU:N	2.23	0.51
3:C:31:ASN:O	3:C:34:ARG:HB3	2.11	0.51
3:C:179:GLU:HG2	3:C:180:TYR:H	1.74	0.51
3:C:239:PRO:HB2	3:C:241:ASP:OD1	2.10	0.51
5:E:78:LEU:CA	5:E:107:THR:HB	2.34	0.51
5:E:136:ASN:OD1	5:E:137:GLU:N	2.43	0.51
8:H:135:LEU:HB3	8:H:137:GLN:HG2	1.92	0.51
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.11	0.51
1:A:688:LYS:CD	1:A:691:LEU:HD23	2.41	0.51
1:A:903:ASN:HD22	1:A:903:ASN:C	2.17	0.51
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.75	0.51
1:A:1435:PRO:O	1:A:1436:ILE:HG13	2.10	0.51
2:B:398:ARG:HH11	2:B:398:ARG:HB3	1.76	0.51
2:B:792:MET:HE2	2:B:857:ARG:NH2	2.25	0.51
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.93	0.51
2:B:1031:LEU:HB2	2:B:1055:ILE:CD1	2.40	0.51
3:C:80:LEU:HD11	3:C:95:CYS:C	2.35	0.51
5:E:31:THR:HG1	5:E:34:GLU:H	1.57	0.51
8:H:10:PHE:N	8:H:10:PHE:CD1	2.78	0.51
9:I:53:GLY:O	9:I:55:THR:N	2.44	0.51
12:L:58:LYS:O	12:L:58:LYS:HG2	2.10	0.51
12:L:66:GLN:HG2	12:L:67:PHE:N	2.25	0.51
1:A:75:ASN:O	1:A:76:GLU:HB2	2.10	0.51
1:A:108:MET:HB3	1:A:210:ILE:HD11	1.91	0.51
1:A:351:THR:HG22	2:B:1103:ILE:HG13	1.91	0.51
1:A:414:ASP:OD1	1:A:416:ARG:HG2	2.10	0.51
1:A:688:LYS:HA	1:A:691:LEU:HB3	1.93	0.51
1:A:696:GLU:OE2	1:A:702:LEU:HD21	2.09	0.51
1:A:720:ARG:HG2	1:A:720:ARG:O	2.11	0.51
1:A:889:SER:CB	1:A:1297:GLU:HG3	2.38	0.51
1:A:915:SER:O	1:A:919:ILE:HB	2.10	0.51
1:A:1141:THR:HG23	1:A:1205:LYS:HZ2	1.76	0.51
1:A:1208:THR:O	1:A:1212:VAL:HG23	2.11	0.51
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.26	0.51
1:A:1315:GLU:C	1:A:1317:MET:N	2.68	0.51
1:A:1349:TYR:O	1:A:1350:LYS:C	2.52	0.51
2:B:67:SER:HB2	2:B:92:PHE:HD1	1.76	0.51
2:B:708:GLU:HG3	2:B:709:ASP:N	2.25	0.51
2:B:976:ILE:O	2:B:990:ILE:HB	2.10	0.51
3:C:118:LEU:HB2	3:C:132:PRO:HG2	1.93	0.51
4:D:13:ARG:C	4:D:15:LEU:N	2.68	0.51
5:E:94:LYS:CE	5:E:98:ILE:HD11	2.33	0.51
7:G:58:ARG:HG3	7:G:58:ARG:NH1	2.25	0.51
1:A:233:TRP:C	1:A:235:ILE:N	2.69	0.51
1:A:247:ARG:NH1	1:A:263:THR:HG23	2.25	0.51
1:A:332:LYS:O	1:A:333:GLU:CB	2.57	0.51
1:A:1402:PHE:CD1	1:A:1403:GLU:HG2	2.46	0.51
2:B:69:LEU:HD13	2:B:429:PHE:HD1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.39	0.51
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.09	0.51
3:C:15:LYS:HZ1	3:C:135:GLN:HG2	1.76	0.51
3:C:186:LEU:N	3:C:186:LEU:HD12	2.25	0.51
4:D:195:ILE:HG22	4:D:195:ILE:O	2.10	0.51
7:G:91:VAL:HG12	7:G:92:VAL:N	2.24	0.51
9:I:34:TYR:CE2	9:I:36:GLU:HB3	2.46	0.51
1:A:33:ALA:HA	1:A:57:ARG:NH1	2.25	0.51
1:A:445:ASN:HB2	1:A:454:SER:O	2.10	0.51
1:A:445:ASN:CB	1:A:455:MET:HG2	2.41	0.51
1:A:650:GLN:HB3	1:A:654:ASN:HD21	1.76	0.51
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.10	0.51
2:B:130:VAL:HG23	2:B:167:ILE:HD13	1.92	0.51
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.46	0.51
2:B:604:ARG:C	2:B:606:LYS:H	2.19	0.51
2:B:637:LEU:HD12	2:B:693:ILE:CD1	2.38	0.51
2:B:770:GLN:HG2	2:B:983:ARG:O	2.11	0.51
2:B:861:ASP:OD1	2:B:862:GLN:N	2.44	0.51
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.46	0.51
2:B:996:ARG:HH12	3:C:175:ALA:N	2.09	0.51
2:B:999:MET:HE3	2:B:999:MET:CA	2.30	0.51
2:B:1095:LEU:H	2:B:1095:LEU:CD1	2.15	0.51
4:D:8:PHE:CD2	7:G:6:ASP:HB2	2.46	0.51
5:E:56:LYS:HZ3	5:E:84:ASP:N	2.09	0.51
6:F:119:ARG:HG3	6:F:119:ARG:NH1	2.19	0.51
11:K:68:PHE:N	11:K:68:PHE:CD2	2.75	0.51
14:T:22:DC:H2''	14:T:23:BRU:OP2	2.10	0.51
1:A:49:LYS:HD3	1:A:55:ASP:HB3	1.93	0.51
1:A:447:GLN:HE22	14:T:20:DG:H4'	1.76	0.51
1:A:483:ASP:O	2:B:979:LYS:HE3	2.11	0.51
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.26	0.51
1:A:737:LEU:HD22	1:A:741:ASN:OD1	2.11	0.51
1:A:1450:LEU:HG	7:G:19:GLY:O	2.11	0.51
2:B:46:GLN:HE21	2:B:539:LEU:HD12	1.76	0.51
2:B:555:ILE:HG22	2:B:556:THR:N	2.26	0.51
2:B:565:PRO:HB2	2:B:567:GLU:CG	2.40	0.51
2:B:839:MET:CE	2:B:980:PHE:HB2	2.40	0.51
3:C:183:TRP:CH2	3:C:203:GLN:NE2	2.78	0.51
5:E:10:SER:O	5:E:13:TRP:HB3	2.11	0.51
5:E:168:TYR:HB3	5:E:170:LEU:HG	1.92	0.51
9:I:75:CYS:SG	9:I:79:HIS:N	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:86:PHE:HE1	9:I:100:PHE:HB2	1.76	0.51
11:K:68:PHE:HD1	11:K:70:ARG:NH1	2.05	0.51
12:L:30:ILE:CG2	12:L:31:CYS:N	2.74	0.51
1:A:583:PRO:O	1:A:610:GLY:HA3	2.11	0.51
1:A:1054:LEU:HD13	6:F:84:TYR:OH	2.11	0.51
1:A:1386:ARG:O	1:A:1391:ARG:HD2	2.10	0.51
2:B:37:PHE:HD2	2:B:542:MET:SD	2.34	0.51
2:B:307:ASP:OD2	2:B:310:MET:HB2	2.09	0.51
2:B:557:PHE:CE1	2:B:603:LEU:HD11	2.46	0.51
2:B:834:ASN:O	2:B:838:SER:O	2.29	0.51
2:B:875:GLU:HG3	2:B:877:PRO:HD3	1.92	0.51
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.41	0.51
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.93	0.51
3:C:140:ASN:O	3:C:141:GLY:O	2.29	0.51
4:D:128:VAL:O	4:D:130:LEU:N	2.44	0.51
8:H:100:THR:HG22	8:H:101:ALA:N	2.26	0.51
1:A:43:GLU:HG3	1:A:46:THR:HB	1.93	0.51
1:A:335:ARG:CZ	2:B:1202:LEU:HD13	2.41	0.51
1:A:610:GLY:O	1:A:611:GLN:NE2	2.45	0.51
1:A:691:LEU:O	1:A:691:LEU:HD12	2.11	0.51
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.11	0.51
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.46	0.51
2:B:361:LEU:O	2:B:363:HIS:O	2.29	0.51
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.41	0.51
2:B:593:PRO:O	2:B:595:ARG:N	2.43	0.51
2:B:1072:MET:HB2	2:B:1085:ILE:HD13	1.92	0.51
2:B:1099:VAL:HG13	2:B:1100:ASP:H	1.76	0.51
2:B:1221:SER:O	2:B:1223:ASP:N	2.43	0.51
4:D:47:LEU:CD1	4:D:48:ILE:N	2.74	0.51
5:E:69:ILE:HD12	5:E:69:ILE:H	1.74	0.51
7:G:48:VAL:HA	7:G:76:ALA:HB2	1.93	0.51
7:G:112:LYS:HA	7:G:115:MET:CE	2.28	0.51
8:H:62:SER:OG	8:H:63:LEU:N	2.43	0.51
11:K:21:ILE:HG22	11:K:31:VAL:CG1	2.40	0.51
11:K:79:GLU:C	11:K:81:TYR:H	2.19	0.51
1:A:7:SER:OG	2:B:1161:HIS:CE1	2.61	0.50
1:A:851:HIS:C	1:A:853:ASP:H	2.19	0.50
1:A:858:ASN:C	1:A:858:ASN:ND2	2.65	0.50
1:A:946:VAL:HG22	5:E:201:LYS:CD	2.41	0.50
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.93	0.50
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1423:GLY:O	1:A:1424:VAL:C	2.54	0.50
1:A:1453:TYR:O	1:A:1454:MET:HB3	2.12	0.50
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.93	0.50
2:B:230:ALA:HB3	2:B:231:PRO:HD3	1.93	0.50
2:B:326:ASP:OD1	2:B:329:THR:HB	2.10	0.50
2:B:393:LYS:HA	2:B:393:LYS:HE3	1.93	0.50
2:B:606:LYS:HD2	2:B:608:ASP:OD2	2.10	0.50
2:B:996:ARG:NH1	3:C:175:ALA:H	2.09	0.50
3:C:104:PHE:HD2	3:C:105:GLY:H	1.57	0.50
6:F:90:ARG:O	6:F:91:ALA:C	2.55	0.50
6:F:111:LEU:HD12	6:F:111:LEU:N	2.25	0.50
7:G:14:HIS:HD2	7:G:16:SER:OG	1.94	0.50
1:A:84:ILE:O	1:A:84:ILE:HG22	2.10	0.50
1:A:706:HIS:O	1:A:708:MET:HE3	2.11	0.50
2:B:205:ILE:N	2:B:205:ILE:CD1	2.74	0.50
2:B:504:ARG:NH2	14:T:15:DG:O6	2.43	0.50
2:B:593:PRO:O	2:B:594:ALA:C	2.54	0.50
2:B:661:LEU:HD23	2:B:679:TYR:O	2.11	0.50
2:B:879:ARG:H	2:B:879:ARG:HD2	1.76	0.50
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.75	0.50
2:B:1197:PRO:O	2:B:1200:ALA:N	2.34	0.50
4:D:52:LEU:HD12	4:D:182:SER:HB2	1.93	0.50
4:D:53:SER:H	4:D:148:LEU:CD2	2.24	0.50
4:D:217:LEU:O	4:D:219:THR:N	2.44	0.50
4:D:220:LEU:CD2	4:D:221:TYR:N	2.63	0.50
11:K:53:ASP:OD1	11:K:55:LYS:HB2	2.12	0.50
1:A:108:MET:SD	1:A:210:ILE:HD13	2.52	0.50
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.46	0.50
1:A:332:LYS:H	1:A:337:ARG:HB2	1.77	0.50
1:A:648:ASN:O	1:A:649:ILE:C	2.55	0.50
1:A:1387:HIS:HA	1:A:1391:ARG:NH1	2.23	0.50
2:B:212:LEU:HD23	2:B:480:SER:HB2	1.93	0.50
2:B:223:VAL:HG11	2:B:381:MET:HG2	1.93	0.50
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.40	0.50
2:B:642:ASP:O	2:B:644:GLU:N	2.38	0.50
2:B:911:ILE:HG22	2:B:966:VAL:HG21	1.94	0.50
3:C:91:HIS:O	3:C:91:HIS:CD2	2.64	0.50
4:D:46:GLU:HG2	4:D:47:LEU:N	2.26	0.50
4:D:60:LYS:HE3	4:D:126:ILE:CD1	2.33	0.50
5:E:65:THR:O	5:E:69:ILE:CD1	2.59	0.50
5:E:129:PRO:HG2	5:E:130:ALA:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:178:ILE:HB	5:E:212:ARG:HB3	1.94	0.50
8:H:11:GLN:C	8:H:28:ALA:HB1	2.35	0.50
1:A:196:GLU:HG2	1:A:197:PRO:CD	2.41	0.50
1:A:285:PRO:O	1:A:287:HIS:N	2.44	0.50
1:A:886:ILE:CG2	1:A:952:ALA:HB2	2.41	0.50
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.11	0.50
1:A:1332:PHE:CE1	1:A:1348:LEU:HD13	2.46	0.50
2:B:365:THR:OG1	2:B:367:LEU:HG	2.11	0.50
2:B:376:PHE:CZ	2:B:569:TYR:HD2	2.29	0.50
2:B:687:GLU:O	2:B:689:LEU:HG	2.11	0.50
2:B:827:ILE:O	2:B:1085:ILE:HG23	2.11	0.50
2:B:847:ASP:O	2:B:849:GLY:N	2.44	0.50
2:B:1106:ARG:HD3	2:B:1126:GLY:C	2.36	0.50
5:E:182:ASP:HB3	5:E:185:ALA:CB	2.41	0.50
6:F:97:ARG:HD3	6:F:130:ILE:HG23	1.94	0.50
10:J:32:GLU:CD	10:J:32:GLU:H	2.18	0.50
10:J:36:LEU:HB2	10:J:47:ARG:HH12	1.76	0.50
1:A:115:LEU:HD13	1:A:141:LEU:HD13	1.93	0.50
1:A:447:GLN:HA	1:A:448:PRO:C	2.37	0.50
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.46	0.50
1:A:1187:GLN:HB2	1:A:1244:ARG:CG	2.30	0.50
1:A:1211:GLN:O	1:A:1214:GLU:HB2	2.12	0.50
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.47	0.50
2:B:293:PRO:C	2:B:294:ASP:O	2.51	0.50
2:B:622:LYS:CE	9:I:59:VAL:HG22	2.31	0.50
4:D:146:GLN:O	4:D:147:TYR:C	2.55	0.50
7:G:1:MET:SD	7:G:1:MET:C	2.95	0.50
7:G:112:LYS:CA	7:G:115:MET:HE3	2.29	0.50
7:G:123:ALA:C	7:G:125:SER:N	2.70	0.50
8:H:55:LEU:HD22	8:H:144:ILE:CG2	2.42	0.50
14:T:18:DC:OP1	14:T:18:DC:H3'	2.11	0.50
1:A:207:ILE:O	1:A:208:LEU:C	2.55	0.50
1:A:298:PHE:O	1:A:302:THR:HB	2.12	0.50
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.42	0.50
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.47	0.50
1:A:901:LEU:HA	1:A:907:THR:OG1	2.11	0.50
1:A:964:ILE:HD13	1:A:1035:TYR:CE1	2.46	0.50
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.26	0.50
1:A:1138:ILE:HG21	1:A:1316:VAL:HG13	1.93	0.50
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.76	0.50
2:B:59:LEU:HD12	2:B:417:PHE:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:PRO:HG2	2:B:234:ILE:HD13	1.94	0.50
2:B:259:TYR:HD1	2:B:259:TYR:H	1.59	0.50
2:B:882:THR:CG2	2:B:884:ARG:N	2.66	0.50
2:B:1017:ILE:H	2:B:1018:PRO:CD	2.24	0.50
4:D:53:SER:C	4:D:55:ALA:N	2.65	0.50
4:D:153:ARG:O	4:D:154:PHE:HD2	1.95	0.50
10:J:24:LEU:O	10:J:30:LEU:HB2	2.11	0.50
1:A:12:ARG:NH2	2:B:1192:TYR:CZ	2.79	0.50
1:A:41:MET:O	1:A:42:ASP:C	2.55	0.50
1:A:401:GLY:C	1:A:435:HIS:CD2	2.89	0.50
1:A:460:VAL:HG12	1:A:461:LYS:N	2.26	0.50
1:A:886:ILE:CG2	1:A:887:GLY:H	2.23	0.50
1:A:1048:ASN:O	1:A:1049:ILE:C	2.53	0.50
1:A:1111:MET:O	1:A:1112:LYS:O	2.30	0.50
1:A:1203:ASN:O	1:A:1204:ASP:C	2.55	0.50
1:A:1212:VAL:O	1:A:1216:ILE:HG13	2.11	0.50
1:A:1244:ARG:CB	1:A:1245:PRO:CD	2.88	0.50
2:B:258:LEU:HG	2:B:258:LEU:O	2.11	0.50
2:B:307:ASP:OD2	2:B:310:MET:HE3	2.11	0.50
2:B:678:GLU:HG2	2:B:679:TYR:N	2.26	0.50
3:C:138:GLU:HB2	3:C:140:ASN:ND2	2.26	0.50
3:C:213:PRO:HG2	3:C:214:ASN:H	1.76	0.50
9:I:7:CYS:C	9:I:8:ARG:O	2.51	0.50
1:A:95:PHE:O	1:A:96:ILE:C	2.55	0.50
1:A:269:ILE:HG23	1:A:300:VAL:HG23	1.94	0.50
1:A:475:THR:CG2	1:A:476:SER:N	2.75	0.50
1:A:690:VAL:HG12	1:A:691:LEU:N	2.26	0.50
2:B:27:ALA:O	2:B:28:GLU:C	2.55	0.50
2:B:292:ILE:HD13	2:B:326:ASP:HA	1.93	0.50
2:B:335:GLY:O	2:B:336:ARG:HG3	2.12	0.50
2:B:345:LYS:C	2:B:347:LYS:H	2.20	0.50
2:B:357:GLN:O	2:B:366:GLN:HA	2.11	0.50
2:B:591:ARG:O	2:B:592:ASN:C	2.55	0.50
2:B:705:MET:HB3	2:B:706:GLN:OE1	2.12	0.50
2:B:842:ASN:HD22	2:B:845:SER:N	2.04	0.50
3:C:204:SER:C	3:C:206:ASN:N	2.69	0.50
3:C:242:GLN:O	3:C:244:VAL:N	2.45	0.50
5:E:37:LEU:HD11	5:E:41:ASP:HB2	1.93	0.50
5:E:211:TYR:N	5:E:211:TYR:CD1	2.79	0.50
7:G:3:PHE:HB2	7:G:78:VAL:HG23	1.94	0.50
1:A:51:GLY:O	1:A:56:PRO:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HG	1:A:142:CYS:HB3	1.94	0.50
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.46	0.50
1:A:590:ARG:HH22	1:A:620:LYS:HB2	1.77	0.50
1:A:666:ILE:HD11	2:B:1086:PHE:CE1	2.46	0.50
2:B:542:MET:HE2	2:B:747:MET:HE2	1.93	0.50
2:B:639:ILE:HD11	2:B:691:GLU:HB3	1.94	0.50
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.92	0.50
5:E:27:GLY:O	5:E:65:THR:HG23	2.12	0.50
7:G:17:PHE:C	7:G:19:GLY:H	2.20	0.50
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.94	0.49
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.12	0.49
1:A:146:MET:HA	1:A:171:GLN:HB2	1.94	0.49
1:A:629:LEU:HD11	1:A:645:LEU:HD21	1.94	0.49
1:A:1003:LYS:O	1:A:1004:ASN:HB3	2.11	0.49
1:A:1280:GLU:O	1:A:1281:ARG:O	2.30	0.49
2:B:987:LYS:HE3	15:P:11:G:H1'	1.94	0.49
2:B:1187:ASN:OD1	2:B:1190:ASP:N	2.45	0.49
3:C:73:GLN:HB3	3:C:131:HIS:H	1.77	0.49
3:C:249:ASP:O	3:C:250:THR:C	2.55	0.49
5:E:33:GLU:C	5:E:35:VAL:H	2.19	0.49
5:E:100:ILE:CG2	5:E:105:PHE:HB2	2.41	0.49
8:H:138:GLU:O	8:H:139:ASN:C	2.55	0.49
9:I:50:THR:HB	9:I:92:ARG:HH22	1.77	0.49
9:I:119:THR:O	9:I:119:THR:HG22	2.11	0.49
10:J:1:MET:H2	10:J:57:ILE:H	1.59	0.49
1:A:108:MET:HA	1:A:210:ILE:HD13	1.93	0.49
1:A:692:ASP:O	1:A:693:VAL:C	2.55	0.49
1:A:1277:GLU:C	1:A:1279:ILE:H	2.20	0.49
4:D:12:ARG:HG2	4:D:12:ARG:NH1	2.26	0.49
4:D:29:LEU:N	4:D:29:LEU:CD2	2.74	0.49
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.92	0.49
6:F:109:VAL:HG12	6:F:110:ASP:H	1.75	0.49
11:K:17:SER:O	11:K:18:LYS:C	2.50	0.49
1:A:40:THR:HB	1:A:41:MET:CE	2.41	0.49
1:A:153:PRO:CD	1:A:161:LEU:HD13	2.41	0.49
1:A:336:ILE:HD13	1:A:340:LEU:HD12	1.93	0.49
1:A:1115:SER:C	1:A:1308:THR:HG22	2.38	0.49
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.93	0.49
2:B:654:ARG:O	2:B:656:GLY:N	2.46	0.49
2:B:916:THR:HB	2:B:935:ARG:CD	2.41	0.49
2:B:1097:HIS:H	2:B:1098:MET:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:20:PHE:CD1	3:C:20:PHE:C	2.90	0.49
3:C:46:ILE:HD13	3:C:157:CYS:SG	2.52	0.49
3:C:97:VAL:HG21	3:C:129:ILE:HG22	1.93	0.49
3:C:193:TYR:C	3:C:193:TYR:CD1	2.89	0.49
3:C:193:TYR:C	3:C:193:TYR:HD1	2.21	0.49
4:D:8:PHE:CE2	7:G:6:ASP:HB2	2.48	0.49
4:D:138:ASN:C	4:D:140:ASP:N	2.67	0.49
4:D:209:ARG:HG2	4:D:209:ARG:NH1	2.27	0.49
9:I:61:ASP:C	9:I:63:GLY:N	2.67	0.49
9:I:118:ARG:HH12	9:I:120:GLN:HB2	1.77	0.49
10:J:32:GLU:O	10:J:34:THR:N	2.45	0.49
1:A:287:HIS:ND1	1:A:290:GLU:HG2	2.28	0.49
1:A:382:PRO:N	1:A:428:TYR:HE2	2.10	0.49
1:A:809:THR:H	1:A:812:GLU:HB2	1.77	0.49
1:A:1206:ASP:O	1:A:1274:ARG:NH2	2.44	0.49
2:B:167:ILE:HD12	2:B:167:ILE:N	2.27	0.49
2:B:958:GLN:C	2:B:960:GLY:H	2.20	0.49
2:B:996:ARG:HH22	3:C:175:ALA:H	1.60	0.49
3:C:105:GLY:O	3:C:149:LYS:O	2.31	0.49
8:H:40:LEU:HD23	8:H:42:ILE:HD11	1.93	0.49
11:K:12:LEU:HD21	11:K:17:SER:C	2.37	0.49
1:A:55:ASP:O	1:A:55:ASP:OD2	2.31	0.49
1:A:670:ILE:HD12	2:B:1067:ARG:NH2	2.27	0.49
1:A:692:ASP:C	1:A:694:THR:N	2.68	0.49
1:A:946:VAL:CG2	5:E:201:LYS:HD2	2.42	0.49
1:A:1129:GLU:OE2	1:A:1132:LYS:HD2	2.12	0.49
2:B:287:ARG:HG3	2:B:292:ILE:HA	1.93	0.49
2:B:363:HIS:O	2:B:364:ILE:CB	2.61	0.49
2:B:458:LYS:O	2:B:459:TYR:C	2.55	0.49
2:B:910:VAL:HG11	2:B:938:SER:HB3	1.94	0.49
3:C:215:GLU:O	3:C:217:ASP:N	2.46	0.49
3:C:239:PRO:O	3:C:241:ASP:N	2.45	0.49
4:D:35:LEU:HA	4:D:47:LEU:HB2	1.92	0.49
4:D:71:LYS:HA	4:D:74:GLN:HB2	1.93	0.49
5:E:61:GLN:HG3	5:E:78:LEU:O	2.11	0.49
1:A:56:PRO:O	1:A:57:ARG:NH1	2.45	0.49
1:A:380:VAL:CG1	1:A:385:ILE:HG12	2.42	0.49
1:A:714:PHE:CG	9:I:97:MET:HE1	2.48	0.49
1:A:888:GLY:O	1:A:940:ARG:NH2	2.45	0.49
2:B:25:ILE:CD1	2:B:653:VAL:O	2.60	0.49
2:B:185:THR:O	2:B:188:ASP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:LEU:HD22	2:B:361:LEU:HD12	1.94	0.49
2:B:575:PRO:HG2	2:B:576:ASP:H	1.76	0.49
2:B:995:ARG:HH12	3:C:165:LYS:HG2	1.77	0.49
4:D:153:ARG:HB3	4:D:154:PHE:CE2	2.48	0.49
5:E:168:TYR:CB	5:E:170:LEU:HG	2.42	0.49
6:F:69:LEU:HB2	6:F:72:LYS:HD2	1.95	0.49
7:G:165:GLU:HB2	7:G:168:LEU:HD12	1.94	0.49
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.42	0.49
2:B:240:ILE:HG23	2:B:254:LEU:HB3	1.94	0.49
2:B:263:GLY:O	2:B:264:SER:C	2.55	0.49
2:B:603:LEU:HD13	2:B:608:ASP:CB	2.35	0.49
2:B:874:PHE:HB3	2:B:896:ASP:O	2.12	0.49
2:B:1065:GLN:NE2	2:B:1066:SER:N	2.61	0.49
3:C:33:LEU:HD12	3:C:37:MET:HG3	1.95	0.49
3:C:124:LEU:O	3:C:125:MET:C	2.55	0.49
4:D:149:THR:HG22	4:D:150:ASN:N	2.27	0.49
8:H:135:LEU:CB	8:H:137:GLN:HG2	2.43	0.49
12:L:61:THR:HG22	12:L:62:LYS:H	1.78	0.49
1:A:2:VAL:HG22	1:A:3:GLY:N	2.26	0.49
1:A:265:LYS:CA	1:A:265:LYS:CE	2.86	0.49
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.47	0.49
1:A:774:ARG:NH1	1:A:797:LYS:HG3	2.27	0.49
1:A:820:GLY:O	1:A:822:GLU:N	2.45	0.49
1:A:846:GLU:OE1	1:A:1425:SER:OG	2.29	0.49
2:B:129:PHE:HA	2:B:165:VAL:O	2.13	0.49
2:B:217:ARG:NE	2:B:405:ARG:HB2	2.26	0.49
2:B:281:PRO:O	2:B:283:VAL:N	2.45	0.49
2:B:313:MET:HE2	2:B:390:LEU:HD11	1.94	0.49
2:B:579:ARG:N	2:B:589:VAL:HG13	2.28	0.49
2:B:579:ARG:CA	2:B:589:VAL:HG13	2.42	0.49
2:B:603:LEU:HD12	2:B:609:ILE:CG2	2.41	0.49
2:B:711:GLU:HB2	2:B:712:PRO:HD2	1.94	0.49
8:H:12:VAL:HG11	8:H:51:ALA:HA	1.95	0.49
11:K:50:LEU:HD11	11:K:75:ILE:HD13	1.94	0.49
15:P:9:C:OP2	15:P:9:C:H6	1.96	0.49
1:A:256:GLN:HE21	2:B:935:ARG:HH12	1.60	0.49
1:A:337:ARG:HD2	2:B:1132:GLU:OE1	2.13	0.49
1:A:378:GLU:CD	1:A:387:ARG:HH22	2.21	0.49
1:A:549:MET:CE	1:A:656:TRP:HD1	2.19	0.49
1:A:993:LEU:HD22	1:A:1046:LEU:CD2	2.42	0.49
1:A:1019:CYS:O	1:A:1020:CYS:C	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:LEU:HD12	2:B:417:PHE:CE2	2.48	0.49
2:B:114:PRO:O	2:B:115:GLN:C	2.55	0.49
2:B:542:MET:CE	2:B:747:MET:HG3	2.43	0.49
3:C:91:HIS:CD2	3:C:91:HIS:C	2.91	0.49
3:C:144:ILE:HG22	3:C:145:CYS:N	2.28	0.49
3:C:167:HIS:N	11:K:6:ARG:NH1	2.61	0.49
4:D:118:THR:CB	4:D:121:LYS:HB3	2.43	0.49
8:H:44:VAL:CG1	8:H:48:PRO:HA	2.41	0.49
8:H:93:TYR:HB3	8:H:144:ILE:O	2.12	0.49
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.94	0.49
1:A:306:ASN:HD22	1:A:322:VAL:HG12	1.78	0.49
1:A:378:GLU:OE2	1:A:387:ARG:NH2	2.46	0.49
1:A:639:PRO:HG2	1:A:640:GLN:HE21	1.77	0.49
1:A:730:GLY:O	1:A:731:ARG:C	2.56	0.49
1:A:919:ILE:HG12	1:A:925:LEU:HD12	1.95	0.49
1:A:1187:GLN:HG2	1:A:1188:GLN:N	2.28	0.49
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.13	0.49
1:A:1436:ILE:O	1:A:1439:GLY:N	2.27	0.49
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.31	0.49
2:B:179:CYS:SG	2:B:181:LEU:HB2	2.53	0.49
2:B:277:LYS:HG2	2:B:336:ARG:HB3	1.94	0.49
2:B:815:ARG:HB2	2:B:815:ARG:NH1	2.28	0.49
3:C:15:LYS:HG2	3:C:15:LYS:O	2.12	0.49
4:D:120:GLU:HA	4:D:123:LEU:HD23	1.95	0.49
5:E:89:GLY:C	5:E:91:LYS:H	2.20	0.49
5:E:119:SER:O	5:E:123:LEU:HD21	2.13	0.49
8:H:82:PRO:HG2	8:H:83:GLN:H	1.78	0.49
12:L:34:CYS:HB3	12:L:51:CYS:SG	2.53	0.49
13:N:4:DA:H2"	13:N:5:DC:C6	2.48	0.49
1:A:12:ARG:CB	2:B:1218:THR:HG22	2.29	0.48
1:A:117:GLU:CD	1:A:117:GLU:N	2.68	0.48
1:A:321:PRO:O	1:A:322:VAL:CB	2.60	0.48
1:A:482:PHE:HB2	2:B:838:SER:OG	2.13	0.48
1:A:1166:ASP:CG	1:A:1194:ARG:HE	2.21	0.48
2:B:753:ALA:O	2:B:756:ILE:HG13	2.13	0.48
2:B:879:ARG:CD	2:B:879:ARG:N	2.75	0.48
2:B:906:SER:O	2:B:907:GLY:C	2.56	0.48
2:B:1094:ARG:HH21	2:B:1098:MET:HG2	1.78	0.48
3:C:208:GLU:C	3:C:210:GLU:H	2.20	0.48
4:D:14:ARG:NH2	4:D:16:LYS:HD2	2.28	0.48
5:E:79:TRP:HB2	5:E:105:PHE:CE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:2:THR:O	9:I:2:THR:HG23	2.13	0.48
1:A:337:ARG:HD2	2:B:1132:GLU:CD	2.38	0.48
1:A:482:PHE:C	1:A:484:GLY:H	2.20	0.48
1:A:774:ARG:CZ	1:A:797:LYS:HB2	2.43	0.48
1:A:889:SER:C	1:A:891:ALA:N	2.69	0.48
2:B:183:GLU:O	2:B:184:ALA:O	2.30	0.48
2:B:247:GLY:H	2:B:249:ARG:HH21	1.61	0.48
2:B:405:ARG:NE	2:B:632:ARG:HG2	2.27	0.48
2:B:839:MET:HG3	2:B:1010:LEU:HD23	1.94	0.48
4:D:136:GLY:HA2	4:D:142:LYS:NZ	2.28	0.48
5:E:157:SER:OG	5:E:160:GLU:HG3	2.13	0.48
8:H:44:VAL:O	8:H:44:VAL:HG12	2.13	0.48
9:I:59:VAL:C	9:I:61:ASP:H	2.21	0.48
11:K:83:PRO:O	11:K:84:LYS:C	2.56	0.48
12:L:34:CYS:SG	12:L:51:CYS:SG	3.11	0.48
1:A:144:THR:O	1:A:146:MET:HG3	2.12	0.48
1:A:336:ILE:HD11	2:B:1203:LEU:HD22	1.94	0.48
1:A:463:ILE:CD1	1:A:469:ARG:HG3	2.43	0.48
1:A:666:ILE:HG23	2:B:1026:LEU:HB3	1.95	0.48
1:A:883:LEU:CD1	1:A:1017:LEU:HD11	2.40	0.48
2:B:218:SER:HB3	2:B:241:ARG:HH12	1.77	0.48
2:B:240:ILE:HG21	2:B:381:MET:HE1	1.94	0.48
2:B:642:ASP:CB	2:B:649:LYS:HA	2.44	0.48
2:B:976:ILE:HD13	2:B:992:ILE:HA	1.95	0.48
2:B:1001:PHE:CD2	3:C:34:ARG:NH2	2.81	0.48
3:C:89:GLU:O	3:C:90:ASP:CB	2.60	0.48
3:C:238:ILE:HD11	3:C:246:ARG:NH1	2.28	0.48
4:D:51:ASN:C	4:D:52:LEU:O	2.55	0.48
4:D:216:ASN:C	4:D:218:GLU:N	2.68	0.48
7:G:30:LEU:HD23	7:G:54:ILE:HD13	1.95	0.48
7:G:87:VAL:CG2	7:G:103:VAL:HG21	2.44	0.48
8:H:6:PHE:C	8:H:6:PHE:CD2	2.91	0.48
9:I:17:ARG:HG3	9:I:28:GLU:HG2	1.95	0.48
9:I:61:ASP:O	9:I:63:GLY:N	2.47	0.48
11:K:45:LEU:HG	11:K:94:ILE:CD1	2.41	0.48
12:L:27:LEU:HD13	12:L:37:LYS:CD	2.43	0.48
12:L:61:THR:HG22	12:L:63:ARG:HG3	1.93	0.48
1:A:901:LEU:HD23	1:A:907:THR:OG1	2.12	0.48
2:B:120:ARG:NH1	12:L:54:ARG:NH1	2.60	0.48
2:B:282:ILE:HG21	2:B:382:ILE:HD11	1.95	0.48
2:B:384:ARG:HA	2:B:387:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:766:ARG:HH11	2:B:769:TYR:HD1	1.61	0.48
3:C:33:LEU:HD12	3:C:33:LEU:C	2.37	0.48
3:C:167:HIS:N	11:K:6:ARG:HH12	2.11	0.48
3:C:177:GLU:CG	3:C:231:ASN:HD22	2.20	0.48
11:K:54:ARG:HG2	11:K:54:ARG:NH1	2.27	0.48
1:A:255:SER:OG	2:B:918:ILE:CG2	2.61	0.48
1:A:381:THR:CG2	1:A:382:PRO:HD2	2.35	0.48
1:A:720:ARG:O	1:A:724:GLU:HB2	2.12	0.48
2:B:416:LEU:HD12	2:B:466:TRP:CE2	2.49	0.48
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.95	0.48
2:B:773:MET:CE	2:B:985:GLY:HA2	2.39	0.48
3:C:35:ARG:NH1	11:K:41:THR:N	2.60	0.48
5:E:42:PHE:O	5:E:43:LYS:C	2.57	0.48
8:H:4:THR:CA	8:H:60:ALA:HB2	2.23	0.48
8:H:56:THR:O	8:H:144:ILE:HA	2.14	0.48
8:H:92:ASP:C	8:H:93:TYR:CD1	2.91	0.48
10:J:27:GLU:C	10:J:29:GLU:N	2.67	0.48
12:L:31:CYS:SG	12:L:34:CYS:N	2.86	0.48
1:A:20:GLY:O	1:A:21:LEU:HD23	2.13	0.48
1:A:34:LYS:HZ2	1:A:57:ARG:HH22	1.59	0.48
1:A:65:LEU:O	1:A:71:GLN:HA	2.13	0.48
1:A:343:LYS:HZ2	2:B:1151:LEU:HG	1.77	0.48
1:A:1029:ARG:CG	1:A:1029:ARG:NH1	2.77	0.48
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.29	0.48
1:A:1094:VAL:HG13	1:A:1113:THR:HB	1.96	0.48
2:B:412:LEU:HB3	2:B:466:TRP:NE1	2.28	0.48
2:B:831:SER:CB	2:B:994:TYR:OH	2.61	0.48
2:B:860:MET:CG	2:B:965:LYS:HG2	2.42	0.48
2:B:882:THR:HG23	2:B:884:ARG:CA	2.44	0.48
3:C:56:THR:HG22	3:C:57:VAL:N	2.26	0.48
5:E:7:ARG:HG3	5:E:8:ASN:H	1.77	0.48
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.49	0.48
7:G:115:MET:O	7:G:164:LYS:HD3	2.14	0.48
9:I:12:ASN:HD22	9:I:12:ASN:HA	1.53	0.48
1:A:49:LYS:CD	1:A:55:ASP:HB3	2.44	0.48
1:A:1230:GLU:C	1:A:1232:ASN:N	2.72	0.48
2:B:190:TYR:CE1	2:B:196:PRO:HG3	2.49	0.48
2:B:199:MET:HE2	2:B:492:LEU:CD2	2.44	0.48
2:B:896:ASP:OD2	12:L:58:LYS:HE3	2.14	0.48
2:B:1000:PRO:O	2:B:1007:VAL:HG23	2.14	0.48
2:B:1115:THR:O	2:B:1116:ARG:CB	2.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:7:THR:HG21	4:D:32:GLU:CD	2.38	0.48
4:D:40:HIS:CE1	7:G:7:LEU:O	2.65	0.48
7:G:88:ASP:CB	7:G:144:ARG:HA	2.34	0.48
8:H:61:SER:O	8:H:62:SER:HB2	2.14	0.48
1:A:26:GLU:O	1:A:29:ALA:HB3	2.14	0.48
1:A:396:PRO:HB3	1:A:402:ALA:O	2.13	0.48
1:A:477:PRO:CG	1:A:521:MET:HG2	2.44	0.48
1:A:526:ASP:HB2	2:B:835:GLN:OE1	2.14	0.48
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.94	0.48
1:A:1134:ILE:O	1:A:1138:ILE:HG12	2.13	0.48
2:B:284:ILE:HG21	2:B:333:PHE:HD2	1.79	0.48
2:B:360:PHE:CE2	2:B:361:LEU:HD13	2.49	0.48
2:B:434:ARG:O	2:B:436:VAL:HG23	2.13	0.48
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.97	0.48
2:B:1170:THR:O	2:B:1172:ILE:HD13	2.13	0.48
4:D:39:ASN:ND2	4:D:41:GLN:HB2	2.28	0.48
4:D:155:ARG:HB3	4:D:155:ARG:HH11	1.79	0.48
5:E:33:GLU:C	5:E:35:VAL:N	2.71	0.48
5:E:153:HIS:C	5:E:154:ILE:HG13	2.39	0.48
8:H:24:CYS:HB2	8:H:44:VAL:CG2	2.43	0.48
10:J:47:ARG:C	10:J:49:MET:N	2.69	0.48
11:K:40:HIS:O	11:K:41:THR:C	2.57	0.48
11:K:111:LEU:N	11:K:111:LEU:HD23	2.29	0.48
12:L:46:VAL:O	12:L:46:VAL:HG12	2.14	0.48
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.59	0.48
1:A:794:PRO:C	1:A:796:SER:H	2.22	0.48
1:A:896:ARG:HD3	1:A:897:TYR:CZ	2.48	0.48
1:A:1376:THR:O	1:A:1377:THR:C	2.56	0.48
2:B:199:MET:HE2	2:B:492:LEU:HD23	1.96	0.48
2:B:405:ARG:HD2	2:B:631:GLY:O	2.14	0.48
2:B:563:MET:HA	2:B:563:MET:HE3	1.96	0.48
2:B:1072:MET:HB2	2:B:1085:ILE:CD1	2.44	0.48
2:B:1154:ALA:O	2:B:1155:SER:HB2	2.13	0.48
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.39	0.48
3:C:186:LEU:N	3:C:186:LEU:CD1	2.77	0.48
3:C:213:PRO:O	3:C:214:ASN:HB3	2.14	0.48
4:D:123:LEU:CD2	4:D:149:THR:HG21	2.44	0.48
8:H:5:LEU:CG	8:H:60:ALA:HA	2.44	0.48
10:J:24:LEU:HA	10:J:28:ASP:HB2	1.96	0.48
11:K:21:ILE:CG2	11:K:33:ILE:HG12	2.37	0.48
1:A:218:ASP:O	1:A:219:PHE:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:ARG:HD2	1:A:825:ILE:HD11	1.96	0.48
1:A:1025:ARG:HG3	1:A:1025:ARG:HH11	1.79	0.48
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.96	0.48
2:B:222:ILE:C	2:B:240:ILE:HD13	2.39	0.48
2:B:701:ILE:HG13	2:B:702:LEU:N	2.29	0.48
3:C:84:ARG:HG3	3:C:85:ASP:OD1	2.14	0.48
3:C:105:GLY:HA3	3:C:149:LYS:O	2.14	0.48
4:D:27:LEU:HD11	4:D:197:SER:HB3	1.96	0.48
4:D:154:PHE:CE2	4:D:218:GLU:HA	2.49	0.48
7:G:31:LEU:HD13	7:G:35:GLU:HG3	1.96	0.48
7:G:111:THR:O	7:G:113:HIS:N	2.47	0.48
8:H:135:LEU:HD13	8:H:137:GLN:NE2	2.29	0.48
9:I:82:GLU:HB3	9:I:104:LEU:CG	2.44	0.48
11:K:8:GLU:O	11:K:37:LYS:HD2	2.14	0.48
11:K:101:LEU:O	11:K:101:LEU:HD23	2.13	0.48
1:A:116:ASP:C	1:A:118:HIS:N	2.71	0.47
1:A:208:LEU:HD22	1:A:212:LYS:HD2	1.96	0.47
1:A:384:ASN:O	1:A:385:ILE:C	2.55	0.47
1:A:443:LEU:HD21	1:A:455:MET:HB3	1.96	0.47
1:A:899:VAL:CB	1:A:929:LEU:HD12	2.44	0.47
1:A:1319:VAL:HG12	1:A:1320:PRO:O	2.14	0.47
2:B:425:THR:HA	2:B:428:ILE:CD1	2.39	0.47
2:B:644:GLU:OE1	2:B:644:GLU:HA	2.14	0.47
2:B:935:ARG:HG3	2:B:935:ARG:O	2.12	0.47
2:B:975:GLN:CG	2:B:976:ILE:N	2.74	0.47
2:B:1223:ASP:O	2:B:1224:PHE:CB	2.60	0.47
3:C:35:ARG:HH12	11:K:41:THR:H	1.62	0.47
4:D:64:VAL:C	4:D:66:ARG:N	2.68	0.47
4:D:124:GLU:CD	4:D:124:GLU:N	2.71	0.47
5:E:35:VAL:C	5:E:37:LEU:H	2.22	0.47
8:H:47:PHE:HB3	8:H:95:TYR:HD1	1.78	0.47
1:A:195:ASP:O	1:A:196:GLU:HB3	2.14	0.47
1:A:200:ARG:HG2	1:A:201:VAL:N	2.28	0.47
1:A:645:LEU:HG	1:A:649:ILE:CD1	2.44	0.47
1:A:817:ALA:O	1:A:818:MET:C	2.54	0.47
1:A:1278:ASN:O	1:A:1310:GLY:HA3	2.13	0.47
1:A:1285:MET:O	1:A:1305:VAL:N	2.39	0.47
2:B:431:TYR:CG	2:B:447:ALA:HB2	2.49	0.47
2:B:434:ARG:O	2:B:436:VAL:N	2.46	0.47
2:B:661:LEU:C	2:B:663:ALA:N	2.70	0.47
2:B:875:GLU:O	2:B:877:PRO:CD	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:49:SER:OG	5:E:50:MET:N	2.47	0.47
5:E:138:ALA:HA	5:E:141:VAL:HG23	1.95	0.47
6:F:119:ARG:HH11	6:F:119:ARG:CG	2.21	0.47
7:G:21:ARG:HD2	7:G:24:GLN:HB2	1.93	0.47
8:H:40:LEU:HD11	8:H:97:MET:HE1	1.96	0.47
9:I:55:THR:HG22	9:I:58:VAL:CG2	2.44	0.47
10:J:16:ASP:OD1	10:J:17:LYS:HD2	2.14	0.47
12:L:26:THR:CG2	12:L:27:LEU:H	2.27	0.47
14:T:19:DT:OP1	14:T:19:DT:H3'	2.14	0.47
1:A:186:LYS:HZ1	1:A:197:PRO:HD3	1.77	0.47
1:A:537:ARG:HB2	8:H:20:TYR:CE2	2.50	0.47
1:A:663:SER:OG	1:A:664:THR:N	2.43	0.47
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.53	0.47
2:B:593:PRO:C	2:B:595:ARG:N	2.71	0.47
4:D:17:LYS:CD	4:D:18:VAL:HG13	2.43	0.47
8:H:11:GLN:O	8:H:28:ALA:CB	2.61	0.47
8:H:41:ASP:O	8:H:42:ILE:HG13	2.15	0.47
10:J:2:ILE:HG12	10:J:57:ILE:CD1	2.44	0.47
14:T:13:DT:H2''	14:T:14:DA:C8	2.48	0.47
1:A:26:GLU:O	1:A:27:VAL:C	2.57	0.47
1:A:106:VAL:CG1	1:A:107:CYS:N	2.77	0.47
1:A:262:LEU:O	1:A:266:LEU:HG	2.14	0.47
1:A:350:ARG:CB	2:B:1128:LEU:HD11	2.45	0.47
1:A:494:SER:O	1:A:498:ARG:HG2	2.14	0.47
1:A:507:VAL:HG13	1:A:521:MET:HE1	1.96	0.47
1:A:717:ASN:O	1:A:718:VAL:C	2.56	0.47
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.44	0.47
2:B:55:VAL:HG13	2:B:97:VAL:HG21	1.97	0.47
2:B:101:MET:HB3	2:B:109:THR:CG2	2.45	0.47
2:B:789:MET:HE3	2:B:965:LYS:HB3	1.96	0.47
3:C:66:ARG:NH2	10:J:5:VAL:HG23	2.28	0.47
3:C:235:VAL:CG1	10:J:13:VAL:HG13	2.44	0.47
4:D:51:ASN:O	4:D:52:LEU:C	2.55	0.47
4:D:220:LEU:HD23	4:D:221:TYR:N	2.17	0.47
5:E:61:GLN:HG2	5:E:62:ALA:N	2.29	0.47
5:E:182:ASP:HB3	5:E:185:ALA:HB2	1.96	0.47
6:F:109:VAL:HG13	6:F:127:GLU:OE1	2.14	0.47
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.95	0.47
9:I:65:ASP:OD1	9:I:67:THR:OG1	2.25	0.47
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.96	0.47
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:GLU:OE1	2:B:1145:SER:N	2.48	0.47
1:A:698:GLN:HE21	9:I:99:LEU:HD21	1.78	0.47
1:A:719:VAL:HG12	1:A:720:ARG:N	2.29	0.47
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.14	0.47
2:B:113:TYR:CE2	2:B:192:LEU:HD21	2.50	0.47
2:B:167:ILE:HG22	2:B:453:ILE:CD1	2.41	0.47
2:B:209:GLU:CD	2:B:485:ARG:HE	2.23	0.47
2:B:291:ILE:CD1	2:B:300:HIS:NE2	2.77	0.47
2:B:635:ARG:HB2	2:B:636:PRO:HD2	1.95	0.47
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.48	0.47
2:B:638:PHE:HD2	2:B:690:VAL:HG22	1.79	0.47
2:B:642:ASP:CA	2:B:649:LYS:HG3	2.43	0.47
2:B:918:ILE:CG2	2:B:935:ARG:NH2	2.74	0.47
2:B:997:GLU:H	2:B:997:GLU:HG3	1.41	0.47
3:C:24:ASN:CG	3:C:24:ASN:O	2.55	0.47
3:C:193:TYR:HD1	3:C:193:TYR:O	1.97	0.47
5:E:145:THR:HG21	5:E:187:TYR:CD2	2.50	0.47
7:G:136:VAL:O	7:G:136:VAL:HG12	2.14	0.47
12:L:26:THR:HG22	12:L:27:LEU:N	2.30	0.47
1:A:671:ALA:H	1:A:676:MET:HE2	1.80	0.47
1:A:829:VAL:O	1:A:830:LYS:C	2.57	0.47
1:A:960:ILE:HA	1:A:963:ILE:HG22	1.97	0.47
1:A:1332:PHE:H	1:A:1332:PHE:HD2	1.63	0.47
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.78	0.47
2:B:29:ASP:CB	2:B:658:ILE:HD13	2.44	0.47
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.49	0.47
2:B:560:GLU:O	2:B:561:TRP:CD1	2.68	0.47
2:B:798:TYR:CE2	3:C:62:PHE:HE2	2.30	0.47
2:B:849:GLY:O	2:B:852:ARG:HG3	2.14	0.47
2:B:850:LEU:HD12	2:B:850:LEU:C	2.39	0.47
4:D:118:THR:O	4:D:119:ARG:C	2.57	0.47
7:G:123:ALA:O	7:G:125:SER:N	2.48	0.47
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.63	0.47
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.97	0.47
1:A:320:ARG:HE	1:A:323:LYS:HZ1	1.63	0.47
1:A:453:MET:HB3	1:A:477:PRO:HB3	1.96	0.47
1:A:548:ASN:O	1:A:549:MET:C	2.57	0.47
1:A:551:TYR:CE2	11:K:62:LYS:HE2	2.50	0.47
1:A:814:PHE:CD2	1:A:814:PHE:O	2.67	0.47
1:A:898:ARG:HD3	1:A:933:TYR:CE1	2.50	0.47
1:A:993:LEU:CD2	1:A:1022:LEU:HD11	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:ASN:HD22	1:A:1048:ASN:N	2.12	0.47
1:A:1375:MET:HE3	1:A:1384:VAL:HG23	1.95	0.47
1:A:1389:PHE:C	1:A:1391:ARG:H	2.22	0.47
1:A:1424:VAL:HG13	1:A:1436:ILE:CD1	2.45	0.47
1:A:1441:PHE:HE1	6:F:92:ARG:HG2	1.79	0.47
2:B:126:SER:HA	2:B:169:ARG:HH12	1.79	0.47
2:B:129:PHE:CD2	2:B:166:PHE:HA	2.49	0.47
2:B:331:LEU:HD23	2:B:353:LYS:HG2	1.97	0.47
2:B:473:MET:C	2:B:475:SER:H	2.23	0.47
2:B:515:HIS:NE2	2:B:517:THR:HG23	2.30	0.47
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.96	0.47
2:B:654:ARG:HG3	2:B:654:ARG:NH1	2.29	0.47
2:B:654:ARG:O	2:B:657:HIS:N	2.47	0.47
2:B:860:MET:SD	2:B:963:PHE:HE1	2.37	0.47
2:B:952:VAL:HG12	2:B:953:LEU:N	2.30	0.47
2:B:996:ARG:HH12	3:C:174:ALA:HA	1.80	0.47
2:B:1065:GLN:CD	2:B:1066:SER:N	2.73	0.47
2:B:1073:TYR:HE2	3:C:180:TYR:CE2	2.32	0.47
3:C:44:LEU:HD21	3:C:159:ALA:CB	2.44	0.47
3:C:59:ALA:O	3:C:62:PHE:HB3	2.13	0.47
3:C:73:GLN:NE2	3:C:75:MET:N	2.62	0.47
3:C:131:HIS:O	3:C:133:ILE:N	2.48	0.47
4:D:8:PHE:HZ	4:D:37:GLN:CD	2.23	0.47
5:E:112:TYR:CE1	5:E:136:ASN:HB2	2.50	0.47
6:F:88:TYR:O	6:F:89:GLU:C	2.58	0.47
8:H:81:PRO:CB	8:H:82:PRO:CD	2.92	0.47
8:H:82:PRO:O	8:H:84:ALA:N	2.33	0.47
8:H:143:LEU:C	8:H:144:ILE:HG13	2.38	0.47
9:I:95:THR:HG22	9:I:96:SER:O	2.15	0.47
10:J:1:MET:H1	10:J:57:ILE:N	2.10	0.47
10:J:7:CYS:CA	10:J:49:MET:HE3	2.43	0.47
10:J:34:THR:O	10:J:35:ALA:C	2.57	0.47
12:L:27:LEU:O	12:L:28:LYS:HB2	2.13	0.47
1:A:23:SER:CB	1:A:233:TRP:NE1	2.78	0.47
1:A:385:ILE:HG22	1:A:386:ASP:N	2.30	0.47
1:A:442:VAL:CG2	1:A:489:LEU:HD11	2.45	0.47
1:A:904:THR:O	1:A:904:THR:CG2	2.62	0.47
1:A:1193:LEU:HD12	1:A:1193:LEU:C	2.38	0.47
2:B:37:PHE:HE1	2:B:41:LYS:CG	2.28	0.47
2:B:98:THR:O	2:B:126:SER:HB2	2.14	0.47
2:B:641:GLU:O	2:B:643:ASP:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:706:GLN:NE2	2:B:730:ARG:HD3	2.29	0.47
2:B:735:ALA:HB3	2:B:738:PHE:CE1	2.50	0.47
2:B:1183:LYS:O	2:B:1183:LYS:HE3	2.14	0.47
3:C:204:SER:C	3:C:206:ASN:H	2.23	0.47
9:I:100:PHE:N	9:I:100:PHE:CD1	2.83	0.47
12:L:60:ARG:HH21	12:L:65:VAL:CG2	2.28	0.47
1:A:130:ASP:O	1:A:131:SER:C	2.58	0.47
1:A:180:LYS:NZ	1:A:294:SER:HB3	2.30	0.47
1:A:1166:ASP:OD2	1:A:1239:ARG:CD	2.62	0.47
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.29	0.47
2:B:126:SER:HB3	2:B:172:ILE:HD11	1.97	0.47
2:B:376:PHE:HB3	2:B:566:LEU:HD21	1.96	0.47
2:B:386:LEU:O	2:B:387:LEU:C	2.55	0.47
2:B:412:LEU:HB3	2:B:466:TRP:CZ2	2.50	0.47
2:B:848:ARG:HD3	10:J:11:GLY:HA2	1.97	0.47
2:B:992:ILE:HG12	2:B:993:THR:H	1.79	0.47
2:B:1167:GLY:O	2:B:1215:ARG:HA	2.15	0.47
2:B:1181:GLU:H	2:B:1188:LYS:HA	1.80	0.47
5:E:12:LEU:HD11	5:E:58:MET:HE1	1.97	0.47
5:E:112:TYR:C	5:E:112:TYR:HD1	2.21	0.47
5:E:162:ARG:CZ	5:E:162:ARG:HB3	2.45	0.47
9:I:99:LEU:C	9:I:100:PHE:HD1	2.23	0.47
12:L:30:ILE:CG2	12:L:31:CYS:H	2.28	0.47
1:A:90:VAL:HG12	1:A:297:GLN:NE2	2.30	0.47
1:A:92:HIS:CD2	1:A:304:MET:HE1	2.50	0.47
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.96	0.47
1:A:960:ILE:HA	1:A:963:ILE:CG2	2.45	0.47
1:A:1410:PHE:HD2	2:B:1212:ILE:HD12	1.80	0.47
2:B:63:ILE:HD12	2:B:421:PHE:CD2	2.49	0.47
2:B:307:ASP:OD1	2:B:309:GLN:HB2	2.15	0.47
2:B:430:ARG:HB3	2:B:434:ARG:CZ	2.45	0.47
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.50	0.47
3:C:101:LEU:HD13	3:C:118:LEU:CD2	2.45	0.47
4:D:39:ASN:ND2	4:D:41:GLN:H	2.13	0.47
4:D:71:LYS:C	4:D:74:GLN:H	2.23	0.47
4:D:139:LYS:HG3	4:D:140:ASP:OD1	2.15	0.47
5:E:89:GLY:C	5:E:91:LYS:N	2.72	0.47
8:H:15:VAL:HG22	8:H:26:ILE:CD1	2.45	0.47
8:H:83:GLN:CD	8:H:87:ARG:NH2	2.73	0.47
8:H:84:ALA:HA	8:H:87:ARG:HG3	1.96	0.47
10:J:21:TYR:HB2	10:J:39:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:15:DG:C8	14:T:16:DT:C7	2.98	0.47
1:A:590:ARG:HG2	1:A:590:ARG:NH1	2.29	0.46
1:A:683:ILE:HG21	1:A:801:GLU:CD	2.40	0.46
1:A:785:PRO:HG2	1:A:786:HIS:CD2	2.51	0.46
1:A:877:HIS:C	1:A:878:ILE:HG13	2.40	0.46
2:B:39:ARG:NH2	2:B:665:GLU:CD	2.73	0.46
2:B:466:TRP:N	2:B:475:SER:OG	2.48	0.46
2:B:528:PRO:HG2	2:B:532:ALA:O	2.15	0.46
2:B:530:GLY:O	2:B:531:GLN:C	2.57	0.46
2:B:797:TYR:HE1	2:B:854:LEU:HD21	1.80	0.46
3:C:196:ASP:HB3	3:C:199:LYS:HD2	1.96	0.46
4:D:15:LEU:O	4:D:15:LEU:HD12	2.15	0.46
4:D:155:ARG:NE	4:D:221:TYR:CE1	2.83	0.46
8:H:138:GLU:C	8:H:138:GLU:OE1	2.58	0.46
9:I:58:VAL:O	9:I:58:VAL:HG12	2.15	0.46
10:J:32:GLU:O	10:J:33:GLY:C	2.57	0.46
1:A:903:ASN:ND2	1:A:903:ASN:C	2.73	0.46
1:A:934:LYS:O	1:A:937:VAL:HG12	2.16	0.46
1:A:1081:LEU:HD21	1:A:1097:GLY:HA3	1.96	0.46
1:A:1208:THR:HG22	1:A:1210:GLY:N	2.29	0.46
2:B:189:LEU:CD1	2:B:196:PRO:HA	2.45	0.46
2:B:269:ILE:O	2:B:282:ILE:HG12	2.15	0.46
2:B:644:GLU:C	2:B:646:LEU:N	2.73	0.46
2:B:649:LYS:HD3	2:B:736:THR:O	2.14	0.46
2:B:706:GLN:HB2	2:B:709:ASP:HB2	1.97	0.46
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.97	0.46
2:B:970:THR:HG22	2:B:971:THR:N	2.30	0.46
2:B:1130:PHE:CE1	2:B:1134:GLU:HB3	2.51	0.46
4:D:138:ASN:C	4:D:140:ASP:H	2.23	0.46
5:E:12:LEU:HD22	5:E:55:ARG:CZ	2.46	0.46
5:E:78:LEU:HD21	5:E:80:VAL:CG2	2.45	0.46
6:F:116:ASP:C	6:F:116:ASP:OD1	2.56	0.46
7:G:126:ASN:HD22	7:G:127:PRO:N	2.13	0.46
8:H:3:ASN:CG	8:H:4:THR:H	2.24	0.46
10:J:41:LEU:HD11	10:J:50:ILE:HG13	1.97	0.46
11:K:12:LEU:HD12	11:K:37:LYS:CG	2.44	0.46
11:K:55:LYS:HB2	11:K:81:TYR:CE1	2.49	0.46
1:A:196:GLU:HG2	1:A:197:PRO:N	2.31	0.46
1:A:398:GLU:O	1:A:399:HIS:O	2.34	0.46
1:A:407:ARG:CD	1:A:413:ILE:HD11	2.40	0.46
1:A:504:LEU:HD13	6:F:91:ALA:CB	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:LEU:C	1:A:740:LEU:HD12	2.41	0.46
1:A:1001:ARG:O	1:A:1002:GLY:C	2.57	0.46
1:A:1169:ILE:HG22	1:A:1169:ILE:O	2.15	0.46
2:B:25:ILE:HD13	2:B:653:VAL:HG12	1.96	0.46
2:B:44:VAL:O	2:B:45:SER:C	2.59	0.46
2:B:377:PHE:C	2:B:379:GLY:N	2.72	0.46
2:B:416:LEU:HD12	2:B:466:TRP:CZ2	2.50	0.46
2:B:696:GLU:O	2:B:699:GLU:HB2	2.15	0.46
2:B:944:THR:HG21	2:B:1122:ARG:CZ	2.45	0.46
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.96	0.46
3:C:215:GLU:O	3:C:216:GLY:C	2.57	0.46
4:D:154:PHE:CD2	4:D:154:PHE:N	2.82	0.46
4:D:218:GLU:O	4:D:219:THR:C	2.58	0.46
4:D:219:THR:HG23	4:D:220:LEU:O	2.16	0.46
6:F:111:LEU:HD12	6:F:111:LEU:H	1.80	0.46
6:F:116:ASP:OD1	6:F:117:PRO:N	2.48	0.46
8:H:12:VAL:HA	8:H:28:ALA:HB2	1.97	0.46
8:H:94:ASP:O	8:H:95:TYR:HB2	2.15	0.46
8:H:109:LYS:HD3	8:H:111:LEU:HD11	1.96	0.46
11:K:67:PHE:C	11:K:68:PHE:CD2	2.93	0.46
12:L:59:ALA:O	12:L:60:ARG:O	2.34	0.46
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	1.97	0.46
1:A:690:VAL:CG1	1:A:691:LEU:N	2.78	0.46
1:A:1076:ALA:HA	1:A:1079:MET:HG3	1.96	0.46
1:A:1420:ASP:CB	1:A:1422:ARG:HG3	2.41	0.46
1:A:1451:VAL:C	1:A:1453:TYR:N	2.73	0.46
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.51	0.46
2:B:96:TYR:N	2:B:129:PHE:O	2.38	0.46
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.50	0.46
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.44	0.46
3:C:10:ILE:HG22	3:C:11:ARG:O	2.16	0.46
3:C:221:TYR:CD1	3:C:222:LYS:HG3	2.50	0.46
4:D:14:ARG:C	4:D:16:LYS:H	2.23	0.46
8:H:9:ILE:HG23	8:H:55:LEU:O	2.15	0.46
9:I:62:ILE:HD11	9:I:86:PHE:CE2	2.50	0.46
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.97	0.46
10:J:48:ARG:HE	10:J:49:MET:CE	2.28	0.46
11:K:33:ILE:HD13	11:K:87:LEU:HD22	1.96	0.46
11:K:85:ASP:O	11:K:88:LYS:HB2	2.15	0.46
1:A:77:CYS:C	1:A:78:PRO:O	2.58	0.46
1:A:100:LYS:O	1:A:104:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:MET:O	1:A:109:HIS:HB3	2.15	0.46
1:A:244:PRO:CB	1:A:245:PRO:CD	2.91	0.46
1:A:699:ALA:HB3	1:A:701:LEU:HG	1.96	0.46
1:A:700:ASN:C	1:A:701:LEU:HD23	2.40	0.46
1:A:751:SER:O	1:A:752:LYS:HG2	2.16	0.46
1:A:1127:ASP:O	1:A:1128:GLN:C	2.58	0.46
1:A:1166:ASP:HA	1:A:1169:ILE:HD12	1.97	0.46
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.96	0.46
1:A:1289:ARG:NH1	1:A:1326:ARG:NH1	2.63	0.46
2:B:427:ASP:OD1	2:B:430:ARG:HD2	2.16	0.46
2:B:602:THR:HA	2:B:605:ARG:HB2	1.97	0.46
2:B:792:MET:H	2:B:857:ARG:HA	1.79	0.46
3:C:29:MET:HE2	11:K:98:LEU:CD2	2.45	0.46
3:C:209:TYR:CD1	3:C:209:TYR:N	2.75	0.46
11:K:53:ASP:HB3	11:K:56:VAL:HG23	1.97	0.46
1:A:40:THR:C	1:A:41:MET:HG3	2.41	0.46
1:A:121:LEU:HD23	1:A:121:LEU:O	2.16	0.46
1:A:295:LEU:O	1:A:298:PHE:HB3	2.16	0.46
1:A:728:LYS:O	1:A:732:LEU:HG	2.15	0.46
1:A:767:GLN:NE2	1:A:774:ARG:CB	2.77	0.46
1:A:845:LEU:O	1:A:846:GLU:C	2.58	0.46
2:B:254:LEU:CD1	2:B:273:LEU:HD23	2.45	0.46
2:B:294:ASP:H	9:I:12:ASN:HD22	1.57	0.46
2:B:347:LYS:CG	2:B:348:ARG:H	2.29	0.46
2:B:417:PHE:O	2:B:420:LEU:HB2	2.16	0.46
2:B:430:ARG:HG2	2:B:430:ARG:NH1	2.31	0.46
2:B:910:VAL:CG1	2:B:938:SER:HB3	2.46	0.46
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.50	0.46
3:C:196:ASP:CB	3:C:199:LYS:HD2	2.45	0.46
4:D:155:ARG:NE	4:D:221:TYR:HE1	2.14	0.46
5:E:22:MET:HE3	5:E:26:ARG:CZ	2.46	0.46
10:J:3:VAL:N	10:J:53:HIS:CE1	2.84	0.46
1:A:284:ALA:HB1	1:A:289:ILE:HD12	1.97	0.46
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.96	0.46
1:A:577:ILE:HA	1:A:580:VAL:HG23	1.98	0.46
1:A:675:THR:HB	1:A:736:ASN:OD1	2.15	0.46
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.49	0.46
1:A:1155:ASP:OD2	1:A:1162:VAL:N	2.48	0.46
2:B:265:SER:O	2:B:266:ALA:HB3	2.16	0.46
2:B:282:ILE:CD1	2:B:382:ILE:HD13	2.46	0.46
2:B:311:LEU:O	2:B:314:LEU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.15	0.46
2:B:615:MET:C	2:B:616:ILE:HD12	2.41	0.46
2:B:914:LYS:HE2	2:B:937:ALA:CB	2.45	0.46
2:B:918:ILE:HD12	2:B:935:ARG:CZ	2.45	0.46
2:B:1072:MET:HE3	2:B:1085:ILE:CB	2.24	0.46
2:B:1182:CYS:C	2:B:1183:LYS:HE3	2.40	0.46
6:F:106:PRO:HG2	7:G:18:PHE:C	2.41	0.46
9:I:8:ARG:HG3	9:I:8:ARG:H	1.59	0.46
1:A:80:HIS:H	1:A:243:PRO:CB	2.28	0.46
1:A:592:ASP:N	1:A:595:THR:OG1	2.49	0.46
1:A:665:GLY:O	1:A:666:ILE:C	2.59	0.46
1:A:853:ASP:OD1	1:A:855:THR:CG2	2.63	0.46
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.48	0.46
1:A:1394:THR:CG2	1:A:1398:MET:SD	3.04	0.46
1:A:1420:ASP:O	1:A:1421:CYS:CB	2.62	0.46
1:A:1433:MET:HE2	2:B:1145:SER:OG	2.16	0.46
2:B:37:PHE:CD2	2:B:542:MET:SD	3.09	0.46
2:B:131:ASP:HA	2:B:164:LYS:HB3	1.98	0.46
2:B:1116:ARG:NE	2:B:1198:TYR:CE1	2.84	0.46
7:G:14:HIS:HD2	7:G:16:SER:CB	2.29	0.46
7:G:154:VAL:HG12	7:G:155:SER:N	2.30	0.46
10:J:3:VAL:HA	10:J:53:HIS:HD1	1.80	0.46
1:A:185:TRP:HE3	1:A:185:TRP:N	1.98	0.46
1:A:516:SER:O	1:A:517:ASN:C	2.59	0.46
1:A:871:ASP:OD2	1:A:873:MET:HB2	2.16	0.46
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.51	0.46
2:B:525:ALA:O	2:B:768:THR:HG23	2.16	0.46
2:B:582:VAL:HG22	2:B:626:ILE:HG22	1.98	0.46
2:B:1001:PHE:CD1	2:B:1001:PHE:C	2.94	0.46
3:C:23:SER:O	3:C:24:ASN:HB3	2.16	0.46
4:D:14:ARG:O	4:D:16:LYS:N	2.40	0.46
4:D:123:LEU:HD13	4:D:149:THR:HG21	1.97	0.46
5:E:22:MET:HE3	5:E:26:ARG:NH2	2.30	0.46
5:E:56:LYS:NZ	5:E:84:ASP:N	2.63	0.46
5:E:186:LEU:HA	5:E:186:LEU:HD23	1.71	0.46
6:F:69:LEU:HD22	6:F:71:GLU:OE2	2.15	0.46
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.97	0.46
6:F:79:ARG:NH2	6:F:150:GLU:OE1	2.35	0.46
10:J:9:SER:OG	10:J:48:ARG:NH2	2.48	0.46
1:A:356:ASP:OD2	11:K:65:HIS:CE1	2.65	0.46
1:A:451:HIS:O	1:A:452:LYS:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:LYS:HB3	1:A:612:ILE:CG2	2.46	0.46
1:A:645:LEU:HG	1:A:649:ILE:HD11	1.98	0.46
1:A:738:LYS:NZ	3:C:194:GLU:O	2.48	0.46
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.98	0.46
1:A:898:ARG:HA	1:A:933:TYR:CD1	2.51	0.46
1:A:1314:SER:C	1:A:1315:GLU:HG2	2.41	0.46
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.84	0.46
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.96	0.46
2:B:169:ARG:CB	2:B:454:THR:HG23	2.45	0.46
2:B:295:GLY:N	2:B:298:LEU:HD23	2.29	0.46
2:B:356:LEU:HD23	2:B:360:PHE:CD1	2.51	0.46
2:B:582:VAL:O	2:B:582:VAL:HG12	2.14	0.46
2:B:710:LEU:HA	2:B:733:HIS:CB	2.29	0.46
2:B:792:MET:O	2:B:793:ALA:HB2	2.16	0.46
2:B:878:GLN:HB2	2:B:879:ARG:NH1	2.30	0.46
2:B:980:PHE:HD2	2:B:1094:ARG:HA	1.81	0.46
2:B:1033:LYS:HA	2:B:1089:PRO:HD2	1.98	0.46
2:B:1034:VAL:O	2:B:1037:LEU:N	2.48	0.46
3:C:100:THR:CG2	3:C:101:LEU:N	2.79	0.46
3:C:124:LEU:C	3:C:126:GLY:N	2.74	0.46
4:D:8:PHE:CG	4:D:38:ILE:O	2.69	0.46
4:D:24:ALA:C	4:D:26:THR:H	2.24	0.46
5:E:19:VAL:HG11	5:E:80:VAL:HG11	1.98	0.46
5:E:108:GLY:HA3	5:E:132:ILE:HG23	1.98	0.46
8:H:15:VAL:HG13	8:H:26:ILE:HD12	1.98	0.46
10:J:2:ILE:C	10:J:53:HIS:CE1	2.94	0.46
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.81	0.46
1:A:120:GLU:C	1:A:122:MET:N	2.73	0.45
1:A:138:ILE:HD12	1:A:221:SER:O	2.16	0.45
1:A:153:PRO:HD3	1:A:161:LEU:CD1	2.46	0.45
1:A:282:ASN:O	1:A:284:ALA:N	2.48	0.45
1:A:321:PRO:O	1:A:322:VAL:HG12	2.16	0.45
1:A:474:VAL:HG22	1:A:478:TYR:HE1	1.81	0.45
1:A:639:PRO:HG2	1:A:640:GLN:N	2.31	0.45
1:A:698:GLN:O	9:I:98:VAL:HA	2.16	0.45
2:B:112:LEU:HD12	2:B:113:TYR:N	2.27	0.45
2:B:210:LYS:HD3	2:B:482:VAL:HG22	1.98	0.45
2:B:582:VAL:O	2:B:582:VAL:CG1	2.63	0.45
2:B:797:TYR:HE1	2:B:854:LEU:HD23	1.81	0.45
2:B:866:TYR:CB	2:B:870:ILE:HD12	2.47	0.45
2:B:1045:SER:HB3	2:B:1046:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:134:ILE:HG21	3:C:139:GLY:HA2	1.97	0.45
9:I:88:SER:C	9:I:90:GLN:N	2.74	0.45
11:K:47:ARG:HH11	11:K:47:ARG:CB	2.23	0.45
12:L:34:CYS:O	12:L:35:SER:C	2.58	0.45
12:L:38:LEU:O	12:L:39:SER:CB	2.63	0.45
1:A:329:LEU:HD21	2:B:1206:GLU:OE1	2.16	0.45
1:A:332:LYS:HB3	1:A:337:ARG:NE	2.31	0.45
1:A:806:ARG:O	2:B:761:HIS:HE1	1.99	0.45
1:A:1081:LEU:CD2	1:A:1097:GLY:HA3	2.46	0.45
2:B:435:THR:HG22	2:B:437:GLU:C	2.41	0.45
2:B:567:GLU:OE1	2:B:567:GLU:HA	2.16	0.45
2:B:773:MET:C	2:B:775:LYS:N	2.74	0.45
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.47	0.45
3:C:34:ARG:HG2	3:C:35:ARG:N	2.31	0.45
7:G:12:THR:HG23	7:G:67:SER:HB3	1.98	0.45
10:J:3:VAL:CA	10:J:53:HIS:CE1	2.98	0.45
1:A:61:ILE:HG22	1:A:62:ASP:N	2.31	0.45
1:A:90:VAL:HG12	1:A:91:PHE:N	2.29	0.45
1:A:492:PRO:O	1:A:493:GLN:NE2	2.49	0.45
1:A:856:THR:O	1:A:856:THR:HG22	2.16	0.45
1:A:858:ASN:HD22	1:A:860:LEU:H	1.62	0.45
1:A:867:ILE:HD11	1:A:1000:LEU:HD21	1.97	0.45
2:B:244:LEU:HD13	2:B:366:GLN:HE22	1.81	0.45
2:B:314:LEU:O	2:B:318:VAL:HG23	2.16	0.45
2:B:722:ASP:HB3	2:B:723:VAL:H	1.62	0.45
2:B:1130:PHE:CD2	2:B:1150:ARG:HG2	2.52	0.45
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.98	0.45
7:G:129:SER:CB	7:G:138:THR:HG1	2.29	0.45
8:H:43:ASN:C	8:H:45:GLU:H	2.24	0.45
8:H:106:GLU:C	8:H:108:SER:H	2.22	0.45
8:H:128:ASN:C	8:H:128:ASN:HD22	2.23	0.45
9:I:55:THR:OG1	9:I:100:PHE:HD2	1.99	0.45
9:I:105:SER:O	9:I:106:CYS:CB	2.52	0.45
1:A:164:ARG:HG3	1:A:165:GLY:N	2.32	0.45
1:A:335:ARG:HH12	2:B:1202:LEU:HD22	1.81	0.45
1:A:381:THR:C	1:A:383:TYR:N	2.73	0.45
1:A:452:LYS:HB3	2:B:1141:HIS:CE1	2.52	0.45
1:A:608:ILE:HG13	1:A:613:ILE:HD12	1.99	0.45
1:A:768:GLN:NE2	1:A:816:HIS:ND1	2.64	0.45
1:A:820:GLY:O	1:A:821:ARG:C	2.58	0.45
1:A:1064:VAL:O	1:A:1064:VAL:HG12	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1141:THR:HG21	1:A:1205:LYS:HD3	1.98	0.45
2:B:390:LEU:O	2:B:391:ASP:C	2.59	0.45
2:B:500:THR:HA	2:B:501:PRO:HD2	1.75	0.45
2:B:1099:VAL:CG1	2:B:1100:ASP:N	2.78	0.45
4:D:153:ARG:C	4:D:154:PHE:HD2	2.24	0.45
5:E:11:ARG:C	5:E:13:TRP:N	2.74	0.45
5:E:135:PHE:HD2	5:E:140:LEU:CD2	2.28	0.45
9:I:85:PHE:HD1	9:I:99:LEU:HD13	1.75	0.45
1:A:35:ILE:HD13	1:A:241:VAL:HG11	1.98	0.45
1:A:146:MET:CA	1:A:171:GLN:HB2	2.47	0.45
1:A:211:PHE:HA	1:A:214:ILE:HG13	1.98	0.45
1:A:255:SER:OG	2:B:918:ILE:HG21	2.16	0.45
1:A:774:ARG:NH2	1:A:797:LYS:HB2	2.31	0.45
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.99	0.45
1:A:1076:ALA:HA	1:A:1079:MET:CE	2.37	0.45
1:A:1110:ASN:HD22	1:A:1110:ASN:N	2.14	0.45
1:A:1187:GLN:CA	1:A:1244:ARG:HB3	2.45	0.45
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.17	0.45
1:A:1444:MET:O	6:F:133:VAL:N	2.47	0.45
2:B:66:ASP:OD1	2:B:422:LYS:HE2	2.15	0.45
2:B:120:ARG:HH11	12:L:54:ARG:HH11	1.63	0.45
2:B:412:LEU:CD2	2:B:479:VAL:HG11	2.45	0.45
2:B:687:GLU:O	2:B:688:GLY:C	2.59	0.45
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.81	0.45
8:H:100:THR:OG1	8:H:138:GLU:HG2	2.16	0.45
12:L:52:GLY:O	12:L:54:ARG:N	2.50	0.45
1:A:96:ILE:HG22	1:A:97:ALA:N	2.32	0.45
1:A:332:LYS:CD	1:A:333:GLU:HG2	2.47	0.45
1:A:409:SER:O	1:A:410:GLY:C	2.59	0.45
1:A:549:MET:SD	1:A:577:ILE:HD12	2.57	0.45
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.52	0.45
1:A:1266:THR:O	1:A:1270:ASN:HB2	2.17	0.45
1:A:1395:GLY:HA3	1:A:1419:ASP:OD2	2.16	0.45
1:A:1454:MET:O	1:A:1454:MET:HG3	2.17	0.45
2:B:46:GLN:HB2	2:B:408:LEU:HD21	1.98	0.45
2:B:101:MET:HB2	2:B:169:ARG:HH22	1.82	0.45
2:B:120:ARG:CG	2:B:955:THR:HG21	2.46	0.45
2:B:288:ALA:HA	2:B:331:LEU:CD1	2.46	0.45
2:B:604:ARG:CA	2:B:609:ILE:HG13	2.47	0.45
2:B:848:ARG:HA	3:C:69:LEU:HD21	1.98	0.45
2:B:1004:GLU:HG2	10:J:42:LYS:HZ3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1214:PRO:O	2:B:1214:PRO:HG2	2.16	0.45
2:B:1221:SER:C	2:B:1223:ASP:H	2.25	0.45
3:C:99:LEU:HD22	3:C:120:ILE:HG12	1.98	0.45
4:D:35:LEU:H	4:D:35:LEU:CD1	2.29	0.45
5:E:69:ILE:N	5:E:69:ILE:CD1	2.79	0.45
11:K:92:ASN:O	11:K:93:SER:C	2.60	0.45
1:A:125:ALA:O	1:A:127:ALA:N	2.50	0.45
1:A:154:SER:C	1:A:156:ASP:H	2.25	0.45
1:A:492:PRO:CB	1:A:497:THR:HG22	2.47	0.45
1:A:860:LEU:HA	1:A:860:LEU:HD23	1.81	0.45
1:A:1062:GLU:HG2	6:F:88:TYR:OH	2.17	0.45
1:A:1120:LEU:C	1:A:1120:LEU:HD12	2.42	0.45
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.31	0.45
1:A:1242:VAL:CG1	1:A:1243:VAL:N	2.43	0.45
2:B:431:TYR:CE1	2:B:447:ALA:HB2	2.52	0.45
2:B:679:TYR:HE1	2:B:687:GLU:OE2	1.98	0.45
2:B:705:MET:HE1	2:B:742:GLU:OE1	2.16	0.45
2:B:729:ILE:O	2:B:729:ILE:HG22	2.16	0.45
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.98	0.45
2:B:856:PHE:CD1	2:B:856:PHE:N	2.84	0.45
3:C:229:TYR:N	3:C:229:TYR:CD1	2.84	0.45
5:E:56:LYS:CE	5:E:84:ASP:H	2.29	0.45
5:E:60:PHE:CD1	5:E:60:PHE:C	2.95	0.45
5:E:90:VAL:CA	5:E:120:ALA:HB2	2.40	0.45
5:E:92:THR:O	5:E:92:THR:HG22	2.15	0.45
5:E:129:PRO:O	5:E:130:ALA:O	2.35	0.45
5:E:145:THR:HG21	5:E:187:TYR:CZ	2.51	0.45
5:E:204:THR:HG23	5:E:205:SER:N	2.32	0.45
6:F:77:ASP:O	6:F:78:GLN:CB	2.49	0.45
8:H:20:TYR:O	8:H:22:LYS:N	2.50	0.45
1:A:208:LEU:C	1:A:208:LEU:CD2	2.90	0.45
1:A:565:ILE:O	1:A:565:ILE:HG22	2.17	0.45
1:A:709:THR:HG21	9:I:93:LYS:O	2.16	0.45
1:A:1259:MET:HE2	1:A:1263:ILE:HD11	1.98	0.45
1:A:1445:ILE:HG21	7:G:22:MET:HE1	1.99	0.45
2:B:542:MET:SD	2:B:747:MET:HE2	2.56	0.45
2:B:621:GLU:HG3	2:B:621:GLU:O	2.17	0.45
2:B:1119:VAL:O	2:B:1126:GLY:HA3	2.15	0.45
2:B:1177:HIS:CB	2:B:1179:GLN:HE21	2.29	0.45
3:C:185:LYS:HE2	3:C:213:PRO:HA	1.99	0.45
4:D:138:ASN:ND2	7:G:35:GLU:HB3	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:112:TYR:HB3	5:E:116:ILE:HD11	1.99	0.45
8:H:7:ASP:O	8:H:8:ASP:HB2	2.17	0.45
8:H:118:PHE:O	8:H:119:GLY:C	2.60	0.45
11:K:37:LYS:HA	11:K:37:LYS:HD3	1.88	0.45
1:A:50:ILE:HG22	1:A:52:GLY:N	2.32	0.45
1:A:55:ASP:N	1:A:56:PRO:CD	2.78	0.45
1:A:313:GLN:O	1:A:314:ALA:C	2.60	0.45
1:A:416:ARG:HG3	1:A:417:TYR:CE1	2.52	0.45
1:A:614:PHE:CD1	1:A:614:PHE:C	2.95	0.45
1:A:687:LYS:O	1:A:690:VAL:HG12	2.16	0.45
1:A:785:PRO:HG2	1:A:786:HIS:HD2	1.81	0.45
1:A:1116:LEU:N	1:A:1308:THR:CG2	2.73	0.45
1:A:1387:HIS:NE2	13:N:4:DA:H5'	2.32	0.45
2:B:349:ILE:O	2:B:353:LYS:HG3	2.17	0.45
2:B:370:PHE:CD2	2:B:373:ARG:HD2	2.52	0.45
2:B:531:GLN:HG3	2:B:532:ALA:H	1.82	0.45
2:B:769:TYR:HB3	2:B:987:LYS:NZ	2.31	0.45
2:B:880:THR:HG22	2:B:880:THR:O	2.17	0.45
2:B:936:ASP:CG	2:B:937:ALA:N	2.74	0.45
3:C:22:LEU:HD22	3:C:230:MET:CE	2.40	0.45
3:C:44:LEU:HD23	3:C:44:LEU:C	2.42	0.45
5:E:154:ILE:HG22	5:E:155:ARG:O	2.17	0.45
8:H:91:ASP:C	8:H:93:TYR:H	2.24	0.45
9:I:34:TYR:CD2	9:I:34:TYR:C	2.94	0.45
10:J:30:LEU:HD11	10:J:38:ARG:NH1	2.32	0.45
1:A:536:LEU:O	1:A:537:ARG:C	2.60	0.45
1:A:728:LYS:O	1:A:729:ALA:C	2.60	0.45
1:A:798:GLY:HA2	1:A:815:PHE:HD1	1.81	0.45
1:A:1072:ILE:HG23	1:A:1356:ILE:HD11	1.99	0.45
1:A:1081:LEU:HD11	1:A:1097:GLY:HA3	1.98	0.45
1:A:1161:THR:CG2	1:A:1163:ILE:HD12	2.46	0.45
1:A:1199:ARG:O	1:A:1203:ASN:ND2	2.50	0.45
1:A:1393:ASN:C	1:A:1394:THR:O	2.60	0.45
2:B:69:LEU:HD13	2:B:429:PHE:CD1	2.52	0.45
2:B:100:PRO:HB2	2:B:180:TYR:HE1	1.82	0.45
2:B:203:PHE:N	2:B:203:PHE:CD1	2.85	0.45
2:B:811:TYR:N	2:B:811:TYR:CD1	2.84	0.45
2:B:889:THR:HG23	2:B:891:ASP:N	2.32	0.45
3:C:239:PRO:O	3:C:240:VAL:C	2.59	0.45
7:G:113:HIS:CD2	7:G:113:HIS:H	2.34	0.45
8:H:55:LEU:HD22	8:H:144:ILE:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:54:ARG:H	12:L:54:ARG:HG3	1.43	0.45
1:A:330:LYS:O	1:A:334:GLY:HA3	2.17	0.44
1:A:451:HIS:HA	1:A:1070:GLN:OE1	2.16	0.44
2:B:294:ASP:H	9:I:12:ASN:HD21	1.60	0.44
2:B:486:TYR:HD1	2:B:775:LYS:O	2.00	0.44
2:B:805:THR:CG2	2:B:806:THR:H	2.20	0.44
2:B:1072:MET:O	2:B:1081:LEU:HB2	2.17	0.44
4:D:29:LEU:HB3	7:G:82:PHE:CE2	2.52	0.44
6:F:89:GLU:OE2	6:F:134:ILE:HG21	2.16	0.44
7:G:111:THR:HG23	7:G:111:THR:O	2.17	0.44
9:I:40:SER:OG	9:I:41:PRO:HD2	2.17	0.44
10:J:53:HIS:CD2	10:J:55:ASP:N	2.85	0.44
10:J:62:ARG:HG2	10:J:62:ARG:O	2.17	0.44
1:A:125:ALA:C	1:A:127:ALA:N	2.74	0.44
1:A:230:ARG:O	1:A:231:PRO:C	2.60	0.44
1:A:352:VAL:O	1:A:467:THR:HB	2.17	0.44
1:A:883:LEU:O	1:A:884:ASP:C	2.60	0.44
1:A:1015:VAL:O	1:A:1016:THR:C	2.59	0.44
1:A:1208:THR:HA	1:A:1231:ASP:OD1	2.17	0.44
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.98	0.44
2:B:412:LEU:HB3	2:B:466:TRP:CE2	2.52	0.44
2:B:1106:ARG:HD2	2:B:1125:ASP:O	2.17	0.44
3:C:67:LEU:HA	3:C:70:ILE:CD1	2.48	0.44
3:C:68:GLY:O	3:C:169:LYS:HB2	2.17	0.44
3:C:79:GLN:HE21	3:C:127:ARG:CD	2.27	0.44
5:E:128:PRO:HA	5:E:129:PRO:O	2.17	0.44
6:F:97:ARG:NH2	6:F:108:PHE:CE1	2.86	0.44
7:G:15:PRO:O	7:G:16:SER:C	2.59	0.44
8:H:2:SER:OG	8:H:3:ASN:N	2.50	0.44
9:I:100:PHE:N	9:I:100:PHE:HD1	2.15	0.44
11:K:55:LYS:HB2	11:K:81:TYR:HE1	1.82	0.44
1:A:102:VAL:HB	1:A:211:PHE:HE1	1.77	0.44
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.52	0.44
1:A:1111:MET:HG3	1:A:1114:PRO:HB3	2.00	0.44
1:A:1147:THR:HB	9:I:48:LEU:HD12	1.98	0.44
1:A:1170:ILE:HG22	1:A:1174:PHE:CZ	2.52	0.44
1:A:1241:ARG:C	1:A:1242:VAL:HG23	2.42	0.44
2:B:234:ILE:HG21	2:B:237:VAL:HG23	1.98	0.44
2:B:579:ARG:HG2	2:B:579:ARG:NH1	2.30	0.44
2:B:806:THR:CG2	2:B:808:ALA:HB3	2.47	0.44
2:B:987:LYS:HE3	15:P:11:G:C2'	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1002:THR:HG23	2:B:1087:PHE:HE1	1.81	0.44
4:D:51:ASN:OD1	4:D:54:GLU:HB2	2.17	0.44
4:D:173:HIS:ND1	4:D:174:PRO:HD2	2.33	0.44
7:G:49:LEU:O	7:G:50:ASP:C	2.60	0.44
8:H:4:THR:O	8:H:5:LEU:HD23	2.17	0.44
1:A:12:ARG:NH2	2:B:1192:TYR:CE2	2.85	0.44
1:A:69:THR:O	1:A:70:CYS:C	2.61	0.44
1:A:108:MET:O	1:A:109:HIS:CB	2.63	0.44
1:A:121:LEU:HD22	1:A:141:LEU:HD21	2.00	0.44
1:A:264:PHE:CB	1:A:265:LYS:NZ	2.81	0.44
1:A:791:ASP:C	1:A:791:ASP:OD1	2.60	0.44
1:A:833:GLU:OE2	1:A:1102:LYS:HE3	2.17	0.44
1:A:939:ASP:O	1:A:942:PHE:HB3	2.18	0.44
1:A:1076:ALA:CB	1:A:1079:MET:HE2	2.47	0.44
1:A:1094:VAL:HG13	1:A:1113:THR:CB	2.48	0.44
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.98	0.44
2:B:67:SER:HB2	2:B:92:PHE:CD1	2.52	0.44
2:B:361:LEU:HD11	2:B:381:MET:HE2	2.00	0.44
2:B:485:ARG:HG3	2:B:781:PHE:HD1	1.83	0.44
2:B:637:LEU:HD22	2:B:742:GLU:HA	2.00	0.44
2:B:1003:ALA:HA	3:C:178:PHE:O	2.17	0.44
2:B:1031:LEU:HD12	2:B:1031:LEU:C	2.42	0.44
3:C:69:LEU:HB3	10:J:6:ARG:HD3	1.99	0.44
5:E:74:ASP:N	5:E:74:ASP:OD1	2.50	0.44
5:E:100:ILE:HG23	5:E:105:PHE:CD1	2.53	0.44
7:G:1:MET:SD	7:G:79:PHE:HD1	2.39	0.44
8:H:83:GLN:CD	8:H:87:ARG:HH21	2.25	0.44
8:H:100:THR:CG2	8:H:101:ALA:N	2.81	0.44
1:A:336:ILE:CD1	2:B:1203:LEU:HD22	2.47	0.44
1:A:377:PRO:O	1:A:377:PRO:HG2	2.18	0.44
1:A:755:PHE:O	1:A:757:ASN:N	2.51	0.44
1:A:858:ASN:ND2	1:A:860:LEU:HB2	2.32	0.44
1:A:1037:LEU:HD13	1:A:1042:PHE:HA	2.00	0.44
1:A:1100:ARG:HD2	1:A:1100:ARG:O	2.17	0.44
1:A:1205:LYS:O	1:A:1206:ASP:C	2.61	0.44
1:A:1424:VAL:HG11	2:B:1139:ILE:HD11	1.98	0.44
2:B:408:LEU:HB3	2:B:409:ALA:H	1.69	0.44
2:B:650:GLU:HG3	2:B:654:ARG:HH21	1.83	0.44
2:B:879:ARG:HD2	2:B:879:ARG:N	2.33	0.44
6:F:135:ARG:HG2	6:F:137:TYR:CE1	2.52	0.44
7:G:114:LEU:HD23	7:G:161:GLY:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:99:GLY:HA3	8:H:117:SER:O	2.17	0.44
1:A:317:LYS:O	1:A:318:SER:HB3	2.18	0.44
1:A:388:LEU:HD13	1:A:432:VAL:CG2	2.48	0.44
1:A:820:GLY:C	1:A:822:GLU:N	2.74	0.44
1:A:821:ARG:HG2	2:B:514:LEU:H	1.82	0.44
1:A:1081:LEU:CD1	1:A:1098:VAL:H	2.29	0.44
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.79	0.44
1:A:1311:VAL:HG21	1:A:1329:THR:HG23	2.00	0.44
2:B:225:VAL:HG11	2:B:385:LEU:HA	1.99	0.44
2:B:273:LEU:HD22	2:B:360:PHE:CD1	2.52	0.44
2:B:781:PHE:CD2	2:B:781:PHE:N	2.83	0.44
3:C:174:ALA:O	3:C:175:ALA:HB3	2.18	0.44
3:C:183:TRP:CZ3	3:C:203:GLN:NE2	2.86	0.44
4:D:155:ARG:CD	4:D:221:TYR:CE1	3.00	0.44
4:D:180:LEU:HD23	4:D:180:LEU:HA	1.89	0.44
5:E:22:MET:HE3	5:E:26:ARG:HH21	1.77	0.44
5:E:111:VAL:HG12	5:E:137:GLU:HG2	1.99	0.44
5:E:124:VAL:HG13	5:E:132:ILE:CB	2.47	0.44
6:F:82:THR:HA	6:F:83:PRO:HD3	1.71	0.44
6:F:119:ARG:NH1	6:F:119:ARG:CG	2.78	0.44
7:G:91:VAL:CG1	7:G:92:VAL:N	2.80	0.44
8:H:83:GLN:C	8:H:85:GLY:N	2.75	0.44
8:H:102:TYR:CD2	8:H:102:TYR:N	2.86	0.44
9:I:88:SER:HB3	9:I:95:THR:HG21	2.00	0.44
1:A:173:THR:HG22	1:A:184:SER:OG	2.18	0.44
1:A:305:ASP:OD1	1:A:305:ASP:C	2.60	0.44
1:A:321:PRO:O	1:A:322:VAL:HB	2.16	0.44
1:A:378:GLU:OE1	1:A:388:LEU:HD21	2.17	0.44
1:A:568:PRO:HB2	3:C:221:TYR:CE1	2.52	0.44
1:A:705:LYS:O	1:A:706:HIS:C	2.61	0.44
1:A:935:GLN:NE2	1:A:938:LYS:HD2	2.32	0.44
1:A:973:ILE:CD1	1:A:1037:LEU:HA	2.47	0.44
2:B:20:ASP:C	2:B:22:SER:N	2.74	0.44
2:B:860:MET:HG2	2:B:861:ASP:N	2.32	0.44
5:E:56:LYS:CE	5:E:84:ASP:HB2	2.29	0.44
5:E:78:LEU:HD11	5:E:109:ILE:HD12	1.99	0.44
8:H:65:LEU:N	8:H:65:LEU:CD2	2.64	0.44
10:J:34:THR:C	10:J:36:LEU:N	2.74	0.44
1:A:273:ASN:O	1:A:274:ILE:C	2.61	0.44
1:A:666:ILE:HD12	1:A:666:ILE:N	2.33	0.44
1:A:722:LEU:HD23	1:A:799:PHE:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:TYR:N	14:T:18:DC:H5'	2.33	0.44
1:A:1131:ALA:O	1:A:1132:LYS:C	2.60	0.44
1:A:1410:PHE:HD2	2:B:1212:ILE:CD1	2.30	0.44
2:B:33:VAL:O	2:B:36:ALA:HB3	2.17	0.44
2:B:599:THR:O	2:B:603:LEU:HB2	2.18	0.44
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.82	0.44
2:B:860:MET:HG3	2:B:965:LYS:CG	2.44	0.44
2:B:1110:PRO:O	2:B:1119:VAL:HG13	2.17	0.44
3:C:114:TYR:HB3	3:C:140:ASN:O	2.18	0.44
5:E:46:TYR:O	5:E:54:GLN:HB2	2.18	0.44
5:E:78:LEU:HD23	5:E:79:TRP:N	2.33	0.44
8:H:26:ILE:CD1	8:H:49:VAL:HG11	2.48	0.44
9:I:74:GLU:O	9:I:74:GLU:HG3	2.17	0.44
1:A:92:HIS:O	1:A:93:VAL:C	2.59	0.44
1:A:277:GLU:O	1:A:277:GLU:HG2	2.18	0.44
1:A:382:PRO:HB3	1:A:428:TYR:CE2	2.53	0.44
1:A:823:GLY:O	1:A:824:LEU:C	2.61	0.44
1:A:884:ASP:HB2	1:A:1024:SER:OG	2.18	0.44
1:A:1067:LEU:O	1:A:1068:ALA:C	2.61	0.44
1:A:1127:ASP:CG	1:A:1130:GLN:CB	2.89	0.44
1:A:1144:LYS:HA	1:A:1268:LEU:HD22	2.00	0.44
1:A:1161:THR:O	1:A:1163:ILE:N	2.51	0.44
2:B:351:TYR:CD1	2:B:355:ILE:HD11	2.52	0.44
2:B:597:MET:SD	2:B:617:ARG:HB2	2.57	0.44
2:B:603:LEU:CD1	2:B:609:ILE:HG23	2.43	0.44
2:B:770:GLN:OE1	2:B:983:ARG:CA	2.53	0.44
2:B:1002:THR:O	2:B:1003:ALA:C	2.59	0.44
3:C:3:GLU:N	11:K:104:ASN:HD21	2.15	0.44
3:C:33:LEU:O	3:C:34:ARG:C	2.61	0.44
3:C:233:GLU:CG	3:C:234:SER:N	2.80	0.44
4:D:130:LEU:C	4:D:132:GLN:N	2.76	0.44
4:D:187:THR:C	4:D:189:ASP:N	2.70	0.44
5:E:114:ASN:O	5:E:115:ASN:CB	2.54	0.44
6:F:120:ILE:O	6:F:124:GLU:HG3	2.18	0.44
9:I:55:THR:OG1	9:I:100:PHE:CD2	2.70	0.44
14:T:16:DT:C2'	14:T:17:DT:C5'	2.94	0.44
1:A:265:LYS:HA	1:A:265:LYS:CE	2.48	0.43
1:A:683:ILE:HG21	1:A:801:GLU:CG	2.48	0.43
1:A:844:ALA:O	1:A:845:LEU:HD23	2.18	0.43
1:A:1118:VAL:HG23	1:A:1118:VAL:O	2.18	0.43
1:A:1241:ARG:O	1:A:1242:VAL:HB	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1259:MET:CE	1:A:1263:ILE:HG13	2.48	0.43
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.35	0.43
2:B:526:GLU:OE1	2:B:752:ALA:CB	2.66	0.43
5:E:20:LYS:O	5:E:21:GLU:C	2.60	0.43
7:G:138:THR:HG22	7:G:139:ILE:HB	2.00	0.43
8:H:130:ARG:HH11	8:H:130:ARG:CA	2.31	0.43
9:I:69:PRO:HG2	9:I:85:PHE:CD2	2.52	0.43
9:I:72:ASP:CG	9:I:72:ASP:O	2.59	0.43
11:K:7:PHE:C	11:K:9:LEU:N	2.76	0.43
11:K:47:ARG:C	11:K:47:ARG:HD2	2.43	0.43
1:A:34:LYS:NZ	1:A:57:ARG:HH21	2.10	0.43
1:A:146:MET:C	1:A:171:GLN:HB2	2.44	0.43
1:A:236:LEU:HD11	1:A:304:MET:HE1	2.00	0.43
1:A:306:ASN:OD1	1:A:306:ASN:O	2.36	0.43
1:A:347:PHE:N	1:A:347:PHE:CD1	2.87	0.43
1:A:495:GLU:O	1:A:498:ARG:HG3	2.17	0.43
1:A:528:LEU:HD23	1:A:751:SER:HA	2.01	0.43
1:A:571:LEU:HD22	8:H:46:LEU:CD1	2.41	0.43
1:A:595:THR:C	1:A:596:THR:CG2	2.90	0.43
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.82	0.43
1:A:901:LEU:H	1:A:926:GLN:CD	2.25	0.43
1:A:1319:VAL:O	1:A:1322:ILE:HG12	2.17	0.43
2:B:235:SER:O	2:B:236:HIS:CD2	2.69	0.43
2:B:240:ILE:HD12	2:B:241:ARG:N	2.33	0.43
2:B:273:LEU:HD12	2:B:280:ILE:HD12	2.00	0.43
2:B:455:SER:O	2:B:456:GLY:C	2.59	0.43
2:B:464:GLY:C	2:B:465:ASN:HD22	2.26	0.43
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.42	0.43
2:B:880:THR:O	2:B:881:ASN:HB2	2.17	0.43
2:B:1002:THR:O	2:B:1004:GLU:N	2.50	0.43
3:C:44:LEU:HD21	3:C:159:ALA:HB1	2.00	0.43
7:G:14:HIS:CE1	7:G:15:PRO:HD2	2.53	0.43
7:G:138:THR:O	7:G:140:LYS:N	2.51	0.43
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.50	0.43
10:J:60:PHE:O	10:J:63:TYR:HD1	2.01	0.43
1:A:184:SER:HB2	1:A:199:LEU:HD23	2.00	0.43
1:A:184:SER:HB3	1:A:199:LEU:HD23	1.99	0.43
1:A:500:GLU:OE1	2:B:1143:ALA:C	2.61	0.43
1:A:528:LEU:HD23	1:A:751:SER:CA	2.48	0.43
1:A:857:ARG:CZ	6:F:139:PRO:HG3	2.48	0.43
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:SER:OG	2:B:411:PRO:HD3	2.17	0.43
2:B:284:ILE:CD1	2:B:324:ILE:HD12	2.48	0.43
2:B:604:ARG:O	2:B:606:LYS:N	2.51	0.43
2:B:885:MET:HA	2:B:936:ASP:HB2	1.98	0.43
2:B:1033:LYS:O	2:B:1037:LEU:HG	2.18	0.43
3:C:236:GLY:O	3:C:237:SER:C	2.59	0.43
5:E:82:PHE:N	5:E:82:PHE:HD1	2.17	0.43
5:E:111:VAL:HG12	5:E:111:VAL:O	2.18	0.43
5:E:177:ARG:C	5:E:212:ARG:HD3	2.43	0.43
6:F:69:LEU:O	6:F:70:LYS:HB2	2.19	0.43
6:F:76:LYS:O	6:F:79:ARG:HD3	2.17	0.43
8:H:40:LEU:CD2	8:H:42:ILE:HD11	2.48	0.43
1:A:207:ILE:CG2	1:A:211:PHE:CE2	3.02	0.43
1:A:523:ILE:C	1:A:524:VAL:CG2	2.91	0.43
1:A:709:THR:CG2	1:A:710:LEU:H	2.28	0.43
1:A:787:PHE:CE1	1:A:796:SER:HA	2.50	0.43
1:A:817:ALA:C	1:A:819:GLY:N	2.76	0.43
1:A:973:ILE:HD11	1:A:1041:ALA:CB	2.48	0.43
1:A:1267:MET:HA	1:A:1271:ILE:HD12	2.00	0.43
1:A:1280:GLU:HB3	1:A:1281:ARG:H	1.64	0.43
1:A:1399:ARG:HB3	1:A:1408:ILE:HD13	2.00	0.43
2:B:69:LEU:HD22	2:B:429:PHE:CE1	2.53	0.43
2:B:546:SER:OG	2:B:631:GLY:N	2.51	0.43
2:B:604:ARG:O	2:B:607:GLY:N	2.51	0.43
2:B:604:ARG:HA	2:B:609:ILE:HG13	1.99	0.43
2:B:887:HIS:CD2	2:B:887:HIS:N	2.85	0.43
2:B:1001:PHE:CE2	3:C:34:ARG:CZ	3.02	0.43
3:C:22:LEU:HD11	11:K:101:LEU:HD21	2.00	0.43
3:C:52:GLU:OE2	3:C:154:LYS:HD2	2.18	0.43
3:C:58:LEU:HD23	3:C:58:LEU:N	2.33	0.43
7:G:26:LEU:HD23	7:G:26:LEU:HA	1.73	0.43
10:J:8:PHE:N	10:J:8:PHE:CD2	2.86	0.43
12:L:68:GLU:CD	12:L:68:GLU:H	2.21	0.43
1:A:298:PHE:HD2	1:A:299:HIS:HD2	1.67	0.43
1:A:688:LYS:C	1:A:690:VAL:N	2.73	0.43
1:A:709:THR:OG1	1:A:712:GLU:HG3	2.17	0.43
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	3.06	0.43
1:A:1077:THR:HB	1:A:1078:GLN:HE21	1.84	0.43
1:A:1332:PHE:O	1:A:1333:ILE:C	2.59	0.43
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.49	0.43
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:ILE:CB	2:B:130:VAL:HG22	2.48	0.43
2:B:261:ARG:HH11	2:B:261:ARG:CB	2.09	0.43
2:B:269:ILE:CG2	2:B:282:ILE:HD13	2.49	0.43
2:B:312:GLU:O	2:B:315:LYS:HB2	2.19	0.43
2:B:846:ILE:HG23	2:B:974:PRO:CG	2.31	0.43
3:C:31:ASN:HA	3:C:34:ARG:HB3	1.99	0.43
4:D:33:PHE:CE1	7:G:80:LYS:HD3	2.52	0.43
4:D:219:THR:CG2	4:D:220:LEU:O	2.67	0.43
5:E:46:TYR:CD2	5:E:58:MET:HG3	2.54	0.43
5:E:116:ILE:HG22	5:E:120:ALA:HB3	2.00	0.43
5:E:161:LYS:HD2	5:E:195:VAL:CG2	2.49	0.43
7:G:142:ARG:C	7:G:143:ILE:HG13	2.44	0.43
8:H:3:ASN:CG	8:H:4:THR:N	2.76	0.43
8:H:40:LEU:HG	8:H:42:ILE:HG13	2.00	0.43
10:J:7:CYS:O	10:J:8:PHE:C	2.60	0.43
10:J:16:ASP:CG	10:J:17:LYS:HD2	2.43	0.43
12:L:38:LEU:HG	12:L:39:SER:N	2.33	0.43
12:L:66:GLN:C	12:L:67:PHE:CD1	2.97	0.43
1:A:2:VAL:CG1	2:B:1157:ALA:O	2.67	0.43
1:A:11:LEU:O	1:A:11:LEU:CD2	2.61	0.43
1:A:47:ARG:NH1	1:A:254:GLU:HG2	2.34	0.43
1:A:343:LYS:NZ	2:B:1151:LEU:O	2.51	0.43
1:A:711:ARG:O	1:A:712:GLU:C	2.62	0.43
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.54	0.43
1:A:1121:GLU:O	1:A:1122:PRO:C	2.61	0.43
1:A:1347:ALA:O	1:A:1348:LEU:C	2.62	0.43
2:B:218:SER:HA	2:B:404:LYS:HA	2.00	0.43
2:B:414:ALA:O	2:B:415:GLN:C	2.62	0.43
2:B:595:ARG:O	2:B:596:LEU:C	2.61	0.43
2:B:882:THR:CG2	2:B:883:LEU:N	2.78	0.43
3:C:123:ASN:CG	3:C:125:MET:H	2.25	0.43
5:E:93:MET:C	5:E:95:THR:N	2.75	0.43
5:E:186:LEU:O	5:E:187:TYR:C	2.62	0.43
9:I:50:THR:CG2	9:I:51:ASN:H	2.32	0.43
9:I:82:GLU:HB3	9:I:104:LEU:HG	2.01	0.43
1:A:351:THR:HG21	2:B:1103:ILE:HG13	2.00	0.43
1:A:396:PRO:HG2	1:A:397:ASN:OD1	2.19	0.43
1:A:632:VAL:O	1:A:633:VAL:C	2.62	0.43
1:A:774:ARG:HG3	1:A:797:LYS:HB3	2.01	0.43
1:A:804:TYR:OH	2:B:763:GLN:HA	2.19	0.43
1:A:833:GLU:CG	1:A:1102:LYS:HE2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.34	0.43
1:A:1124:HIS:HB2	1:A:1130:GLN:HG2	2.01	0.43
1:A:1308:THR:HG21	1:A:1310:GLY:O	2.19	0.43
1:A:1367:HIS:O	1:A:1368:MET:C	2.60	0.43
2:B:46:GLN:HB2	2:B:408:LEU:CD2	2.48	0.43
2:B:46:GLN:OE1	2:B:47:GLN:N	2.50	0.43
2:B:205:ILE:O	2:B:206:ASN:C	2.62	0.43
2:B:605:ARG:NE	2:B:639:ILE:HD13	2.33	0.43
2:B:883:LEU:O	2:B:885:MET:N	2.52	0.43
2:B:1068:GLY:O	2:B:1069:PHE:C	2.62	0.43
3:C:76:ASP:O	3:C:77:ILE:C	2.60	0.43
3:C:136:ASP:OD2	3:C:137:LYS:N	2.52	0.43
3:C:265:MET:HE1	11:K:19:LEU:HB2	2.00	0.43
4:D:29:LEU:HD12	7:G:82:PHE:CE1	2.52	0.43
4:D:35:LEU:HD11	4:D:173:HIS:NE2	2.33	0.43
4:D:38:ILE:H	4:D:38:ILE:HG12	1.47	0.43
4:D:53:SER:H	4:D:148:LEU:HD22	1.84	0.43
4:D:119:ARG:HD2	4:D:221:TYR:CG	2.53	0.43
4:D:155:ARG:NH1	4:D:155:ARG:CB	2.82	0.43
7:G:20:PRO:CD	7:G:21:ARG:N	2.82	0.43
8:H:15:VAL:HG22	8:H:26:ILE:HD11	2.00	0.43
8:H:130:ARG:HD3	8:H:130:ARG:H	1.79	0.43
10:J:1:MET:HB2	10:J:56:LEU:HD12	1.99	0.43
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.54	0.43
10:J:48:ARG:HD2	10:J:48:ARG:C	2.44	0.43
11:K:55:LYS:CB	11:K:81:TYR:CD1	3.01	0.43
1:A:108:MET:CB	1:A:210:ILE:HD13	2.49	0.43
1:A:141:LEU:HD23	1:A:141:LEU:HA	1.86	0.43
1:A:239:LEU:HA	1:A:240:PRO:HD2	1.82	0.43
1:A:360:GLU:HB2	1:A:363:GLN:HG3	2.01	0.43
1:A:382:PRO:CB	1:A:428:TYR:HE2	2.32	0.43
1:A:565:ILE:O	1:A:570:PRO:HA	2.19	0.43
2:B:259:TYR:N	2:B:259:TYR:CD1	2.87	0.43
2:B:294:ASP:C	2:B:296:GLU:N	2.76	0.43
2:B:317:CYS:O	2:B:320:ASP:HB3	2.19	0.43
2:B:570:VAL:HG21	2:B:573:GLN:NE2	2.34	0.43
2:B:686:ASN:C	2:B:688:GLY:H	2.26	0.43
2:B:766:ARG:NH1	2:B:769:TYR:CE1	2.87	0.43
2:B:821:GLN:OE1	2:B:850:LEU:CD1	2.67	0.43
2:B:1023:VAL:O	2:B:1026:LEU:HB2	2.18	0.43
2:B:1198:TYR:CD2	2:B:1198:TYR:O	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:142:VAL:H	10:J:16:ASP:HB3	1.83	0.43
4:D:53:SER:HA	4:D:56:ARG:HB3	2.00	0.43
5:E:55:ARG:C	5:E:57:MET:N	2.74	0.43
1:A:69:THR:HG22	2:B:1174:LYS:HD3	2.01	0.43
1:A:567:LYS:HZ1	8:H:46:LEU:C	2.26	0.43
1:A:785:PRO:O	2:B:702:LEU:HD12	2.18	0.43
1:A:889:SER:HA	1:A:1297:GLU:N	2.33	0.43
1:A:1189:SER:HB2	1:A:1256:GLU:OE1	2.18	0.43
1:A:1450:LEU:CD1	6:F:108:PHE:CZ	3.02	0.43
2:B:308:TRP:CZ3	9:I:45:ARG:HG2	2.54	0.43
2:B:370:PHE:C	2:B:372:SER:N	2.75	0.43
2:B:449:ASN:C	2:B:451:LYS:H	2.27	0.43
2:B:460:ALA:O	2:B:462:ALA:N	2.52	0.43
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.90	0.43
3:C:99:LEU:N	3:C:99:LEU:CD2	2.74	0.43
3:C:184:ASN:ND2	3:C:189:THR:HB	2.34	0.43
3:C:220:ASP:OD1	3:C:223:ALA:HB2	2.18	0.43
5:E:2:ASP:C	5:E:3:GLN:HG2	2.44	0.43
11:K:12:LEU:HD12	11:K:12:LEU:HA	1.88	0.43
11:K:41:THR:HG22	11:K:42:LEU:N	2.33	0.43
1:A:151:ASP:HA	1:A:162:VAL:O	2.19	0.43
1:A:423:ASP:OD1	1:A:424:ILE:N	2.52	0.43
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.49	0.43
1:A:919:ILE:CG1	1:A:925:LEU:HD12	2.49	0.43
1:A:1110:ASN:N	1:A:1110:ASN:ND2	2.66	0.43
1:A:1115:SER:OG	1:A:1116:LEU:N	2.51	0.43
2:B:345:LYS:C	2:B:347:LYS:HG2	2.43	0.43
2:B:376:PHE:CE1	2:B:569:TYR:HB3	2.53	0.43
2:B:479:VAL:O	2:B:480:SER:HB3	2.17	0.43
2:B:1224:PHE:CE1	5:E:171:LYS:HG3	2.54	0.43
4:D:12:ARG:HH12	4:D:14:ARG:HA	1.81	0.43
4:D:64:VAL:C	4:D:66:ARG:H	2.26	0.43
4:D:71:LYS:C	4:D:73:SER:N	2.74	0.43
4:D:138:ASN:O	4:D:142:LYS:HG2	2.19	0.43
4:D:173:HIS:CG	4:D:174:PRO:HD2	2.54	0.43
5:E:24:LYS:HE3	5:E:24:LYS:HB2	1.88	0.43
7:G:49:LEU:HD21	7:G:77:VAL:HG23	2.00	0.43
11:K:79:GLU:HG3	11:K:80:GLY:H	1.83	0.43
1:A:71:GLN:O	1:A:73:GLY:N	2.45	0.42
1:A:78:PRO:CB	2:B:1201:LYS:HE3	2.49	0.42
1:A:114:LEU:HB2	1:A:142:CYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:LEU:HD21	6:F:88:TYR:HD2	1.83	0.42
1:A:814:PHE:CD2	1:A:814:PHE:C	2.97	0.42
1:A:1035:TYR:CD2	1:A:1035:TYR:N	2.85	0.42
1:A:1153:TYR:HA	9:I:41:PRO:O	2.19	0.42
2:B:345:LYS:C	2:B:347:LYS:N	2.77	0.42
2:B:576:ASP:HB3	2:B:622:LYS:NZ	2.34	0.42
2:B:822:ASN:HD22	10:J:52:THR:HG21	1.83	0.42
3:C:167:HIS:CA	11:K:6:ARG:HH12	2.32	0.42
3:C:214:ASN:O	3:C:217:ASP:OD2	2.36	0.42
3:C:235:VAL:HG21	10:J:6:ARG:HH22	1.83	0.42
5:E:135:PHE:CD2	5:E:140:LEU:HD21	2.52	0.42
8:H:42:ILE:O	8:H:44:VAL:HG23	2.18	0.42
8:H:94:ASP:OD1	8:H:94:ASP:N	2.51	0.42
9:I:82:GLU:HB3	9:I:104:LEU:CD1	2.49	0.42
11:K:82:ASP:OD1	11:K:82:ASP:C	2.62	0.42
1:A:64:ASN:C	1:A:66:LYS:N	2.74	0.42
1:A:67:CYS:O	1:A:68:GLN:HG3	2.19	0.42
1:A:310:GLY:C	1:A:312:PRO:HD2	2.43	0.42
1:A:463:ILE:HD11	1:A:469:ARG:HG3	2.01	0.42
1:A:482:PHE:CB	2:B:838:SER:OG	2.66	0.42
1:A:583:PRO:HG2	1:A:586:ILE:HG13	2.01	0.42
1:A:636:GLU:OE2	1:A:962:ARG:NH1	2.52	0.42
1:A:690:VAL:CG2	1:A:718:VAL:HG13	2.48	0.42
1:A:754:SER:O	1:A:757:ASN:HB2	2.19	0.42
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.34	0.42
1:A:1152:ILE:HG23	1:A:1260:LEU:CD2	2.49	0.42
2:B:309:GLN:OE1	9:I:52:ILE:HD11	2.18	0.42
2:B:405:ARG:CD	2:B:631:GLY:O	2.67	0.42
2:B:522:VAL:CG1	2:B:537:LYS:HB3	2.50	0.42
2:B:522:VAL:HG11	2:B:537:LYS:HB3	2.01	0.42
2:B:604:ARG:NH2	2:B:613:VAL:O	2.41	0.42
2:B:785:TYR:CD1	2:B:786:ASN:N	2.87	0.42
2:B:1004:GLU:CG	10:J:42:LYS:HZ3	2.32	0.42
2:B:1207:LEU:HD23	2:B:1207:LEU:HA	1.73	0.42
3:C:20:PHE:CZ	3:C:230:MET:HE3	2.54	0.42
3:C:101:LEU:CD1	3:C:118:LEU:HD23	2.47	0.42
7:G:1:MET:O	7:G:2:PHE:C	2.62	0.42
10:J:14:VAL:O	10:J:14:VAL:CG1	2.66	0.42
10:J:64:ASN:CB	10:J:65:PRO:CD	2.78	0.42
11:K:27:ALA:HB1	11:K:28:PRO:HD2	2.02	0.42
1:A:443:LEU:CD1	2:B:1146:PHE:CE2	3.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:ARG:HH12	2:B:729:ILE:CD1	2.33	0.42
1:A:874:ASP:N	1:A:1058:VAL:HG23	2.34	0.42
1:A:1094:VAL:O	1:A:1095:THR:C	2.63	0.42
2:B:233:PRO:HD3	14:T:11:DA:OP1	2.18	0.42
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.83	0.42
2:B:636:PRO:O	2:B:636:PRO:HG2	2.20	0.42
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.99	0.42
2:B:1220:ARG:NH1	2:B:1220:ARG:HB3	2.34	0.42
3:C:97:VAL:CG1	3:C:99:LEU:HD21	2.48	0.42
3:C:183:TRP:CZ2	3:C:212:PRO:HG3	2.54	0.42
3:C:236:GLY:C	3:C:238:ILE:H	2.24	0.42
7:G:21:ARG:HH11	7:G:24:GLN:HB2	1.81	0.42
7:G:101:VAL:CG1	7:G:102:GLN:N	2.83	0.42
7:G:125:SER:O	7:G:126:ASN:HB2	2.20	0.42
11:K:63:VAL:O	11:K:63:VAL:CG2	2.66	0.42
1:A:27:VAL:O	1:A:28:ARG:C	2.62	0.42
1:A:722:LEU:HB3	1:A:799:PHE:CD1	2.54	0.42
1:A:851:HIS:C	1:A:853:ASP:N	2.75	0.42
1:A:1044:TRP:O	1:A:1045:VAL:C	2.62	0.42
1:A:1081:LEU:CD1	1:A:1097:GLY:HA3	2.49	0.42
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.54	0.42
1:A:1332:PHE:CD2	1:A:1332:PHE:N	2.86	0.42
1:A:1334:ASP:C	1:A:1336:MET:N	2.75	0.42
2:B:172:ILE:HD13	2:B:178:ASN:ND2	2.24	0.42
2:B:412:LEU:HD21	2:B:479:VAL:HG11	2.02	0.42
2:B:542:MET:HG2	2:B:747:MET:CE	2.48	0.42
2:B:788:ARG:O	2:B:967:ARG:NH1	2.53	0.42
2:B:1079:LYS:HA	3:C:27:LEU:HD21	2.01	0.42
3:C:66:ARG:HH21	10:J:5:VAL:HG23	1.85	0.42
5:E:5:ASN:O	5:E:5:ASN:ND2	2.52	0.42
8:H:89:LEU:CD1	8:H:91:ASP:OD1	2.68	0.42
10:J:46:CYS:O	10:J:49:MET:HB3	2.20	0.42
1:A:54:ASN:C	1:A:56:PRO:HD3	2.44	0.42
1:A:61:ILE:O	1:A:62:ASP:C	2.61	0.42
1:A:69:THR:HB	2:B:1174:LYS:HZ3	1.84	0.42
1:A:364:VAL:O	1:A:364:VAL:HG13	2.17	0.42
1:A:674:PRO:HG2	1:A:675:THR:H	1.84	0.42
1:A:962:ARG:C	1:A:964:ILE:N	2.77	0.42
1:A:1263:ILE:O	1:A:1263:ILE:HG22	2.19	0.42
1:A:1385:THR:CG2	1:A:1386:ARG:H	2.29	0.42
2:B:244:LEU:CD2	2:B:366:GLN:NE2	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:384:ARG:HE	2:B:384:ARG:HB3	1.34	0.42
2:B:431:TYR:CG	2:B:447:ALA:CB	3.02	0.42
2:B:700:SER:C	2:B:701:ILE:CG2	2.93	0.42
2:B:700:SER:O	2:B:701:ILE:HG22	2.20	0.42
2:B:794:ASN:C	2:B:795:ILE:HD12	2.44	0.42
4:D:213:GLU:O	4:D:217:LEU:HG	2.18	0.42
5:E:13:TRP:CZ3	5:E:39:LEU:HB2	2.54	0.42
5:E:121:MET:C	5:E:123:LEU:H	2.27	0.42
8:H:106:GLU:C	8:H:108:SER:N	2.78	0.42
12:L:61:THR:CG2	12:L:62:LYS:N	2.82	0.42
1:A:66:LYS:HD3	1:A:67:CYS:H	1.84	0.42
1:A:283:GLY:O	1:A:285:PRO:CD	2.67	0.42
1:A:517:ASN:ND2	1:A:1364:ASN:HD22	2.16	0.42
1:A:639:PRO:CD	1:A:640:GLN:H	2.32	0.42
1:A:774:ARG:CZ	1:A:797:LYS:CB	2.98	0.42
1:A:816:HIS:HE2	2:B:764:SER:H	1.68	0.42
1:A:889:SER:OG	1:A:891:ALA:HB3	2.20	0.42
1:A:993:LEU:CD2	1:A:1022:LEU:HD21	2.49	0.42
2:B:51:PHE:CD2	2:B:173:MET:HB3	2.55	0.42
2:B:244:LEU:CD1	2:B:366:GLN:HE22	2.32	0.42
2:B:345:LYS:HA	2:B:348:ARG:NE	2.33	0.42
2:B:600:LEU:HD13	2:B:626:ILE:HD11	2.02	0.42
2:B:604:ARG:HG3	2:B:611:PRO:HA	2.01	0.42
2:B:831:SER:HB2	2:B:833:TYR:CD1	2.54	0.42
2:B:1168:LEU:C	2:B:1170:THR:H	2.27	0.42
2:B:1202:LEU:HD22	2:B:1206:GLU:OE2	2.19	0.42
3:C:11:ARG:NH2	3:C:206:ASN:OD1	2.52	0.42
3:C:46:ILE:HG13	3:C:72:LEU:HD11	2.02	0.42
4:D:138:ASN:O	4:D:140:ASP:N	2.52	0.42
5:E:22:MET:HG3	5:E:187:TYR:CD1	2.55	0.42
6:F:132:LEU:HD23	6:F:132:LEU:HA	1.82	0.42
7:G:26:LEU:C	7:G:28:THR:N	2.75	0.42
9:I:93:LYS:H	9:I:93:LYS:CD	2.12	0.42
1:A:178:GLY:C	1:A:179:LEU:HD23	2.44	0.42
1:A:385:ILE:CG2	1:A:386:ASP:N	2.82	0.42
1:A:596:THR:O	1:A:597:LEU:C	2.62	0.42
1:A:626:ASN:O	1:A:631:HIS:HD2	2.02	0.42
1:A:719:VAL:C	1:A:721:PHE:N	2.75	0.42
1:A:914:GLU:C	1:A:916:GLY:H	2.27	0.42
1:A:925:LEU:C	1:A:927:VAL:H	2.26	0.42
1:A:1371:LEU:HD12	1:A:1375:MET:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1407:GLU:CD	1:A:1407:GLU:N	2.77	0.42
2:B:56:ASP:CB	2:B:57:TYR:HD1	2.32	0.42
2:B:123:THR:HA	2:B:204:ILE:O	2.19	0.42
2:B:418:LYS:C	2:B:420:LEU:N	2.75	0.42
2:B:473:MET:HE3	2:B:474:SER:CA	2.48	0.42
2:B:526:GLU:OE1	2:B:752:ALA:HB3	2.20	0.42
2:B:889:THR:CG2	2:B:891:ASP:HB2	2.50	0.42
2:B:995:ARG:CB	2:B:997:GLU:OE2	2.67	0.42
2:B:1050:ILE:CG2	2:B:1051:THR:N	2.82	0.42
2:B:1082:MET:HA	3:C:189:THR:HA	2.02	0.42
6:F:133:VAL:HG13	6:F:146:TRP:O	2.19	0.42
7:G:35:GLU:HG2	7:G:48:VAL:HG23	2.02	0.42
8:H:39:THR:O	8:H:123:MET:HG3	2.19	0.42
11:K:47:ARG:HD2	11:K:47:ARG:O	2.19	0.42
1:A:219:PHE:O	1:A:222:LEU:N	2.51	0.42
1:A:244:PRO:CB	1:A:245:PRO:HD3	2.31	0.42
1:A:555:ASP:O	1:A:556:TRP:O	2.36	0.42
1:A:709:THR:CG2	1:A:710:LEU:N	2.80	0.42
1:A:719:VAL:O	1:A:721:PHE:N	2.53	0.42
1:A:758:ILE:H	1:A:758:ILE:HG13	1.72	0.42
1:A:994:GLN:C	1:A:996:ASN:N	2.77	0.42
1:A:1339:LEU:HD13	5:E:147:HIS:CG	2.55	0.42
2:B:44:VAL:HG11	2:B:495:LEU:HD13	2.02	0.42
2:B:100:PRO:HG2	2:B:124:TYR:CE1	2.55	0.42
2:B:311:LEU:O	2:B:312:GLU:C	2.61	0.42
2:B:558:LEU:HD11	2:B:596:LEU:CD2	2.48	0.42
2:B:637:LEU:HD23	2:B:637:LEU:HA	1.80	0.42
2:B:659:ALA:HA	2:B:662:MET:HE3	2.02	0.42
2:B:992:ILE:HD11	11:K:66:PRO:HB2	2.00	0.42
3:C:44:LEU:HD13	3:C:129:ILE:HG23	2.01	0.42
3:C:136:ASP:CB	3:C:141:GLY:H	2.33	0.42
5:E:61:GLN:HB2	5:E:79:TRP:HE3	1.85	0.42
5:E:78:LEU:HB2	5:E:107:THR:HG21	2.02	0.42
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.78	0.42
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.85	0.42
6:F:97:ARG:NH2	6:F:108:PHE:HE1	2.17	0.42
7:G:53:ASN:HD22	7:G:53:ASN:N	2.15	0.42
8:H:27:GLU:HG2	8:H:38:LEU:O	2.20	0.42
9:I:25:LEU:HG	9:I:38:ALA:HB2	2.02	0.42
11:K:78:THR:HG22	11:K:79:GLU:N	2.35	0.42
12:L:34:CYS:CB	12:L:51:CYS:HG	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:ASP:O	1:A:695:LYS:N	2.53	0.42
1:A:870:GLU:CB	5:E:204:THR:HG21	2.49	0.42
1:A:913:LEU:CD1	1:A:914:GLU:N	2.78	0.42
1:A:923:LEU:HD23	1:A:923:LEU:HA	1.88	0.42
1:A:1225:PHE:CE2	1:A:1227:ILE:HD11	2.55	0.42
1:A:1297:GLU:N	1:A:1297:GLU:OE1	2.53	0.42
2:B:638:PHE:CD2	2:B:690:VAL:HG22	2.54	0.42
2:B:779:GLY:O	2:B:795:ILE:HA	2.20	0.42
2:B:859:TYR:N	2:B:859:TYR:CD1	2.88	0.42
2:B:885:MET:HG2	2:B:936:ASP:HB2	2.02	0.42
2:B:973:ILE:HG23	2:B:974:PRO:HD2	2.02	0.42
2:B:1198:TYR:CD2	2:B:1198:TYR:C	2.98	0.42
3:C:248:ILE:CD1	11:K:101:LEU:HD22	2.49	0.42
4:D:8:PHE:HZ	4:D:37:GLN:NE2	2.17	0.42
4:D:155:ARG:HB3	4:D:155:ARG:NH1	2.34	0.42
4:D:196:PRO:O	4:D:197:SER:C	2.62	0.42
5:E:58:MET:O	5:E:59:SER:C	2.63	0.42
5:E:124:VAL:H	5:E:125:PRO:HD2	1.82	0.42
7:G:132:SER:HB3	7:G:135:ASP:N	2.32	0.42
11:K:49:GLU:C	11:K:51:LEU:N	2.75	0.42
1:A:10:PRO:HG2	2:B:1192:TYR:HD2	1.85	0.42
1:A:65:LEU:O	1:A:66:LYS:O	2.38	0.42
1:A:148:CYS:HB3	1:A:167:CYS:O	2.19	0.42
1:A:442:VAL:HB	1:A:489:LEU:HD11	2.01	0.42
1:A:547:LEU:HD21	1:A:560:ILE:CD1	2.50	0.42
1:A:850:VAL:HG21	1:A:1058:VAL:HG11	2.01	0.42
2:B:512:ARG:HG2	2:B:512:ARG:HH11	1.83	0.42
2:B:516:ASN:C	2:B:518:HIS:N	2.77	0.42
2:B:580:VAL:CG2	2:B:624:LEU:HB3	2.49	0.42
2:B:619:ILE:O	2:B:620:ARG:C	2.63	0.42
2:B:642:ASP:N	2:B:649:LYS:HG3	2.35	0.42
2:B:1124:ARG:NH2	15:P:2:A:OP2	2.52	0.42
3:C:22:LEU:HB2	3:C:230:MET:CE	2.50	0.42
3:C:38:ILE:H	3:C:38:ILE:HG13	1.61	0.42
3:C:123:ASN:C	3:C:125:MET:N	2.77	0.42
4:D:16:LYS:O	4:D:18:VAL:N	2.50	0.42
5:E:22:MET:O	5:E:26:ARG:HG2	2.20	0.42
8:H:12:VAL:HB	8:H:52:GLN:N	2.34	0.42
8:H:40:LEU:HD22	8:H:123:MET:CE	2.50	0.42
11:K:53:ASP:HB3	11:K:56:VAL:CG2	2.50	0.42
1:A:718:VAL:HG12	1:A:722:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:ASP:OD2	1:A:1030:ARG:NH2	2.53	0.41
1:A:1025:ARG:HG3	1:A:1025:ARG:NH1	2.33	0.41
1:A:1189:SER:OG	1:A:1191:TRP:HB2	2.20	0.41
2:B:25:ILE:HG22	2:B:29:ASP:CG	2.45	0.41
2:B:69:LEU:CD1	2:B:432:MET:HE1	2.50	0.41
2:B:594:ALA:HA	2:B:617:ARG:NH1	2.35	0.41
2:B:797:TYR:C	2:B:798:TYR:CD2	2.98	0.41
2:B:865:LYS:HD3	2:B:866:TYR:H	1.85	0.41
3:C:59:ALA:O	3:C:60:ASP:C	2.63	0.41
4:D:27:LEU:CD1	4:D:197:SER:HB3	2.50	0.41
4:D:176:GLU:C	4:D:178:ALA:N	2.75	0.41
5:E:19:VAL:HG22	5:E:140:LEU:HD12	2.00	0.41
5:E:93:MET:HE1	5:E:110:PHE:CD2	2.55	0.41
5:E:110:PHE:CD1	5:E:110:PHE:C	2.98	0.41
5:E:120:ALA:C	5:E:123:LEU:HG	2.44	0.41
5:E:191:LYS:O	5:E:192:ARG:C	2.63	0.41
7:G:132:SER:O	7:G:133:SER:C	2.63	0.41
8:H:9:ILE:HA	8:H:55:LEU:O	2.20	0.41
8:H:110:ASP:O	8:H:128:ASN:OD1	2.38	0.41
10:J:47:ARG:NH1	10:J:47:ARG:HG2	2.34	0.41
1:A:150:THR:O	1:A:150:THR:HG22	2.20	0.41
1:A:821:ARG:HH11	1:A:821:ARG:CB	2.27	0.41
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.53	0.41
1:A:1104:ILE:C	1:A:1106:ASN:N	2.78	0.41
1:A:1129:GLU:O	1:A:1130:GLN:C	2.62	0.41
2:B:205:ILE:C	2:B:207:GLY:N	2.78	0.41
2:B:557:PHE:HE1	2:B:603:LEU:HD11	1.84	0.41
3:C:69:LEU:O	10:J:6:ARG:HD2	2.20	0.41
3:C:88:CYS:SG	3:C:91:HIS:HA	2.61	0.41
3:C:113:VAL:HG23	3:C:147:LEU:HD21	2.01	0.41
5:E:56:LYS:HZ1	5:E:85:GLU:HG3	1.82	0.41
7:G:122:ASN:HB2	7:G:131:GLN:NE2	2.35	0.41
1:A:41:MET:O	1:A:42:ASP:O	2.38	0.41
1:A:150:THR:HA	1:A:165:GLY:O	2.20	0.41
1:A:253:ASN:HB3	1:A:254:GLU:H	1.70	0.41
1:A:260:ASP:OD1	1:A:261:ASP:N	2.53	0.41
1:A:347:PHE:HE2	1:A:375:THR:CG2	2.32	0.41
1:A:481:ASP:O	1:A:485:ASP:HB2	2.21	0.41
1:A:553:VAL:HA	1:A:554:PRO:HD2	1.90	0.41
1:A:1037:LEU:HD11	1:A:1045:VAL:HG21	2.00	0.41
2:B:430:ARG:HG2	2:B:430:ARG:HH11	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:570:VAL:HA	2:B:571:PRO:HD2	1.82	0.41
4:D:7:THR:HG21	4:D:32:GLU:OE2	2.20	0.41
4:D:50:LEU:HD21	7:G:4:ILE:CD1	2.49	0.41
4:D:156:ASP:O	4:D:157:GLN:C	2.63	0.41
5:E:7:ARG:HG3	5:E:8:ASN:N	2.35	0.41
11:K:79:GLU:O	11:K:81:TYR:N	2.54	0.41
1:A:54:ASN:HB3	1:A:247:ARG:NH2	2.33	0.41
1:A:120:GLU:C	1:A:122:MET:H	2.27	0.41
1:A:332:LYS:HB3	1:A:337:ARG:CZ	2.50	0.41
1:A:341:MET:HE2	1:A:843:LYS:HZ3	1.78	0.41
1:A:348:SER:HA	1:A:489:LEU:O	2.21	0.41
1:A:697:ALA:CB	1:A:702:LEU:HD12	2.41	0.41
1:A:855:THR:HG21	1:A:857:ARG:HE	1.85	0.41
2:B:114:PRO:HG2	2:B:115:GLN:N	2.30	0.41
2:B:604:ARG:C	2:B:606:LYS:N	2.76	0.41
2:B:661:LEU:C	2:B:663:ALA:H	2.28	0.41
2:B:766:ARG:NH1	2:B:769:TYR:CD1	2.87	0.41
3:C:44:LEU:CD2	3:C:159:ALA:HB1	2.50	0.41
3:C:234:SER:OG	3:C:235:VAL:N	2.54	0.41
4:D:29:LEU:CD2	4:D:29:LEU:H	2.33	0.41
4:D:60:LYS:O	4:D:61:GLU:C	2.63	0.41
4:D:118:THR:HB	4:D:121:LYS:HB3	2.00	0.41
5:E:195:VAL:HG22	5:E:213:ILE:HG13	2.01	0.41
6:F:105:ALA:HB1	6:F:106:PRO:CD	2.50	0.41
7:G:26:LEU:O	7:G:28:THR:N	2.52	0.41
7:G:126:ASN:HA	7:G:127:PRO:HA	1.95	0.41
10:J:13:VAL:C	10:J:14:VAL:HG23	2.44	0.41
10:J:34:THR:O	10:J:37:SER:N	2.54	0.41
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.35	0.41
11:K:68:PHE:CD1	11:K:70:ARG:NH1	2.81	0.41
1:A:139:TRP:C	1:A:141:LEU:N	2.78	0.41
1:A:382:PRO:CD	1:A:428:TYR:CE2	3.04	0.41
1:A:382:PRO:N	1:A:428:TYR:CE2	2.89	0.41
1:A:525:GLN:O	1:A:526:ASP:C	2.64	0.41
1:A:557:ASP:O	1:A:559:VAL:HG23	2.20	0.41
1:A:767:GLN:NE2	1:A:768:GLN:O	2.53	0.41
1:A:774:ARG:CZ	1:A:797:LYS:HG3	2.51	0.41
1:A:830:LYS:HG3	1:A:1098:VAL:HG21	2.02	0.41
2:B:313:MET:CE	2:B:386:LEU:HB3	2.50	0.41
2:B:597:MET:CE	2:B:624:LEU:HD21	2.49	0.41
2:B:613:VAL:HG13	2:B:627:PHE:C	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:877:PRO:O	2:B:878:GLN:HB3	2.20	0.41
2:B:1002:THR:OG1	2:B:1006:ILE:CG1	2.66	0.41
3:C:29:MET:HE2	11:K:98:LEU:HD21	2.02	0.41
4:D:124:GLU:HA	4:D:127:ASP:HB2	2.01	0.41
8:H:38:LEU:HD12	8:H:38:LEU:HA	1.84	0.41
8:H:84:ALA:O	8:H:86:ASP:N	2.53	0.41
9:I:60:GLN:OE1	9:I:107:SER:OG	2.35	0.41
9:I:78:CYS:O	9:I:80:SER:N	2.53	0.41
10:J:37:SER:OG	10:J:47:ARG:NH2	2.53	0.41
11:K:47:ARG:HB3	11:K:47:ARG:NH1	2.23	0.41
12:L:27:LEU:N	12:L:27:LEU:HD23	2.36	0.41
12:L:29:TYR:C	12:L:30:ILE:HG13	2.45	0.41
1:A:255:SER:OG	2:B:918:ILE:HD13	2.20	0.41
1:A:392:VAL:HG13	1:A:415:LEU:HD11	2.03	0.41
1:A:425:GLN:HG2	1:A:425:GLN:O	2.20	0.41
1:A:526:ASP:O	1:A:527:THR:C	2.62	0.41
1:A:618:GLU:O	1:A:619:LYS:C	2.63	0.41
1:A:974:ASP:C	1:A:976:THR:N	2.77	0.41
1:A:1063:MET:HB3	1:A:1063:MET:HE3	1.76	0.41
1:A:1147:THR:O	9:I:48:LEU:HD12	2.20	0.41
1:A:1451:VAL:C	1:A:1453:TYR:H	2.27	0.41
1:A:1454:MET:HA	1:A:1455:PRO:HD2	1.94	0.41
2:B:54:PHE:CZ	2:B:59:LEU:HD13	2.56	0.41
2:B:63:ILE:HG12	2:B:130:VAL:HG21	2.03	0.41
2:B:113:TYR:CE2	2:B:192:LEU:CD2	3.03	0.41
2:B:515:HIS:O	2:B:518:HIS:HB2	2.20	0.41
2:B:1175:LEU:O	2:B:1176:ASN:CB	2.66	0.41
3:C:73:GLN:CB	3:C:131:HIS:H	2.34	0.41
3:C:258:ILE:N	3:C:258:ILE:CD1	2.83	0.41
4:D:170:THR:HB	4:D:172:LEU:HG	2.02	0.41
8:H:83:GLN:O	8:H:85:GLY:N	2.54	0.41
9:I:46:HIS:CE1	9:I:48:LEU:CD2	3.03	0.41
9:I:62:ILE:HD11	9:I:86:PHE:HE2	1.86	0.41
9:I:73:ARG:NH1	9:I:101:PHE:CZ	2.89	0.41
1:A:219:PHE:HB2	1:A:220:THR:H	1.46	0.41
1:A:396:PRO:HB3	1:A:403:LYS:HA	2.02	0.41
1:A:593:GLU:HB3	1:A:594:GLY:H	1.48	0.41
1:A:715:GLU:CD	1:A:774:ARG:HH11	2.28	0.41
1:A:820:GLY:O	1:A:823:GLY:N	2.54	0.41
1:A:946:VAL:HG12	1:A:947:PHE:CE2	2.56	0.41
1:A:1040:GLN:O	1:A:1041:ALA:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1407:GLU:CD	1:A:1407:GLU:H	2.29	0.41
2:B:361:LEU:N	2:B:362:PRO:CD	2.84	0.41
2:B:541:LEU:HB2	2:B:747:MET:HE3	2.03	0.41
2:B:618:ASP:O	2:B:622:LYS:N	2.53	0.41
2:B:745:PRO:O	2:B:746:SER:C	2.64	0.41
2:B:1003:ALA:O	3:C:177:GLU:HA	2.21	0.41
3:C:62:PHE:C	3:C:62:PHE:CD2	2.98	0.41
3:C:138:GLU:HB2	3:C:140:ASN:HD21	1.86	0.41
4:D:126:ILE:C	4:D:128:VAL:N	2.79	0.41
4:D:154:PHE:HE1	4:D:163:VAL:HG11	1.85	0.41
4:D:198:LEU:O	4:D:200:ASN:N	2.54	0.41
6:F:98:ALA:O	6:F:99:LEU:C	2.64	0.41
7:G:104:GLY:HA3	7:G:105:PRO:HD2	1.93	0.41
9:I:16:PRO:HB3	9:I:27:PHE:CE2	2.56	0.41
9:I:17:ARG:HG3	9:I:28:GLU:CD	2.46	0.41
9:I:45:ARG:HG3	9:I:46:HIS:N	2.36	0.41
11:K:51:LEU:CD1	11:K:59:ALA:HB3	2.51	0.41
11:K:53:ASP:C	11:K:55:LYS:N	2.78	0.41
11:K:85:ASP:O	11:K:88:LYS:N	2.54	0.41
1:A:93:VAL:HG21	1:A:301:ALA:HA	2.01	0.41
1:A:224:PHE:CE2	1:A:234:MET:HE2	2.56	0.41
1:A:343:LYS:NZ	2:B:1151:LEU:HG	2.35	0.41
1:A:460:VAL:CG1	1:A:461:LYS:N	2.83	0.41
1:A:473:SER:O	1:A:521:MET:HB3	2.21	0.41
1:A:549:MET:HE1	1:A:656:TRP:CB	2.51	0.41
1:A:639:PRO:CG	1:A:640:GLN:N	2.83	0.41
1:A:800:VAL:HA	1:A:812:GLU:OE2	2.20	0.41
1:A:1158:PRO:C	1:A:1159:ARG:HD2	2.45	0.41
1:A:1273:LEU:N	1:A:1273:LEU:CD1	2.84	0.41
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.60	0.41
2:B:189:LEU:O	2:B:190:TYR:C	2.64	0.41
2:B:205:ILE:O	2:B:207:GLY:N	2.54	0.41
2:B:259:TYR:O	2:B:260:GLY:O	2.39	0.41
2:B:365:THR:O	2:B:365:THR:HG23	2.20	0.41
2:B:500:THR:O	2:B:501:PRO:C	2.63	0.41
2:B:654:ARG:C	2:B:656:GLY:N	2.79	0.41
2:B:707:PRO:CG	2:B:708:GLU:N	2.75	0.41
2:B:976:ILE:CD1	2:B:992:ILE:HA	2.51	0.41
2:B:1084:GLN:OE1	3:C:189:THR:CG2	2.69	0.41
4:D:20:GLU:CD	4:D:20:GLU:N	2.79	0.41
4:D:150:ASN:HB3	7:G:142:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:45:LYS:HD3	5:E:46:TYR:CE1	2.56	0.41
5:E:175:LEU:HA	5:E:176:PRO:HD3	1.81	0.41
6:F:97:ARG:NE	6:F:124:GLU:OE1	2.54	0.41
6:F:152:ILE:HG22	6:F:153:VAL:N	2.35	0.41
9:I:54:GLU:HB3	9:I:100:PHE:HE2	1.85	0.41
10:J:5:VAL:C	10:J:6:ARG:HG3	2.46	0.41
1:A:63:ARG:HA	1:A:74:MET:CE	2.33	0.41
1:A:298:PHE:CD2	1:A:299:HIS:HD2	2.38	0.41
1:A:479:ASN:HD22	1:A:479:ASN:HA	1.62	0.41
1:A:526:ASP:OD1	2:B:1013:ASN:ND2	2.52	0.41
1:A:542:GLU:H	1:A:542:GLU:HG2	1.63	0.41
1:A:559:VAL:O	1:A:561:PRO:HD3	2.20	0.41
1:A:575:LYS:HB3	1:A:612:ILE:HG21	2.01	0.41
1:A:690:VAL:HG11	1:A:794:PRO:HD3	2.03	0.41
1:A:805:LEU:CD1	2:B:1052:VAL:HG21	2.51	0.41
1:A:1038:THR:H	1:A:1041:ALA:HB3	1.85	0.41
1:A:1230:GLU:C	1:A:1232:ASN:H	2.29	0.41
1:A:1279:ILE:O	1:A:1279:ILE:HG22	2.21	0.41
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.49	0.41
2:B:25:ILE:HG21	2:B:658:ILE:CD1	2.49	0.41
2:B:326:ASP:OD1	2:B:329:THR:CB	2.68	0.41
2:B:401:PHE:HB2	2:B:517:THR:OG1	2.20	0.41
2:B:467:GLY:N	2:B:475:SER:OG	2.54	0.41
2:B:571:PRO:HG2	2:B:572:HIS:H	1.86	0.41
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.50	0.41
2:B:912:ILE:O	2:B:938:SER:CB	2.67	0.41
2:B:913:GLY:HA2	2:B:938:SER:OG	2.20	0.41
2:B:918:ILE:HG21	2:B:935:ARG:HH22	1.83	0.41
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.21	0.41
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.56	0.41
2:B:1084:GLN:HE21	2:B:1084:GLN:H	1.67	0.41
2:B:1135:ARG:O	2:B:1136:ASP:C	2.64	0.41
3:C:133:ILE:HD12	3:C:236:GLY:C	2.42	0.41
3:C:133:ILE:CD1	3:C:237:SER:N	2.82	0.41
3:C:138:GLU:N	3:C:138:GLU:CD	2.79	0.41
3:C:154:LYS:HB2	3:C:154:LYS:HE3	1.85	0.41
3:C:168:ALA:C	3:C:170:TRP:N	2.78	0.41
3:C:177:GLU:HB2	3:C:231:ASN:HB3	2.02	0.41
4:D:66:ARG:NH2	7:G:31:LEU:HD11	2.35	0.41
4:D:122:GLU:HA	4:D:125:SER:HB3	2.02	0.41
5:E:99:HIS:ND1	5:E:103:LYS:HG3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:116:ASP:HB3	6:F:119:ARG:HB2	2.02	0.41
6:F:138:LEU:HD23	6:F:138:LEU:HA	1.84	0.41
7:G:44:TYR:OH	7:G:156:SER:HB2	2.20	0.41
7:G:122:ASN:CG	7:G:125:SER:HB3	2.43	0.41
7:G:145:VAL:HG12	7:G:146:LYS:N	2.36	0.41
9:I:15:TYR:CD1	9:I:30:ARG:HD2	2.56	0.41
9:I:54:GLU:OE1	9:I:118:ARG:NH2	2.53	0.41
10:J:57:ILE:HG23	10:J:58:GLU:N	2.35	0.41
11:K:31:VAL:CG1	11:K:32:VAL:N	2.81	0.41
1:A:64:ASN:O	1:A:66:LYS:N	2.54	0.41
1:A:89:PRO:C	1:A:204:THR:HG21	2.46	0.41
1:A:134:ARG:C	1:A:136:ALA:N	2.79	0.41
1:A:371:ALA:HB2	1:A:462:VAL:HG13	2.03	0.41
1:A:650:GLN:HB3	1:A:654:ASN:ND2	2.36	0.41
1:A:722:LEU:HD23	1:A:799:PHE:CG	2.56	0.41
1:A:994:GLN:C	1:A:996:ASN:H	2.29	0.41
1:A:996:ASN:O	1:A:998:LEU:N	2.49	0.41
1:A:1053:PHE:O	1:A:1056:SER:N	2.54	0.41
1:A:1116:LEU:HG	1:A:1308:THR:HB	2.03	0.41
1:A:1138:ILE:HG13	1:A:1139:GLU:N	2.36	0.41
2:B:205:ILE:HG12	2:B:461:LEU:HB3	2.03	0.41
2:B:251:ILE:O	2:B:251:ILE:CG2	2.67	0.41
2:B:307:ASP:C	2:B:309:GLN:N	2.77	0.41
2:B:333:PHE:O	2:B:334:ILE:HG13	2.20	0.41
2:B:798:TYR:CE2	3:C:62:PHE:CZ	3.07	0.41
2:B:1032:SER:HB3	2:B:1089:PRO:HG2	2.03	0.41
3:C:22:LEU:HD11	11:K:101:LEU:HD11	2.03	0.41
5:E:164:LEU:HD22	5:E:211:TYR:HD2	1.77	0.41
7:G:1:MET:CE	7:G:80:LYS:O	2.69	0.41
7:G:59:GLY:CA	7:G:70:PHE:CD2	3.04	0.41
7:G:61:ILE:HG22	7:G:62:LEU:O	2.21	0.41
8:H:130:ARG:N	8:H:130:ARG:CD	2.80	0.41
12:L:49:LYS:O	12:L:50:ASP:CB	2.58	0.41
1:A:53:LEU:O	1:A:54:ASN:C	2.64	0.40
1:A:152:VAL:HG12	1:A:153:PRO:CD	2.51	0.40
1:A:220:THR:O	1:A:221:SER:C	2.61	0.40
1:A:347:PHE:CE2	2:B:1107:ALA:HB1	2.56	0.40
1:A:663:SER:OG	2:B:827:ILE:O	2.35	0.40
1:A:683:ILE:HG21	1:A:801:GLU:OE1	2.21	0.40
1:A:909:ASP:OD1	1:A:911:SER:N	2.46	0.40
2:B:310:MET:HB2	2:B:310:MET:HE3	1.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:PHE:O	2:B:334:ILE:CG1	2.69	0.40
2:B:408:LEU:C	2:B:411:PRO:HD2	2.46	0.40
2:B:806:THR:HG21	2:B:808:ALA:HB3	2.03	0.40
2:B:1026:LEU:HA	2:B:1026:LEU:HD23	1.86	0.40
3:C:216:GLY:O	3:C:217:ASP:C	2.63	0.40
4:D:40:HIS:C	4:D:42:GLY:H	2.29	0.40
4:D:53:SER:HA	4:D:56:ARG:CB	2.51	0.40
4:D:134:THR:CG2	4:D:135:GLY:N	2.84	0.40
5:E:29:PHE:HD1	5:E:30:ILE:N	2.19	0.40
5:E:98:ILE:HG22	5:E:102:GLU:HG3	2.03	0.40
6:F:86:THR:HG23	6:F:89:GLU:CD	2.46	0.40
8:H:8:ASP:OD1	8:H:30:SER:OG	2.31	0.40
11:K:47:ARG:HD3	11:K:59:ALA:C	2.46	0.40
12:L:38:LEU:CG	12:L:39:SER:N	2.83	0.40
1:A:34:LYS:CB	1:A:36:ARG:NH2	2.85	0.40
1:A:101:LYS:HA	1:A:104:GLU:OE1	2.22	0.40
1:A:546:VAL:HG21	1:A:572:TRP:HB2	2.03	0.40
1:A:589:GLN:HG3	1:A:606:LEU:HD13	2.04	0.40
1:A:598:LEU:HA	8:H:122:LEU:CD1	2.48	0.40
1:A:688:LYS:O	1:A:689:LYS:C	2.65	0.40
1:A:752:LYS:HD3	1:A:752:LYS:HA	1.77	0.40
1:A:760:GLN:OE1	2:B:1021:MET:HE1	2.21	0.40
1:A:786:HIS:HE1	2:B:519:TRP:CZ2	2.39	0.40
1:A:857:ARG:NH1	6:F:139:PRO:CB	2.84	0.40
1:A:897:TYR:CD1	1:A:897:TYR:N	2.89	0.40
1:A:1097:GLY:O	1:A:1098:VAL:C	2.64	0.40
2:B:104:GLU:OE2	12:L:47:ARG:NH2	2.55	0.40
2:B:186:GLU:HB3	2:B:187:SER:H	1.71	0.40
2:B:224:GLN:HA	2:B:396:ASP:OD2	2.20	0.40
2:B:276:ILE:HG22	2:B:336:ARG:HB2	2.02	0.40
2:B:769:TYR:HA	15:P:11:G:H22	1.87	0.40
2:B:854:LEU:HD23	2:B:854:LEU:HA	1.91	0.40
2:B:955:THR:HG23	12:L:54:ARG:O	2.21	0.40
2:B:1031:LEU:HB2	2:B:1055:ILE:HD13	2.03	0.40
3:C:3:GLU:HB3	11:K:104:ASN:OD1	2.21	0.40
4:D:154:PHE:HA	4:D:219:THR:HB	2.02	0.40
4:D:190:GLU:O	4:D:193:THR:CG2	2.67	0.40
6:F:84:TYR:N	6:F:84:TYR:CD1	2.90	0.40
7:G:62:LEU:HD13	7:G:62:LEU:HA	1.89	0.40
9:I:8:ARG:O	9:I:9:ASP:HB2	2.21	0.40
10:J:12:LYS:O	10:J:13:VAL:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:53:HIS:HD2	10:J:54:VAL:H	1.58	0.40
10:J:56:LEU:O	10:J:57:ILE:C	2.63	0.40
11:K:102:LYS:O	11:K:103:THR:C	2.62	0.40
12:L:44:ASP:O	12:L:45:ALA:HB3	2.21	0.40
1:A:47:ARG:CZ	1:A:254:GLU:HG2	2.51	0.40
1:A:424:ILE:C	1:A:425:GLN:OE1	2.64	0.40
1:A:524:VAL:CG1	1:A:525:GLN:H	2.25	0.40
1:A:600:PRO:HG2	1:A:601:LYS:H	1.87	0.40
1:A:604:GLY:O	1:A:605:MET:HB2	2.21	0.40
1:A:665:GLY:HA2	2:B:1026:LEU:CD2	2.50	0.40
1:A:738:LYS:HD3	1:A:738:LYS:H	1.85	0.40
1:A:984:LYS:HG2	1:A:988:LEU:HD12	2.02	0.40
1:A:1006:ILE:HD12	5:E:167:ARG:CG	2.50	0.40
1:A:1030:ARG:NH1	1:A:1035:TYR:OH	2.54	0.40
1:A:1134:ILE:HG13	1:A:1134:ILE:H	1.66	0.40
1:A:1170:ILE:H	1:A:1170:ILE:CD1	2.16	0.40
1:A:1333:ILE:H	1:A:1333:ILE:HG12	1.48	0.40
1:A:1368:MET:O	1:A:1369:ALA:C	2.64	0.40
2:B:58:THR:HG22	2:B:62:ILE:HD11	2.02	0.40
2:B:282:ILE:HG21	2:B:382:ILE:CD1	2.51	0.40
2:B:326:ASP:CG	2:B:329:THR:H	2.29	0.40
2:B:624:LEU:HD12	2:B:624:LEU:HA	1.57	0.40
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.86	0.40
2:B:969:ARG:HG2	2:B:970:THR:N	2.36	0.40
3:C:77:ILE:HG23	3:C:161:LYS:HE3	2.03	0.40
4:D:176:GLU:O	4:D:178:ALA:N	2.54	0.40
6:F:109:VAL:CG2	6:F:124:GLU:HA	2.51	0.40
8:H:37:LYS:H	8:H:126:GLU:HB2	1.87	0.40
9:I:5:ARG:CZ	9:I:36:GLU:OE1	2.69	0.40
1:A:89:PRO:HG2	1:A:204:THR:HB	2.04	0.40
1:A:135:PHE:HD1	1:A:222:LEU:HD22	1.79	0.40
1:A:253:ASN:ND2	2:B:884:ARG:HD2	2.35	0.40
1:A:276:LEU:HD13	1:A:293:GLU:HA	2.03	0.40
1:A:543:LEU:O	1:A:544:ASP:C	2.63	0.40
1:A:588:LEU:HD23	1:A:607:ILE:HD12	2.02	0.40
1:A:889:SER:O	1:A:890:ASP:C	2.64	0.40
1:A:1030:ARG:HG2	1:A:1034:GLU:CD	2.44	0.40
1:A:1104:ILE:O	1:A:1106:ASN:N	2.55	0.40
1:A:1334:ASP:O	1:A:1336:MET:N	2.54	0.40
2:B:129:PHE:HE2	2:B:166:PHE:CD1	2.38	0.40
2:B:185:THR:N	2:B:188:ASP:OD2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:231:PRO:O	2:B:231:PRO:HG2	2.21	0.40
2:B:327:ARG:HH22	2:B:371:GLU:HG2	1.79	0.40
2:B:345:LYS:CG	2:B:346:GLU:N	2.70	0.40
2:B:620:ARG:NH1	9:I:68:LEU:HD21	2.37	0.40
2:B:655:LYS:HA	2:B:655:LYS:HD2	1.90	0.40
2:B:871:THR:CG2	2:B:872:GLU:N	2.85	0.40
2:B:950:ASP:HB3	2:B:967:ARG:O	2.21	0.40
3:C:148:ARG:CG	3:C:149:LYS:H	2.34	0.40
4:D:173:HIS:O	4:D:177:VAL:HG23	2.21	0.40
4:D:187:THR:HB	4:D:190:GLU:H	1.86	0.40
7:G:80:LYS:O	7:G:82:PHE:CE1	2.75	0.40
7:G:138:THR:O	7:G:141:SER:OG	2.37	0.40
10:J:7:CYS:SG	10:J:49:MET:HE3	2.61	0.40
11:K:93:SER:O	11:K:97:LYS:HG3	2.21	0.40
1:A:249:SER:O	1:A:250:ILE:CG1	2.66	0.40
1:A:599:SER:HB2	1:A:603:ASN:H	1.87	0.40
1:A:671:ALA:CB	1:A:676:MET:HG3	2.40	0.40
1:A:699:ALA:O	1:A:700:ASN:HB3	2.22	0.40
1:A:856:THR:HG21	1:A:1370:LEU:HD21	2.04	0.40
1:A:1211:GLN:O	1:A:1212:VAL:C	2.64	0.40
2:B:273:LEU:HA	2:B:274:PRO:HD2	1.95	0.40
2:B:286:PHE:HB3	2:B:297:ILE:HG12	2.02	0.40
2:B:390:LEU:O	2:B:392:ARG:HG3	2.21	0.40
2:B:515:HIS:CD2	2:B:517:THR:CG2	3.02	0.40
2:B:557:PHE:CZ	2:B:603:LEU:HG	2.56	0.40
2:B:570:VAL:HB	2:B:573:GLN:HB3	2.02	0.40
2:B:642:ASP:C	2:B:644:GLU:N	2.80	0.40
2:B:796:LEU:HD12	2:B:852:ARG:O	2.21	0.40
2:B:825:VAL:HG21	2:B:1092:TYR:HE1	1.87	0.40
2:B:878:GLN:HB2	2:B:879:ARG:HH11	1.87	0.40
2:B:1017:ILE:H	2:B:1018:PRO:HD2	1.87	0.40
2:B:1030:LEU:HD11	2:B:1059:LEU:HD22	2.04	0.40
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.50	0.40
3:C:265:MET:HB2	3:C:265:MET:HE3	1.81	0.40
5:E:80:VAL:HG12	5:E:82:PHE:CE1	2.57	0.40
6:F:138:LEU:HB3	6:F:139:PRO:HD2	2.03	0.40
7:G:28:THR:O	7:G:29:LYS:C	2.64	0.40
8:H:12:VAL:HG11	8:H:15:VAL:HG22	2.03	0.40
9:I:11:ASN:OD1	9:I:11:ASN:C	2.65	0.40
9:I:50:THR:H	9:I:92:ARG:HH12	1.69	0.40
11:K:65:HIS:CD2	11:K:65:HIS:C	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1408/1733 (81%)	1012 (72%)	262 (19%)	134 (10%)	0	5
2	B	1089/1224 (89%)	779 (72%)	201 (18%)	109 (10%)	0	5
3	C	264/347 (76%)	186 (70%)	51 (19%)	27 (10%)	0	4
4	D	175/221 (79%)	121 (69%)	39 (22%)	15 (9%)	0	6
5	E	212/215 (99%)	154 (73%)	42 (20%)	16 (8%)	1	8
6	F	85/155 (55%)	69 (81%)	14 (16%)	2 (2%)	4	25
7	G	169/171 (99%)	145 (86%)	13 (8%)	11 (6%)	1	11
8	H	132/146 (90%)	85 (64%)	23 (17%)	24 (18%)	0	1
9	I	117/122 (96%)	79 (68%)	29 (25%)	9 (8%)	1	7
10	J	63/70 (90%)	39 (62%)	11 (18%)	13 (21%)	0	1
11	K	113/120 (94%)	87 (77%)	22 (20%)	4 (4%)	3	20
12	L	44/70 (63%)	23 (52%)	9 (20%)	12 (27%)	0	0
All	All	3871/4594 (84%)	2779 (72%)	716 (18%)	376 (10%)	0	5

All (376) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	41	MET
1	A	43	GLU
1	A	48	ALA
1	A	54	ASN
1	A	57	ARG
1	A	58	LEU
1	A	62	ASP
1	A	63	ARG

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Mol	Chain	Res	Type
1	A	67	CYS
1	A	70	CYS
1	A	128	ILE
1	A	130	ASP
1	A	154	SER
1	A	167	CYS
1	A	250	ILE
1	A	286	HIS
1	A	311	GLN
1	A	312	PRO
1	A	332	LYS
1	A	399	HIS
1	A	423	ASP
1	A	567	LYS
1	A	666	ILE
1	A	1112	LYS
1	A	1114	PRO
1	A	1120	LEU
1	A	1124	HIS
1	A	1223	ASP
1	A	1233	ASP
1	A	1242	VAL
1	A	1255	GLU
1	A	1281	ARG
1	A	1314	SER
1	A	1405	THR
2	B	21	GLU
2	B	67	SER
2	B	68	THR
2	B	108	VAL
2	B	184	ALA
2	B	186	GLU
2	B	282	ILE
2	B	365	THR
2	B	367	LEU
2	B	435	THR
2	B	467	GLY
2	B	619	ILE
2	B	708	GLU
2	B	709	ASP
2	B	731	VAL
2	B	850	LEU

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Mol	Chain	Res	Type
2	B	879	ARG
2	B	907	GLY
2	B	958	GLN
2	B	1041	GLU
2	B	1046	PRO
2	B	1069	PHE
2	B	1097	HIS
2	B	1103	ILE
2	B	1108	ARG
2	B	1155	SER
2	B	1157	ALA
2	B	1181	GLU
2	B	1188	LYS
2	B	1222	ARG
3	C	56	THR
3	C	90	ASP
3	C	110	THR
3	C	125	MET
3	C	141	GLY
3	C	149	LYS
3	C	161	LYS
3	C	184	ASN
3	C	209	TYR
3	C	215	GLU
3	C	216	GLY
3	C	237	SER
4	D	5	THR
4	D	8	PHE
4	D	17	LYS
4	D	52	LEU
4	D	198	LEU
4	D	218	GLU
5	E	45	LYS
5	E	74	ASP
5	E	106	GLN
5	E	115	ASN
7	G	112	LYS
7	G	139	ILE
8	H	62	SER
8	H	77	ARG
8	H	82	PRO
8	H	108	SER

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Mol	Chain	Res	Type
8	H	128	ASN
8	H	134	ASN
8	H	140	ALA
9	I	11	ASN
9	I	79	HIS
10	J	2	ILE
10	J	28	ASP
10	J	42	LYS
10	J	55	ASP
10	J	64	ASN
12	L	50	ASP
12	L	53	HIS
12	L	59	ALA
12	L	60	ARG
1	A	5	GLN
1	A	76	GLU
1	A	93	VAL
1	A	126	LEU
1	A	249	SER
1	A	253	ASN
1	A	318	SER
1	A	400	PRO
1	A	410	GLY
1	A	424	ILE
1	A	556	TRP
1	A	576	GLN
1	A	591	PHE
1	A	592	ASP
1	A	597	LEU
1	A	628	GLY
1	A	718	VAL
1	A	821	ARG
1	A	846	GLU
1	A	852	TYR
1	A	884	ASP
1	A	885	THR
1	A	891	ALA
1	A	963	ILE
1	A	968	GLN
1	A	986	ILE
1	A	1002	GLY
1	A	1123	GLY

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Mol	Chain	Res	Type
1	A	1127	ASP
1	A	1139	GLU
1	A	1187	GLN
1	A	1231	ASP
1	A	1280	GLU
1	A	1309	ASP
1	A	1438	THR
2	B	58	THR
2	B	65	GLU
2	B	100	PRO
2	B	221	ASN
2	B	249	ARG
2	B	258	LEU
2	B	259	TYR
2	B	260	GLY
2	B	295	GLY
2	B	333	PHE
2	B	334	ILE
2	B	448	ILE
2	B	461	LEU
2	B	466	TRP
2	B	468	GLU
2	B	474	SER
2	B	501	PRO
2	B	575	PRO
2	B	591	ARG
2	B	642	ASP
2	B	643	ASP
2	B	655	LYS
2	B	746	SER
2	B	751	VAL
2	B	792	MET
2	B	869	SER
2	B	943	SER
2	B	1175	LEU
2	B	1176	ASN
2	B	1214	PRO
3	C	60	ASP
3	C	173	ALA
3	C	240	VAL
4	D	14	ARG
4	D	19	GLU

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Mol	Chain	Res	Type
4	D	119	ARG
4	D	131	GLU
4	D	199	ASN
5	E	36	GLU
5	E	130	ALA
5	E	158	SER
7	G	63	PRO
7	G	154	VAL
8	H	12	VAL
8	H	17	PRO
8	H	21	ASN
8	H	32	THR
8	H	51	ALA
8	H	59	ILE
8	H	84	ALA
8	H	90	ALA
8	H	92	ASP
8	H	95	TYR
8	H	107	VAL
9	I	54	GLU
9	I	57	GLY
9	I	106	CYS
10	J	6	ARG
10	J	17	LYS
10	J	33	GLY
10	J	62	ARG
11	K	53	ASP
11	K	80	GLY
12	L	28	LYS
12	L	40	LEU
12	L	54	ARG
1	A	51	GLY
1	A	61	ILE
1	A	66	LYS
1	A	74	MET
1	A	131	SER
1	A	169	ASN
1	A	219	PHE
1	A	283	GLY
1	A	313	GLN
1	A	322	VAL
1	A	426	LEU

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Mol	Chain	Res	Type
1	A	517	ASN
1	A	755	PHE
1	A	975	HIS
1	A	1122	PRO
1	A	1206	ASP
1	A	1221	LYS
1	A	1308	THR
1	A	1378	GLN
1	A	1390	ASN
2	B	24	PRO
2	B	27	ALA
2	B	206	ASN
2	B	309	GLN
2	B	531	GLN
2	B	561	TRP
2	B	594	ALA
2	B	605	ARG
2	B	641	GLU
2	B	711	GLU
2	B	728	ARG
2	B	734	HIS
2	B	752	ALA
2	B	881	ASN
2	B	892	LYS
2	B	906	SER
2	B	959	ASP
2	B	1003	ALA
2	B	1100	ASP
3	C	132	PRO
3	C	169	LYS
3	C	172	PRO
3	C	208	GLU
4	D	157	GLN
5	E	76	GLY
6	F	128	LYS
7	G	2	PHE
7	G	20	PRO
8	H	44	VAL
8	H	63	LEU
9	I	8	ARG
9	I	9	ASP
10	J	14	VAL

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Mol	Chain	Res	Type
10	J	24	LEU
12	L	27	LEU
12	L	35	SER
1	A	69	THR
1	A	159	THR
1	A	294	SER
1	A	331	GLY
1	A	466	SER
1	A	510	GLN
1	A	526	ASP
1	A	789	LYS
1	A	875	ALA
1	A	1278	ASN
2	B	114	PRO
2	B	257	LYS
2	B	264	SER
2	B	277	LYS
2	B	294	ASP
2	B	509	ALA
2	B	680	THR
2	B	810	GLU
2	B	848	ARG
2	B	937	ALA
2	B	1017	ILE
2	B	1082	MET
3	C	11	ARG
3	C	142	VAL
3	C	213	PRO
3	C	227	THR
3	C	243	VAL
4	D	118	THR
5	E	95	THR
5	E	129	PRO
7	G	27	LYS
7	G	136	VAL
8	H	81	PRO
8	H	139	ASN
9	I	62	ILE
11	K	54	ARG
11	K	79	GLU
12	L	39	SER
1	A	35	ILE

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Mol	Chain	Res	Type
1	A	42	ASP
1	A	244	PRO
1	A	465	TYR
1	A	543	LEU
1	A	619	LYS
1	A	673	GLY
1	A	693	VAL
1	A	704	ALA
1	A	720	ARG
1	A	958	VAL
1	A	995	GLU
1	A	1067	LEU
1	A	1105	LEU
1	A	1158	PRO
1	A	1244	ARG
1	A	1270	ASN
1	A	1365	TYR
1	A	1454	MET
2	B	45	SER
2	B	245	GLU
2	B	291	ILE
2	B	449	ASN
2	B	460	ALA
2	B	738	PHE
2	B	878	GLN
2	B	1075	GLY
2	B	1171	VAL
2	B	1183	LYS
3	C	12	GLU
4	D	30	GLY
4	D	53	SER
5	E	66	GLU
5	E	73	PRO
5	E	92	THR
6	F	150	GLU
8	H	8	ASP
9	I	95	THR
10	J	27	GLU
12	L	45	ALA
12	L	56	LEU
1	A	599	SER
1	A	605	MET

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Mol	Chain	Res	Type
1	A	922	ASP
1	A	1211	GLN
2	B	793	ALA
3	C	78	GLU
5	E	38	PRO
5	E	44	ALA
10	J	13	VAL
1	A	1437	GLY
2	B	818	PRO
2	B	1167	GLY
5	E	183	PRO
8	H	47	PHE
1	A	719	VAL
1	A	1335	ILE
2	B	593	PRO
7	G	126	ASN
1	A	775	ILE
2	B	707	PRO
2	B	764	SER
2	B	867	GLY
7	G	163	ILE
1	A	84	ILE
1	A	568	PRO
1	A	583	PRO
1	A	756	ILE
1	A	973	ILE
2	B	364	ILE
3	C	18	VAL
7	G	128	PRO
1	A	96	ILE
1	A	1006	ILE

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1241/1520 (82%)	1108 (89%)	133 (11%)	6 26
2	B	963/1061 (91%)	834 (87%)	129 (13%)	4 19
3	C	234/299 (78%)	205 (88%)	29 (12%)	4 20
4	D	161/200 (80%)	135 (84%)	26 (16%)	2 13
5	E	196/197 (100%)	182 (93%)	14 (7%)	13 38
6	F	77/137 (56%)	71 (92%)	6 (8%)	11 36
7	G	152/152 (100%)	135 (89%)	17 (11%)	6 24
8	H	120/128 (94%)	105 (88%)	15 (12%)	4 20
9	I	113/116 (97%)	97 (86%)	16 (14%)	3 17
10	J	60/65 (92%)	54 (90%)	6 (10%)	7 28
11	K	99/102 (97%)	91 (92%)	8 (8%)	11 34
12	L	40/57 (70%)	36 (90%)	4 (10%)	7 28
All	All	3456/4034 (86%)	3053 (88%)	403 (12%)	5 23

All (403) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	18	GLN
1	A	32	VAL
1	A	34	LYS
1	A	37	PHE
1	A	41	MET
1	A	46	THR
1	A	54	ASN
1	A	68	GLN
1	A	70	CYS
1	A	93	VAL
1	A	121	LEU
1	A	141	LEU
1	A	145	LYS
1	A	154	SER
1	A	160	GLN
1	A	161	LEU
1	A	162	VAL
1	A	185	TRP

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Mol	Chain	Res	Type
1	A	196	GLU
1	A	203	SER
1	A	208	LEU
1	A	221	SER
1	A	244	PRO
1	A	245	PRO
1	A	250	ILE
1	A	265	LYS
1	A	289	ILE
1	A	290	GLU
1	A	302	THR
1	A	312	PRO
1	A	320	ARG
1	A	321	PRO
1	A	322	VAL
1	A	324	SER
1	A	332	LYS
1	A	337	ARG
1	A	344	ARG
1	A	385	ILE
1	A	396	PRO
1	A	432	VAL
1	A	443	LEU
1	A	445	ASN
1	A	451	HIS
1	A	454	SER
1	A	462	VAL
1	A	475	THR
1	A	479	ASN
1	A	481	ASP
1	A	483	ASP
1	A	493	GLN
1	A	497	THR
1	A	505	CYS
1	A	513	SER
1	A	518	LYS
1	A	539	THR
1	A	545	GLN
1	A	547	LEU
1	A	549	MET
1	A	562	THR
1	A	565	ILE

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Mol	Chain	Res	Type
1	A	571	LEU
1	A	582	ILE
1	A	593	GLU
1	A	618	GLU
1	A	629	LEU
1	A	664	THR
1	A	666	ILE
1	A	670	ILE
1	A	676	MET
1	A	680	THR
1	A	690	VAL
1	A	691	LEU
1	A	701	LEU
1	A	710	LEU
1	A	735	VAL
1	A	738	LYS
1	A	768	GLN
1	A	774	ARG
1	A	810	PRO
1	A	821	ARG
1	A	822	GLU
1	A	827	THR
1	A	838	GLN
1	A	858	ASN
1	A	871	ASP
1	A	920	LEU
1	A	923	LEU
1	A	941	LYS
1	A	961	ARG
1	A	970	THR
1	A	978	PRO
1	A	983	ILE
1	A	992	ASP
1	A	1029	ARG
1	A	1067	LEU
1	A	1096	SER
1	A	1110	ASN
1	A	1116	LEU
1	A	1120	LEU
1	A	1122	PRO
1	A	1124	HIS
1	A	1135	ARG

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Mol	Chain	Res	Type
1	A	1146	VAL
1	A	1169	ILE
1	A	1170	ILE
1	A	1171	GLN
1	A	1193	LEU
1	A	1217	LYS
1	A	1257	ASP
1	A	1265	ASN
1	A	1276	VAL
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1305	VAL
1	A	1308	THR
1	A	1315	GLU
1	A	1325	THR
1	A	1333	ILE
1	A	1349	TYR
1	A	1353	TYR
1	A	1368	MET
1	A	1370	LEU
1	A	1371	LEU
1	A	1393	ASN
1	A	1394	THR
1	A	1400	CYS
1	A	1405	THR
1	A	1420	ASP
1	A	1424	VAL
1	A	1436	ILE
1	A	1445	ILE
2	B	21	GLU
2	B	25	ILE
2	B	46	GLN
2	B	57	TYR
2	B	63	ILE
2	B	91	SER
2	B	98	THR
2	B	100	PRO
2	B	128	LEU
2	B	167	ILE
2	B	169	ARG
2	B	194	GLU

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Mol	Chain	Res	Type
2	B	217	ARG
2	B	222	ILE
2	B	225	VAL
2	B	240	ILE
2	B	249	ARG
2	B	261	ARG
2	B	262	GLU
2	B	272	THR
2	B	297	ILE
2	B	298	LEU
2	B	303	TYR
2	B	323	VAL
2	B	325	GLN
2	B	348	ARG
2	B	360	PHE
2	B	361	LEU
2	B	364	ILE
2	B	371	GLU
2	B	376	PHE
2	B	378	LEU
2	B	393	LYS
2	B	394	ASP
2	B	416	LEU
2	B	419	THR
2	B	425	THR
2	B	427	ASP
2	B	429	PHE
2	B	455	SER
2	B	465	ASN
2	B	466	TRP
2	B	473	MET
2	B	476	ARG
2	B	485	ARG
2	B	487	THR
2	B	493	SER
2	B	502	ILE
2	B	513	GLN
2	B	516	ASN
2	B	529	GLU
2	B	555	ILE
2	B	557	PHE
2	B	558	LEU

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Mol	Chain	Res	Type
2	B	570	VAL
2	B	576	ASP
2	B	580	VAL
2	B	582	VAL
2	B	585	VAL
2	B	597	MET
2	B	598	GLU
2	B	603	LEU
2	B	615	MET
2	B	616	ILE
2	B	626	ILE
2	B	635	ARG
2	B	636	PRO
2	B	678	GLU
2	B	682	SER
2	B	691	GLU
2	B	693	ILE
2	B	730	ARG
2	B	737	THR
2	B	742	GLU
2	B	748	ILE
2	B	776	GLN
2	B	786	ASN
2	B	790	ASP
2	B	794	ASN
2	B	805	THR
2	B	830	TYR
2	B	835	GLN
2	B	839	MET
2	B	859	TYR
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	883	LEU
2	B	884	ARG
2	B	889	THR
2	B	909	ASP
2	B	918	ILE
2	B	939	THR
2	B	944	THR
2	B	953	LEU
2	B	956	THR

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Mol	Chain	Res	Type
2	B	959	ASP
2	B	966	VAL
2	B	987	LYS
2	B	997	GLU
2	B	999	MET
2	B	1006	ILE
2	B	1010	LEU
2	B	1031	LEU
2	B	1046	PRO
2	B	1047	PHE
2	B	1049	ASP
2	B	1060	ARG
2	B	1077	THR
2	B	1081	LEU
2	B	1084	GLN
2	B	1087	PHE
2	B	1095	LEU
2	B	1098	MET
2	B	1108	ARG
2	B	1122	ARG
2	B	1124	ARG
2	B	1147	LEU
2	B	1149	GLU
2	B	1150	ARG
2	B	1159	ARG
2	B	1160	VAL
2	B	1175	LEU
2	B	1183	LYS
2	B	1185	CYS
2	B	1202	LEU
2	B	1212	ILE
2	B	1218	THR
2	B	1220	ARG
3	C	7	GLN
3	C	11	ARG
3	C	23	SER
3	C	25	VAL
3	C	26	ASP
3	C	53	THR
3	C	55	THR
3	C	57	VAL
3	C	77	ILE

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Mol	Chain	Res	Type
3	C	78	GLU
3	C	99	LEU
3	C	108	GLU
3	C	111	THR
3	C	115	SER
3	C	124	LEU
3	C	133	ILE
3	C	138	GLU
3	C	145	CYS
3	C	147	LEU
3	C	155	LEU
3	C	156	THR
3	C	166	GLU
3	C	177	GLU
3	C	193	TYR
3	C	209	TYR
3	C	238	ILE
3	C	245	VAL
3	C	262	LEU
3	C	266	ASP
4	D	11	ARG
4	D	14	ARG
4	D	15	LEU
4	D	16	LYS
4	D	17	LYS
4	D	20	GLU
4	D	22	GLU
4	D	23	ASN
4	D	29	LEU
4	D	38	ILE
4	D	41	GLN
4	D	47	LEU
4	D	63	LEU
4	D	70	PHE
4	D	118	THR
4	D	120	GLU
4	D	124	GLU
4	D	138	ASN
4	D	149	THR
4	D	187	THR
4	D	206	GLU
4	D	207	LEU

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Mol	Chain	Res	Type
4	D	213	GLU
4	D	214	LEU
4	D	219	THR
4	D	221	TYR
5	E	31	THR
5	E	37	LEU
5	E	65	THR
5	E	69	ILE
5	E	72	PHE
5	E	78	LEU
5	E	82	PHE
5	E	112	TYR
5	E	123	LEU
5	E	131	THR
5	E	132	ILE
5	E	134	THR
5	E	140	LEU
5	E	150	VAL
6	F	79	ARG
6	F	93	ILE
6	F	103	MET
6	F	112	GLU
6	F	119	ARG
6	F	123	LYS
7	G	1	MET
7	G	12	THR
7	G	13	LEU
7	G	21	ARG
7	G	31	LEU
7	G	51	TYR
7	G	58	ARG
7	G	62	LEU
7	G	74	TYR
7	G	114	LEU
7	G	120	THR
7	G	128	PRO
7	G	133	SER
7	G	134	GLU
7	G	139	ILE
7	G	151	ILE
7	G	165	GLU
8	H	10	PHE

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Mol	Chain	Res	Type
8	H	14	GLU
8	H	15	VAL
8	H	17	PRO
8	H	65	LEU
8	H	88	SER
8	H	89	LEU
8	H	91	ASP
8	H	94	ASP
8	H	102	TYR
8	H	107	VAL
8	H	129	TYR
8	H	130	ARG
8	H	138	GLU
8	H	143	LEU
9	I	2	THR
9	I	4	PHE
9	I	6	PHE
9	I	8	ARG
9	I	12	ASN
9	I	31	THR
9	I	44	TYR
9	I	52	ILE
9	I	59	VAL
9	I	72	ASP
9	I	85	PHE
9	I	86	PHE
9	I	93	LYS
9	I	94	ASP
9	I	100	PHE
9	I	101	PHE
10	J	2	ILE
10	J	13	VAL
10	J	22	LEU
10	J	24	LEU
10	J	43	ARG
10	J	44	TYR
11	K	21	ILE
11	K	25	THR
11	K	34	THR
11	K	47	ARG
11	K	50	LEU
11	K	103	THR

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Mol	Chain	Res	Type
11	K	107	THR
11	K	111	LEU
12	L	26	THR
12	L	27	LEU
12	L	55	ILE
12	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	71	GLN
1	A	75	ASN
1	A	169	ASN
1	A	225	ASN
1	A	253	ASN
1	A	256	GLN
1	A	282	ASN
1	A	299	HIS
1	A	316	GLN
1	A	339	ASN
1	A	358	ASN
1	A	390	GLN
1	A	394	ASN
1	A	435	HIS
1	A	447	GLN
1	A	451	HIS
1	A	479	ASN
1	A	490	HIS
1	A	493	GLN
1	A	503	GLN
1	A	515	GLN
1	A	517	ASN
1	A	611	GLN
1	A	640	GLN
1	A	650	GLN
1	A	654	ASN
1	A	723	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	767	GLN

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Mol	Chain	Res	Type
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	972	HIS
1	A	1048	ASN
1	A	1078	GLN
1	A	1110	ASN
1	A	1140	HIS
1	A	1203	ASN
1	A	1211	GLN
1	A	1218	GLN
1	A	1258	HIS
1	A	1265	ASN
1	A	1312	ASN
1	A	1390	ASN
1	A	1393	ASN
1	A	1432	GLN
2	B	47	GLN
2	B	103	ASN
2	B	115	GLN
2	B	121	ASN
2	B	178	ASN
2	B	236	HIS
2	B	255	GLN
2	B	366	GLN
2	B	383	ASN
2	B	465	ASN
2	B	469	GLN
2	B	499	ASN
2	B	515	HIS
2	B	518	HIS
2	B	657	HIS
2	B	667	GLN
2	B	686	ASN
2	B	762	ASN
2	B	794	ASN
2	B	842	ASN
2	B	862	GLN
2	B	887	HIS
2	B	957	ASN

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Mol	Chain	Res	Type
2	B	975	GLN
2	B	984	HIS
2	B	1065	GLN
2	B	1161	HIS
2	B	1178	ASN
2	B	1179	GLN
2	B	1193	GLN
3	C	65	HIS
3	C	73	GLN
3	C	79	GLN
3	C	91	HIS
3	C	102	GLN
3	C	112	ASN
3	C	123	ASN
3	C	135	GLN
3	C	140	ASN
3	C	231	ASN
4	D	23	ASN
4	D	28	GLN
4	D	39	ASN
4	D	40	HIS
4	D	41	GLN
4	D	74	GLN
4	D	138	ASN
4	D	199	ASN
5	E	54	GLN
5	E	61	GLN
5	E	101	GLN
5	E	104	ASN
5	E	115	ASN
5	E	147	HIS
6	F	104	ASN
7	G	10	ASN
7	G	14	HIS
7	G	53	ASN
7	G	102	GLN
7	G	113	HIS
7	G	122	ASN
7	G	126	ASN
7	G	131	GLN
8	H	52	GLN
8	H	128	ASN

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Mol	Chain	Res	Type
8	H	131	ASN
8	H	133	ASN
9	I	12	ASN
9	I	46	HIS
9	I	90	GLN
9	I	108	HIS
10	J	53	HIS
11	K	29	ASN
11	K	44	ASN
11	K	65	HIS
11	K	76	GLN
11	K	89	ASN

5.3.3 RNA ⓘ

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

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	3	A
15	P	11	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	2	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BRU	T	23	14,15	18,21,22	3.91	1 (5%)	25,30,33	0.87	1 (4%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	23	BRU	BR-C5	-16.56	1.50	1.88

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	23	BRU	C6-C5-C4	-2.60	118.04	120.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	23	BRU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	1418/1733 (81%)	0.05	34 (2%) 59 35	23, 70, 112, 141	0
2	B	1109/1224 (90%)	0.31	51 (4%) 37 23	23, 81, 123, 141	0
3	C	266/347 (76%)	-0.03	0 100 100	34, 69, 105, 119	0
4	D	179/221 (80%)	0.40	12 (6%) 24 16	37, 79, 118, 131	0
5	E	214/215 (99%)	0.42	6 (2%) 55 32	41, 97, 128, 137	0
6	F	87/155 (56%)	-0.37	1 (1%) 78 52	19, 46, 77, 86	0
7	G	171/171 (100%)	0.04	0 100 100	48, 64, 104, 113	0
8	H	136/146 (93%)	0.86	14 (10%) 12 11	80, 106, 127, 135	0
9	I	119/122 (97%)	0.62	3 (2%) 58 35	65, 100, 125, 143	0
10	J	65/70 (92%)	-0.06	0 100 100	49, 65, 92, 105	0
11	K	115/120 (95%)	-0.23	1 (0%) 81 57	34, 73, 93, 122	0
12	L	46/70 (65%)	0.92	4 (8%) 16 12	48, 108, 125, 132	0
13	N	7/12 (58%)	2.04	3 (42%) 0 1	135, 140, 151, 157	0
14	T	18/26 (69%)	1.99	8 (44%) 0 1	117, 144, 155, 155	0
15	P	11/18 (61%)	1.90	5 (45%) 0 1	125, 133, 152, 156	0
All	All	3961/4650 (85%)	0.21	142 (3%) 46 27	19, 76, 121, 157	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1081	LEU	4.9
2	B	883	LEU	4.7
15	P	1	C	4.6
15	P	11	G	4.5
1	A	1254	ALA	4.4
14	T	28	DA	4.2
4	D	24	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	715	ALA	4.1
11	K	115	ALA	4.1
1	A	3	GLY	4.1
2	B	710	LEU	4.1
2	B	446	LEU	4.0
2	B	70	ILE	3.9
1	A	69	THR	3.9
1	A	2	VAL	3.9
1	A	255	SER	3.8
1	A	483	ASP	3.7
8	H	83	GLN	3.6
2	B	733	HIS	3.5
8	H	65	LEU	3.5
2	B	709	ASP	3.4
8	H	84	ALA	3.4
2	B	250	PHE	3.4
4	D	18	VAL	3.4
2	B	882	THR	3.4
2	B	734	HIS	3.4
14	T	10	DA	3.3
2	B	934	LYS	3.2
2	B	265	SER	3.2
8	H	139	ASN	3.2
1	A	251	SER	3.2
2	B	249	ARG	3.2
2	B	24	PRO	3.2
1	A	253	ASN	3.1
2	B	509	ALA	3.1
1	A	1455	PRO	3.1
12	L	43	THR	3.1
12	L	27	LEU	3.0
1	A	256	GLN	3.0
1	A	51	GLY	3.0
1	A	65	LEU	3.0
13	N	1	DA	3.0
4	D	3	VAL	2.9
2	B	108	VAL	2.8
13	N	7	DT	2.8
9	I	120	GLN	2.8
2	B	866	TYR	2.8
1	A	153	PRO	2.8
2	B	731	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
4	D	19	GLU	2.8
8	H	86	ASP	2.7
6	F	69	LEU	2.7
1	A	187	LYS	2.7
8	H	82	PRO	2.7
1	A	44	THR	2.7
8	H	85	GLY	2.6
2	B	712	PRO	2.6
1	A	159	THR	2.6
2	B	263	GLY	2.6
1	A	66	LYS	2.6
14	T	24	DG	2.6
2	B	473	MET	2.6
1	A	1204	ASP	2.6
2	B	251	ILE	2.5
2	B	246	LYS	2.5
15	P	9	C	2.5
2	B	1224	PHE	2.5
2	B	508	LEU	2.5
14	T	18	DC	2.5
2	B	335	GLY	2.5
2	B	723	VAL	2.5
12	L	26	THR	2.5
2	B	164	LYS	2.5
1	A	1188	GLN	2.5
2	B	115	GLN	2.5
2	B	66	ASP	2.5
2	B	468	GLU	2.4
4	D	137	ASN	2.4
1	A	1245	PRO	2.4
4	D	136	GLY	2.4
9	I	117	LYS	2.4
13	N	5	DC	2.4
2	B	266	ALA	2.4
1	A	1080	THR	2.4
2	B	643	ASP	2.4
2	B	648	HIS	2.4
2	B	933	SER	2.4
2	B	577	ALA	2.4
1	A	587	HIS	2.3
2	B	918	ILE	2.3
8	H	132	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
14	T	25	DG	2.3
5	E	41	ASP	2.3
2	B	262	GLU	2.3
5	E	90	VAL	2.3
8	H	90	ALA	2.3
1	A	286	HIS	2.3
1	A	154	SER	2.3
5	E	126	SER	2.3
2	B	885	MET	2.3
1	A	1173	HIS	2.3
4	D	12	ARG	2.3
5	E	93	MET	2.3
8	H	87	ARG	2.3
15	P	10	U	2.3
2	B	431	TYR	2.3
2	B	241	ARG	2.3
2	B	598	GLU	2.2
1	A	1321	GLY	2.2
2	B	917	PRO	2.2
4	D	11	ARG	2.2
1	A	1144	LYS	2.2
1	A	257	ARG	2.2
2	B	467	GLY	2.2
5	E	4	GLU	2.2
2	B	958	GLN	2.2
2	B	532	ALA	2.2
2	B	133	LYS	2.1
14	T	22	DC	2.1
2	B	880	THR	2.1
8	H	1	MET	2.1
1	A	63	ARG	2.1
9	I	58	VAL	2.1
15	P	2	A	2.1
1	A	265	LYS	2.1
5	E	77	SER	2.1
14	T	27	DC	2.1
4	D	20	GLU	2.1
8	H	35	GLN	2.1
4	D	13	ARG	2.0
2	B	502	ILE	2.0
14	T	11	DA	2.0
1	A	292	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
4	D	25	ALA	2.0
2	B	878	GLN	2.0
12	L	52	GLY	2.0
8	H	129	TYR	2.0
1	A	1217	LYS	2.0
2	B	370	PHE	2.0
8	H	135	LEU	2.0
1	A	1158	PRO	2.0
4	D	4	SER	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å ²)	Q<0.9
14	BRU	T	23	20/21	0.64	0.24	136,142,145,146	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å ²)	Q<0.9
17	MG	P	2458	1/1	0.85	0.18	180,180,180,180	0
16	ZN	I	1122	1/1	0.95	0.07	135,135,135,135	0
16	ZN	A	2456	1/1	0.99	0.03	88,88,88,88	0
16	ZN	L	1071	1/1	0.99	0.02	100,100,100,100	0
16	ZN	I	1121	1/1	0.99	0.02	76,76,76,76	0
16	ZN	B	2225	1/1	1.00	0.01	30,30,30,30	0
16	ZN	J	1066	1/1	1.00	0.02	53,53,53,53	0
16	ZN	C	1269	1/1	1.00	0.02	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	ZN	A	2457	1/1	1.00	0.02	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.