



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:22 AM UTC

PDB ID : 3I4N / pdb_00003i4n
Title : 8-oxoguanine containing RNA polymerase II elongation complex E
Authors : Damsma, G.E.; Cramer, P.
Deposited on : 2009-07-02
Resolution : 3.90 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

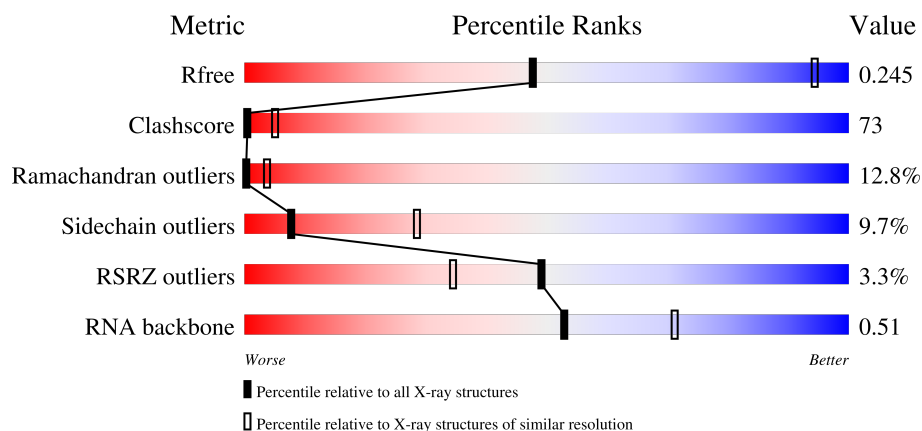
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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.



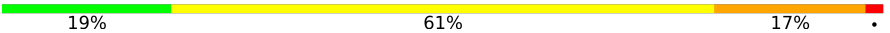
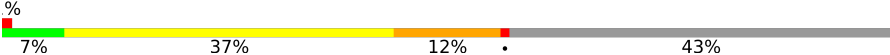
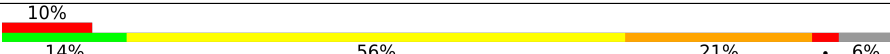
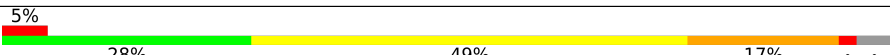
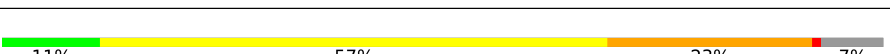
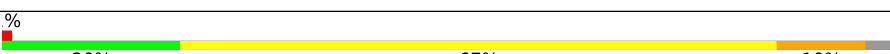
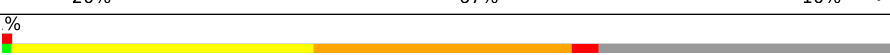
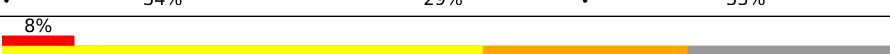
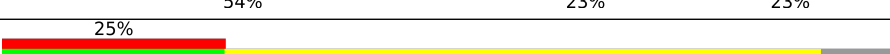
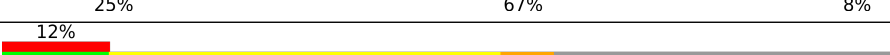
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)
RNA backbone	3983	1014 (4.70-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	1733	14% 51% 16% • 18%
2	B	1224	5% 19% 55% 16% • 8%
3	C	324	17% 50% 15% • 17%
4	D	221	5% 18% 48% 14% • 18%

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

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32307 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	1429	Total	C	N	O	S	0	0	0
			11240	7079	1966	2133	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1125	Total	C	N	O	S	0	0	0
			8942	5659	1571	1657	55			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	270	Total	C	N	O	S	0	0	0
			2125	1336	353	422	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	expression tag	UNP P16370
C	-4	HIS	-	expression tag	UNP P16370
C	-3	HIS	-	expression tag	UNP P16370
C	-2	HIS	-	expression tag	UNP P16370
C	-1	HIS	-	expression tag	UNP P16370
C	0	HIS	-	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	182	Total	C	N	O	S	0	0	0
			1465	904	262	296	3			

- 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	88	Total	C	N	O	S	0	0	0
			712	455	120	134	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	137	Total	C	N	O	S	0	0	0
			1101	693	185	218	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	117	Total	C	N	O	S	0	0	0
			952	586	173	182	11			

- 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	116	Total	C	N	O	S	0	0	0
			929	596	158	173	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	47	Total	C	N	O	S	0	0	0
			370	228	73	65	4			

- Molecule 13 is a DNA chain called DNA (5'-D(*AP*G*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP*(8OG)P*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	T	20	Total	Br	C	N	O	P	0	0	0
			407	1	194	72	121	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	11	Total	C	N	O	P	0	0	0
			224	108	42	64	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	10	Total	C	N	O	P	0	0	0
			207	94	35	69	9			

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	2	Total	Zn	0	0
			2	2		
17	B	1	Total	Zn	0	0
			1	1		
17	C	1	Total	Zn	0	0
			1	1		
17	I	2	Total	Zn	0	0
			2	2		

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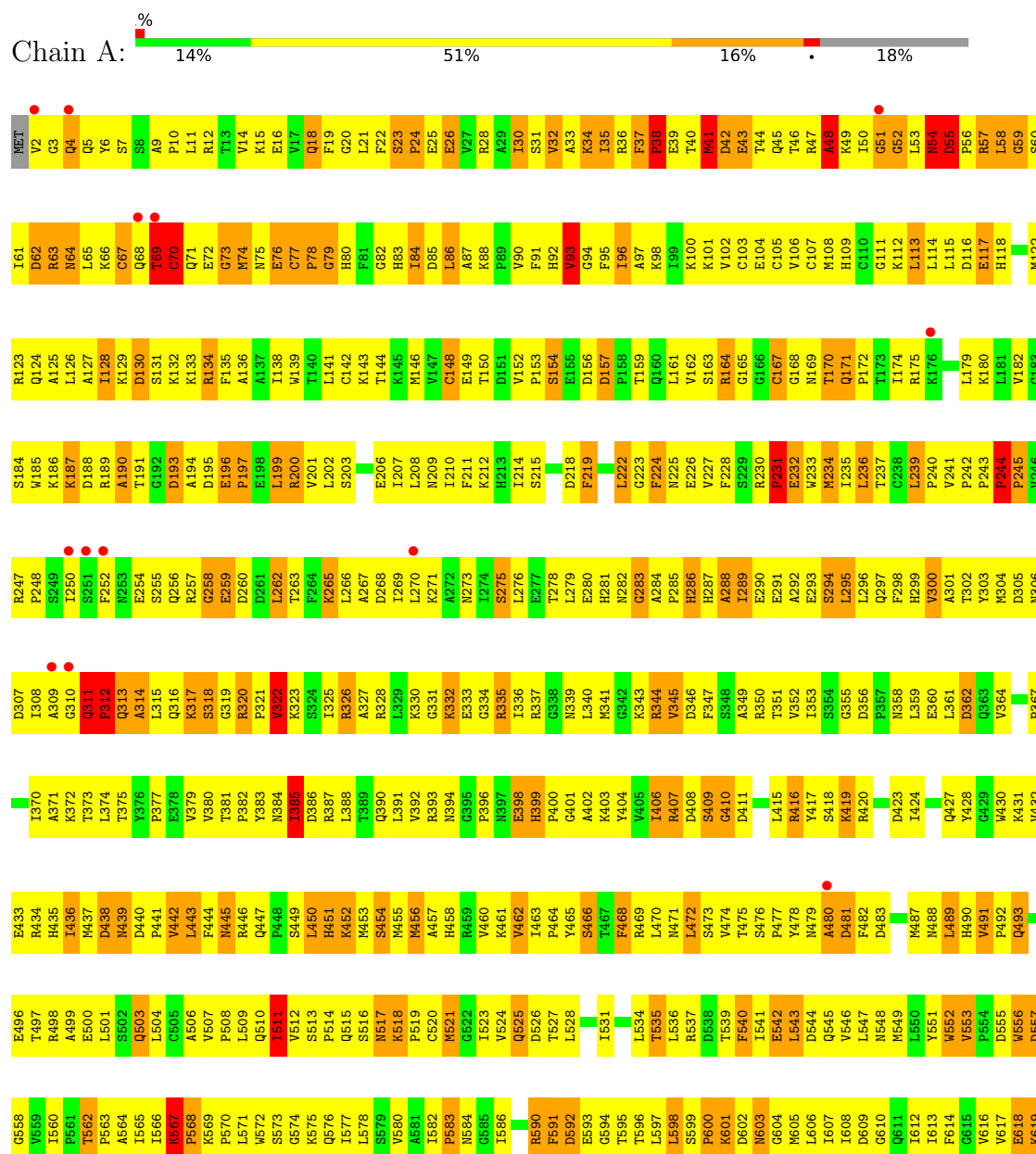
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	J	1	Total 1	Zn 1	0	0
17	L	1	Total 1	Zn 1	0	0

3 Residue-property plots

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

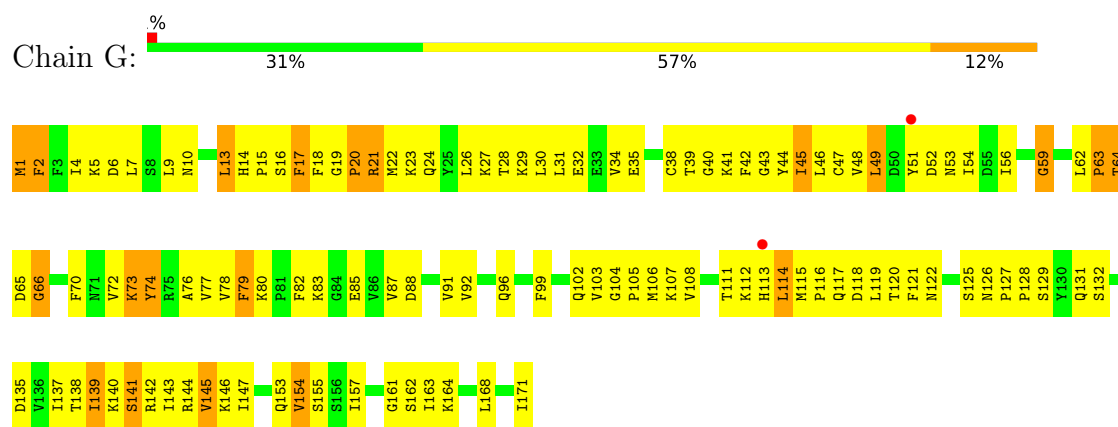
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



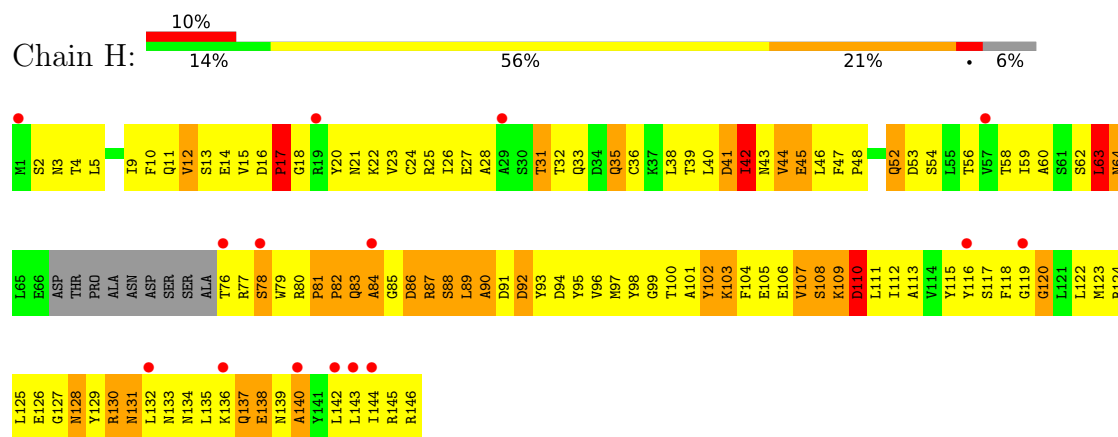




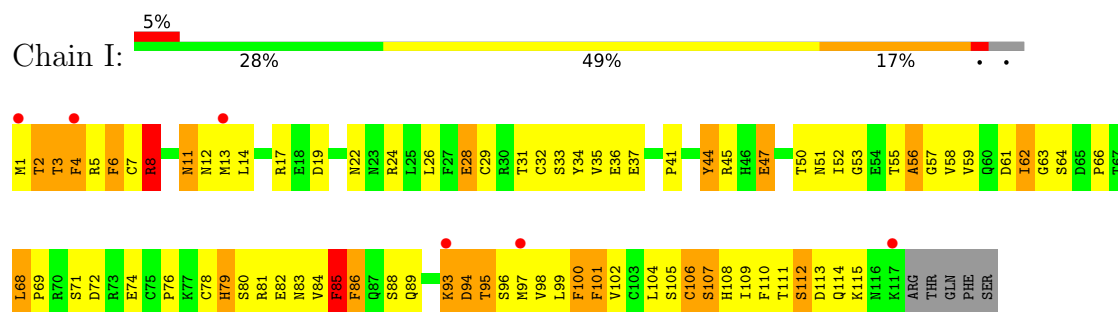




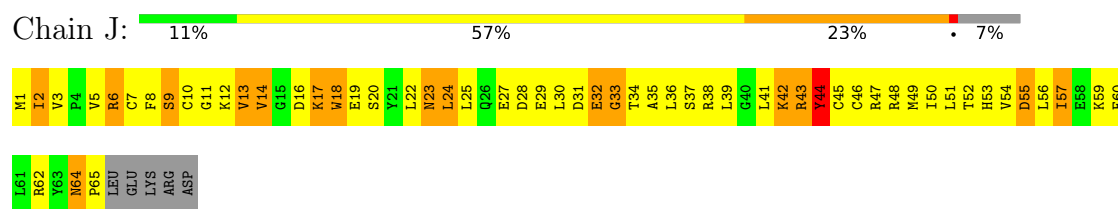
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



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

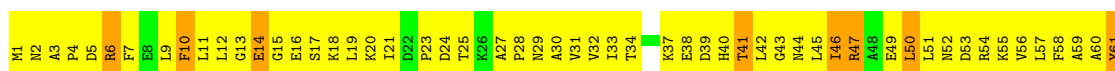


• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

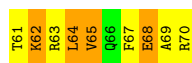
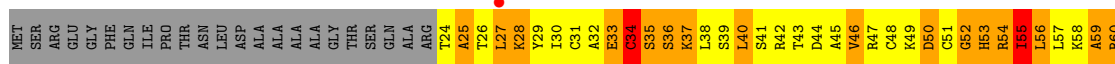


• Molecule 11: DNA-directed RNA polymerase II subunit RPB11





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



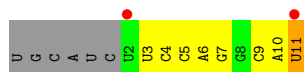
- Molecule 13: DNA (5'-D(*AP*G*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP*(8OG)P*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3')



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	221.17Å 394.15Å 282.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.90 50.00 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-3.90) 99.9 (50.00-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 3.88Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.228 , 0.266 0.208 , 0.245	Depositor DCC
R_{free} test set	4364 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	128.1	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 99.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.019 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32307	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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: BRU, ZN, 8OG, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.53	0/11441	1.10	92/15473 (0.6%)
2	B	0.49	0/9116	1.02	53/12291 (0.4%)
3	C	0.52	0/2163	1.11	17/2930 (0.6%)
4	D	0.46	0/1475	1.01	6/1976 (0.3%)
5	E	0.46	0/1788	1.04	12/2406 (0.5%)
6	F	0.60	0/724	1.28	9/977 (0.9%)
7	G	0.50	0/1368	0.99	5/1844 (0.3%)
8	H	0.45	0/1119	1.06	10/1514 (0.7%)
9	I	0.42	0/970	0.97	6/1305 (0.5%)
10	J	0.50	0/541	0.93	1/727 (0.1%)
11	K	0.50	0/947	1.04	5/1279 (0.4%)
12	L	0.54	0/372	1.06	3/495 (0.6%)
13	T	0.39	0/405	0.91	4/618 (0.6%)
14	N	0.43	0/251	0.84	0/386
15	P	0.41	0/230	0.78	0/356
All	All	0.50	0/32910	1.06	223/44577 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1185	CYS	N-CA-C	-11.56	98.89	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	SER	N-CA-C	-11.08	98.72	114.12
3	C	148	ARG	N-CA-C	10.98	117.78	108.78
1	A	950	GLY	N-CA-C	-10.28	102.58	113.58
1	A	3	GLY	N-CA-C	-10.15	100.82	115.64
1	A	288	ALA	N-CA-C	-9.95	101.48	114.31
5	E	5	ASN	N-CA-C	-9.91	98.74	113.61
1	A	452	LYS	N-CA-C	-9.82	99.61	111.69
8	H	130	ARG	N-CA-C	-9.56	101.76	112.57
3	C	40	GLU	N-CA-C	9.42	122.96	112.97
1	A	219	PHE	N-CA-C	-9.29	99.69	111.02
1	A	710	LEU	N-CA-C	-9.16	101.19	111.82
6	F	70	LYS	N-CA-C	-9.15	102.11	113.18
2	B	628	THR	N-CA-C	-9.02	102.28	113.28
2	B	555	ILE	N-CA-C	-8.96	102.00	110.42
6	F	82	THR	CA-C-N	8.81	128.46	119.56
6	F	82	THR	C-N-CA	8.81	128.46	119.56
3	C	194	GLU	N-CA-C	-8.39	103.63	114.04
2	B	1052	VAL	N-CA-C	-8.33	102.42	110.42
1	A	639	PRO	N-CA-C	-7.99	103.10	113.57
2	B	1009	ASP	N-CA-C	-7.98	103.68	113.50
2	B	296	GLU	N-CA-C	-7.78	103.92	113.41
3	C	172	PRO	N-CA-C	-7.76	104.16	113.86
4	D	188	ALA	N-CA-C	-7.73	103.74	113.01
2	B	681	TRP	N-CA-C	-7.70	102.22	111.69
1	A	344	ARG	N-CA-C	-7.61	98.22	110.32
6	F	103	MET	N-CA-C	-7.59	104.01	113.20
2	B	1201	LYS	N-CA-C	-7.56	101.79	111.02
2	B	807	ARG	N-CA-C	-7.32	103.33	111.82
1	A	1311	VAL	N-CA-C	7.32	118.68	107.78
2	B	714	GLU	N-CA-C	7.30	117.61	108.19
1	A	964	ILE	N-CA-C	-7.29	105.54	111.81
1	A	682	THR	N-CA-C	-7.25	104.40	113.18
1	A	567	LYS	CA-C-N	-7.24	110.79	119.84
1	A	567	LYS	C-N-CA	-7.24	110.79	119.84
2	B	882	THR	N-CA-C	7.20	126.14	110.80
1	A	1422	ARG	N-CA-C	-7.19	104.54	113.38
1	A	689	LYS	N-CA-C	-7.19	104.48	113.18
6	F	130	ILE	N-CA-C	-7.11	100.14	107.89
5	E	132	ILE	N-CA-C	7.09	118.04	108.11
1	A	562	THR	CA-C-N	7.09	127.13	119.90
1	A	562	THR	C-N-CA	7.09	127.13	119.90
2	B	1078	GLY	N-CA-C	-7.05	105.75	114.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	PHE	N-CA-C	7.04	119.21	109.29
8	H	138	GLU	N-CA-C	-6.99	103.27	111.03
10	J	44	TYR	N-CA-C	6.96	120.66	111.75
2	B	66	ASP	N-CA-C	-6.95	102.85	112.30
3	C	62	PHE	N-CA-C	-6.93	103.34	111.03
1	A	244	PRO	N-CA-C	6.92	119.15	110.70
1	A	987	VAL	N-CA-C	6.89	117.59	110.36
7	G	66	GLY	N-CA-C	6.88	122.48	114.16
3	C	96	SER	N-CA-C	6.83	119.55	109.24
1	A	663	SER	N-CA-C	6.78	116.81	107.73
1	A	472	LEU	N-CA-C	6.77	119.66	111.40
1	A	32	VAL	N-CA-C	-6.69	106.97	113.53
1	A	199	LEU	N-CA-C	6.67	119.90	109.96
1	A	543	LEU	N-CA-C	6.67	119.12	111.11
1	A	946	VAL	N-CA-C	-6.67	106.08	111.81
5	E	150	VAL	CA-C-N	6.65	126.83	120.31
5	E	150	VAL	C-N-CA	6.65	126.83	120.31
1	A	778	GLY	N-CA-C	-6.64	107.07	115.31
1	A	553	VAL	CA-C-N	6.64	128.14	119.84
1	A	553	VAL	C-N-CA	6.64	128.14	119.84
1	A	566	ILE	N-CA-C	-6.62	105.08	113.22
13	T	24	DG	C2'-C3'-O3'	-6.60	101.60	111.50
1	A	1421	CYS	N-CA-C	-6.58	103.10	111.92
3	C	225	ALA	N-CA-C	6.58	119.44	108.13
4	D	75	LYS	N-CA-C	-6.58	105.82	114.31
1	A	1155	ASP	CA-C-N	6.58	126.71	119.87
1	A	1155	ASP	C-N-CA	6.58	126.71	119.87
1	A	1256	GLU	N-CA-C	6.49	119.32	111.40
1	A	1261	LYS	N-CA-C	-6.49	107.22	114.62
8	H	45	GLU	N-CA-C	-6.48	105.68	113.97
5	E	103	LYS	N-CA-C	-6.44	105.28	113.01
1	A	1345	ARG	N-CA-C	-6.44	103.38	111.11
2	B	498	THR	N-CA-C	6.42	118.90	107.80
11	K	46	ILE	N-CA-C	-6.39	103.62	112.50
12	L	62	LYS	N-CA-C	-6.37	104.38	111.71
6	F	77	ASP	N-CA-C	-6.36	100.21	110.32
1	A	23	SER	N-CA-C	-6.34	100.42	109.62
4	D	171	GLY	N-CA-C	-6.33	107.04	115.40
2	B	366	GLN	N-CA-C	-6.33	104.72	112.88
2	B	211	VAL	N-CA-C	6.29	115.40	106.53
12	L	34	CYS	N-CA-C	-6.28	105.89	112.93
2	B	1177	HIS	N-CA-C	-6.28	105.26	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	180	ARG	N-CA-C	-6.26	105.46	113.23
1	A	511	ILE	N-CA-C	6.24	117.73	110.62
5	E	149	LEU	N-CA-C	6.23	117.94	111.03
5	E	25	ASP	N-CA-C	-6.23	103.64	111.11
1	A	171	GLN	CA-C-N	6.22	126.43	119.90
1	A	171	GLN	C-N-CA	6.22	126.43	119.90
2	B	1025	HIS	N-CA-C	-6.21	103.23	111.24
2	B	680	THR	N-CA-C	6.12	117.94	110.41
1	A	311	GLN	N-CA-C	6.11	123.31	109.81
1	A	491	VAL	N-CA-C	6.11	114.69	107.73
7	G	129	SER	N-CA-C	6.08	117.42	108.86
1	A	79	GLY	N-CA-C	6.07	118.91	111.93
3	C	38	ILE	CB-CA-C	-6.07	104.20	111.97
8	H	62	SER	N-CA-C	6.06	117.36	108.14
3	C	81	GLU	N-CA-C	6.03	118.07	110.24
1	A	143	LYS	N-CA-C	-6.02	105.98	113.15
2	B	208	SER	N-CA-C	6.02	118.78	110.35
2	B	363	HIS	N-CA-C	-6.01	102.05	110.35
2	B	307	ASP	N-CA-C	-6.00	101.41	110.70
2	B	288	ALA	N-CA-C	-5.98	104.76	111.28
9	I	85	PHE	N-CA-C	5.97	118.23	110.53
3	C	39	ALA	N-CA-C	5.94	123.45	110.80
1	A	117	GLU	N-CA-C	-5.94	104.62	112.34
1	A	1039	LYS	N-CA-C	-5.93	104.16	111.40
1	A	993	LEU	N-CA-C	-5.93	104.16	111.33
6	F	154	ASP	N-CA-C	-5.92	105.64	112.92
11	K	65	HIS	CA-C-N	5.92	127.23	119.84
11	K	65	HIS	C-N-CA	5.92	127.23	119.84
1	A	1262	LYS	N-CA-C	-5.91	104.42	111.69
1	A	480	ALA	N-CA-C	5.91	118.87	109.24
11	K	77	THR	N-CA-C	5.90	117.94	109.14
1	A	242	PRO	CA-C-N	5.85	126.40	120.38
1	A	242	PRO	C-N-CA	5.85	126.40	120.38
3	C	131	HIS	CA-C-N	5.84	127.14	119.84
3	C	131	HIS	C-N-CA	5.84	127.14	119.84
12	L	52	GLY	N-CA-C	-5.76	105.61	113.27
2	B	213	ILE	N-CA-C	5.72	116.72	108.48
13	T	25	DG	C2'-C3'-O3'	-5.71	102.93	111.50
1	A	398	GLU	N-CA-C	-5.70	100.70	109.76
7	G	59	GLY	N-CA-C	-5.69	104.97	112.82
2	B	292	ILE	N-CA-C	5.67	121.12	108.88
1	A	55	ASP	CA-C-N	-5.67	112.76	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	ASP	C-N-CA	-5.67	112.76	119.84
2	B	834	ASN	N-CA-C	-5.63	106.25	113.01
2	B	734	HIS	N-CA-C	5.63	117.86	109.25
2	B	902	GLY	N-CA-C	5.59	120.56	113.24
1	A	1343	ALA	N-CA-C	-5.59	105.96	112.89
2	B	473	MET	N-CA-C	-5.58	103.91	111.55
2	B	763	GLN	N-CA-C	-5.57	102.65	110.50
3	C	23	SER	N-CA-C	5.56	117.63	109.24
9	I	28	GLU	N-CA-C	5.56	115.88	108.38
8	H	103	LYS	N-CA-C	5.55	119.10	110.17
1	A	927	VAL	N-CA-C	-5.54	105.45	110.82
5	E	105	PHE	CB-CA-C	-5.54	108.39	116.53
7	G	45	ILE	N-CA-C	-5.54	101.58	108.89
2	B	535	LEU	N-CA-C	-5.53	106.37	113.23
9	I	68	LEU	CA-C-N	5.53	125.50	120.03
9	I	68	LEU	C-N-CA	5.53	125.50	120.03
2	B	774	GLY	N-CA-C	-5.52	106.92	113.99
2	B	833	TYR	N-CA-C	-5.51	106.92	113.97
11	K	39	ASP	N-CA-C	5.51	114.83	108.49
6	F	127	GLU	N-CA-C	-5.49	106.17	112.92
5	E	84	ASP	N-CA-C	-5.48	106.91	113.21
1	A	890	ASP	N-CA-C	-5.47	105.70	112.38
4	D	38	ILE	N-CA-C	5.47	115.52	107.15
2	B	873	THR	N-CA-C	5.44	117.53	108.99
1	A	468	PHE	N-CA-C	-5.42	99.69	108.41
5	E	147	HIS	N-CA-C	5.42	118.09	109.96
2	B	876	LYS	CA-C-N	5.42	125.41	120.21
2	B	876	LYS	C-N-CA	5.42	125.41	120.21
2	B	91	SER	N-CA-C	5.41	117.74	109.95
2	B	1144	ALA	N-CA-C	5.37	116.82	111.07
1	A	62	ASP	N-CA-C	5.36	118.52	111.28
3	C	226	ASP	N-CA-C	-5.33	101.61	109.18
1	A	598	LEU	N-CA-C	-5.33	104.21	111.56
2	B	560	GLU	N-CA-C	-5.31	105.07	112.03
2	B	297	ILE	N-CA-C	-5.31	104.45	111.09
2	B	1044	ALA	N-CA-C	-5.31	107.46	114.31
1	A	852	TYR	N-CA-C	5.30	122.09	110.80
2	B	831	SER	N-CA-C	-5.29	105.59	111.36
2	B	195	CYS	CA-C-N	5.28	124.47	118.97
2	B	195	CYS	C-N-CA	5.28	124.47	118.97
3	C	27	LEU	N-CA-C	-5.28	105.52	111.28
2	B	839	MET	N-CA-C	5.26	116.28	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1096	SER	N-CA-C	5.26	117.18	109.24
3	C	148	ARG	CB-CA-C	-5.25	109.50	117.07
1	A	998	LEU	N-CA-C	5.22	117.80	109.96
8	H	35	GLN	N-CA-C	-5.22	106.86	114.12
4	D	70	PHE	N-CA-C	-5.22	106.59	113.17
1	A	756	ILE	N-CA-C	5.22	115.66	110.23
2	B	805	THR	N-CA-C	5.22	116.59	109.18
13	T	21	DC	C2'-C3'-O3'	-5.20	103.70	111.50
1	A	698	GLN	N-CA-C	-5.19	106.80	113.02
13	T	22	DC	C2'-C3'-O3'	-5.19	103.72	111.50
1	A	1226	VAL	N-CA-C	5.18	116.12	108.45
1	A	999	VAL	N-CA-C	-5.18	107.53	111.62
2	B	1101	ASP	N-CA-C	-5.16	106.22	112.88
6	F	143	PHE	N-CA-C	5.15	116.64	108.96
1	A	1113	THR	CA-C-N	-5.15	113.40	119.84
1	A	1113	THR	C-N-CA	-5.15	113.40	119.84
5	E	177	ARG	N-CA-C	5.15	118.51	110.32
1	A	416	ARG	N-CA-C	5.14	119.13	113.21
7	G	145	VAL	N-CA-C	5.14	117.01	108.99
1	A	134	ARG	N-CA-C	-5.14	105.33	111.03
9	I	44	TYR	N-CA-C	5.13	116.32	108.52
1	A	239	LEU	N-CA-C	5.13	117.72	109.15
1	A	624	SER	N-CA-C	-5.13	107.53	112.97
1	A	1283	VAL	N-CA-C	5.13	115.87	108.48
1	A	1434	ALA	CA-C-N	5.13	126.25	119.84
1	A	1434	ALA	C-N-CA	5.13	126.25	119.84
2	B	294	ASP	N-CA-C	-5.13	101.75	109.60
1	A	60	SER	N-CA-C	5.13	116.09	108.86
1	A	26	GLU	N-CA-C	-5.12	104.96	111.11
2	B	379	GLY	N-CA-C	-5.11	106.31	112.49
1	A	31	SER	N-CA-C	5.10	117.63	110.23
1	A	436	ILE	N-CA-C	-5.10	102.48	109.37
2	B	736	THR	N-CA-C	-5.10	105.42	113.02
1	A	362	ASP	N-CA-C	5.08	119.34	113.20
1	A	289	ILE	N-CA-C	-5.07	106.13	110.74
1	A	1038	THR	N-CA-C	-5.07	101.98	109.94
1	A	4	GLN	N-CA-C	5.07	121.59	110.80
8	H	13	SER	N-CA-C	-5.06	105.76	111.28
1	A	865	GLN	N-CA-C	-5.06	100.03	110.80
9	I	112	SER	N-CA-C	-5.05	106.42	112.59
1	A	30	ILE	CB-CA-C	-5.05	105.32	112.14
1	A	48	ALA	N-CA-C	-5.04	100.06	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ASN	N-CA-C	5.03	116.50	107.80
3	C	186	LEU	N-CA-C	-5.03	107.19	113.38
4	D	169	SER	N-CA-C	-5.02	100.10	110.80
8	H	31	THR	N-CA-C	-5.02	107.65	112.97
2	B	803	LEU	N-CA-C	-5.02	105.28	111.40
8	H	16	ASP	CA-C-N	5.02	126.11	119.84
8	H	16	ASP	C-N-CA	5.02	126.11	119.84
1	A	521	MET	N-CA-C	-5.01	101.77	108.34
2	B	1015	HIS	N-CA-C	5.01	118.65	112.54
1	A	582	ILE	CA-C-N	5.00	126.09	119.84
1	A	582	ILE	C-N-CA	5.00	126.09	119.84
2	B	192	LEU	N-CA-C	-5.00	107.15	113.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	797	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11240	0	11313	1848	0
2	B	8942	0	8987	1396	0
3	C	2125	0	2090	346	0
4	D	1465	0	1489	222	0
5	E	1752	0	1776	243	0
6	F	712	0	738	137	0
7	G	1340	0	1357	176	0
8	H	1101	0	1075	220	0
9	I	952	0	913	145	0
10	J	532	0	542	121	0
11	K	929	0	939	142	0
12	L	370	0	394	92	0
13	T	407	0	225	43	0
14	N	224	0	126	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	P	207	0	109	9	0
16	A	1	0	0	0	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
All	All	32307	0	32073	4724	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 73.

All (4724) 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:577:ALA:HB1	2:B:589:VAL:HG11	1.19	1.14
1:A:320:ARG:HB2	1:A:320:ARG:HH11	1.07	1.14
8:H:33:GLN:HE21	8:H:35:GLN:HB2	1.12	1.13
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.25	1.12
1:A:590:ARG:HH21	1:A:620:LYS:HB3	1.06	1.12
7:G:138:THR:HG22	7:G:139:ILE:H	1.05	1.12
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.32	1.12
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.29	1.11
2:B:638:PHE:HA	2:B:690:VAL:HG22	1.31	1.11
3:C:66:ARG:HH12	10:J:2:ILE:HG21	0.96	1.10
7:G:122:ASN:HD22	7:G:125:SER:HB3	1.11	1.10
2:B:806:THR:HG22	2:B:808:ALA:H	1.11	1.10
1:A:1244:ARG:HB3	1:A:1245:PRO:HA	1.21	1.09
1:A:567:LYS:HG3	8:H:95:TYR:HA	1.32	1.08
6:F:109:VAL:HG12	6:F:110:ASP:H	1.13	1.08
1:A:41:MET:HB2	1:A:49:LYS:HA	1.35	1.08
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.12	1.08
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.35	1.08
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.33	1.07
2:B:1095:LEU:H	2:B:1095:LEU:HD12	1.14	1.07
6:F:103:MET:HE2	7:G:66:GLY:H	1.16	1.07
1:A:1006:ILE:HD11	5:E:163:GLU:HG3	1.38	1.06
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.30	1.05
2:B:642:ASP:HA	2:B:649:LYS:HA	1.36	1.05
1:A:1017:LEU:HB2	5:E:206:GLY:H	1.14	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1424:VAL:HG13	1:A:1436:ILE:HD11	1.38	1.04
2:B:165:VAL:HG11	2:B:448:ILE:HD12	1.36	1.04
3:C:66:ARG:NH1	10:J:2:ILE:HG21	1.72	1.04
2:B:186:GLU:HG3	10:J:62:ARG:HH22	1.22	1.04
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.39	1.03
2:B:340:ALA:HB3	2:B:343:ILE:HG12	1.33	1.03
6:F:130:ILE:O	6:F:148:VAL:HG21	1.58	1.03
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.41	1.02
10:J:64:ASN:HB3	10:J:65:PRO:CD	1.88	1.02
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.42	1.02
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.41	1.01
1:A:108:MET:HB3	1:A:210:ILE:HD13	1.40	1.01
2:B:603:LEU:HB3	2:B:609:ILE:HD11	1.40	1.01
1:A:901:LEU:H	1:A:926:GLN:NE2	1.59	1.01
2:B:1099:VAL:HG13	2:B:1100:ASP:H	1.25	1.00
2:B:934:LYS:HG2	2:B:934:LYS:O	1.62	0.99
12:L:34:CYS:HB3	12:L:51:CYS:SG	2.03	0.99
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	1.97	0.99
5:E:22:MET:HE1	5:E:26:ARG:HH11	1.27	0.99
1:A:53:LEU:HD23	1:A:54:ASN:N	1.77	0.99
3:C:43:THR:HG22	3:C:44:LEU:H	1.25	0.98
1:A:1409:LEU:HD13	2:B:1207:LEU:HD11	1.42	0.98
11:K:46:ILE:O	11:K:50:LEU:HB2	1.64	0.98
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.42	0.98
12:L:32:ALA:HB2	12:L:55:ILE:HG13	1.43	0.98
2:B:999:MET:HA	2:B:999:MET:HE3	1.45	0.98
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.12	0.97
1:A:1258:HIS:HB3	1:A:1259:MET:HE3	1.46	0.97
2:B:882:THR:HG22	2:B:884:ARG:HB2	1.45	0.97
7:G:62:LEU:HB3	7:G:63:PRO:HD2	1.45	0.97
12:L:61:THR:HG22	12:L:63:ARG:H	1.26	0.97
4:D:134:THR:HG22	4:D:135:GLY:H	1.28	0.97
1:A:567:LYS:HE2	8:H:47:PHE:HB2	1.45	0.97
1:A:763:ALA:O	1:A:803:SER:HB3	1.65	0.97
2:B:746:SER:HB2	2:B:1046:PRO:HG2	1.46	0.97
2:B:1002:THR:CG2	2:B:1006:ILE:HG13	1.94	0.97
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.45	0.96
2:B:497:ARG:HH22	2:B:775:LYS:HE2	1.26	0.96
1:A:1445:ILE:H	1:A:1445:ILE:HD12	1.31	0.96
1:A:1254:ALA:O	1:A:1255:GLU:HB2	1.66	0.95
11:K:65:HIS:HD2	11:K:67:PHE:H	1.01	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:LYS:HB3	1:A:641:VAL:HG21	1.48	0.95
2:B:723:VAL:HG12	2:B:724:ASP:H	1.28	0.95
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.47	0.94
8:H:25:ARG:HA	8:H:41:ASP:HA	1.47	0.94
1:A:855:THR:HG21	1:A:857:ARG:HE	1.33	0.94
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.48	0.94
2:B:542:MET:HE3	2:B:636:PRO:HG3	1.49	0.94
1:A:49:LYS:HZ1	1:A:61:ILE:H	1.11	0.94
11:K:65:HIS:CD2	11:K:67:PHE:H	1.85	0.94
3:C:244:VAL:O	3:C:248:ILE:HG13	1.68	0.94
2:B:611:PRO:HG2	2:B:685:LEU:HD21	1.50	0.94
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.33	0.93
1:A:666:ILE:HD12	1:A:667:GLY:H	1.31	0.93
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.32	0.93
4:D:47:LEU:HD13	4:D:48:ILE:H	1.32	0.93
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.29	0.93
2:B:559:SER:HA	2:B:563:MET:HB3	1.48	0.93
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.48	0.92
1:A:1100:ARG:HH12	1:A:1111:MET:HE3	1.32	0.92
8:H:64:ASN:HB2	8:H:88:SER:HB2	1.50	0.92
1:A:754:SER:H	1:A:757:ASN:HD22	1.17	0.92
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.50	0.92
1:A:40:THR:HG22	1:A:41:MET:HG3	1.52	0.92
1:A:390:GLN:O	1:A:394:ASN:HB2	1.69	0.92
1:A:1369:ALA:O	1:A:1372:VAL:HG12	1.68	0.91
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.52	0.91
1:A:1160:SER:HA	1:A:1170:ILE:HD13	1.52	0.91
1:A:808:LEU:HD23	1:A:813:PHE:HA	1.52	0.91
2:B:944:THR:HG21	2:B:1122:ARG:NH2	1.85	0.91
1:A:1116:LEU:HB3	1:A:1308:THR:CG2	2.01	0.91
1:A:590:ARG:NH2	1:A:620:LYS:HB3	1.86	0.91
2:B:430:ARG:O	2:B:434:ARG:HD2	1.71	0.91
4:D:53:SER:H	4:D:148:LEU:CD2	1.84	0.90
5:E:22:MET:CE	5:E:26:ARG:HH11	1.83	0.90
12:L:26:THR:HG23	12:L:62:LYS:NZ	1.86	0.90
3:C:33:LEU:HG	3:C:37:MET:HE2	1.53	0.90
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.52	0.90
13:T:16:DT:H2''	13:T:17:DT:H5'	1.51	0.90
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.52	0.90
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.72	0.90
12:L:40:LEU:HD13	12:L:44:ASP:HB3	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:1:MET:HE2	9:I:4:PHE:HB3	1.54	0.90
1:A:49:LYS:HZ1	1:A:61:ILE:N	1.70	0.90
1:A:1332:PHE:H	1:A:1332:PHE:HD2	1.13	0.90
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.07	0.90
11:K:31:VAL:HG12	11:K:32:VAL:H	1.36	0.90
2:B:654:ARG:H	2:B:657:HIS:HD2	1.17	0.89
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.53	0.89
10:J:64:ASN:HB3	10:J:65:PRO:HD2	1.51	0.89
1:A:567:LYS:CG	8:H:95:TYR:HA	2.02	0.89
10:J:1:MET:H1	10:J:57:ILE:H	1.21	0.89
2:B:1150:ARG:HG3	2:B:1150:ARG:HH11	1.37	0.89
3:C:73:GLN:HE21	3:C:75:MET:H	1.21	0.89
4:D:168:LYS:HG3	4:D:177:VAL:HG11	1.53	0.89
1:A:567:LYS:HB2	8:H:96:VAL:H	1.38	0.89
1:A:665:GLY:O	1:A:667:GLY:N	2.06	0.89
1:A:1343:ALA:HB2	5:E:150:VAL:HG22	1.54	0.89
12:L:30:ILE:O	12:L:56:LEU:HA	1.72	0.89
1:A:1057:VAL:HG12	1:A:1058:VAL:H	1.38	0.88
2:B:664:THR:HG1	2:B:678:GLU:N	1.70	0.88
2:B:515:HIS:H	2:B:518:HIS:HD2	1.18	0.88
3:C:61:GLU:HA	3:C:64:ALA:HB3	1.54	0.88
3:C:66:ARG:HH12	10:J:2:ILE:CG2	1.84	0.88
6:F:111:LEU:HD12	6:F:111:LEU:H	1.38	0.88
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.56	0.88
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.54	0.88
1:A:1244:ARG:HB3	1:A:1245:PRO:CA	2.03	0.88
2:B:364:ILE:O	2:B:365:THR:HB	1.72	0.88
2:B:882:THR:CG2	2:B:884:ARG:HB2	2.02	0.88
10:J:12:LYS:O	10:J:14:VAL:HG23	1.74	0.88
8:H:135:LEU:HD13	8:H:137:GLN:NE2	1.89	0.88
1:A:565:ILE:O	1:A:570:PRO:HA	1.74	0.88
2:B:658:ILE:HG22	2:B:662:MET:HE2	1.53	0.88
1:A:308:ILE:HG22	1:A:309:ALA:H	1.39	0.88
1:A:320:ARG:HB2	1:A:320:ARG:NH1	1.89	0.87
1:A:946:VAL:HG13	5:E:201:LYS:HB3	1.54	0.87
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.56	0.87
4:D:11:ARG:HD2	4:D:31:GLN:HE22	1.38	0.87
7:G:18:PHE:HA	7:G:22:MET:HE3	1.56	0.87
9:I:111:THR:HG22	9:I:113:ASP:H	1.39	0.87
1:A:600:PRO:HG2	1:A:601:LYS:H	1.38	0.87
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:114:ASN:O	5:E:115:ASN:HB3	1.73	0.87
1:A:42:ASP:O	1:A:44:THR:N	2.08	0.87
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.57	0.87
1:A:962:ARG:HA	1:A:965:GLN:HB2	1.56	0.87
8:H:102:TYR:H	8:H:102:TYR:HD2	1.15	0.87
2:B:168:GLY:H	2:B:450:ALA:HB1	1.40	0.87
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.56	0.87
1:A:43:GLU:HB2	1:A:46:THR:HB	1.57	0.86
2:B:637:LEU:O	2:B:690:VAL:HG13	1.75	0.86
6:F:136:ARG:O	6:F:143:PHE:HB2	1.74	0.86
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	1.75	0.86
5:E:117:THR:HG22	5:E:119:SER:H	1.37	0.86
2:B:46:GLN:HG3	2:B:47:GLN:H	1.39	0.86
11:K:12:LEU:H	11:K:12:LEU:HD12	1.40	0.86
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.39	0.86
3:C:148:ARG:H	3:C:151:GLN:HG3	1.40	0.86
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.57	0.86
3:C:38:ILE:HA	3:C:173:ALA:HB2	1.58	0.86
1:A:666:ILE:H	2:B:1026:LEU:HD13	1.39	0.86
4:D:71:LYS:HG2	4:D:74:GLN:NE2	1.89	0.86
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.55	0.86
1:A:466:SER:HB3	2:B:1103:ILE:HG12	1.57	0.86
2:B:1165:ILE:HD11	4:D:17:LYS:HD3	1.57	0.86
2:B:126:SER:OG	2:B:172:ILE:HD11	1.75	0.85
2:B:842:ASN:HD22	2:B:845:SER:HB3	1.40	0.85
13:T:13:DT:H2''	13:T:14:DA:OP2	1.74	0.85
6:F:109:VAL:HG12	6:F:110:ASP:N	1.89	0.85
2:B:880:THR:HB	2:B:934:LYS:HD3	1.57	0.85
7:G:122:ASN:ND2	7:G:125:SER:HB3	1.91	0.85
1:A:537:ARG:HD2	8:H:20:TYR:HE1	1.41	0.85
1:A:1261:LYS:O	1:A:1264:GLU:HB3	1.76	0.85
2:B:776:GLN:OE1	15:P:9:C:H4'	1.76	0.85
7:G:138:THR:HG22	7:G:139:ILE:N	1.88	0.85
14:N:3:DT:H1'	14:N:4:DA:C8	2.12	0.85
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.57	0.85
1:A:180:LYS:NZ	1:A:294:SER:HB3	1.92	0.85
12:L:61:THR:HG21	12:L:63:ARG:HE	1.42	0.85
1:A:30:ILE:HG23	2:B:1170:THR:HG23	1.59	0.85
12:L:32:ALA:CB	12:L:55:ILE:HG13	2.07	0.85
1:A:196:GLU:HB2	1:A:197:PRO:HD2	1.58	0.85
2:B:1181:GLU:O	2:B:1182:CYS:HB3	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:VAL:HG11	2:B:1157:ALA:HB1	1.59	0.84
1:A:70:CYS:O	1:A:72:GLU:HG2	1.77	0.84
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.59	0.84
6:F:103:MET:CE	7:G:66:GLY:H	1.88	0.84
1:A:98:LYS:O	1:A:102:VAL:HG23	1.77	0.84
6:F:86:THR:OG1	6:F:89:GLU:HG3	1.77	0.84
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.11	0.84
8:H:128:ASN:H	8:H:130:ARG:NH1	1.75	0.84
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.59	0.84
1:A:372:LYS:HA	1:A:435:HIS:ND1	1.91	0.84
3:C:6:PRO:HB2	11:K:101:LEU:HD12	1.57	0.84
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.57	0.84
12:L:55:ILE:HD13	12:L:55:ILE:H	1.41	0.84
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	1.78	0.84
4:D:118:THR:HG21	4:D:121:LYS:HD2	1.57	0.84
13:T:15:DC:H2"	13:T:16:DT:H71	1.57	0.84
2:B:597:MET:HA	2:B:597:MET:HE3	1.57	0.84
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.57	0.84
2:B:882:THR:HG21	2:B:935:ARG:HA	1.59	0.84
1:A:35:ILE:HG22	1:A:84:ILE:HD12	1.58	0.84
1:A:746:MET:CE	2:B:1018:PRO:HG2	2.07	0.84
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.59	0.84
8:H:15:VAL:HG13	8:H:26:ILE:HG12	1.60	0.84
1:A:225:ASN:ND2	1:A:228:PHE:H	1.75	0.84
1:A:1047:SER:O	1:A:1050:GLU:HB3	1.77	0.84
1:A:117:GLU:H	1:A:117:GLU:CD	1.86	0.83
1:A:442:VAL:HG12	1:A:490:HIS:O	1.78	0.83
5:E:180:ARG:NH2	5:E:192:ARG:HB2	1.94	0.83
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.60	0.83
2:B:824:ILE:HG22	2:B:1087:PHE:HE2	1.41	0.83
1:A:470:LEU:HD23	1:A:470:LEU:H	1.44	0.83
2:B:515:HIS:HD2	2:B:517:THR:H	1.22	0.83
2:B:1159:ARG:HB3	2:B:1159:ARG:NH1	1.93	0.83
4:D:139:LYS:HE2	4:D:143:ASN:HD21	1.42	0.83
10:J:48:ARG:HD2	10:J:49:MET:N	1.92	0.83
1:A:188:ASP:HB3	1:A:191:THR:HB	1.60	0.83
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.42	0.83
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.78	0.83
1:A:384:ASN:OD1	1:A:388:LEU:HD12	1.78	0.82
2:B:469:GLN:HG3	2:B:470:LYS:H	1.45	0.82
3:C:43:THR:HG22	3:C:44:LEU:N	1.92	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:197:LYS:HE2	5:E:199:ILE:HD11	1.60	0.82
2:B:515:HIS:H	2:B:518:HIS:CD2	1.96	0.82
13:T:24:DG:H2'	13:T:25:DG:C8	2.14	0.82
1:A:84:ILE:HD11	1:A:270:LEU:HD13	1.62	0.82
3:C:32:SER:O	3:C:36:VAL:HG23	1.80	0.82
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.61	0.82
2:B:852:ARG:HH22	12:L:70:ARG:C	1.88	0.82
1:A:49:LYS:NZ	1:A:61:ILE:H	1.78	0.81
1:A:857:ARG:HD3	1:A:861:GLY:O	1.79	0.81
4:D:34:GLN:O	4:D:47:LEU:HD23	1.79	0.81
8:H:26:ILE:HG22	8:H:27:GLU:H	1.45	0.81
5:E:78:LEU:HA	5:E:107:THR:HB	1.63	0.81
1:A:567:LYS:HB3	1:A:568:PRO:HD3	1.62	0.81
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.44	0.81
2:B:706:GLN:HE21	2:B:730:ARG:HH11	1.29	0.81
4:D:18:VAL:O	4:D:19:GLU:HB2	1.79	0.81
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.11	0.81
10:J:35:ALA:O	10:J:39:LEU:HD12	1.80	0.81
1:A:255:SER:OG	2:B:918:ILE:CG2	2.27	0.81
2:B:193:LYS:NZ	12:L:32:ALA:HB1	1.96	0.81
13:T:9:DC:H2''	13:T:10:DA:C8	2.15	0.81
2:B:794:ASN:C	2:B:795:ILE:HD12	2.06	0.81
3:C:20:PHE:HE1	3:C:22:LEU:HB2	1.45	0.81
4:D:8:PHE:HZ	4:D:37:GLN:HB2	1.46	0.81
8:H:100:THR:OG1	8:H:138:GLU:HG3	1.81	0.81
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.61	0.81
2:B:288:ALA:HA	2:B:331:LEU:HD12	1.62	0.81
2:B:1099:VAL:HG13	2:B:1100:ASP:N	1.96	0.81
2:B:1165:ILE:CD1	4:D:17:LYS:HD3	2.10	0.81
3:C:142:VAL:H	10:J:16:ASP:HB3	1.46	0.81
1:A:55:ASP:C	1:A:57:ARG:H	1.84	0.81
2:B:378:LEU:O	2:B:382:ILE:HG13	1.81	0.81
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.11	0.81
1:A:320:ARG:HH11	1:A:320:ARG:CB	1.91	0.81
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.62	0.81
4:D:155:ARG:HD3	4:D:221:TYR:CZ	2.16	0.81
5:E:17:ARG:HB2	5:E:17:ARG:HH11	1.43	0.81
12:L:55:ILE:O	12:L:56:LEU:HB2	1.81	0.81
2:B:503:GLY:HA3	2:B:507:LYS:HE2	1.61	0.80
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.61	0.80
4:D:8:PHE:HD2	7:G:6:ASP:HB2	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:24:ALA:C	4:D:26:THR:H	1.88	0.80
1:A:535:THR:HG21	1:A:616:VAL:HA	1.63	0.80
3:C:66:ARG:HH21	10:J:5:VAL:HG23	1.46	0.80
1:A:903:ASN:HD22	1:A:904:THR:H	1.26	0.80
1:A:1435:PRO:HA	1:A:1439:GLY:O	1.82	0.80
2:B:1115:THR:HG22	2:B:1117:GLN:HG3	1.63	0.80
5:E:178:ILE:HB	5:E:212:ARG:HD2	1.63	0.80
1:A:741:ASN:ND2	1:A:744:LYS:H	1.80	0.80
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.46	0.80
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.46	0.80
5:E:17:ARG:HB2	5:E:17:ARG:NH1	1.97	0.80
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.63	0.80
1:A:855:THR:CG2	1:A:857:ARG:HE	1.94	0.80
1:A:1187:GLN:O	1:A:1244:ARG:HG3	1.81	0.80
1:A:1187:GLN:HG3	1:A:1188:GLN:HG3	1.64	0.80
4:D:71:LYS:HG2	4:D:74:GLN:HE21	1.45	0.80
11:K:21:ILE:HG22	11:K:31:VAL:HG11	1.64	0.80
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.22	0.80
1:A:470:LEU:HD13	1:A:487:MET:HE1	1.61	0.80
13:T:10:DA:H2"	13:T:11:DA:C8	2.16	0.80
4:D:40:HIS:CD2	7:G:73:LYS:HG2	2.17	0.80
5:E:156:LEU:HD12	5:E:195:VAL:HB	1.62	0.79
10:J:23:ASN:C	10:J:25:LEU:H	1.90	0.79
1:A:41:MET:CB	1:A:49:LYS:HA	2.11	0.79
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.64	0.79
2:B:186:GLU:HG3	10:J:62:ARG:NH2	1.97	0.79
2:B:193:LYS:HD3	2:B:787:VAL:HG11	1.65	0.79
2:B:746:SER:CB	2:B:1046:PRO:HG2	2.13	0.79
1:A:577:ILE:O	1:A:580:VAL:HG23	1.83	0.79
5:E:19:VAL:O	5:E:23:VAL:HG23	1.82	0.79
1:A:323:LYS:H	1:A:323:LYS:HD2	1.47	0.79
1:A:825:ILE:HD11	2:B:512:ARG:HD3	1.65	0.79
1:A:1447:GLU:OE2	7:G:23:LYS:HB2	1.83	0.79
3:C:8:VAL:O	3:C:9:LYS:HG3	1.81	0.79
4:D:180:LEU:HD23	4:D:195:ILE:HD12	1.63	0.79
6:F:82:THR:HG22	6:F:84:TYR:H	1.47	0.79
1:A:809:THR:H	1:A:812:GLU:HB2	1.46	0.79
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.65	0.79
3:C:265:MET:HE1	11:K:19:LEU:HB2	1.64	0.79
4:D:71:LYS:HA	4:D:74:GLN:HG3	1.65	0.79
1:A:829:VAL:HG11	2:B:508:LEU:HD22	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	1.97	0.79
2:B:778:MET:HE1	2:B:853:SER:HB3	1.65	0.79
2:B:792:MET:HE2	2:B:857:ARG:HH22	1.48	0.79
5:E:31:THR:HG23	5:E:34:GLU:HB2	1.65	0.79
8:H:100:THR:HG23	8:H:138:GLU:HA	1.65	0.79
1:A:472:LEU:O	1:A:475:THR:HB	1.82	0.79
2:B:1183:LYS:O	2:B:1185:CYS:N	2.15	0.78
2:B:745:PRO:O	2:B:748:ILE:HG12	1.84	0.78
12:L:30:ILE:O	12:L:56:LEU:HD23	1.83	0.78
2:B:821:GLN:HE22	2:B:851:PHE:H	1.30	0.78
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.48	0.78
6:F:99:LEU:O	6:F:103:MET:HG2	1.83	0.78
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.65	0.78
2:B:516:ASN:HD22	2:B:516:ASN:N	1.77	0.78
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.64	0.78
10:J:44:TYR:H	10:J:44:TYR:HD2	1.29	0.78
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.65	0.78
1:A:590:ARG:HB3	1:A:605:MET:H	1.48	0.78
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.63	0.78
1:A:524:VAL:HG12	1:A:525:GLN:N	1.97	0.78
2:B:830:TYR:HE2	2:B:1000:PRO:HD3	1.48	0.78
2:B:860:MET:HE2	2:B:965:LYS:HE2	1.65	0.78
1:A:1057:VAL:HG12	1:A:1058:VAL:N	1.98	0.78
2:B:277:LYS:HG3	2:B:338:GLY:HA2	1.66	0.78
1:A:341:MET:HE3	1:A:843:LYS:HZ1	1.49	0.78
1:A:1030:ARG:HG3	1:A:1034:GLU:OE2	1.83	0.78
4:D:213:GLU:O	4:D:217:LEU:HG	1.84	0.78
1:A:560:ILE:HD11	8:H:79:TRP:H	1.47	0.78
2:B:217:ARG:NE	2:B:405:ARG:HB2	1.98	0.78
2:B:345:LYS:O	2:B:347:LYS:HG2	1.84	0.78
1:A:372:LYS:HA	1:A:435:HIS:HD1	1.48	0.78
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.17	0.78
13:T:21:DC:H2''	13:T:22:DC:H5'	1.64	0.78
1:A:1130:GLN:HG3	1:A:1134:ILE:HD11	1.65	0.77
2:B:345:LYS:O	2:B:347:LYS:N	2.17	0.77
3:C:98:VAL:C	3:C:99:LEU:HD23	2.09	0.77
4:D:8:PHE:CD2	7:G:6:ASP:HB2	2.18	0.77
7:G:13:LEU:HD23	7:G:14:HIS:H	1.49	0.77
1:A:266:LEU:HD21	1:A:303:TYR:CE1	2.20	0.77
7:G:128:PRO:O	7:G:138:THR:HG23	1.83	0.77
1:A:745:GLN:HA	1:A:748:MET:HE3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:GLN:HB2	2:B:408:LEU:HD21	1.64	0.77
2:B:826:ALA:HB2	2:B:1008:PRO:HB3	1.67	0.77
1:A:1008:GLN:O	1:A:1011:GLN:HB3	1.85	0.77
2:B:244:LEU:HD11	2:B:366:GLN:HE22	1.49	0.77
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.10	0.77
2:B:879:ARG:NH1	2:B:883:LEU:HD23	1.98	0.77
4:D:8:PHE:CZ	4:D:37:GLN:HB2	2.19	0.77
1:A:896:ARG:NH2	1:A:1030:ARG:HE	1.82	0.77
2:B:212:LEU:HD23	2:B:480:SER:HB2	1.65	0.77
13:T:15:DC:C2'	13:T:16:DT:H71	2.14	0.77
1:A:93:VAL:HG23	1:A:304:MET:HE3	1.66	0.77
1:A:305:ASP:OD2	1:A:326:ARG:HD2	1.84	0.77
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.32	0.77
7:G:127:PRO:HG2	7:G:138:THR:HG21	1.67	0.77
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.65	0.77
1:A:1027:ALA:O	1:A:1031:VAL:HG23	1.84	0.77
2:B:430:ARG:O	2:B:434:ARG:CD	2.32	0.77
4:D:173:HIS:HD2	4:D:174:PRO:HD2	1.48	0.77
1:A:1081:LEU:HD11	1:A:1098:VAL:H	1.48	0.77
1:A:1268:LEU:O	1:A:1269:GLU:HG3	1.85	0.77
2:B:879:ARG:O	2:B:934:LYS:HE2	1.85	0.77
5:E:22:MET:HE1	5:E:26:ARG:NH1	1.99	0.77
1:A:382:PRO:HD3	1:A:428:TYR:HD2	1.49	0.77
2:B:120:ARG:NE	2:B:955:THR:HG21	1.99	0.77
3:C:238:ILE:HD13	3:C:246:ARG:HH11	1.50	0.77
7:G:115:MET:HB2	7:G:116:PRO:HD2	1.66	0.77
11:K:50:LEU:HD11	11:K:75:ILE:HD13	1.67	0.77
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.11	0.76
2:B:497:ARG:NH2	2:B:775:LYS:HE2	2.00	0.76
5:E:23:VAL:HG13	5:E:78:LEU:HD13	1.66	0.76
8:H:91:ASP:O	8:H:93:TYR:N	2.16	0.76
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.50	0.76
1:A:995:GLU:HA	1:A:995:GLU:OE1	1.84	0.76
1:A:1116:LEU:HB3	1:A:1308:THR:HG22	1.66	0.76
1:A:1315:GLU:C	1:A:1317:MET:H	1.92	0.76
2:B:810:GLU:HB2	2:B:815:ARG:HH22	1.48	0.76
8:H:89:LEU:C	8:H:91:ASP:H	1.91	0.76
2:B:661:LEU:HD23	2:B:679:TYR:O	1.85	0.76
4:D:134:THR:HG22	4:D:135:GLY:N	1.99	0.76
1:A:55:ASP:CG	1:A:55:ASP:O	2.29	0.76
2:B:549:THR:HB	2:B:628:THR:OG1	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:579:ARG:HA	2:B:589:VAL:HG22	1.68	0.76
4:D:57:LEU:HD11	4:D:160:VAL:HG21	1.66	0.76
5:E:180:ARG:HH21	5:E:192:ARG:CB	1.97	0.76
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.67	0.76
1:A:230:ARG:H	1:A:233:TRP:HE3	1.34	0.76
1:A:903:ASN:HD22	1:A:904:THR:N	1.84	0.76
2:B:430:ARG:O	2:B:434:ARG:HG3	1.86	0.76
9:I:74:GLU:HA	9:I:80:SER:O	1.86	0.76
1:A:7:SER:HB3	2:B:1175:LEU:HD22	1.68	0.76
9:I:105:SER:O	9:I:106:CYS:HB3	1.85	0.76
1:A:534:LEU:O	1:A:574:GLY:HA3	1.86	0.76
7:G:153:GLN:HG2	7:G:154:VAL:HG23	1.68	0.76
8:H:130:ARG:HB3	8:H:134:ASN:HB2	1.66	0.76
1:A:103:CYS:SG	1:A:108:MET:HE1	2.26	0.76
1:A:1325:THR:O	5:E:148:GLU:HB2	1.86	0.76
2:B:1150:ARG:HH11	2:B:1150:ARG:CG	1.99	0.76
12:L:40:LEU:HD22	12:L:44:ASP:CG	2.11	0.76
1:A:672:ASP:HB3	1:A:675:THR:HB	1.68	0.75
2:B:123:THR:OG1	2:B:458:LYS:HE2	1.86	0.75
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.00	0.75
3:C:101:LEU:O	3:C:102:GLN:HG3	1.85	0.75
1:A:317:LYS:HA	2:B:471:LYS:HE2	1.68	0.75
1:A:910:PRO:HB3	1:A:917:SER:H	1.51	0.75
1:A:1130:GLN:O	1:A:1134:ILE:HG13	1.85	0.75
7:G:138:THR:CG2	7:G:139:ILE:H	1.89	0.75
8:H:26:ILE:O	8:H:27:GLU:HG3	1.86	0.75
10:J:64:ASN:HD22	10:J:65:PRO:HD3	1.48	0.75
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	1.99	0.75
2:B:806:THR:HG22	2:B:808:ALA:N	1.95	0.75
2:B:1095:LEU:HD12	2:B:1095:LEU:N	1.98	0.75
1:A:107:CYS:N	1:A:114:LEU:HD21	2.01	0.75
2:B:168:GLY:HA2	2:B:454:THR:OG1	1.87	0.75
2:B:866:TYR:O	2:B:868:MET:N	2.19	0.75
4:D:144:THR:O	4:D:148:LEU:HB2	1.86	0.75
8:H:84:ALA:HB2	8:H:87:ARG:HD2	1.68	0.75
1:A:23:SER:HA	1:A:233:TRP:NE1	2.02	0.75
1:A:695:LYS:HA	1:A:698:GLN:HB2	1.67	0.75
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.69	0.75
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.22	0.75
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.68	0.75
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:ARG:HD2	1:A:899:VAL:H	1.52	0.75
1:A:1148:ILE:HD11	1:A:1198:ASP:HA	1.69	0.75
2:B:577:ALA:CB	2:B:589:VAL:HG11	2.10	0.75
1:A:135:PHE:HD1	1:A:222:LEU:HD22	1.51	0.75
2:B:101:MET:HB2	2:B:169:ARG:HH22	1.52	0.75
2:B:293:PRO:HG2	2:B:296:GLU:HB3	1.68	0.75
1:A:380:VAL:HG12	1:A:428:TYR:HA	1.69	0.75
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.67	0.75
1:A:302:THR:HA	1:A:305:ASP:O	1.87	0.74
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	2.01	0.74
1:A:1227:ILE:HG22	1:A:1228:TRP:N	1.99	0.74
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.87	0.74
3:C:7:GLN:HG2	11:K:104:ASN:ND2	2.01	0.74
9:I:6:PHE:HB3	9:I:12:ASN:O	1.86	0.74
1:A:12:ARG:HB2	2:B:1218:THR:HG22	1.68	0.74
1:A:148:CYS:O	1:A:168:GLY:HA2	1.86	0.74
1:A:697:ALA:HB2	1:A:702:LEU:HD12	1.69	0.74
9:I:111:THR:HG22	9:I:113:ASP:N	2.01	0.74
13:T:18:DA:H1'	13:T:19:8OG:H5'	1.69	0.74
2:B:326:ASP:OD2	2:B:328:GLU:HB3	1.86	0.74
2:B:497:ARG:HH22	2:B:775:LYS:CE	1.99	0.74
2:B:636:PRO:O	2:B:743:ILE:HD11	1.88	0.74
4:D:148:LEU:O	4:D:152:SER:HB3	1.87	0.74
11:K:107:THR:O	11:K:111:LEU:HG	1.87	0.74
1:A:438:ASP:O	1:A:439:ASN:HB2	1.85	0.74
4:D:159:THR:O	4:D:163:VAL:HG23	1.87	0.74
5:E:97:VAL:HG13	5:E:127:ILE:HD13	1.69	0.74
1:A:1193:LEU:HB2	1:A:1260:LEU:HD11	1.69	0.74
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.17	0.74
3:C:174:ALA:O	10:J:10:CYS:HB2	1.88	0.74
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.68	0.74
2:B:1002:THR:HG23	2:B:1006:ILE:HG13	1.68	0.74
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	1.87	0.74
1:A:403:LYS:O	1:A:415:LEU:HB2	1.88	0.74
1:A:591:PHE:HA	1:A:595:THR:HG21	1.70	0.74
2:B:807:ARG:HG2	2:B:1045:SER:OG	1.86	0.74
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.70	0.74
14:N:3:DT:H4'	14:N:4:DA:H5'	1.70	0.74
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.70	0.74
3:C:76:ASP:O	3:C:78:GLU:N	2.21	0.74
3:C:259:LEU:HD21	11:K:91:CYS:HB3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:PHE:CD1	1:A:222:LEU:HD22	2.22	0.74
1:A:808:LEU:HG	1:A:812:GLU:HB3	1.70	0.74
1:A:933:TYR:O	1:A:937:VAL:HG23	1.88	0.74
6:F:75:PRO:HG2	6:F:77:ASP:O	1.87	0.74
1:A:40:THR:HB	1:A:41:MET:HE2	1.70	0.73
1:A:1009:ASN:HA	1:A:1012:ARG:NH1	2.02	0.73
10:J:48:ARG:HE	10:J:49:MET:HE2	1.51	0.73
1:A:567:LYS:HG3	8:H:94:ASP:O	1.88	0.73
1:A:825:ILE:HD11	2:B:512:ARG:HB3	1.70	0.73
2:B:351:TYR:O	2:B:355:ILE:HG13	1.89	0.73
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.68	0.73
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.23	0.73
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.23	0.73
8:H:99:GLY:HA3	8:H:118:PHE:HA	1.69	0.73
1:A:596:THR:C	1:A:598:LEU:H	1.97	0.73
2:B:60:GLN:O	2:B:63:ILE:HG22	1.88	0.73
3:C:115:SER:HB3	3:C:142:VAL:HB	1.69	0.73
8:H:130:ARG:N	8:H:130:ARG:HD2	2.03	0.73
1:A:71:GLN:HG3	1:A:72:GLU:H	1.54	0.73
1:A:215:SER:HB3	1:A:218:ASP:OD2	1.87	0.73
2:B:193:LYS:HZ3	12:L:32:ALA:HB1	1.54	0.73
2:B:326:ASP:C	2:B:328:GLU:H	1.95	0.73
2:B:526:GLU:HG2	2:B:538:ASN:HD22	1.54	0.73
3:C:101:LEU:CD1	3:C:118:LEU:HD23	2.15	0.73
3:C:148:ARG:N	3:C:151:GLN:HG3	2.02	0.73
11:K:82:ASP:OD1	11:K:84:LYS:HG3	1.88	0.73
8:H:81:PRO:HG2	8:H:82:PRO:HD2	1.69	0.73
11:K:65:HIS:HD2	11:K:67:PHE:N	1.84	0.73
1:A:825:ILE:CD1	2:B:512:ARG:HB3	2.18	0.73
1:A:87:ALA:HB1	1:A:276:LEU:HD23	1.70	0.73
1:A:849:MET:HB2	1:A:1062:GLU:O	1.89	0.73
1:A:896:ARG:HH21	1:A:1030:ARG:NE	1.87	0.73
1:A:919:ILE:HG23	1:A:925:LEU:HD12	1.70	0.73
7:G:102:GLN:HG3	7:G:106:MET:O	1.88	0.73
13:T:7:DC:H2"	13:T:8:DT:C5	2.24	0.73
1:A:709:THR:HG22	1:A:711:ARG:H	1.54	0.73
2:B:220:GLY:O	2:B:222:ILE:HG13	1.89	0.73
4:D:60:LYS:O	4:D:64:VAL:HG23	1.88	0.73
8:H:129:TYR:HA	8:H:131:ASN:ND2	2.04	0.73
2:B:216:GLU:HB3	2:B:500:THR:HG23	1.70	0.73
2:B:613:VAL:HG22	2:B:628:THR:HA	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:778:MET:HE2	2:B:1094:ARG:HG2	1.70	0.73
1:A:701:LEU:HD21	9:I:114:GLN:HB2	1.71	0.73
2:B:230:ALA:N	2:B:231:PRO:HD2	2.04	0.73
4:D:137:ASN:ND2	4:D:137:ASN:H	1.87	0.73
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.71	0.73
1:A:1198:ASP:HB3	1:A:1201:ALA:HB3	1.71	0.72
2:B:906:SER:O	2:B:941:LEU:HD23	1.89	0.72
5:E:92:THR:O	5:E:95:THR:HB	1.89	0.72
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.70	0.72
1:A:284:ALA:C	1:A:286:HIS:H	1.96	0.72
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.71	0.72
1:A:963:ILE:HD13	1:A:1049:ILE:HG12	1.71	0.72
2:B:95:ILE:HB	2:B:130:VAL:HG22	1.71	0.72
2:B:326:ASP:CG	2:B:328:GLU:HB3	2.14	0.72
2:B:335:GLY:HA3	2:B:348:ARG:HB2	1.71	0.72
3:C:62:PHE:O	3:C:66:ARG:HG3	1.89	0.72
11:K:21:ILE:HG23	11:K:33:ILE:HG12	1.71	0.72
1:A:167:CYS:HB2	1:A:169:ASN:ND2	2.03	0.72
1:A:847:ASP:OD2	1:A:858:ASN:HB2	1.89	0.72
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.71	0.72
7:G:88:ASP:HB3	7:G:144:ARG:HA	1.70	0.72
1:A:37:PHE:HD1	1:A:37:PHE:H	1.38	0.72
1:A:855:THR:HG21	1:A:857:ARG:NE	2.04	0.72
5:E:61:GLN:HG3	5:E:78:LEU:O	1.90	0.72
1:A:774:ARG:NH1	1:A:797:LYS:HG3	2.04	0.72
1:A:866:PHE:C	1:A:867:ILE:HD12	2.14	0.72
1:A:1002:GLY:HA3	1:A:1007:ILE:CG2	2.19	0.72
4:D:139:LYS:HE2	4:D:143:ASN:ND2	2.03	0.72
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.72	0.72
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.70	0.72
1:A:567:LYS:HD2	8:H:95:TYR:CD2	2.25	0.72
1:A:1308:THR:HG23	1:A:1309:ASP:N	2.03	0.72
2:B:112:LEU:HD12	2:B:113:TYR:H	1.54	0.72
6:F:109:VAL:CG1	6:F:110:ASP:H	1.97	0.72
1:A:100:LYS:HE2	1:A:104:GLU:OE2	1.89	0.72
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.15	0.72
1:A:646:PHE:O	1:A:650:GLN:HB2	1.90	0.72
1:A:1332:PHE:N	1:A:1332:PHE:CD2	2.55	0.72
1:A:332:LYS:H	1:A:337:ARG:HB3	1.55	0.72
1:A:524:VAL:HG12	1:A:525:GLN:H	1.54	0.72
2:B:23:ALA:H	2:B:654:ARG:HB3	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.70	0.72
1:A:53:LEU:HD23	1:A:54:ASN:H	1.53	0.72
1:A:751:SER:O	1:A:752:LYS:HG2	1.89	0.72
1:A:885:THR:O	1:A:940:ARG:HD2	1.88	0.72
1:A:1045:VAL:O	1:A:1049:ILE:HG13	1.90	0.72
2:B:118:ARG:HG2	2:B:204:ILE:HD13	1.72	0.72
7:G:40:GLY:HA2	7:G:157:ILE:HD11	1.72	0.72
8:H:36:CYS:HA	8:H:126:GLU:O	1.89	0.72
12:L:26:THR:HG23	12:L:62:LYS:HZ1	1.52	0.72
1:A:71:GLN:CG	1:A:72:GLU:H	2.00	0.72
2:B:435:THR:O	2:B:435:THR:HG22	1.89	0.72
2:B:801:LYS:O	10:J:52:THR:HG23	1.89	0.72
5:E:49:SER:OG	5:E:50:MET:HE3	1.90	0.72
5:E:52:ARG:HB3	5:E:53:PRO:HD2	1.71	0.72
8:H:38:LEU:HD12	8:H:124:ARG:O	1.90	0.72
12:L:32:ALA:HB3	12:L:33:GLU:OE2	1.89	0.72
1:A:1111:MET:HE2	1:A:1330:ASN:OD1	1.89	0.71
1:A:1237:ILE:HG22	1:A:1238:ILE:N	2.05	0.71
3:C:75:MET:HE1	3:C:239:PRO:HG2	1.71	0.71
3:C:128:ASN:O	3:C:129:ILE:HG13	1.90	0.71
1:A:265:LYS:HE2	1:A:302:THR:HG23	1.72	0.71
1:A:341:MET:CE	1:A:843:LYS:HZ1	2.03	0.71
1:A:567:LYS:HG3	8:H:95:TYR:CA	2.17	0.71
1:A:849:MET:HE3	1:A:1061:GLY:HA2	1.73	0.71
2:B:315:LYS:NZ	9:I:1:MET:HE1	2.05	0.71
2:B:1085:ILE:N	2:B:1085:ILE:HD12	2.05	0.71
1:A:32:VAL:HG21	1:A:68:GLN:NE2	2.05	0.71
1:A:34:LYS:CB	1:A:36:ARG:HH21	2.03	0.71
1:A:71:GLN:HG3	1:A:72:GLU:N	2.04	0.71
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.20	0.71
2:B:1183:LYS:HA	2:B:1186:ASP:HA	1.70	0.71
6:F:72:LYS:HA	6:F:72:LYS:HE3	1.72	0.71
1:A:629:LEU:O	1:A:633:VAL:HG23	1.89	0.71
1:A:1127:ASP:CG	1:A:1130:GLN:HB2	2.15	0.71
2:B:277:LYS:O	2:B:278:GLN:HB2	1.88	0.71
7:G:62:LEU:HB3	7:G:63:PRO:CD	2.18	0.71
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.55	0.71
2:B:954:VAL:HG13	2:B:964:VAL:HG22	1.72	0.71
3:C:20:PHE:CE1	3:C:22:LEU:HB2	2.25	0.71
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.25	0.71
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:268:ASP:O	3:C:269:LYS:HB2	1.90	0.71
7:G:9:LEU:HD12	7:G:10:ASN:N	2.04	0.71
1:A:822:GLU:O	1:A:825:ILE:HG22	1.90	0.71
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.73	0.71
2:B:179:CYS:SG	2:B:181:LEU:HD12	2.30	0.71
5:E:124:VAL:N	5:E:125:PRO:HD2	2.04	0.71
6:F:80:ALA:HB3	6:F:144:GLU:OE2	1.91	0.71
1:A:590:ARG:HH21	1:A:620:LYS:CB	1.96	0.71
1:A:873:MET:C	1:A:1058:VAL:HG23	2.16	0.71
2:B:1215:ARG:C	2:B:1216:LEU:HD23	2.15	0.71
8:H:128:ASN:H	8:H:130:ARG:HH11	1.39	0.71
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.55	0.71
1:A:901:LEU:H	1:A:926:GLN:HE21	1.37	0.71
2:B:313:MET:O	2:B:316:PRO:HD2	1.91	0.71
2:B:563:MET:HE1	2:B:580:VAL:HB	1.72	0.71
2:B:603:LEU:HD12	2:B:609:ILE:HG12	1.73	0.71
4:D:208:GLU:HG3	4:D:212:LYS:HE3	1.73	0.71
11:K:68:PHE:HB3	11:K:70:ARG:HH11	1.55	0.71
2:B:359:GLU:O	2:B:362:PRO:HD3	1.91	0.71
2:B:999:MET:HA	2:B:999:MET:CE	2.20	0.71
6:F:135:ARG:HG2	6:F:137:TYR:CE1	2.26	0.71
7:G:143:ILE:HG22	7:G:144:ARG:N	2.05	0.71
1:A:92:HIS:HB2	1:A:236:LEU:HD21	1.71	0.70
1:A:853:ASP:O	1:A:854:ASN:HB2	1.91	0.70
1:A:868:TYR:OH	1:A:1366:ARG:HD3	1.90	0.70
3:C:193:TYR:HD2	3:C:197:SER:HB3	1.54	0.70
3:C:256:ALA:HA	3:C:259:LEU:HD23	1.72	0.70
1:A:332:LYS:CA	1:A:337:ARG:HD2	2.21	0.70
1:A:888:GLY:O	1:A:940:ARG:NH2	2.24	0.70
2:B:900:ALA:HB3	12:L:61:THR:OG1	1.91	0.70
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.56	0.70
2:B:1215:ARG:NH1	4:D:15:LEU:HD21	2.05	0.70
6:F:97:ARG:O	6:F:101:ILE:HG13	1.92	0.70
1:A:7:SER:CB	2:B:1175:LEU:HD22	2.20	0.70
1:A:10:PRO:HB3	4:D:3:VAL:HA	1.73	0.70
1:A:315:LEU:HD13	2:B:471:LYS:HB3	1.72	0.70
1:A:896:ARG:HH21	1:A:1030:ARG:HE	1.35	0.70
3:C:56:THR:HG21	3:C:145:CYS:SG	2.32	0.70
9:I:58:VAL:HG13	9:I:62:ILE:HD12	1.72	0.70
2:B:898:LEU:HD13	2:B:952:VAL:HG11	1.73	0.70
5:E:55:ARG:C	5:E:57:MET:H	1.99	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1183:LYS:C	2:B:1186:ASP:H	1.99	0.70
8:H:32:THR:HG22	8:H:33:GLN:H	1.57	0.70
1:A:353:ILE:CD1	1:A:487:MET:HE2	2.22	0.70
3:C:242:GLN:C	3:C:244:VAL:H	1.98	0.70
7:G:1:MET:SD	7:G:79:PHE:HD1	2.14	0.70
11:K:68:PHE:HB3	11:K:70:ARG:NH1	2.06	0.70
1:A:526:ASP:HB2	2:B:835:GLN:OE1	1.91	0.70
2:B:464:GLY:O	2:B:477:ALA:HA	1.91	0.70
3:C:239:PRO:HB2	3:C:241:ASP:OD1	1.90	0.70
7:G:34:VAL:HG11	7:G:74:TYR:HE1	1.56	0.70
1:A:35:ILE:CG2	1:A:84:ILE:HD12	2.21	0.70
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.22	0.70
2:B:589:VAL:HG12	2:B:590:HIS:N	2.06	0.70
6:F:90:ARG:HG3	6:F:91:ALA:N	2.06	0.70
2:B:101:MET:HB2	2:B:169:ARG:NH2	2.07	0.70
2:B:824:ILE:HG22	2:B:1087:PHE:CE2	2.27	0.70
8:H:64:ASN:CG	8:H:90:ALA:H	1.99	0.70
8:H:64:ASN:HD22	8:H:88:SER:CB	2.04	0.70
1:A:49:LYS:NZ	1:A:61:ILE:HG13	2.06	0.70
2:B:850:LEU:HD12	2:B:851:PHE:N	2.06	0.70
2:B:978:ASP:OD2	2:B:1098:MET:HG2	1.91	0.70
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.73	0.70
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.27	0.69
2:B:54:PHE:O	2:B:58:THR:HB	1.92	0.69
2:B:60:GLN:HE22	2:B:94:LYS:HA	1.57	0.69
4:D:47:LEU:HD13	4:D:48:ILE:N	2.04	0.69
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.27	0.69
6:F:106:PRO:HB2	6:F:108:PHE:CE2	2.27	0.69
1:A:84:ILE:O	1:A:84:ILE:HG23	1.92	0.69
1:A:447:GLN:HE22	13:T:20:DG:H4'	1.55	0.69
1:A:705:LYS:HB2	1:A:708:MET:HE3	1.73	0.69
1:A:852:TYR:CD1	6:F:136:ARG:HB3	2.28	0.69
1:A:1006:ILE:CD1	5:E:163:GLU:HG3	2.20	0.69
1:A:1210:GLY:O	1:A:1214:GLU:HG2	1.92	0.69
3:C:73:GLN:HE21	3:C:75:MET:N	1.89	0.69
6:F:73:ALA:HB1	6:F:143:PHE:O	1.91	0.69
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.73	0.69
1:A:474:VAL:HA	1:A:521:MET:HE2	1.72	0.69
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.87	0.69
1:A:602:ASP:HB3	1:A:616:VAL:HG23	1.74	0.69
1:A:1074:GLU:C	1:A:1076:ALA:H	2.01	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.07	0.69
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.89	0.69
3:C:18:VAL:HG23	3:C:240:VAL:HG12	1.74	0.69
3:C:89:GLU:O	3:C:90:ASP:HB3	1.90	0.69
12:L:60:ARG:HH21	12:L:65:VAL:HG21	1.57	0.69
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.23	0.69
1:A:825:ILE:HG23	1:A:826:ASP:N	2.08	0.69
1:A:1120:LEU:H	1:A:1120:LEU:HD12	1.57	0.69
2:B:243:ALA:HB2	2:B:251:ILE:HG12	1.74	0.69
2:B:465:ASN:HD22	2:B:465:ASN:N	1.89	0.69
2:B:821:GLN:HE22	2:B:851:PHE:N	1.90	0.69
5:E:168:TYR:HB3	5:E:170:LEU:HG	1.74	0.69
1:A:443:LEU:HD23	1:A:501:LEU:CD2	2.22	0.69
1:A:1420:ASP:O	1:A:1421:CYS:HB2	1.93	0.69
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.28	0.69
5:E:124:VAL:HG13	5:E:132:ILE:HG13	1.73	0.69
5:E:190:LEU:HD12	5:E:214:CYS:HB2	1.75	0.69
1:A:53:LEU:HD23	1:A:54:ASN:HB3	1.74	0.69
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.74	0.69
2:B:1202:LEU:O	2:B:1206:GLU:HG3	1.92	0.69
3:C:166:GLU:C	11:K:6:ARG:HH11	2.01	0.69
3:C:261:ALA:O	3:C:265:MET:HB2	1.92	0.69
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.73	0.69
7:G:96:GLN:O	7:G:112:LYS:HD3	1.92	0.69
7:G:125:SER:OG	7:G:128:PRO:HA	1.92	0.69
8:H:14:GLU:HG2	8:H:15:VAL:N	2.08	0.69
8:H:82:PRO:HG3	11:K:54:ARG:HH11	1.56	0.69
1:A:72:GLU:HB3	1:A:76:GLU:HG2	1.75	0.69
1:A:106:VAL:HG13	1:A:112:LYS:O	1.93	0.69
2:B:121:ASN:HA	2:B:207:GLY:HA2	1.75	0.69
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.75	0.69
2:B:637:LEU:C	2:B:690:VAL:HG13	2.18	0.69
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.75	0.69
8:H:97:MET:HE3	8:H:142:LEU:HD23	1.73	0.69
1:A:49:LYS:HZ3	1:A:61:ILE:HG13	1.58	0.69
1:A:356:ASP:HB2	1:A:469:ARG:HH12	1.58	0.69
1:A:1151:GLU:HG2	9:I:45:ARG:HB2	1.75	0.69
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.93	0.69
2:B:25:ILE:HD11	2:B:653:VAL:O	1.92	0.69
2:B:563:MET:CE	2:B:580:VAL:HB	2.23	0.69
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:58:VAL:HG13	9:I:62:ILE:CD1	2.23	0.69
1:A:567:LYS:CE	8:H:47:PHE:HB2	2.23	0.68
1:A:898:ARG:HD2	1:A:899:VAL:N	2.08	0.68
1:A:1032:LEU:O	1:A:1036:ARG:HD3	1.94	0.68
2:B:289:LEU:HD13	2:B:375:ALA:CB	2.23	0.68
2:B:613:VAL:HG13	2:B:627:PHE:O	1.92	0.68
3:C:36:VAL:HG21	3:C:251:LEU:HD13	1.74	0.68
3:C:251:LEU:O	3:C:255:VAL:HG23	1.94	0.68
11:K:61:TYR:C	11:K:61:TYR:CD2	2.70	0.68
1:A:12:ARG:HD2	2:B:1218:THR:HB	1.73	0.68
1:A:1208:THR:HB	1:A:1211:GLN:HG3	1.75	0.68
2:B:658:ILE:CG2	2:B:662:MET:HE2	2.23	0.68
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.28	0.68
7:G:119:LEU:HD12	7:G:131:GLN:O	1.93	0.68
1:A:382:PRO:HB3	1:A:428:TYR:HE2	1.56	0.68
1:A:442:VAL:O	1:A:457:ALA:HA	1.92	0.68
1:A:722:LEU:HD23	1:A:799:PHE:CD1	2.28	0.68
1:A:1081:LEU:HD11	1:A:1097:GLY:HA3	1.75	0.68
1:A:1116:LEU:HB3	1:A:1308:THR:HG21	1.75	0.68
2:B:309:GLN:OE1	9:I:52:ILE:HD11	1.93	0.68
5:E:202:SER:OG	5:E:204:THR:HG22	1.94	0.68
1:A:11:LEU:HD12	2:B:1193:GLN:O	1.92	0.68
1:A:547:LEU:HD22	11:K:58:PHE:CE1	2.28	0.68
1:A:1348:LEU:O	1:A:1352:VAL:HG23	1.93	0.68
7:G:44:TYR:HE1	7:G:157:ILE:H	1.40	0.68
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.24	0.68
1:A:1202:MET:HE1	1:A:1212:VAL:HG21	1.75	0.68
1:A:573:SER:O	1:A:576:GLN:HB2	1.93	0.68
1:A:1345:ARG:NH1	5:E:200:ARG:HH22	1.92	0.68
2:B:90:ILE:HG23	2:B:133:LYS:O	1.93	0.68
2:B:127:GLY:C	2:B:128:LEU:HD12	2.19	0.68
2:B:253:THR:HG22	2:B:254:LEU:H	1.58	0.68
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.74	0.68
2:B:1095:LEU:H	2:B:1095:LEU:CD1	1.96	0.68
4:D:40:HIS:HD2	7:G:73:LYS:HG2	1.57	0.68
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.28	0.68
1:A:69:THR:C	1:A:71:GLN:N	2.49	0.68
2:B:620:ARG:NH1	9:I:68:LEU:HD21	2.08	0.68
8:H:109:LYS:HD2	8:H:111:LEU:HD11	1.76	0.68
9:I:99:LEU:O	9:I:111:THR:HG23	1.94	0.68
1:A:741:ASN:HD22	1:A:744:LYS:H	1.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:ILE:HA	1:A:963:ILE:HG22	1.76	0.68
2:B:763:GLN:NE2	2:B:1021:MET:HE2	2.09	0.68
2:B:1069:PHE:HA	2:B:1085:ILE:O	1.94	0.68
2:B:1084:GLN:OE1	3:C:189:THR:HG22	1.92	0.68
3:C:43:THR:CG2	3:C:44:LEU:H	1.95	0.68
3:C:238:ILE:CD1	3:C:246:ARG:HH11	2.07	0.68
11:K:31:VAL:HG12	11:K:32:VAL:N	2.06	0.68
1:A:456:MET:HE2	1:A:507:VAL:HG22	1.76	0.68
1:A:717:ASN:HA	1:A:720:ARG:NH1	2.09	0.68
2:B:558:LEU:C	2:B:560:GLU:H	2.01	0.68
2:B:824:ILE:CG2	2:B:1087:PHE:HE2	2.06	0.68
4:D:47:LEU:O	4:D:48:ILE:HD13	1.92	0.68
6:F:84:TYR:CE2	6:F:152:ILE:HD12	2.29	0.68
1:A:1081:LEU:CD1	1:A:1098:VAL:H	2.07	0.68
2:B:219:ALA:HB2	2:B:405:ARG:NH1	2.08	0.68
2:B:1099:VAL:CG1	2:B:1100:ASP:H	2.05	0.68
6:F:74:ILE:HG23	6:F:75:PRO:HD2	1.75	0.68
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.76	0.67
2:B:654:ARG:H	2:B:657:HIS:CD2	2.08	0.67
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.74	0.67
1:A:528:LEU:O	1:A:531:ILE:HG22	1.95	0.67
1:A:903:ASN:ND2	1:A:904:THR:N	2.41	0.67
1:A:1115:SER:C	1:A:1308:THR:HG22	2.19	0.67
1:A:1308:THR:HG23	1:A:1310:GLY:H	1.59	0.67
2:B:1224:PHE:CE1	5:E:171:LYS:HG3	2.29	0.67
9:I:4:PHE:CD1	9:I:4:PHE:C	2.70	0.67
1:A:102:VAL:HB	1:A:211:PHE:CZ	2.30	0.67
1:A:1223:ASP:HA	1:A:1243:VAL:HG11	1.76	0.67
1:A:1276:VAL:HG12	1:A:1277:GLU:H	1.58	0.67
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.28	0.67
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.75	0.67
1:A:33:ALA:HB3	1:A:82:GLY:HA3	1.77	0.67
1:A:709:THR:HG21	9:I:93:LYS:O	1.95	0.67
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.29	0.67
12:L:26:THR:HG23	12:L:62:LYS:HZ3	1.58	0.67
1:A:129:LYS:O	1:A:130:ASP:HB2	1.93	0.67
3:C:3:GLU:CB	11:K:104:ASN:HD21	2.07	0.67
9:I:71:SER:OG	9:I:83:ASN:HB2	1.93	0.67
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.76	0.67
1:A:732:LEU:O	1:A:736:ASN:HB2	1.95	0.67
2:B:289:LEU:HD13	2:B:375:ALA:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:942:ARG:HH22	13:T:23:BRU:H5''	1.58	0.67
2:B:1098:MET:HE3	2:B:1098:MET:H	1.59	0.67
1:A:265:LYS:HE2	1:A:302:THR:CG2	2.24	0.67
1:A:1144:LYS:HB2	1:A:1268:LEU:O	1.94	0.67
1:A:1224:LEU:HD11	1:A:1240:CYS:HB2	1.76	0.67
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.56	0.67
2:B:755:ILE:HG23	2:B:809:MET:HE3	1.76	0.67
2:B:1174:LYS:O	2:B:1176:ASN:N	2.28	0.67
14:N:2:DG:H4'	14:N:3:DT:OP1	1.93	0.67
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.25	0.67
1:A:1175:SER:O	1:A:1176:LEU:HB2	1.94	0.67
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.24	0.67
5:E:136:ASN:O	5:E:140:LEU:HG	1.95	0.67
11:K:21:ILE:HG22	11:K:31:VAL:CG1	2.24	0.67
1:A:335:ARG:CD	2:B:1202:LEU:HD23	2.25	0.67
1:A:1259:MET:HG3	1:A:1262:LYS:HZ2	1.60	0.67
2:B:430:ARG:O	2:B:434:ARG:CG	2.43	0.67
2:B:1150:ARG:HA	2:B:1154:ALA:HB3	1.77	0.67
1:A:2:VAL:HG11	2:B:1157:ALA:CB	2.25	0.67
1:A:58:LEU:HD22	1:A:80:HIS:O	1.95	0.67
1:A:630:ILE:HD11	1:A:646:PHE:HZ	1.60	0.67
1:A:647:GLY:O	1:A:651:LYS:HG3	1.94	0.67
1:A:1372:VAL:O	1:A:1376:THR:HG22	1.95	0.67
2:B:20:ASP:C	2:B:22:SER:H	2.01	0.67
2:B:35:SER:O	2:B:39:ARG:HG3	1.94	0.67
3:C:184:ASN:ND2	3:C:187:LYS:HA	2.09	0.67
7:G:23:LYS:HG3	7:G:56:ILE:CD1	2.24	0.67
2:B:769:TYR:CE1	15:P:11:U:H2'	2.30	0.66
2:B:785:TYR:CE1	2:B:795:ILE:HG12	2.30	0.66
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.24	0.66
1:A:406:ILE:HG13	1:A:431:LYS:HB2	1.75	0.66
1:A:504:LEU:HD11	6:F:91:ALA:HB1	1.77	0.66
1:A:1052:GLN:HA	1:A:1055:ARG:NH1	2.10	0.66
1:A:869:GLY:O	5:E:204:THR:HG21	1.95	0.66
2:B:102:VAL:HG11	12:L:54:ARG:NH2	2.09	0.66
2:B:294:ASP:O	2:B:296:GLU:N	2.29	0.66
2:B:416:LEU:HD11	2:B:466:TRP:CZ2	2.30	0.66
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.29	0.66
4:D:117:GLU:O	4:D:118:THR:HG23	1.94	0.66
11:K:42:LEU:HD23	11:K:42:LEU:C	2.19	0.66
1:A:335:ARG:HH11	2:B:1202:LEU:CD2	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:575:PRO:HG2	2:B:576:ASP:H	1.59	0.66
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.60	0.66
2:B:792:MET:HA	2:B:856:PHE:O	1.96	0.66
8:H:26:ILE:HG22	8:H:27:GLU:N	2.10	0.66
2:B:114:PRO:HG2	2:B:115:GLN:H	1.61	0.66
2:B:465:ASN:N	2:B:465:ASN:ND2	2.40	0.66
2:B:639:ILE:HD11	2:B:691:GLU:CG	2.26	0.66
3:C:8:VAL:HG12	3:C:9:LYS:H	1.60	0.66
8:H:125:LEU:HG	8:H:126:GLU:H	1.59	0.66
11:K:53:ASP:HB3	11:K:56:VAL:HG23	1.75	0.66
1:A:310:GLY:O	1:A:312:PRO:HD2	1.94	0.66
1:A:1120:LEU:HD22	1:A:1124:HIS:O	1.96	0.66
2:B:25:ILE:HD11	2:B:653:VAL:C	2.20	0.66
7:G:23:LYS:HG3	7:G:56:ILE:HD11	1.78	0.66
1:A:64:ASN:H	1:A:74:MET:HE3	1.59	0.66
1:A:68:GLN:C	1:A:70:CYS:H	2.04	0.66
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	1.94	0.66
2:B:164:LYS:HE2	2:B:164:LYS:N	2.11	0.66
2:B:253:THR:HG22	2:B:254:LEU:N	2.11	0.66
2:B:313:MET:HE2	2:B:390:LEU:HD11	1.76	0.66
2:B:343:ILE:HD12	2:B:347:LYS:HE2	1.77	0.66
2:B:1048:THR:OG1	2:B:1050:ILE:HD13	1.96	0.66
5:E:156:LEU:HA	5:E:160:GLU:OE1	1.95	0.66
1:A:265:LYS:HD3	1:A:303:TYR:HA	1.76	0.66
2:B:276:ILE:HA	2:B:337:ARG:O	1.95	0.66
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.76	0.66
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.77	0.66
5:E:153:HIS:HB3	5:E:196:VAL:CG1	2.26	0.66
9:I:35:VAL:HG12	9:I:36:GLU:N	2.11	0.66
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.60	0.66
10:J:64:ASN:CB	10:J:65:PRO:CD	2.71	0.66
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.31	0.66
1:A:832:ALA:HA	13:T:18:DA:C8	2.30	0.66
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.77	0.66
4:D:32:GLU:OE1	7:G:41:LYS:HE2	1.96	0.66
2:B:723:VAL:HG12	2:B:724:ASP:N	2.08	0.66
2:B:934:LYS:O	2:B:934:LYS:CG	2.41	0.66
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.30	0.66
1:A:356:ASP:OD1	1:A:358:ASN:N	2.27	0.65
2:B:57:TYR:H	2:B:57:TYR:HD1	1.41	0.65
2:B:314:LEU:O	2:B:318:VAL:HG23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:546:SER:OG	2:B:631:GLY:N	2.27	0.65
2:B:599:THR:O	2:B:603:LEU:HB2	1.96	0.65
2:B:847:ASP:C	2:B:849:GLY:H	2.02	0.65
2:B:980:PHE:HE2	2:B:1094:ARG:HB2	1.61	0.65
4:D:53:SER:H	4:D:148:LEU:HD21	1.59	0.65
4:D:134:THR:CG2	4:D:135:GLY:H	2.07	0.65
13:T:9:DC:H2"	13:T:10:DA:H8	1.58	0.65
1:A:43:GLU:HG3	1:A:48:ALA:HB3	1.78	0.65
1:A:528:LEU:HD23	1:A:751:SER:HB3	1.78	0.65
1:A:575:LYS:HD2	8:H:120:GLY:HA2	1.79	0.65
1:A:666:ILE:HD12	1:A:667:GLY:N	2.06	0.65
1:A:858:ASN:C	1:A:858:ASN:HD22	2.04	0.65
2:B:604:ARG:C	2:B:606:LYS:H	2.03	0.65
4:D:155:ARG:HH11	4:D:155:ARG:HG3	1.62	0.65
4:D:180:LEU:CD2	4:D:195:ILE:HD12	2.26	0.65
5:E:124:VAL:N	5:E:125:PRO:CD	2.59	0.65
8:H:33:GLN:NE2	8:H:35:GLN:HB2	1.98	0.65
9:I:82:GLU:O	9:I:104:LEU:HG	1.97	0.65
1:A:572:TRP:HA	1:A:576:GLN:OE1	1.96	0.65
3:C:176:ILE:HG22	3:C:177:GLU:N	2.11	0.65
4:D:173:HIS:CD2	4:D:174:PRO:HD2	2.31	0.65
8:H:81:PRO:CG	8:H:82:PRO:HD2	2.26	0.65
1:A:12:ARG:O	2:B:1194:ILE:HG22	1.96	0.65
1:A:321:PRO:O	1:A:322:VAL:HG12	1.96	0.65
1:A:1114:PRO:C	1:A:1330:ASN:HD21	2.05	0.65
2:B:243:ALA:HA	2:B:250:PHE:O	1.95	0.65
2:B:460:ALA:HB1	2:B:466:TRP:CZ3	2.30	0.65
2:B:473:MET:O	2:B:473:MET:HE3	1.97	0.65
4:D:137:ASN:HD22	4:D:137:ASN:N	1.94	0.65
4:D:155:ARG:HD3	4:D:221:TYR:CE1	2.32	0.65
9:I:4:PHE:HE1	9:I:6:PHE:HE2	1.43	0.65
1:A:682:THR:CG2	1:A:728:LYS:HE3	2.27	0.65
2:B:708:GLU:HG3	2:B:709:ASP:H	1.61	0.65
2:B:857:ARG:HH21	2:B:942:ARG:NH2	1.92	0.65
10:J:14:VAL:O	10:J:14:VAL:HG12	1.96	0.65
1:A:313:GLN:O	1:A:314:ALA:C	2.40	0.65
1:A:1424:VAL:HG13	1:A:1436:ILE:CD1	2.20	0.65
3:C:68:GLY:O	3:C:169:LYS:HB2	1.97	0.65
10:J:30:LEU:HD11	10:J:38:ARG:NH1	2.11	0.65
1:A:851:HIS:O	1:A:853:ASP:N	2.30	0.65
1:A:1036:ARG:HG2	1:A:1036:ARG:HH11	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:THR:OG1	2:B:101:MET:HE2	1.97	0.65
2:B:578:THR:H	2:B:589:VAL:CG1	2.10	0.65
2:B:872:GLU:OE1	2:B:914:LYS:HE3	1.96	0.65
2:B:1180:PHE:HB3	2:B:1191:ILE:HD12	1.78	0.65
3:C:82:TYR:CZ	3:C:161:LYS:HG2	2.32	0.65
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.32	0.65
1:A:477:PRO:HG2	1:A:521:MET:HE3	1.79	0.65
2:B:1069:PHE:H	2:B:1069:PHE:HD1	1.44	0.65
3:C:107:SER:C	3:C:109:SER:H	2.03	0.65
9:I:4:PHE:C	9:I:4:PHE:HD1	2.04	0.65
1:A:35:ILE:HA	1:A:52:GLY:O	1.97	0.65
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.26	0.65
1:A:280:GLU:C	1:A:282:ASN:H	2.04	0.65
1:A:743:VAL:O	1:A:747:VAL:HG23	1.97	0.65
2:B:387:LEU:O	2:B:392:ARG:HB2	1.97	0.65
6:F:75:PRO:O	6:F:77:ASP:O	2.15	0.65
1:A:174:ILE:HG22	1:A:175:ARG:N	2.11	0.65
1:A:227:VAL:C	1:A:228:PHE:HD2	2.05	0.65
1:A:306:ASN:ND2	1:A:322:VAL:HG12	2.12	0.65
1:A:332:LYS:HA	1:A:337:ARG:HD2	1.79	0.65
1:A:401:GLY:C	1:A:435:HIS:HD2	2.05	0.65
1:A:416:ARG:HG3	1:A:417:TYR:CE2	2.32	0.65
1:A:666:ILE:N	2:B:1026:LEU:HD13	2.08	0.65
1:A:832:ALA:HA	13:T:18:DA:N7	2.11	0.65
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.31	0.65
1:A:886:ILE:HG23	1:A:887:GLY:N	2.11	0.65
1:A:1223:ASP:HA	1:A:1243:VAL:CG1	2.27	0.65
2:B:25:ILE:HG23	2:B:658:ILE:HD11	1.79	0.65
2:B:172:ILE:HD13	2:B:178:ASN:HD22	1.61	0.65
2:B:1072:MET:HE3	2:B:1085:ILE:HD13	1.79	0.65
3:C:39:ALA:O	3:C:164:ALA:HB3	1.97	0.65
4:D:180:LEU:HD21	4:D:198:LEU:HD11	1.79	0.65
7:G:13:LEU:HD23	7:G:14:HIS:N	2.11	0.65
9:I:111:THR:HG22	9:I:112:SER:N	2.12	0.65
2:B:283:VAL:HG21	2:B:317:CYS:O	1.97	0.64
2:B:999:MET:HG3	2:B:1000:PRO:CD	2.20	0.64
3:C:181:ASP:OD2	3:C:185:LYS:N	2.30	0.64
4:D:22:GLU:H	4:D:22:GLU:CD	2.05	0.64
5:E:114:ASN:O	5:E:115:ASN:CB	2.45	0.64
6:F:118:LEU:HD12	6:F:118:LEU:O	1.97	0.64
8:H:80:ARG:HH11	11:K:57:LEU:HD21	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:13:MET:HE3	9:I:14:LEU:H	1.61	0.64
1:A:144:THR:O	1:A:146:MET:HE2	1.98	0.64
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.23	0.64
8:H:40:LEU:HB2	8:H:123:MET:HE3	1.79	0.64
1:A:65:LEU:HD22	1:A:71:GLN:OE1	1.97	0.64
1:A:233:TRP:C	1:A:235:ILE:H	2.04	0.64
1:A:356:ASP:HB2	1:A:469:ARG:NH1	2.11	0.64
1:A:384:ASN:O	1:A:386:ASP:N	2.31	0.64
2:B:956:THR:HG22	2:B:957:ASN:H	1.63	0.64
3:C:5:GLY:O	3:C:7:GLN:HG3	1.98	0.64
5:E:55:ARG:C	5:E:57:MET:N	2.55	0.64
6:F:79:ARG:HG2	6:F:79:ARG:NH1	2.11	0.64
6:F:103:MET:HE2	7:G:66:GLY:N	2.01	0.64
10:J:2:ILE:CG2	10:J:3:VAL:N	2.59	0.64
11:K:19:LEU:HD22	11:K:33:ILE:HG21	1.79	0.64
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.32	0.64
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.27	0.64
9:I:76:PRO:HD2	9:I:108:HIS:CD2	2.32	0.64
2:B:516:ASN:N	2:B:516:ASN:ND2	2.45	0.64
2:B:854:LEU:O	2:B:855:PHE:HB2	1.96	0.64
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.31	0.64
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.62	0.64
8:H:42:ILE:HG12	8:H:95:TYR:CE1	2.32	0.64
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.33	0.64
1:A:182:VAL:HG22	1:A:201:VAL:HA	1.78	0.64
1:A:903:ASN:ND2	1:A:904:THR:H	1.94	0.64
1:A:1155:ASP:OD2	1:A:1161:THR:HA	1.98	0.64
2:B:68:THR:OG1	2:B:91:SER:HB3	1.98	0.64
3:C:232:VAL:HG21	3:C:244:VAL:HG22	1.78	0.64
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.32	0.64
9:I:50:THR:HG22	9:I:51:ASN:N	2.11	0.64
1:A:62:ASP:O	1:A:63:ARG:C	2.41	0.64
1:A:233:TRP:C	1:A:235:ILE:N	2.55	0.64
2:B:1084:GLN:N	2:B:1084:GLN:NE2	2.46	0.64
1:A:567:LYS:HD3	1:A:568:PRO:HD3	1.80	0.64
1:A:1072:ILE:HD11	1:A:1368:MET:HA	1.80	0.64
1:A:1315:GLU:C	1:A:1317:MET:N	2.55	0.64
2:B:383:ASN:C	2:B:387:LEU:HD13	2.22	0.64
2:B:542:MET:HE3	2:B:636:PRO:CG	2.23	0.64
2:B:706:GLN:NE2	2:B:730:ARG:HH11	1.94	0.64
3:C:88:CYS:SG	3:C:91:HIS:C	2.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:40:LEU:HD22	8:H:123:MET:HE3	1.80	0.64
1:A:68:GLN:O	1:A:70:CYS:N	2.28	0.64
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.80	0.64
1:A:1211:GLN:O	1:A:1214:GLU:HB2	1.98	0.64
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.78	0.64
2:B:165:VAL:HG11	2:B:448:ILE:CD1	2.18	0.64
3:C:24:ASN:HA	3:C:226:ASP:HB3	1.79	0.64
4:D:68:ARG:O	4:D:72:ARG:HG3	1.98	0.64
1:A:567:LYS:HZ2	8:H:95:TYR:N	1.96	0.64
1:A:1066:VAL:O	1:A:1070:GLN:HG3	1.98	0.64
1:A:1293:SER:OG	1:A:1295:THR:HG23	1.98	0.64
2:B:53:GLN:HG2	2:B:547:VAL:CG2	2.28	0.64
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.28	0.64
2:B:755:ILE:HG23	2:B:809:MET:CE	2.28	0.64
2:B:882:THR:HG22	2:B:884:ARG:H	1.61	0.64
1:A:947:PHE:CE2	1:A:954:TRP:CE2	2.86	0.63
1:A:1141:THR:OG1	1:A:1205:LYS:HD3	1.97	0.63
1:A:1441:PHE:CE2	6:F:89:GLU:HG2	2.34	0.63
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.80	0.63
5:E:167:ARG:O	5:E:168:TYR:HD2	1.81	0.63
1:A:993:LEU:HD23	1:A:1022:LEU:HD11	1.79	0.63
1:A:1343:ALA:O	1:A:1346:ALA:HB3	1.97	0.63
2:B:865:LYS:HD2	2:B:961:LEU:HD21	1.80	0.63
5:E:124:VAL:HG13	5:E:132:ILE:CG1	2.28	0.63
1:A:1404:GLU:HB2	1:A:1408:ILE:CD1	2.29	0.63
1:A:1444:MET:HB3	7:G:59:GLY:O	1.97	0.63
2:B:520:GLY:H	2:B:748:ILE:HG22	1.62	0.63
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.80	0.63
3:C:66:ARG:HH22	10:J:2:ILE:CG2	2.12	0.63
3:C:169:LYS:NZ	12:L:69:ALA:HB3	2.12	0.63
7:G:106:MET:HG2	7:G:107:LYS:N	2.13	0.63
10:J:1:MET:H1	10:J:57:ILE:N	1.95	0.63
1:A:111:GLY:O	1:A:214:ILE:HA	1.98	0.63
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.80	0.63
1:A:443:LEU:HD11	1:A:455:MET:HB3	1.81	0.63
1:A:860:LEU:HD13	1:A:1393:ASN:HD22	1.63	0.63
2:B:130:VAL:HG23	2:B:167:ILE:HD13	1.80	0.63
2:B:363:HIS:O	2:B:364:ILE:HB	1.97	0.63
2:B:806:THR:HG23	2:B:1046:PRO:HD3	1.81	0.63
2:B:955:THR:CG2	2:B:956:THR:N	2.60	0.63
8:H:100:THR:HG22	8:H:101:ALA:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLU:O	1:A:78:PRO:HD3	1.98	0.63
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.79	0.63
1:A:93:VAL:CG2	1:A:304:MET:HE3	2.28	0.63
1:A:986:ILE:HD12	1:A:1032:LEU:HD11	1.80	0.63
2:B:53:GLN:HG2	2:B:547:VAL:HG23	1.79	0.63
2:B:785:TYR:HA	2:B:788:ARG:HG3	1.80	0.63
2:B:1178:ASN:O	2:B:1179:GLN:C	2.42	0.63
3:C:75:MET:HE1	3:C:239:PRO:CG	2.29	0.63
3:C:112:ASN:HB2	3:C:114:TYR:HE1	1.63	0.63
4:D:40:HIS:HB2	7:G:73:LYS:HD3	1.80	0.63
5:E:93:MET:HE3	5:E:123:LEU:HB2	1.78	0.63
10:J:7:CYS:O	10:J:11:GLY:HA2	1.97	0.63
1:A:1260:LEU:HD12	1:A:1260:LEU:O	1.97	0.63
2:B:860:MET:HG2	2:B:861:ASP:N	2.12	0.63
2:B:1050:ILE:HD12	2:B:1050:ILE:N	2.14	0.63
7:G:28:THR:O	7:G:32:GLU:HG3	1.98	0.63
8:H:89:LEU:O	8:H:91:ASP:N	2.29	0.63
1:A:825:ILE:CG2	1:A:826:ASP:N	2.61	0.63
2:B:469:GLN:CG	2:B:470:LYS:H	2.11	0.63
2:B:810:GLU:HA	2:B:815:ARG:HH12	1.64	0.63
5:E:106:GLN:HA	5:E:130:ALA:CB	2.29	0.63
1:A:103:CYS:SG	1:A:207:ILE:HD12	2.39	0.63
1:A:1276:VAL:HG12	1:A:1277:GLU:N	2.14	0.63
2:B:542:MET:HG2	2:B:747:MET:HE2	1.81	0.63
2:B:593:PRO:HA	2:B:596:LEU:HB3	1.81	0.63
3:C:80:LEU:HD11	3:C:95:CYS:C	2.24	0.63
3:C:241:ASP:O	3:C:245:VAL:HG23	1.99	0.63
5:E:15:ALA:O	5:E:19:VAL:HG23	1.99	0.63
5:E:128:PRO:HA	5:E:129:PRO:O	1.99	0.63
1:A:767:GLN:HB2	1:A:799:PHE:HD1	1.64	0.63
1:A:1152:ILE:HD11	9:I:44:TYR:HD2	1.63	0.63
2:B:123:THR:O	2:B:125:SER:N	2.32	0.63
2:B:186:GLU:CG	10:J:62:ARG:HH22	2.05	0.63
2:B:527:THR:OG1	2:B:528:PRO:HD2	1.99	0.63
2:B:615:MET:HB3	2:B:626:ILE:HG12	1.80	0.63
2:B:839:MET:HE2	2:B:1010:LEU:HD11	1.81	0.63
2:B:841:MET:HE1	2:B:980:PHE:CE1	2.34	0.63
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.80	0.63
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.78	0.63
4:D:66:ARG:HD2	4:D:133:THR:HB	1.80	0.63
5:E:100:ILE:HG22	5:E:100:ILE:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:82:PRO:HG3	11:K:54:ARG:HD2	1.81	0.63
12:L:68:GLU:H	12:L:68:GLU:CD	2.07	0.63
1:A:69:THR:C	1:A:71:GLN:H	2.05	0.62
1:A:504:LEU:HD11	6:F:91:ALA:CB	2.29	0.62
1:A:630:ILE:HG23	1:A:631:HIS:N	2.13	0.62
1:A:913:LEU:HD12	1:A:914:GLU:H	1.62	0.62
2:B:579:ARG:HG2	2:B:579:ARG:HH11	1.64	0.62
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.28	0.62
2:B:847:ASP:OD2	3:C:167:HIS:HD2	1.82	0.62
10:J:64:ASN:ND2	10:J:65:PRO:HD3	2.14	0.62
1:A:35:ILE:HD12	1:A:241:VAL:HG21	1.81	0.62
1:A:325:ILE:CG2	2:B:1210:MET:HE2	2.29	0.62
1:A:523:ILE:HD12	1:A:622:VAL:HG21	1.82	0.62
1:A:590:ARG:HB3	1:A:605:MET:N	2.13	0.62
1:A:814:PHE:CE1	2:B:519:TRP:HA	2.34	0.62
1:A:849:MET:HE3	1:A:1061:GLY:CA	2.28	0.62
1:A:1158:PRO:HB2	1:A:1188:GLN:HE22	1.64	0.62
2:B:878:GLN:O	2:B:934:LYS:HE2	1.99	0.62
4:D:25:ALA:C	4:D:27:LEU:H	2.06	0.62
7:G:143:ILE:CG2	7:G:144:ARG:N	2.62	0.62
8:H:84:ALA:CB	8:H:87:ARG:HD2	2.29	0.62
9:I:50:THR:HG22	9:I:51:ASN:H	1.64	0.62
10:J:48:ARG:HD2	10:J:48:ARG:C	2.23	0.62
12:L:61:THR:HG21	12:L:63:ARG:NE	2.14	0.62
1:A:25:GLU:OE1	1:A:25:GLU:N	2.32	0.62
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.32	0.62
2:B:281:PRO:O	2:B:283:VAL:N	2.33	0.62
9:I:17:ARG:HG3	9:I:28:GLU:OE1	1.99	0.62
1:A:768:GLN:CG	1:A:816:HIS:HA	2.23	0.62
1:A:902:LEU:HD11	1:A:923:LEU:HD21	1.79	0.62
1:A:1017:LEU:HB2	5:E:206:GLY:N	2.00	0.62
1:A:1412:ALA:HA	1:A:1417:GLU:OE2	1.99	0.62
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.35	0.62
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.81	0.62
7:G:114:LEU:HG	7:G:162:SER:HB3	1.81	0.62
1:A:180:LYS:HZ2	1:A:294:SER:HB3	1.64	0.62
1:A:754:SER:N	1:A:757:ASN:HD22	1.96	0.62
1:A:1340:GLY:O	1:A:1342:GLU:N	2.32	0.62
2:B:244:LEU:HD21	2:B:366:GLN:NE2	2.14	0.62
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.35	0.62
3:C:6:PRO:HB3	3:C:25:VAL:HG12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:PRO:O	3:C:134:ILE:HG13	2.00	0.62
13:T:21:DC:H2''	13:T:22:DC:C5'	2.30	0.62
1:A:50:ILE:O	1:A:52:GLY:N	2.33	0.62
1:A:115:LEU:CD1	1:A:141:LEU:HB3	2.30	0.62
1:A:259:GLU:OE1	1:A:263:THR:HG21	1.99	0.62
1:A:427:GLN:HB2	1:A:430:TRP:CD2	2.34	0.62
1:A:1279:ILE:HG22	1:A:1279:ILE:O	1.99	0.62
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.14	0.62
2:B:1002:THR:HG21	2:B:1006:ILE:HG13	1.80	0.62
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.81	0.62
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.81	0.62
7:G:1:MET:SD	7:G:79:PHE:CD1	2.92	0.62
1:A:255:SER:OG	2:B:918:ILE:HG21	1.98	0.62
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.82	0.62
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.29	0.62
1:A:1293:SER:HB2	1:A:1299:VAL:HG23	1.82	0.62
1:A:1445:ILE:H	1:A:1445:ILE:CD1	1.99	0.62
2:B:244:LEU:HD13	2:B:247:GLY:O	2.00	0.62
2:B:997:GLU:CD	2:B:997:GLU:H	2.08	0.62
2:B:1115:THR:O	2:B:1116:ARG:HB2	1.99	0.62
5:E:31:THR:CG2	5:E:34:GLU:HB2	2.29	0.62
5:E:54:GLN:O	5:E:57:MET:HB3	1.99	0.62
5:E:138:ALA:HA	5:E:141:VAL:HG23	1.82	0.62
8:H:93:TYR:HB3	8:H:144:ILE:O	2.00	0.62
13:T:10:DA:H2''	13:T:11:DA:H8	1.61	0.62
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.64	0.62
1:A:463:ILE:HD11	1:A:469:ARG:HG3	1.82	0.62
1:A:606:LEU:HG	1:A:613:ILE:HD12	1.81	0.62
1:A:857:ARG:NH2	6:F:139:PRO:HG3	2.14	0.62
2:B:331:LEU:HD23	2:B:353:LYS:HG2	1.81	0.62
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.29	0.62
4:D:59:ILE:O	4:D:63:LEU:HB2	2.00	0.62
6:F:103:MET:O	6:F:104:ASN:HB2	2.00	0.62
12:L:53:HIS:HB3	12:L:55:ILE:CD1	2.30	0.62
13:T:24:DG:H2'	13:T:25:DG:H8	1.65	0.62
1:A:438:ASP:OD1	1:A:462:VAL:HG23	2.00	0.62
1:A:744:LYS:O	1:A:748:MET:HG3	2.00	0.62
1:A:834:THR:HG21	1:A:1077:THR:HG23	1.81	0.62
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.80	0.62
2:B:211:VAL:CG2	2:B:483:LEU:HB2	2.29	0.62
2:B:276:ILE:HD13	2:B:280:ILE:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:MET:HE3	11:K:98:LEU:CD2	2.30	0.62
1:A:1140:HIS:HA	1:A:1275:GLY:HA3	1.82	0.62
2:B:521:LEU:HD13	2:B:633:VAL:HB	1.80	0.62
3:C:100:THR:HG22	3:C:101:LEU:H	1.64	0.62
3:C:258:ILE:HD11	11:K:42:LEU:HD11	1.81	0.62
6:F:70:LYS:C	6:F:72:LYS:H	2.07	0.62
7:G:1:MET:SD	7:G:2:PHE:N	2.72	0.62
7:G:153:GLN:O	7:G:154:VAL:C	2.42	0.62
8:H:109:LYS:HD2	8:H:111:LEU:CD1	2.30	0.62
12:L:34:CYS:O	12:L:34:CYS:SG	2.58	0.62
1:A:335:ARG:O	1:A:339:ASN:HB2	1.99	0.61
1:A:954:TRP:HB3	1:A:955:PRO:HD2	1.82	0.61
2:B:838:SER:HB2	2:B:989:THR:O	1.99	0.61
3:C:123:ASN:CG	3:C:125:MET:H	2.08	0.61
3:C:124:LEU:O	3:C:127:ARG:HG2	2.00	0.61
11:K:7:PHE:O	11:K:11:LEU:HD23	1.99	0.61
1:A:335:ARG:HD2	2:B:1202:LEU:HD23	1.82	0.61
1:A:1160:SER:HA	1:A:1170:ILE:CD1	2.28	0.61
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.36	0.61
2:B:167:ILE:HD12	2:B:167:ILE:N	2.14	0.61
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.15	0.61
9:I:78:CYS:O	9:I:80:SER:N	2.32	0.61
10:J:27:GLU:C	10:J:29:GLU:H	2.08	0.61
1:A:1187:GLN:HG3	1:A:1188:GLN:N	2.15	0.61
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.82	0.61
2:B:611:PRO:CG	2:B:685:LEU:HD21	2.27	0.61
2:B:882:THR:C	2:B:884:ARG:H	2.09	0.61
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.46	0.61
4:D:118:THR:OG1	4:D:121:LYS:HB2	2.00	0.61
11:K:93:SER:O	11:K:97:LYS:HG3	2.00	0.61
1:A:184:SER:HB3	1:A:199:LEU:HD23	1.83	0.61
2:B:1215:ARG:O	2:B:1216:LEU:HD23	2.00	0.61
4:D:13:ARG:O	4:D:13:ARG:HD3	1.99	0.61
1:A:40:THR:HB	1:A:41:MET:CE	2.30	0.61
1:A:65:LEU:O	1:A:71:GLN:HA	2.00	0.61
1:A:224:PHE:CE2	1:A:231:PRO:HG3	2.35	0.61
1:A:1353:TYR:CD1	1:A:1368:MET:HE1	2.35	0.61
2:B:882:THR:HG22	2:B:884:ARG:CB	2.26	0.61
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.81	0.61
6:F:77:ASP:O	6:F:78:GLN:HB2	2.01	0.61
6:F:85:MET:O	6:F:155:LEU:HD21	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:32:THR:HG22	8:H:33:GLN:N	2.15	0.61
2:B:860:MET:HG3	2:B:965:LYS:HG2	1.82	0.61
10:J:7:CYS:HA	10:J:49:MET:HE3	1.83	0.61
1:A:18:GLN:HG2	1:A:1418:LEU:HD13	1.83	0.61
1:A:93:VAL:HG21	1:A:301:ALA:O	2.01	0.61
2:B:20:ASP:O	2:B:22:SER:N	2.30	0.61
2:B:485:ARG:NH2	2:B:782:LEU:HD11	2.16	0.61
2:B:686:ASN:C	2:B:688:GLY:H	2.09	0.61
2:B:766:ARG:HG2	2:B:766:ARG:NH1	2.15	0.61
2:B:842:ASN:HD22	2:B:845:SER:CB	2.10	0.61
3:C:50:GLU:HG2	12:L:64:LEU:HD22	1.82	0.61
3:C:101:LEU:C	3:C:102:GLN:HG3	2.26	0.61
3:C:112:ASN:HB2	3:C:114:TYR:CE1	2.36	0.61
5:E:42:PHE:CZ	5:E:58:MET:HE3	2.35	0.61
7:G:30:LEU:HD13	7:G:72:VAL:HG11	1.83	0.61
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.82	0.61
8:H:81:PRO:CB	8:H:82:PRO:CD	2.77	0.61
1:A:825:ILE:HD11	2:B:512:ARG:CB	2.31	0.61
1:A:1100:ARG:NH1	1:A:1111:MET:HE3	2.11	0.61
1:A:1214:GLU:OE1	1:A:1214:GLU:HA	2.00	0.61
1:A:1308:THR:HG21	1:A:1310:GLY:O	2.01	0.61
2:B:169:ARG:HB3	2:B:169:ARG:HH11	1.65	0.61
2:B:980:PHE:CE2	2:B:1094:ARG:HB2	2.34	0.61
1:A:332:LYS:H	1:A:337:ARG:CB	2.13	0.61
1:A:531:ILE:CD1	1:A:653:VAL:HG21	2.30	0.61
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.83	0.61
1:A:1420:ASP:CB	1:A:1422:ARG:HG3	2.22	0.61
3:C:58:LEU:HD22	3:C:58:LEU:N	2.16	0.61
5:E:69:ILE:HA	5:E:72:PHE:O	2.01	0.61
8:H:12:VAL:HB	8:H:52:GLN:N	2.15	0.61
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.36	0.61
1:A:438:ASP:OD2	1:A:461:LYS:HD2	2.00	0.61
1:A:560:ILE:CD1	8:H:79:TRP:H	2.12	0.61
1:A:726:ARG:O	1:A:729:ALA:HB3	2.00	0.61
1:A:1213:GLY:HA2	1:A:1216:ILE:HG13	1.82	0.61
4:D:130:LEU:C	4:D:132:GLN:H	2.08	0.61
7:G:49:LEU:HG	7:G:76:ALA:HA	1.82	0.61
12:L:49:LYS:O	12:L:50:ASP:HB2	1.99	0.61
1:A:30:ILE:HG23	2:B:1170:THR:CG2	2.30	0.60
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.83	0.60
1:A:1343:ALA:CB	5:E:150:VAL:HG22	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:TYR:HD1	2:B:180:TYR:H	1.48	0.60
2:B:190:TYR:CE1	2:B:196:PRO:HG3	2.36	0.60
2:B:244:LEU:O	2:B:249:ARG:HG2	2.01	0.60
2:B:591:ARG:O	2:B:593:PRO:HD3	2.01	0.60
3:C:193:TYR:CD2	3:C:197:SER:HB3	2.35	0.60
3:C:242:GLN:C	3:C:244:VAL:N	2.58	0.60
5:E:173:SER:O	5:E:175:LEU:N	2.33	0.60
7:G:7:LEU:HB2	7:G:74:TYR:HE2	1.64	0.60
7:G:39:THR:HG22	7:G:41:LYS:H	1.66	0.60
1:A:418:SER:O	1:A:420:ARG:N	2.28	0.60
1:A:709:THR:HB	1:A:712:GLU:H	1.65	0.60
1:A:885:THR:O	1:A:885:THR:HG22	2.01	0.60
2:B:571:PRO:HG2	2:B:572:HIS:ND1	2.15	0.60
5:E:44:ALA:O	5:E:45:LYS:HB2	2.00	0.60
1:A:299:HIS:HA	1:A:302:THR:HG22	1.81	0.60
1:A:340:LEU:HD21	2:B:1199:ALA:HB3	1.83	0.60
1:A:666:ILE:HD11	2:B:1067:ARG:O	2.01	0.60
1:A:809:THR:HG23	1:A:812:GLU:OE1	2.00	0.60
1:A:996:ASN:O	1:A:998:LEU:HD12	2.02	0.60
2:B:57:TYR:CD1	2:B:57:TYR:N	2.70	0.60
2:B:294:ASP:C	2:B:296:GLU:H	2.09	0.60
2:B:485:ARG:CZ	2:B:782:LEU:HD11	2.31	0.60
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.31	0.60
5:E:179:GLN:HB2	5:E:182:ASP:HB2	1.83	0.60
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.37	0.60
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.65	0.60
1:A:1244:ARG:CB	1:A:1245:PRO:HA	2.14	0.60
2:B:29:ASP:CG	2:B:658:ILE:HD13	2.25	0.60
2:B:273:LEU:HD12	2:B:280:ILE:HD12	1.83	0.60
2:B:309:GLN:CD	9:I:52:ILE:HD11	2.26	0.60
3:C:46:ILE:CG2	3:C:157:CYS:HB3	2.31	0.60
3:C:261:ALA:HA	3:C:264:GLN:OE1	2.02	0.60
6:F:106:PRO:HB2	6:F:108:PHE:HE2	1.66	0.60
7:G:146:LYS:HB2	7:G:168:LEU:HD11	1.83	0.60
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.37	0.60
1:A:69:THR:O	1:A:71:GLN:N	2.34	0.60
1:A:523:ILE:HG23	1:A:527:THR:HB	1.83	0.60
2:B:850:LEU:HD12	2:B:851:PHE:H	1.67	0.60
5:E:111:VAL:HG12	5:E:137:GLU:HG2	1.83	0.60
11:K:47:ARG:HH11	11:K:47:ARG:CB	2.13	0.60
1:A:87:ALA:HB2	1:A:273:ASN:OD1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:VAL:CG1	1:A:525:GLN:H	2.15	0.60
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.01	0.60
1:A:925:LEU:HD13	1:A:983:ILE:HD12	1.84	0.60
1:A:1220:PHE:CE2	1:A:1263:ILE:HG23	2.36	0.60
1:A:1424:VAL:O	1:A:1428:VAL:HG23	2.00	0.60
1:A:1445:ILE:HD12	1:A:1445:ILE:N	2.09	0.60
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.83	0.60
2:B:288:ALA:HA	2:B:331:LEU:CD1	2.32	0.60
2:B:467:GLY:O	2:B:469:GLN:N	2.35	0.60
2:B:542:MET:SD	2:B:747:MET:HE2	2.42	0.60
2:B:766:ARG:HG3	2:B:1022:THR:HG23	1.82	0.60
3:C:102:GLN:HG2	3:C:154:LYS:HG2	1.82	0.60
12:L:61:THR:HG22	12:L:63:ARG:N	2.08	0.60
2:B:190:TYR:HD2	10:J:62:ARG:O	1.85	0.60
2:B:258:LEU:HG	2:B:258:LEU:O	2.02	0.60
2:B:393:LYS:HA	2:B:393:LYS:HE3	1.83	0.60
2:B:603:LEU:HD13	2:B:608:ASP:HB3	1.82	0.60
2:B:770:GLN:CD	2:B:983:ARG:HA	2.27	0.60
2:B:1000:PRO:O	2:B:1007:VAL:HG23	2.02	0.60
2:B:1186:ASP:O	4:D:17:LYS:HE2	2.01	0.60
3:C:13:ALA:O	11:K:114:LEU:HD22	2.01	0.60
9:I:7:CYS:HB2	9:I:34:TYR:CD2	2.37	0.60
1:A:105:CYS:O	1:A:114:LEU:HG	2.02	0.60
1:A:567:LYS:HD2	8:H:95:TYR:CG	2.36	0.60
1:A:993:LEU:CD2	1:A:1022:LEU:HD11	2.32	0.60
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.82	0.60
2:B:638:PHE:HA	2:B:690:VAL:CG2	2.20	0.60
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.83	0.60
2:B:882:THR:O	2:B:883:LEU:HB2	2.02	0.60
7:G:112:LYS:HA	7:G:115:MET:HE3	1.83	0.60
12:L:38:LEU:HD23	12:L:56:LEU:HD21	1.84	0.60
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.37	0.60
1:A:282:ASN:O	1:A:284:ALA:N	2.35	0.60
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.83	0.60
1:A:542:GLU:HG3	1:A:544:ASP:OD1	2.02	0.60
1:A:590:ARG:HG3	1:A:590:ARG:NH1	2.17	0.60
1:A:918:GLU:HG3	1:A:918:GLU:O	2.02	0.60
1:A:1161:THR:C	1:A:1163:ILE:H	2.08	0.60
2:B:95:ILE:CB	2:B:130:VAL:HG22	2.31	0.60
2:B:230:ALA:N	2:B:231:PRO:CD	2.64	0.60
2:B:327:ARG:O	2:B:331:LEU:HD13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:641:GLU:HB2	2:B:643:ASP:OD2	2.02	0.60
2:B:882:THR:CG2	2:B:935:ARG:HA	2.32	0.60
3:C:236:GLY:O	3:C:238:ILE:N	2.35	0.60
6:F:89:GLU:O	6:F:93:ILE:HG13	2.01	0.60
12:L:27:LEU:HD23	12:L:27:LEU:N	2.16	0.60
1:A:12:ARG:CZ	2:B:1192:TYR:HE2	2.15	0.60
1:A:67:CYS:O	1:A:68:GLN:HB2	2.00	0.60
1:A:262:LEU:HD21	1:A:303:TYR:CE1	2.36	0.60
1:A:845:LEU:O	1:A:846:GLU:C	2.45	0.60
1:A:1030:ARG:HG3	1:A:1034:GLU:CD	2.27	0.60
1:A:1063:MET:SD	1:A:1436:ILE:HG23	2.42	0.60
1:A:1081:LEU:CD1	1:A:1098:VAL:HG23	2.32	0.60
1:A:1202:MET:HE1	1:A:1212:VAL:CG2	2.31	0.60
5:E:17:ARG:HH11	5:E:17:ARG:CB	2.14	0.60
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.83	0.60
7:G:91:VAL:HG23	7:G:141:SER:O	2.02	0.60
7:G:145:VAL:HG12	7:G:146:LYS:N	2.15	0.60
8:H:104:PHE:CE2	8:H:136:LYS:HG2	2.37	0.60
9:I:58:VAL:O	9:I:58:VAL:HG12	1.99	0.60
1:A:276:LEU:HD13	1:A:293:GLU:HA	1.83	0.59
1:A:471:ASN:OD1	1:A:472:LEU:N	2.35	0.59
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.15	0.59
2:B:365:THR:OG1	2:B:367:LEU:HG	2.02	0.59
4:D:123:LEU:HD11	4:D:150:ASN:OD1	2.02	0.59
5:E:100:ILE:CG2	5:E:105:PHE:HB2	2.31	0.59
7:G:6:ASP:HB3	7:G:73:LYS:HZ1	1.66	0.59
8:H:139:ASN:O	8:H:140:ALA:HB2	2.02	0.59
10:J:1:MET:N	10:J:56:LEU:HB2	2.17	0.59
1:A:116:ASP:C	1:A:118:HIS:N	2.55	0.59
1:A:248:PRO:O	1:A:260:ASP:HB2	2.02	0.59
1:A:322:VAL:O	1:A:322:VAL:CG1	2.50	0.59
1:A:1315:GLU:O	1:A:1317:MET:N	2.35	0.59
2:B:596:LEU:O	2:B:600:LEU:HG	2.02	0.59
2:B:870:ILE:HG22	2:B:917:PRO:HG2	1.83	0.59
3:C:18:VAL:HG12	3:C:18:VAL:O	2.02	0.59
4:D:170:THR:CG2	4:D:172:LEU:HG	2.32	0.59
8:H:81:PRO:HB2	8:H:82:PRO:HD2	1.84	0.59
1:A:12:ARG:HB2	2:B:1218:THR:CG2	2.32	0.59
1:A:19:PHE:O	1:A:1416:ALA:HA	2.01	0.59
1:A:24:PRO:HB3	1:A:237:THR:HB	1.84	0.59
1:A:49:LYS:NZ	1:A:61:ILE:N	2.41	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:PRO:O	1:A:57:ARG:HG3	2.03	0.59
1:A:507:VAL:HG13	1:A:521:MET:HE1	1.83	0.59
1:A:865:GLN:HE21	1:A:1370:LEU:HA	1.67	0.59
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.33	0.59
1:A:1272:THR:C	1:A:1273:LEU:HD12	2.27	0.59
2:B:51:PHE:O	2:B:55:VAL:HG23	2.02	0.59
2:B:638:PHE:CB	2:B:651:LEU:HD22	2.32	0.59
8:H:12:VAL:HB	8:H:52:GLN:H	1.66	0.59
1:A:55:ASP:N	1:A:56:PRO:HD3	2.16	0.59
1:A:524:VAL:CG1	1:A:525:GLN:N	2.64	0.59
1:A:1116:LEU:HD13	1:A:1329:THR:HB	1.84	0.59
2:B:217:ARG:HD2	2:B:217:ARG:C	2.27	0.59
2:B:821:GLN:HE22	2:B:850:LEU:HD12	1.66	0.59
2:B:955:THR:OG1	12:L:55:ILE:HA	2.03	0.59
3:C:36:VAL:CG2	3:C:251:LEU:HD13	2.32	0.59
4:D:40:HIS:HB2	7:G:73:LYS:NZ	2.17	0.59
4:D:71:LYS:HA	4:D:74:GLN:CG	2.32	0.59
4:D:137:ASN:ND2	4:D:137:ASN:N	2.48	0.59
5:E:22:MET:HE3	5:E:26:ARG:HD2	1.85	0.59
5:E:180:ARG:NH2	5:E:192:ARG:HD2	2.18	0.59
7:G:138:THR:HG22	7:G:139:ILE:HG13	1.83	0.59
1:A:341:MET:CE	1:A:843:LYS:NZ	2.66	0.59
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.84	0.59
1:A:434:ARG:HG2	1:A:434:ARG:HH11	1.68	0.59
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.37	0.59
1:A:1375:MET:HE3	1:A:1384:VAL:HG23	1.84	0.59
2:B:555:ILE:HD11	2:B:587:HIS:CE1	2.38	0.59
1:A:172:PRO:HG3	1:A:185:TRP:CZ2	2.38	0.59
1:A:466:SER:O	2:B:1103:ILE:HD11	2.02	0.59
1:A:645:LEU:O	1:A:649:ILE:HG13	2.02	0.59
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	1.83	0.59
1:A:1373:ASP:HA	1:A:1376:THR:CG2	2.32	0.59
1:A:1402:PHE:O	1:A:1403:GLU:HB2	2.03	0.59
2:B:579:ARG:N	2:B:589:VAL:HG13	2.17	0.59
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.84	0.59
3:C:166:GLU:HB3	3:C:170:TRP:HZ3	1.67	0.59
4:D:52:LEU:HD12	4:D:182:SER:HB2	1.83	0.59
5:E:198:ILE:N	5:E:198:ILE:HD12	2.18	0.59
12:L:55:ILE:O	12:L:56:LEU:CB	2.48	0.59
1:A:37:PHE:N	1:A:37:PHE:CD1	2.68	0.59
1:A:418:SER:C	1:A:420:ARG:H	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1259:MET:C	1:A:1261:LYS:H	2.09	0.59
1:A:1290:LYS:O	1:A:1291:VAL:HG23	2.02	0.59
1:A:1313:LEU:O	1:A:1315:GLU:N	2.35	0.59
1:A:1345:ARG:NH1	5:E:200:ARG:NH2	2.50	0.59
1:A:1353:TYR:HD1	1:A:1368:MET:HE1	1.65	0.59
2:B:410:GLY:HA2	2:B:413:LEU:HD12	1.85	0.59
2:B:853:SER:O	2:B:854:LEU:HD23	2.02	0.59
2:B:1040:ASN:O	2:B:1042:GLY:N	2.35	0.59
3:C:137:LYS:HB2	3:C:138:GLU:OE1	2.03	0.59
8:H:118:PHE:O	8:H:120:GLY:N	2.35	0.59
11:K:18:LYS:NZ	11:K:38:GLU:HG2	2.17	0.59
1:A:445:ASN:CB	1:A:455:MET:HG2	2.32	0.59
1:A:590:ARG:O	1:A:591:PHE:HB2	2.02	0.59
1:A:825:ILE:HD11	2:B:512:ARG:CD	2.31	0.59
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.68	0.59
1:A:1377:THR:OG1	1:A:1378:GLN:N	2.36	0.59
1:A:1389:PHE:CD1	1:A:1389:PHE:C	2.80	0.59
2:B:174:LEU:HD22	2:B:202:TYR:CE1	2.37	0.59
2:B:175:ARG:HG2	2:B:175:ARG:HH11	1.67	0.59
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.33	0.59
2:B:1049:ASP:C	2:B:1050:ILE:HD12	2.28	0.59
3:C:93:ASP:OD1	3:C:122:SER:HB2	2.03	0.59
3:C:165:LYS:O	11:K:6:ARG:NH1	2.36	0.59
5:E:129:PRO:O	5:E:130:ALA:C	2.46	0.59
5:E:198:ILE:HD11	5:E:212:ARG:HB2	1.85	0.59
8:H:44:VAL:O	8:H:44:VAL:HG12	2.03	0.59
9:I:102:VAL:HA	9:I:108:HIS:O	2.03	0.59
1:A:186:LYS:O	1:A:187:LYS:HB3	2.01	0.59
1:A:466:SER:HB2	2:B:1099:VAL:CG2	2.33	0.59
1:A:468:PHE:CZ	1:A:489:LEU:HD23	2.37	0.59
1:A:477:PRO:HG2	1:A:521:MET:CE	2.33	0.59
1:A:541:ILE:N	1:A:572:TRP:O	2.35	0.59
2:B:188:ASP:O	2:B:192:LEU:HD12	2.02	0.59
2:B:326:ASP:C	2:B:328:GLU:N	2.61	0.59
2:B:1006:ILE:HD13	10:J:44:TYR:CE2	2.37	0.59
4:D:204:ASP:O	4:D:208:GLU:HB2	2.02	0.59
11:K:102:LYS:O	11:K:106:GLU:HG3	2.03	0.59
1:A:346:ASP:OD1	2:B:1108:ARG:HA	2.02	0.59
1:A:531:ILE:HD12	1:A:653:VAL:HG21	1.83	0.59
1:A:738:LYS:NZ	3:C:194:GLU:HA	2.18	0.59
1:A:898:ARG:HD3	1:A:933:TYR:CD1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1404:GLU:CB	1:A:1408:ILE:HG13	2.33	0.59
2:B:388:CYS:C	2:B:390:LEU:N	2.59	0.59
2:B:642:ASP:CA	2:B:649:LYS:HG3	2.33	0.59
2:B:773:MET:CE	2:B:985:GLY:HA2	2.32	0.59
3:C:169:LYS:HZ3	12:L:69:ALA:HB3	1.67	0.59
4:D:49:ALA:HB1	4:D:178:ALA:HB2	1.84	0.59
9:I:6:PHE:HD1	9:I:11:ASN:OD1	1.86	0.59
9:I:99:LEU:C	9:I:100:PHE:HD1	2.10	0.59
1:A:219:PHE:CD2	1:A:231:PRO:HD2	2.37	0.58
1:A:323:LYS:HD2	1:A:323:LYS:N	2.17	0.58
1:A:848:ILE:HA	1:A:857:ARG:O	2.03	0.58
1:A:1057:VAL:CG1	1:A:1058:VAL:H	2.14	0.58
1:A:1146:VAL:HG11	1:A:1207:LEU:HD12	1.86	0.58
2:B:601:ARG:C	2:B:603:LEU:H	2.11	0.58
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.33	0.58
3:C:186:LEU:HD21	3:C:224:GLN:O	2.04	0.58
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.83	0.58
11:K:23:PRO:HA	11:K:31:VAL:HG13	1.83	0.58
11:K:45:LEU:HG	11:K:94:ILE:CD1	2.32	0.58
1:A:56:PRO:O	1:A:57:ARG:CG	2.51	0.58
1:A:345:VAL:HG21	2:B:1150:ARG:NH2	2.17	0.58
1:A:744:LYS:HG2	1:A:748:MET:CE	2.31	0.58
2:B:335:GLY:CA	2:B:348:ARG:HB2	2.32	0.58
2:B:582:VAL:HG22	2:B:626:ILE:CG2	2.33	0.58
2:B:839:MET:HG3	2:B:1010:LEU:HD11	1.83	0.58
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.38	0.58
8:H:40:LEU:HD13	8:H:123:MET:HE3	1.84	0.58
10:J:32:GLU:CD	10:J:32:GLU:H	2.11	0.58
10:J:44:TYR:CD2	10:J:44:TYR:N	2.68	0.58
12:L:30:ILE:HD11	12:L:59:ALA:HB2	1.85	0.58
1:A:746:MET:HE3	2:B:1018:PRO:HG2	1.81	0.58
1:A:845:LEU:CD2	1:A:1374:VAL:HG21	2.33	0.58
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.84	0.58
1:A:1107:VAL:HG12	1:A:1107:VAL:O	2.03	0.58
2:B:336:ARG:HE	2:B:348:ARG:NH1	2.00	0.58
2:B:781:PHE:HE2	2:B:793:ALA:HB1	1.69	0.58
2:B:1002:THR:HG21	2:B:1006:ILE:CD1	2.33	0.58
3:C:107:SER:O	3:C:109:SER:N	2.30	0.58
3:C:167:HIS:CE1	12:L:70:ARG:HA	2.38	0.58
4:D:40:HIS:CB	7:G:73:LYS:NZ	2.65	0.58
1:A:107:CYS:H	1:A:114:LEU:HD21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:CG	1:A:568:PRO:HD3	2.34	0.58
2:B:171:PRO:HD2	2:B:457:LEU:CD1	2.33	0.58
2:B:519:TRP:HE1	2:B:635:ARG:NH2	2.02	0.58
2:B:622:LYS:HE2	9:I:59:VAL:CG2	2.31	0.58
2:B:811:TYR:N	2:B:811:TYR:CD1	2.70	0.58
3:C:105:GLY:HA3	3:C:148:ARG:O	2.02	0.58
8:H:23:VAL:HG22	8:H:43:ASN:HA	1.85	0.58
8:H:129:TYR:H	8:H:130:ARG:HH11	1.52	0.58
9:I:13:MET:CE	9:I:14:LEU:H	2.16	0.58
1:A:450:LEU:HD13	1:A:1074:GLU:HG2	1.84	0.58
1:A:506:ALA:HB1	1:A:508:PRO:HD2	1.85	0.58
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.69	0.58
1:A:1239:ARG:C	1:A:1240:CYS:SG	2.86	0.58
2:B:65:GLU:HG3	2:B:66:ASP:N	2.18	0.58
2:B:121:ASN:HA	2:B:207:GLY:CA	2.34	0.58
2:B:654:ARG:N	2:B:657:HIS:HD2	1.97	0.58
3:C:166:GLU:HB3	3:C:170:TRP:CZ3	2.38	0.58
3:C:238:ILE:HG22	3:C:243:VAL:HG23	1.85	0.58
14:N:4:DA:H2"	14:N:5:DC:C6	2.39	0.58
1:A:332:LYS:HG3	1:A:333:GLU:HG2	1.85	0.58
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.39	0.58
2:B:120:ARG:HE	2:B:955:THR:HG21	1.68	0.58
2:B:648:HIS:CG	2:B:649:LYS:H	2.20	0.58
2:B:1222:ARG:O	2:B:1223:ASP:HB2	2.03	0.58
3:C:3:GLU:HG3	11:K:104:ASN:OD1	2.03	0.58
3:C:173:ALA:O	3:C:174:ALA:CB	2.52	0.58
4:D:167:LEU:O	4:D:170:THR:OG1	2.21	0.58
10:J:23:ASN:O	10:J:25:LEU:N	2.36	0.58
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.33	0.58
1:A:115:LEU:O	1:A:122:MET:HG2	2.04	0.58
1:A:212:LYS:HG2	1:A:232:GLU:HB2	1.85	0.58
1:A:243:PRO:HB2	1:A:244:PRO:HD2	1.86	0.58
1:A:332:LYS:N	1:A:337:ARG:HB3	2.19	0.58
1:A:396:PRO:HB3	1:A:403:LYS:HA	1.84	0.58
1:A:1201:ALA:O	1:A:1203:ASN:N	2.35	0.58
2:B:115:GLN:HG2	2:B:193:LYS:CB	2.30	0.58
2:B:857:ARG:NH2	2:B:942:ARG:CZ	2.67	0.58
6:F:147:SER:OG	6:F:150:GLU:HG3	2.04	0.58
7:G:34:VAL:HG11	7:G:74:TYR:CE1	2.37	0.58
8:H:4:THR:HA	8:H:60:ALA:HB2	1.85	0.58
1:A:20:GLY:O	1:A:21:LEU:HD23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:LYS:HD2	1:A:750:GLY:O	2.04	0.58
1:A:1454:MET:HE3	1:A:1454:MET:O	2.03	0.58
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.69	0.58
3:C:15:LYS:HG2	3:C:15:LYS:O	2.03	0.58
3:C:174:ALA:O	3:C:175:ALA:HB2	2.04	0.58
3:C:243:VAL:O	3:C:243:VAL:HG12	2.03	0.58
4:D:130:LEU:O	4:D:132:GLN:N	2.35	0.58
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.33	0.58
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.85	0.58
1:A:385:ILE:HG22	1:A:386:ASP:N	2.18	0.58
1:A:590:ARG:CG	1:A:590:ARG:HH11	2.17	0.58
1:A:596:THR:O	1:A:598:LEU:N	2.33	0.58
1:A:1227:ILE:CG2	1:A:1228:TRP:H	2.12	0.58
2:B:229:ALA:CB	2:B:231:PRO:HD2	2.33	0.58
2:B:331:LEU:CD2	2:B:353:LYS:HG2	2.33	0.58
13:T:11:DA:H2''	13:T:12:DG:H8	1.69	0.58
1:A:115:LEU:HG	1:A:142:CYS:HB3	1.85	0.58
1:A:125:ALA:C	1:A:127:ALA:H	2.12	0.58
1:A:447:GLN:NE2	13:T:20:DG:H4'	2.19	0.58
2:B:284:ILE:HD13	2:B:333:PHE:CD2	2.39	0.58
2:B:310:MET:HE1	2:B:387:LEU:HD12	1.86	0.58
2:B:639:ILE:CG2	2:B:641:GLU:HG2	2.34	0.58
2:B:842:ASN:ND2	2:B:845:SER:HB3	2.14	0.58
2:B:866:TYR:HD1	2:B:870:ILE:O	1.86	0.58
2:B:1065:GLN:HB2	3:C:201:TRP:CZ3	2.39	0.58
2:B:1084:GLN:HG2	3:C:201:TRP:HZ2	1.66	0.58
3:C:100:THR:HG22	3:C:101:LEU:N	2.19	0.58
3:C:174:ALA:O	10:J:10:CYS:O	2.22	0.58
6:F:152:ILE:HG22	6:F:153:VAL:H	1.68	0.58
8:H:15:VAL:HG22	8:H:26:ILE:HD13	1.85	0.58
1:A:306:ASN:HD22	1:A:322:VAL:HG12	1.68	0.57
1:A:714:PHE:CB	9:I:97:MET:HE1	2.33	0.57
1:A:794:PRO:HG2	1:A:795:GLU:OE2	2.03	0.57
1:A:1201:ALA:C	1:A:1203:ASN:H	2.11	0.57
1:A:1377:THR:O	1:A:1379:GLY:N	2.36	0.57
2:B:801:LYS:N	10:J:52:THR:HG23	2.18	0.57
6:F:79:ARG:HG2	6:F:79:ARG:HH11	1.69	0.57
1:A:286:HIS:C	1:A:288:ALA:H	2.11	0.57
2:B:31:TRP:CE3	2:B:31:TRP:HA	2.39	0.57
2:B:133:LYS:HE3	2:B:135:ARG:HH21	1.70	0.57
2:B:181:LEU:HD23	2:B:189:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:TYR:CZ	2:B:355:ILE:HD11	2.39	0.57
2:B:446:LEU:O	2:B:447:ALA:HB3	2.03	0.57
2:B:508:LEU:O	2:B:509:ALA:HB2	2.03	0.57
2:B:975:GLN:O	2:B:990:ILE:HD12	2.04	0.57
3:C:236:GLY:O	3:C:237:SER:C	2.46	0.57
4:D:153:ARG:HB3	4:D:154:PHE:CD1	2.39	0.57
5:E:99:HIS:CE1	5:E:103:LYS:HG3	2.39	0.57
5:E:111:VAL:CG1	5:E:137:GLU:HG2	2.34	0.57
6:F:111:LEU:HD12	6:F:111:LEU:N	2.15	0.57
8:H:100:THR:HG23	8:H:138:GLU:CA	2.33	0.57
9:I:100:PHE:HD1	9:I:100:PHE:N	2.02	0.57
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.39	0.57
2:B:570:VAL:HG21	2:B:573:GLN:HB3	1.85	0.57
8:H:14:GLU:O	8:H:26:ILE:HG23	2.03	0.57
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.34	0.57
8:H:89:LEU:C	8:H:91:ASP:N	2.62	0.57
1:A:79:GLY:CA	1:A:243:PRO:HG3	2.34	0.57
1:A:372:LYS:HA	1:A:435:HIS:CE1	2.38	0.57
1:A:503:GLN:C	1:A:504:LEU:HD12	2.29	0.57
1:A:709:THR:HG22	1:A:710:LEU:N	2.19	0.57
1:A:729:ALA:HA	1:A:732:LEU:HD12	1.87	0.57
1:A:804:TYR:HE1	2:B:1021:MET:HE3	1.69	0.57
1:A:1152:ILE:CD1	9:I:44:TYR:HD2	2.17	0.57
1:A:1213:GLY:HA2	1:A:1216:ILE:CG1	2.34	0.57
1:A:1394:THR:CG2	1:A:1398:MET:SD	2.92	0.57
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.39	0.57
2:B:498:THR:O	2:B:536:VAL:HA	2.05	0.57
5:E:83:CYS:C	5:E:85:GLU:H	2.11	0.57
8:H:127:GLY:O	8:H:128:ASN:HB2	2.04	0.57
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.37	0.57
1:A:53:LEU:CD2	1:A:54:ASN:HB3	2.34	0.57
1:A:740:LEU:HD12	1:A:741:ASN:N	2.20	0.57
1:A:1187:GLN:HG3	1:A:1188:GLN:H	1.68	0.57
2:B:278:GLN:HG2	2:B:279:ASP:H	1.69	0.57
2:B:309:GLN:O	2:B:312:GLU:HB3	2.04	0.57
2:B:333:PHE:CE1	2:B:337:ARG:NH2	2.73	0.57
5:E:91:LYS:C	5:E:93:MET:H	2.13	0.57
10:J:23:ASN:C	10:J:25:LEU:N	2.59	0.57
1:A:469:ARG:NH1	1:A:469:ARG:HB3	2.19	0.57
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.86	0.57
1:A:1284:MET:O	1:A:1285:MET:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:899:ILE:HD11	2:B:910:VAL:O	2.05	0.57
2:B:1200:ALA:HA	2:B:1203:LEU:HB3	1.87	0.57
6:F:111:LEU:H	6:F:111:LEU:CD1	2.13	0.57
7:G:116:PRO:HG2	7:G:119:LEU:HB2	1.86	0.57
10:J:24:LEU:HA	10:J:28:ASP:HB2	1.86	0.57
1:A:335:ARG:HH11	2:B:1202:LEU:HD23	1.68	0.57
1:A:537:ARG:HH12	8:H:122:LEU:HG	1.70	0.57
1:A:786:HIS:HE1	2:B:519:TRP:CZ2	2.22	0.57
2:B:167:ILE:HG22	2:B:453:ILE:CD1	2.33	0.57
2:B:188:ASP:C	2:B:192:LEU:HD12	2.30	0.57
2:B:589:VAL:HG12	2:B:590:HIS:H	1.69	0.57
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.35	0.57
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.37	0.57
3:C:58:LEU:H	3:C:58:LEU:CD2	2.18	0.57
7:G:59:GLY:HA3	7:G:70:PHE:CD2	2.39	0.57
7:G:140:LYS:O	7:G:141:SER:C	2.47	0.57
10:J:7:CYS:SG	10:J:49:MET:HE3	2.44	0.57
11:K:6:ARG:O	11:K:9:LEU:HG	2.05	0.57
1:A:594:GLY:H	1:A:603:ASN:ND2	2.02	0.57
1:A:774:ARG:NH2	1:A:797:LYS:HB2	2.19	0.57
1:A:913:LEU:HD11	1:A:981:LEU:O	2.04	0.57
1:A:1103:GLU:O	1:A:1108:ALA:HB2	2.05	0.57
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.05	0.57
6:F:86:THR:HG23	6:F:89:GLU:OE1	2.04	0.57
7:G:119:LEU:HD12	7:G:132:SER:HB2	1.86	0.57
8:H:125:LEU:HG	8:H:126:GLU:N	2.20	0.57
11:K:63:VAL:HG23	11:K:63:VAL:O	2.05	0.57
1:A:325:ILE:HG21	2:B:1210:MET:HE2	1.87	0.57
1:A:409:SER:O	1:A:411:ASP:N	2.38	0.57
1:A:808:LEU:HD23	1:A:813:PHE:CA	2.33	0.57
1:A:947:PHE:N	1:A:947:PHE:CD1	2.73	0.57
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.05	0.57
2:B:601:ARG:HD3	2:B:605:ARG:HH21	1.69	0.57
2:B:638:PHE:HB3	2:B:651:LEU:HD22	1.87	0.57
3:C:241:ASP:O	3:C:244:VAL:HB	2.04	0.57
5:E:17:ARG:O	5:E:21:GLU:HG3	2.04	0.57
5:E:182:ASP:O	5:E:185:ALA:HB3	2.05	0.57
9:I:69:PRO:HG2	9:I:85:PHE:CD2	2.39	0.57
10:J:1:MET:N	10:J:56:LEU:N	2.53	0.57
1:A:108:MET:HA	1:A:210:ILE:CG2	2.35	0.57
1:A:1005:GLU:HG3	1:A:1006:ILE:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:LEU:HD23	2:B:189:LEU:CD2	2.35	0.57
2:B:635:ARG:HB2	2:B:636:PRO:HD2	1.86	0.57
3:C:33:LEU:O	3:C:34:ARG:C	2.48	0.57
4:D:51:ASN:OD1	4:D:54:GLU:HB3	2.05	0.57
5:E:144:ILE:HG13	5:E:145:THR:H	1.69	0.57
12:L:26:THR:HG22	12:L:27:LEU:N	2.20	0.57
1:A:564:ALA:O	8:H:97:MET:HA	2.05	0.56
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.34	0.56
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.29	0.56
2:B:299:GLU:HG2	2:B:571:PRO:HG3	1.87	0.56
2:B:594:ALA:HA	2:B:617:ARG:NH1	2.18	0.56
2:B:1095:LEU:C	2:B:1096:ARG:O	2.46	0.56
2:B:1146:PHE:CE1	2:B:1150:ARG:HD3	2.39	0.56
3:C:25:VAL:HG22	3:C:228:PHE:HE1	1.70	0.56
4:D:51:ASN:O	4:D:52:LEU:C	2.48	0.56
1:A:2:VAL:HG11	2:B:1157:ALA:C	2.31	0.56
1:A:32:VAL:HG21	1:A:68:GLN:HE22	1.70	0.56
1:A:52:GLY:O	1:A:56:PRO:HG2	2.05	0.56
1:A:157:ASP:C	1:A:159:THR:H	2.12	0.56
1:A:340:LEU:CD2	2:B:1199:ALA:HB3	2.36	0.56
1:A:899:VAL:HG13	1:A:908:LEU:HD21	1.87	0.56
2:B:315:LYS:HZ2	9:I:1:MET:HE1	1.69	0.56
2:B:613:VAL:HG13	2:B:627:PHE:C	2.30	0.56
2:B:615:MET:HA	2:B:625:LYS:O	2.05	0.56
2:B:847:ASP:C	2:B:849:GLY:N	2.63	0.56
2:B:980:PHE:HD2	2:B:1094:ARG:HA	1.70	0.56
3:C:2:SER:O	3:C:3:GLU:HB2	2.06	0.56
3:C:51:VAL:HB	12:L:65:VAL:HG23	1.85	0.56
10:J:2:ILE:O	10:J:53:HIS:NE2	2.38	0.56
1:A:78:PRO:HB2	2:B:1201:LYS:HE3	1.87	0.56
1:A:150:THR:HG22	1:A:150:THR:O	2.05	0.56
1:A:186:LYS:O	1:A:194:ALA:HB1	2.05	0.56
1:A:252:PHE:O	1:A:256:GLN:HB2	2.06	0.56
1:A:427:GLN:HB2	1:A:430:TRP:CD1	2.39	0.56
1:A:446:ARG:HB2	1:A:487:MET:SD	2.45	0.56
1:A:833:GLU:HG3	1:A:1102:LYS:HZ2	1.69	0.56
1:A:889:SER:HA	1:A:1297:GLU:N	2.21	0.56
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.69	0.56
1:A:947:PHE:N	1:A:947:PHE:HD1	2.02	0.56
1:A:979:SER:OG	1:A:980:ASP:N	2.37	0.56
2:B:364:ILE:CG1	2:B:585:VAL:HG13	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:750:GLY:O	2:B:751:VAL:C	2.47	0.56
2:B:1034:VAL:C	2:B:1036:ALA:H	2.13	0.56
3:C:66:ARG:NH1	10:J:2:ILE:CG2	2.56	0.56
3:C:73:GLN:HB3	3:C:131:HIS:H	1.70	0.56
3:C:146:LYS:C	3:C:147:LEU:HD23	2.30	0.56
4:D:126:ILE:HD13	4:D:145:MET:HE3	1.85	0.56
5:E:9:ILE:HD11	5:E:53:PRO:HD3	1.85	0.56
5:E:180:ARG:HB2	5:E:215:MET:OXT	2.04	0.56
7:G:9:LEU:HD12	7:G:10:ASN:H	1.70	0.56
7:G:85:GLU:HB3	7:G:147:ILE:HD12	1.87	0.56
8:H:64:ASN:HD22	8:H:88:SER:HB2	1.68	0.56
10:J:36:LEU:HB2	10:J:47:ARG:NH1	2.20	0.56
13:T:15:DC:H2''	13:T:16:DT:C7	2.33	0.56
1:A:22:PHE:HE2	1:A:30:ILE:HD12	1.71	0.56
1:A:90:VAL:HG12	1:A:297:GLN:NE2	2.21	0.56
1:A:401:GLY:C	1:A:435:HIS:CD2	2.83	0.56
1:A:767:GLN:OE1	1:A:799:PHE:HB2	2.04	0.56
1:A:871:ASP:OD2	1:A:873:MET:HB2	2.06	0.56
1:A:1042:PHE:CE2	1:A:1046:LEU:HD11	2.41	0.56
2:B:224:GLN:NE2	2:B:403:LYS:HD3	2.20	0.56
1:A:358:ASN:ND2	2:B:833:TYR:OH	2.39	0.56
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.86	0.56
1:A:466:SER:HB2	2:B:1099:VAL:HG21	1.87	0.56
1:A:717:ASN:HA	1:A:720:ARG:HH12	1.70	0.56
1:A:818:MET:HA	2:B:514:LEU:HB3	1.88	0.56
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.36	0.56
2:B:360:PHE:O	2:B:361:LEU:C	2.49	0.56
2:B:365:THR:HG23	2:B:367:LEU:H	1.70	0.56
2:B:766:ARG:HG2	2:B:766:ARG:HH11	1.70	0.56
3:C:57:VAL:HG11	10:J:60:PHE:CB	2.31	0.56
3:C:112:ASN:CB	3:C:114:TYR:CE1	2.89	0.56
3:C:167:HIS:HA	11:K:6:ARG:HH12	1.71	0.56
5:E:171:LYS:HG2	5:E:174:GLN:OE1	2.06	0.56
6:F:138:LEU:O	6:F:140:ASP:N	2.38	0.56
7:G:48:VAL:HA	7:G:76:ALA:HB2	1.86	0.56
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.69	0.56
1:A:860:LEU:CD1	1:A:1393:ASN:HD22	2.18	0.56
1:A:986:ILE:CD1	1:A:1032:LEU:HD11	2.36	0.56
2:B:562:GLY:HA3	2:B:590:HIS:ND1	2.20	0.56
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.87	0.56
3:C:213:PRO:HG2	3:C:214:ASN:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:50:LEU:HD11	7:G:4:ILE:HD11	1.88	0.56
7:G:14:HIS:ND1	7:G:15:PRO:HD2	2.20	0.56
1:A:41:MET:SD	1:A:42:ASP:N	2.78	0.56
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.36	0.56
1:A:180:LYS:HZ1	1:A:294:SER:HB3	1.69	0.56
1:A:583:PRO:HG2	1:A:586:ILE:HG13	1.87	0.56
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.71	0.56
2:B:652:LYS:O	2:B:689:LEU:HD22	2.05	0.56
2:B:1159:ARG:NE	2:B:1193:GLN:HE21	2.04	0.56
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.35	0.56
5:E:181:ALA:O	5:E:182:ASP:C	2.49	0.56
11:K:18:LYS:HZ2	11:K:38:GLU:HG2	1.70	0.56
1:A:244:PRO:HG2	1:A:245:PRO:HD3	1.86	0.56
1:A:560:ILE:HD11	8:H:79:TRP:N	2.18	0.56
3:C:11:ARG:H	3:C:20:PHE:HA	1.69	0.56
3:C:123:ASN:HD21	3:C:125:MET:HA	1.70	0.56
4:D:24:ALA:C	4:D:26:THR:N	2.58	0.56
4:D:27:LEU:HD22	4:D:173:HIS:ND1	2.21	0.56
4:D:118:THR:CG2	4:D:121:LYS:HD2	2.32	0.56
5:E:145:THR:HG21	5:E:187:TYR:CD2	2.41	0.56
1:A:427:GLN:HB2	1:A:430:TRP:CG	2.40	0.56
1:A:446:ARG:HB3	1:A:478:TYR:HB3	1.88	0.56
1:A:993:LEU:HD22	1:A:1046:LEU:CD2	2.36	0.56
1:A:1019:CYS:O	1:A:1022:LEU:HB3	2.05	0.56
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.87	0.56
3:C:123:ASN:C	3:C:125:MET:H	2.12	0.56
5:E:144:ILE:HG13	5:E:145:THR:N	2.20	0.56
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.87	0.56
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.45	0.56
1:A:901:LEU:N	1:A:926:GLN:NE2	2.43	0.56
1:A:1198:ASP:HB3	1:A:1201:ALA:CB	2.35	0.56
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.06	0.56
1:A:1313:LEU:C	1:A:1315:GLU:H	2.14	0.56
2:B:32:ALA:O	2:B:35:SER:HB2	2.05	0.56
2:B:405:ARG:HA	2:B:631:GLY:O	2.06	0.56
5:E:124:VAL:H	5:E:125:PRO:HD2	1.69	0.56
5:E:156:LEU:HD12	5:E:195:VAL:CB	2.33	0.56
7:G:106:MET:HE3	7:G:108:VAL:CG2	2.36	0.56
8:H:111:LEU:HA	8:H:127:GLY:O	2.06	0.56
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.28	0.55
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:GLN:HG2	1:A:549:MET:HE2	1.87	0.55
1:A:696:GLU:OE2	1:A:702:LEU:HD21	2.06	0.55
1:A:1009:ASN:HA	1:A:1012:ARG:HH11	1.68	0.55
1:A:1120:LEU:HD11	1:A:1304:TRP:O	2.05	0.55
2:B:555:ILE:HG22	2:B:556:THR:N	2.19	0.55
2:B:844:SER:O	2:B:847:ASP:HB2	2.05	0.55
8:H:102:TYR:OH	8:H:122:LEU:HD22	2.06	0.55
1:A:613:ILE:O	1:A:614:PHE:HB3	2.04	0.55
1:A:960:ILE:O	1:A:963:ILE:HG22	2.06	0.55
1:A:1107:VAL:CG2	1:A:1383:SER:HB3	2.36	0.55
2:B:510:LYS:CB	2:B:511:PRO:HD3	2.36	0.55
2:B:604:ARG:C	2:B:606:LYS:N	2.64	0.55
2:B:1192:TYR:CD2	2:B:1218:THR:HG21	2.41	0.55
3:C:37:MET:HE3	3:C:176:ILE:HD13	1.88	0.55
3:C:42:PRO:HB3	3:C:161:LYS:HE3	1.89	0.55
3:C:66:ARG:CZ	10:J:2:ILE:HG21	2.34	0.55
4:D:156:ASP:HB3	4:D:159:THR:OG1	2.06	0.55
6:F:136:ARG:O	6:F:143:PHE:CB	2.52	0.55
8:H:102:TYR:CD2	8:H:102:TYR:N	2.68	0.55
9:I:100:PHE:N	9:I:100:PHE:CD1	2.72	0.55
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.36	0.55
13:T:19:8OG:H2"	13:T:19:8OG:N3	2.20	0.55
1:A:189:ARG:O	1:A:190:ALA:HB3	2.06	0.55
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.40	0.55
1:A:1267:MET:O	1:A:1271:ILE:HB	2.07	0.55
2:B:102:VAL:O	2:B:102:VAL:HG12	2.06	0.55
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.36	0.55
2:B:773:MET:SD	2:B:987:LYS:HG2	2.46	0.55
2:B:778:MET:HE2	2:B:1094:ARG:CG	2.34	0.55
2:B:873:THR:O	2:B:914:LYS:HA	2.05	0.55
5:E:98:ILE:O	5:E:102:GLU:HG3	2.07	0.55
5:E:109:ILE:HG22	5:E:110:PHE:N	2.21	0.55
12:L:53:HIS:O	12:L:55:ILE:HD13	2.07	0.55
1:A:606:LEU:HB3	1:A:614:PHE:CD2	2.42	0.55
1:A:675:THR:O	1:A:679:ILE:HG13	2.07	0.55
1:A:719:VAL:O	1:A:720:ARG:C	2.48	0.55
1:A:825:ILE:CG2	1:A:826:ASP:H	2.18	0.55
2:B:785:TYR:CD1	2:B:795:ILE:HG12	2.42	0.55
5:E:23:VAL:HG13	5:E:78:LEU:CD1	2.36	0.55
5:E:78:LEU:HD23	5:E:79:TRP:N	2.21	0.55
8:H:118:PHE:C	8:H:120:GLY:H	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:GLU:C	1:A:282:ASN:N	2.65	0.55
1:A:511:ILE:HG21	1:A:634:THR:HG21	1.87	0.55
2:B:185:THR:O	2:B:186:GLU:C	2.49	0.55
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.71	0.55
2:B:705:MET:HA	2:B:705:MET:HE3	1.89	0.55
3:C:73:GLN:NE2	3:C:74:SER:H	2.04	0.55
3:C:100:THR:HG22	3:C:102:GLN:HE21	1.71	0.55
6:F:103:MET:HE1	7:G:65:ASP:HB2	1.87	0.55
9:I:95:THR:HG22	9:I:96:SER:O	2.07	0.55
12:L:38:LEU:CD1	12:L:49:LYS:HG2	2.36	0.55
1:A:144:THR:O	1:A:146:MET:HG3	2.07	0.55
1:A:310:GLY:C	1:A:312:PRO:HD2	2.31	0.55
1:A:1076:ALA:HA	1:A:1079:MET:HE2	1.89	0.55
2:B:243:ALA:CB	2:B:251:ILE:HG12	2.36	0.55
2:B:289:LEU:HD22	2:B:371:GLU:O	2.07	0.55
2:B:345:LYS:HA	2:B:348:ARG:HG2	1.88	0.55
2:B:616:ILE:CD1	2:B:625:LYS:HB2	2.36	0.55
2:B:773:MET:HE2	2:B:985:GLY:HA2	1.89	0.55
3:C:50:GLU:HG2	3:C:50:GLU:O	2.06	0.55
3:C:166:GLU:C	11:K:6:ARG:NH1	2.64	0.55
5:E:167:ARG:O	5:E:168:TYR:CD2	2.60	0.55
9:I:85:PHE:CD2	9:I:85:PHE:N	2.63	0.55
11:K:79:GLU:HG3	11:K:80:GLY:H	1.72	0.55
1:A:108:MET:HB3	1:A:210:ILE:CD1	2.27	0.55
1:A:1057:VAL:CG1	1:A:1058:VAL:N	2.70	0.55
2:B:590:HIS:CD2	2:B:596:LEU:HD22	2.42	0.55
4:D:19:GLU:O	4:D:20:GLU:C	2.50	0.55
5:E:128:PRO:HA	5:E:129:PRO:C	2.31	0.55
13:T:7:DC:H2''	13:T:8:DT:C7	2.36	0.55
13:T:18:DA:H3'	13:T:18:DA:OP1	2.06	0.55
1:A:34:LYS:HB3	1:A:36:ARG:HH21	1.72	0.55
1:A:381:THR:CG2	1:A:382:PRO:HD2	2.37	0.55
1:A:496:GLU:O	1:A:499:ALA:HB3	2.06	0.55
1:A:506:ALA:HB3	1:A:509:LEU:HD12	1.88	0.55
1:A:512:VAL:HA	1:A:519:PRO:HA	1.88	0.55
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.69	0.55
3:C:178:PHE:HE1	3:C:230:MET:HE2	1.72	0.55
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.87	0.55
4:D:40:HIS:HB2	7:G:73:LYS:CD	2.37	0.55
4:D:138:ASN:HD21	7:G:35:GLU:HB3	1.71	0.55
5:E:103:LYS:HB3	5:E:105:PHE:CE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:79:GLU:HG3	11:K:80:GLY:N	2.22	0.55
12:L:43:THR:HG22	12:L:43:THR:O	2.07	0.55
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.29	0.55
1:A:470:LEU:H	1:A:470:LEU:CD2	2.18	0.55
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.46	0.55
1:A:1130:GLN:HG3	1:A:1134:ILE:CD1	2.36	0.55
1:A:1341:ILE:O	1:A:1344:GLY:N	2.40	0.55
1:A:1396:ALA:HA	1:A:1399:ARG:NH2	2.22	0.55
2:B:565:PRO:O	2:B:567:GLU:N	2.39	0.55
2:B:1159:ARG:HE	2:B:1193:GLN:HE21	1.54	0.55
3:C:175:ALA:HB2	10:J:10:CYS:CB	2.37	0.55
5:E:13:TRP:CZ3	5:E:39:LEU:HB2	2.41	0.55
5:E:117:THR:HG22	5:E:119:SER:N	2.14	0.55
6:F:108:PHE:HE1	6:F:131:PRO:HG3	1.72	0.55
7:G:17:PHE:N	7:G:17:PHE:CD2	2.74	0.55
1:A:42:ASP:C	1:A:44:THR:N	2.65	0.55
1:A:267:ALA:O	1:A:271:LYS:HG3	2.06	0.55
1:A:555:ASP:O	1:A:556:TRP:C	2.50	0.55
1:A:1067:LEU:O	1:A:1068:ALA:C	2.48	0.55
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.42	0.55
2:B:343:ILE:O	2:B:345:LYS:N	2.39	0.55
2:B:449:ASN:O	2:B:451:LYS:N	2.40	0.55
2:B:562:GLY:O	2:B:590:HIS:ND1	2.38	0.55
2:B:570:VAL:CG2	2:B:573:GLN:HB3	2.37	0.55
2:B:839:MET:HG3	2:B:1010:LEU:CD1	2.37	0.55
2:B:948:ILE:CD1	12:L:67:PHE:HE2	2.20	0.55
2:B:1122:ARG:HB3	13:T:22:DC:OP1	2.06	0.55
3:C:7:GLN:HG2	11:K:104:ASN:HD22	1.72	0.55
3:C:107:SER:C	3:C:109:SER:N	2.65	0.55
5:E:42:PHE:HZ	5:E:58:MET:HE3	1.72	0.55
6:F:99:LEU:HD11	6:F:103:MET:HE2	1.88	0.55
1:A:18:GLN:NE2	1:A:228:PHE:CE1	2.75	0.54
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.43	0.54
1:A:598:LEU:O	1:A:599:SER:C	2.50	0.54
1:A:734:GLU:C	1:A:736:ASN:H	2.14	0.54
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.72	0.54
1:A:1404:GLU:HB2	1:A:1408:ILE:HG13	1.88	0.54
2:B:378:LEU:O	2:B:378:LEU:HD12	2.07	0.54
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.88	0.54
2:B:515:HIS:CD2	2:B:517:THR:H	2.14	0.54
2:B:542:MET:HG2	2:B:747:MET:CE	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:641:GLU:C	2:B:643:ASP:H	2.14	0.54
2:B:696:GLU:O	2:B:699:GLU:HB2	2.06	0.54
2:B:776:GLN:O	2:B:1095:LEU:HB3	2.07	0.54
2:B:792:MET:HE2	2:B:857:ARG:NH2	2.21	0.54
2:B:857:ARG:HH21	2:B:942:ARG:CZ	2.20	0.54
2:B:898:LEU:HD13	2:B:952:VAL:CG1	2.36	0.54
2:B:1063:GLY:O	3:C:202:PRO:HG2	2.07	0.54
3:C:215:GLU:O	3:C:216:GLY:C	2.49	0.54
6:F:117:PRO:C	6:F:119:ARG:H	2.15	0.54
9:I:6:PHE:N	9:I:6:PHE:CD2	2.71	0.54
10:J:1:MET:H3	10:J:56:LEU:HB2	1.72	0.54
2:B:405:ARG:NE	2:B:629:ASP:OD2	2.37	0.54
2:B:488:TYR:CE2	2:B:813:LYS:HB2	2.42	0.54
2:B:520:GLY:N	2:B:748:ILE:HG22	2.22	0.54
2:B:1031:LEU:HA	2:B:1055:ILE:HD13	1.90	0.54
2:B:1038:SER:O	10:J:33:GLY:HA3	2.07	0.54
8:H:83:GLN:C	8:H:85:GLY:H	2.15	0.54
9:I:106:CYS:O	9:I:107:SER:HB2	2.05	0.54
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.36	0.54
1:A:279:LEU:HB3	1:A:289:ILE:HG12	1.89	0.54
1:A:548:ASN:HA	11:K:60:ALA:HB1	1.90	0.54
1:A:1028:THR:O	1:A:1032:LEU:HD12	2.07	0.54
1:A:1054:LEU:O	1:A:1057:VAL:HG23	2.07	0.54
1:A:1158:PRO:O	1:A:1159:ARG:HG2	2.08	0.54
2:B:284:ILE:HG23	2:B:324:ILE:CD1	2.36	0.54
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.42	0.54
2:B:906:SER:HA	2:B:946:ASN:HB2	1.90	0.54
2:B:953:LEU:HD23	2:B:965:LYS:O	2.07	0.54
4:D:70:PHE:O	4:D:74:GLN:HG3	2.07	0.54
5:E:52:ARG:HB3	5:E:53:PRO:CD	2.38	0.54
5:E:134:THR:C	5:E:135:PHE:HD1	2.15	0.54
8:H:82:PRO:HG3	11:K:54:ARG:NH1	2.23	0.54
1:A:7:SER:C	1:A:9:ALA:H	2.16	0.54
1:A:40:THR:CB	1:A:41:MET:HE2	2.35	0.54
1:A:54:ASN:HB2	1:A:247:ARG:HH12	1.73	0.54
1:A:233:TRP:O	1:A:235:ILE:N	2.40	0.54
1:A:456:MET:HE1	1:A:521:MET:CE	2.37	0.54
2:B:948:ILE:HD11	12:L:67:PHE:HE2	1.73	0.54
2:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.88	0.54
2:B:1182:CYS:O	2:B:1183:LYS:O	2.24	0.54
3:C:13:ALA:O	11:K:114:LEU:HD13	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:ARG:HG2	3:C:149:LYS:H	1.71	0.54
7:G:47:CYS:O	7:G:76:ALA:HB1	2.07	0.54
8:H:11:GLN:O	8:H:28:ALA:HB1	2.08	0.54
1:A:963:ILE:HD13	1:A:1049:ILE:CG1	2.36	0.54
1:A:1265:ASN:O	1:A:1266:THR:C	2.51	0.54
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.89	0.54
2:B:65:GLU:HG3	2:B:66:ASP:OD1	2.06	0.54
2:B:648:HIS:CG	2:B:649:LYS:N	2.76	0.54
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.41	0.54
5:E:124:VAL:HA	5:E:132:ILE:CD1	2.36	0.54
9:I:35:VAL:HG12	9:I:36:GLU:H	1.71	0.54
1:A:254:GLU:HB2	2:B:935:ARG:NH2	2.22	0.54
1:A:663:SER:OG	1:A:664:THR:N	2.40	0.54
1:A:711:ARG:O	1:A:714:PHE:HB3	2.07	0.54
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.38	0.54
2:B:455:SER:O	2:B:456:GLY:C	2.49	0.54
2:B:1133:MET:HE2	2:B:1133:MET:HA	1.90	0.54
3:C:43:THR:O	3:C:77:ILE:HG13	2.08	0.54
3:C:147:LEU:HD23	3:C:147:LEU:N	2.23	0.54
10:J:7:CYS:CA	10:J:49:MET:HE3	2.38	0.54
11:K:27:ALA:HB1	11:K:28:PRO:HD2	1.90	0.54
12:L:36:SER:O	12:L:37:LYS:C	2.51	0.54
1:A:61:ILE:HG22	1:A:62:ASP:H	1.73	0.54
1:A:383:TYR:N	1:A:383:TYR:CD2	2.74	0.54
1:A:630:ILE:HD11	1:A:646:PHE:CZ	2.43	0.54
1:A:683:ILE:HG21	1:A:801:GLU:CD	2.32	0.54
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.43	0.54
1:A:1370:LEU:O	1:A:1373:ASP:HB2	2.08	0.54
3:C:132:PRO:O	3:C:133:ILE:C	2.49	0.54
7:G:49:LEU:CD2	7:G:77:VAL:HG23	2.21	0.54
7:G:88:ASP:HB3	7:G:144:ARG:CB	2.38	0.54
1:A:113:LEU:C	1:A:114:LEU:HD23	2.32	0.54
1:A:1151:GLU:HG2	9:I:45:ARG:CB	2.37	0.54
2:B:215:GLN:OE1	2:B:479:VAL:HG22	2.07	0.54
2:B:266:ALA:O	2:B:268:THR:HG22	2.08	0.54
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.89	0.54
7:G:88:ASP:HB3	7:G:144:ARG:CA	2.36	0.54
8:H:82:PRO:O	8:H:84:ALA:N	2.38	0.54
10:J:2:ILE:HG22	10:J:3:VAL:N	2.23	0.54
14:N:6:DT:H2"	14:N:7:DT:OP2	2.06	0.54
1:A:193:ASP:O	1:A:194:ALA:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:GLN:O	1:A:312:PRO:C	2.50	0.54
1:A:345:VAL:HG21	2:B:1150:ARG:HH22	1.73	0.54
1:A:488:ASN:OD1	2:B:1128:LEU:HD13	2.08	0.54
1:A:489:LEU:C	1:A:489:LEU:HD12	2.32	0.54
1:A:783:THR:HG21	1:A:815:PHE:CZ	2.42	0.54
1:A:1158:PRO:CB	1:A:1188:GLN:HE22	2.20	0.54
2:B:44:VAL:O	2:B:45:SER:C	2.51	0.54
4:D:60:LYS:CE	4:D:126:ILE:HD11	2.38	0.54
6:F:70:LYS:O	6:F:72:LYS:HD2	2.08	0.54
11:K:53:ASP:OD1	11:K:55:LYS:HB2	2.07	0.54
12:L:30:ILE:HG22	12:L:31:CYS:H	1.71	0.54
15:P:3:U:H2'	15:P:4:C:C6	2.43	0.54
1:A:9:ALA:HB3	2:B:1193:GLN:HB2	1.89	0.54
1:A:24:PRO:HD3	1:A:233:TRP:CD1	2.42	0.54
1:A:41:MET:O	1:A:42:ASP:O	2.26	0.54
1:A:741:ASN:ND2	1:A:744:LYS:N	2.54	0.54
1:A:1015:VAL:O	1:A:1017:LEU:N	2.41	0.54
1:A:1104:ILE:HG21	1:A:1352:VAL:HG22	1.90	0.54
1:A:1344:GLY:O	1:A:1345:ARG:C	2.50	0.54
2:B:613:VAL:CG2	2:B:628:THR:HA	2.38	0.54
3:C:191:TYR:HB3	3:C:201:TRP:CD1	2.43	0.54
4:D:64:VAL:HG22	4:D:129:LEU:HD22	1.89	0.54
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.32	0.54
7:G:87:VAL:HB	7:G:103:VAL:HG11	1.90	0.54
7:G:127:PRO:HG3	7:G:139:ILE:CD1	2.38	0.54
8:H:10:PHE:O	8:H:54:SER:HA	2.08	0.54
13:T:18:DA:HI'	13:T:19:8OG:C5'	2.37	0.54
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.90	0.53
1:A:537:ARG:HD2	8:H:20:TYR:CE1	2.31	0.53
1:A:547:LEU:HB3	11:K:58:PHE:CE1	2.43	0.53
1:A:863:VAL:HG11	1:A:866:PHE:CE2	2.42	0.53
2:B:484:ASN:ND2	2:B:486:TYR:HE1	2.06	0.53
2:B:503:GLY:CA	2:B:507:LYS:HE2	2.35	0.53
2:B:510:LYS:CG	2:B:511:PRO:HD3	2.37	0.53
2:B:895:ASP:C	2:B:897:GLY:H	2.16	0.53
5:E:22:MET:HG3	5:E:187:TYR:CD1	2.43	0.53
7:G:41:LYS:HD3	7:G:42:PHE:CE1	2.42	0.53
8:H:76:THR:HG23	8:H:77:ARG:HG3	1.88	0.53
11:K:49:GLU:HA	11:K:52:ASN:HD22	1.72	0.53
1:A:211:PHE:HA	1:A:214:ILE:HG13	1.90	0.53
1:A:798:GLY:HA2	1:A:815:PHE:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:993:LEU:HD22	1:A:1046:LEU:HD23	1.90	0.53
2:B:67:SER:OG	2:B:68:THR:N	2.42	0.53
2:B:311:LEU:O	2:B:312:GLU:C	2.51	0.53
2:B:701:ILE:HB	2:B:739:THR:OG1	2.07	0.53
2:B:756:ILE:O	2:B:759:PRO:HD3	2.08	0.53
2:B:992:ILE:HD11	11:K:66:PRO:HB2	1.90	0.53
3:C:50:GLU:CG	12:L:64:LEU:HD22	2.39	0.53
10:J:36:LEU:HB2	10:J:47:ARG:HH12	1.72	0.53
11:K:67:PHE:C	11:K:68:PHE:HD2	2.16	0.53
1:A:83:HIS:C	1:A:83:HIS:CD2	2.87	0.53
1:A:98:LYS:HE2	1:A:224:PHE:CZ	2.42	0.53
1:A:231:PRO:C	1:A:233:TRP:H	2.15	0.53
1:A:798:GLY:HA2	1:A:815:PHE:HD1	1.73	0.53
1:A:1050:GLU:O	1:A:1053:PHE:HB3	2.08	0.53
1:A:1081:LEU:CD1	1:A:1097:GLY:HA3	2.38	0.53
2:B:583:ASN:HD21	2:B:628:THR:CG2	2.21	0.53
2:B:651:LEU:C	2:B:653:VAL:H	2.17	0.53
2:B:1219:ASP:C	2:B:1219:ASP:OD1	2.52	0.53
3:C:25:VAL:HG22	3:C:228:PHE:CE1	2.43	0.53
8:H:100:THR:HG23	8:H:138:GLU:CB	2.38	0.53
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.38	0.53
1:A:9:ALA:O	1:A:10:PRO:C	2.49	0.53
1:A:923:LEU:O	1:A:927:VAL:HG23	2.09	0.53
1:A:1215:ARG:HG2	1:A:1215:ARG:HH11	1.73	0.53
1:A:1423:GLY:HA3	1:A:1426:GLU:HG2	1.90	0.53
2:B:46:GLN:HG3	2:B:47:GLN:N	2.18	0.53
2:B:642:ASP:N	2:B:649:LYS:HG3	2.24	0.53
4:D:141:LEU:HD22	7:G:46:LEU:O	2.07	0.53
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.89	0.53
5:E:138:ALA:HA	5:E:141:VAL:CG2	2.39	0.53
1:A:40:THR:CG2	1:A:41:MET:HE2	2.38	0.53
1:A:102:VAL:HB	1:A:211:PHE:HZ	1.71	0.53
1:A:317:LYS:O	1:A:318:SER:CB	2.56	0.53
1:A:475:THR:HG23	1:A:476:SER:N	2.24	0.53
1:A:556:TRP:C	1:A:558:GLY:H	2.16	0.53
1:A:567:LYS:CB	1:A:568:PRO:CD	2.87	0.53
1:A:1178:ASP:O	1:A:1179:GLU:HG3	2.09	0.53
1:A:1373:ASP:HA	1:A:1376:THR:HG22	1.90	0.53
1:A:1451:VAL:C	1:A:1453:TYR:H	2.15	0.53
2:B:459:TYR:C	2:B:459:TYR:CD2	2.87	0.53
2:B:843:GLN:O	2:B:844:SER:C	2.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:864:LYS:HB2	2:B:872:GLU:CD	2.33	0.53
2:B:891:ASP:C	2:B:893:LEU:H	2.16	0.53
2:B:1001:PHE:CD1	2:B:1001:PHE:C	2.87	0.53
2:B:1003:ALA:HA	3:C:178:PHE:O	2.09	0.53
2:B:1081:LEU:C	2:B:1083:ALA:N	2.65	0.53
2:B:1138:MET:HE2	2:B:1146:PHE:CD2	2.43	0.53
2:B:1166:CYS:SG	2:B:1185:CYS:SG	3.06	0.53
3:C:133:ILE:HG21	3:C:236:GLY:HA3	1.90	0.53
11:K:108:GLU:O	11:K:112:GLN:HG2	2.08	0.53
13:T:11:DA:H2"	13:T:12:DG:C8	2.43	0.53
1:A:286:HIS:O	1:A:288:ALA:N	2.41	0.53
1:A:322:VAL:O	1:A:322:VAL:HG13	2.08	0.53
1:A:535:THR:CG2	1:A:616:VAL:HA	2.38	0.53
1:A:756:ILE:O	1:A:759:ALA:HB3	2.09	0.53
1:A:1153:TYR:HB2	1:A:1192:LEU:HD23	1.91	0.53
1:A:1366:ARG:HG2	1:A:1366:ARG:HH11	1.73	0.53
2:B:435:THR:C	2:B:437:GLU:H	2.16	0.53
2:B:549:THR:HG22	2:B:550:ASP:N	2.23	0.53
2:B:603:LEU:CD1	2:B:608:ASP:HB3	2.39	0.53
2:B:616:ILE:CG2	2:B:700:SER:OG	2.56	0.53
2:B:711:GLU:HB2	2:B:712:PRO:CD	2.38	0.53
9:I:85:PHE:N	9:I:85:PHE:HD2	2.04	0.53
10:J:57:ILE:O	10:J:60:PHE:HB2	2.09	0.53
1:A:289:ILE:O	1:A:292:ALA:N	2.31	0.53
1:A:777:PHE:C	1:A:779:PHE:H	2.16	0.53
1:A:1075:PRO:O	1:A:1079:MET:HG3	2.09	0.53
1:A:1161:THR:C	1:A:1163:ILE:N	2.65	0.53
1:A:1220:PHE:CD1	1:A:1224:LEU:HD23	2.44	0.53
1:A:1291:VAL:HG13	1:A:1292:PRO:CD	2.39	0.53
2:B:216:GLU:HA	2:B:406:LEU:HD23	1.91	0.53
2:B:706:GLN:NE2	2:B:730:ARG:HD3	2.24	0.53
5:E:185:ALA:O	5:E:190:LEU:HB2	2.09	0.53
11:K:30:ALA:HB2	11:K:76:GLN:HG3	1.90	0.53
11:K:42:LEU:HD21	11:K:46:ILE:CD1	2.39	0.53
12:L:30:ILE:HG22	12:L:31:CYS:N	2.24	0.53
1:A:75:ASN:O	1:A:76:GLU:CB	2.57	0.53
1:A:265:LYS:CE	1:A:302:THR:HG23	2.39	0.53
1:A:456:MET:CE	1:A:507:VAL:HG13	2.39	0.53
1:A:658:LEU:HD23	1:A:659:HIS:CE1	2.44	0.53
1:A:699:ALA:HB1	9:I:114:GLN:HE21	1.74	0.53
1:A:1005:GLU:O	1:A:1006:ILE:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:616:ILE:HG23	2:B:700:SER:OG	2.09	0.53
4:D:63:LEU:O	4:D:129:LEU:HD11	2.08	0.53
5:E:182:ASP:HB3	5:E:185:ALA:HB2	1.91	0.53
9:I:11:ASN:C	9:I:12:ASN:HD22	2.17	0.53
9:I:55:THR:HG23	9:I:86:PHE:HZ	1.73	0.53
10:J:20:SER:O	10:J:24:LEU:HG	2.08	0.53
1:A:42:ASP:OD2	1:A:45:GLN:HA	2.09	0.53
1:A:57:ARG:O	1:A:58:LEU:O	2.27	0.53
1:A:150:THR:HG23	1:A:165:GLY:O	2.09	0.53
1:A:219:PHE:CE1	1:A:230:ARG:HD3	2.44	0.53
1:A:427:GLN:O	1:A:428:TYR:C	2.52	0.53
1:A:453:MET:HE3	1:A:520:CYS:SG	2.49	0.53
1:A:537:ARG:HH22	8:H:122:LEU:CD1	2.22	0.53
1:A:600:PRO:C	1:A:602:ASP:H	2.16	0.53
2:B:29:ASP:OD1	2:B:658:ILE:HD13	2.09	0.53
2:B:203:PHE:N	2:B:203:PHE:CD1	2.77	0.53
2:B:340:ALA:C	2:B:342:GLY:H	2.17	0.53
2:B:597:MET:HA	2:B:597:MET:CE	2.33	0.53
2:B:687:GLU:HB3	2:B:689:LEU:HG	1.91	0.53
2:B:705:MET:HE1	2:B:742:GLU:HG2	1.90	0.53
2:B:999:MET:HG2	2:B:1007:VAL:HG22	1.91	0.53
4:D:70:PHE:O	4:D:74:GLN:NE2	2.42	0.53
5:E:91:LYS:C	5:E:93:MET:N	2.65	0.53
5:E:176:PRO:O	5:E:212:ARG:HA	2.09	0.53
1:A:71:GLN:C	1:A:73:GLY:H	2.16	0.53
1:A:266:LEU:HD21	1:A:303:TYR:CZ	2.44	0.53
1:A:341:MET:HE3	2:B:1135:ARG:NH1	2.24	0.53
1:A:600:PRO:CG	1:A:601:LYS:H	2.13	0.53
1:A:777:PHE:CD1	1:A:781:ASP:HA	2.44	0.53
1:A:1264:GLU:HG3	1:A:1265:ASN:N	2.24	0.53
1:A:1449:SER:HB2	1:A:1453:TYR:CE1	2.44	0.53
2:B:190:TYR:CE2	10:J:62:ARG:HD3	2.44	0.53
2:B:221:ASN:N	2:B:241:ARG:O	2.41	0.53
2:B:284:ILE:HG23	2:B:324:ILE:HD13	1.91	0.53
3:C:66:ARG:NH2	10:J:3:VAL:O	2.42	0.53
3:C:182:PRO:HD2	3:C:210:GLU:OE1	2.09	0.53
4:D:126:ILE:HD13	4:D:145:MET:CE	2.39	0.53
5:E:110:PHE:HE2	5:E:112:TYR:HB3	1.73	0.53
7:G:13:LEU:CD2	7:G:14:HIS:N	2.73	0.53
12:L:33:GLU:C	12:L:35:SER:H	2.17	0.53
13:T:22:DC:H2'	13:T:23:BRU:H6	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LYS:HE3	1:A:280:GLU:OE2	2.09	0.52
1:A:108:MET:CB	1:A:210:ILE:HD13	2.26	0.52
1:A:569:LYS:O	1:A:571:LEU:HD13	2.09	0.52
1:A:605:MET:HE1	1:A:612:ILE:HG23	1.91	0.52
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.44	0.52
2:B:863:GLU:OE2	2:B:873:THR:HA	2.09	0.52
2:B:1165:ILE:HD13	4:D:17:LYS:HD3	1.90	0.52
3:C:89:GLU:O	3:C:90:ASP:CB	2.57	0.52
4:D:118:THR:CB	4:D:121:LYS:HB2	2.38	0.52
5:E:78:LEU:HD23	5:E:78:LEU:C	2.34	0.52
6:F:148:VAL:O	6:F:149:GLU:C	2.51	0.52
10:J:48:ARG:HE	10:J:49:MET:CE	2.18	0.52
1:A:21:LEU:HD21	1:A:1413:GLY:C	2.34	0.52
1:A:57:ARG:HG2	1:A:57:ARG:HH11	1.74	0.52
1:A:299:HIS:C	1:A:301:ALA:H	2.18	0.52
1:A:350:ARG:HH11	1:A:350:ARG:HG3	1.73	0.52
1:A:452:LYS:HE3	2:B:1141:HIS:CE1	2.44	0.52
1:A:664:THR:HG22	1:A:665:GLY:N	2.24	0.52
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.90	0.52
2:B:291:ILE:HG22	2:B:291:ILE:O	2.08	0.52
2:B:582:VAL:HB	2:B:587:HIS:HD2	1.74	0.52
2:B:990:ILE:HG22	2:B:991:GLY:N	2.24	0.52
2:B:1084:GLN:HE21	2:B:1084:GLN:H	1.57	0.52
2:B:1150:ARG:CG	2:B:1150:ARG:NH1	2.67	0.52
2:B:1167:GLY:HA3	2:B:1216:LEU:H	1.74	0.52
3:C:152:GLU:HG2	3:C:153:LEU:H	1.72	0.52
5:E:22:MET:O	5:E:26:ARG:HB2	2.09	0.52
8:H:40:LEU:HD22	8:H:123:MET:CE	2.39	0.52
8:H:142:LEU:C	8:H:143:LEU:HD12	2.34	0.52
9:I:109:ILE:HG22	9:I:109:ILE:O	2.07	0.52
1:A:164:ARG:HG3	1:A:165:GLY:N	2.24	0.52
1:A:279:LEU:O	1:A:289:ILE:HD11	2.09	0.52
1:A:315:LEU:HD22	1:A:319:GLY:O	2.08	0.52
1:A:689:LYS:HE2	1:A:721:PHE:CZ	2.45	0.52
1:A:971:PHE:C	1:A:973:ILE:H	2.17	0.52
2:B:65:GLU:HG3	2:B:66:ASP:H	1.74	0.52
2:B:227:LYS:HB2	2:B:395:GLN:OE1	2.08	0.52
2:B:549:THR:HG22	2:B:550:ASP:H	1.75	0.52
2:B:723:VAL:CG1	2:B:724:ASP:H	2.11	0.52
3:C:1:MET:N	3:C:1:MET:HE2	2.25	0.52
3:C:75:MET:O	3:C:246:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:99:LEU:C	6:F:99:LEU:HD12	2.34	0.52
6:F:119:ARG:HG3	6:F:119:ARG:NH1	2.24	0.52
13:T:10:DA:C2	13:T:11:DA:C4	2.97	0.52
1:A:16:GLU:HG3	2:B:1220:ARG:HA	1.91	0.52
1:A:390:GLN:O	1:A:394:ASN:N	2.42	0.52
1:A:567:LYS:HG2	1:A:568:PRO:N	2.23	0.52
1:A:774:ARG:O	1:A:775:ILE:C	2.52	0.52
1:A:897:TYR:N	1:A:897:TYR:CD1	2.77	0.52
2:B:546:SER:HA	2:B:612:GLU:OE2	2.10	0.52
2:B:559:SER:CA	2:B:563:MET:HB3	2.29	0.52
3:C:167:HIS:ND1	3:C:169:LYS:HG2	2.25	0.52
4:D:52:LEU:HA	4:D:148:LEU:HD21	1.91	0.52
5:E:110:PHE:CE2	5:E:112:TYR:HB3	2.44	0.52
5:E:207:ARG:HB3	5:E:207:ARG:HH11	1.75	0.52
6:F:116:ASP:O	6:F:120:ILE:HG13	2.09	0.52
7:G:45:ILE:HD13	7:G:78:VAL:CG1	2.40	0.52
8:H:44:VAL:CG1	8:H:48:PRO:HA	2.40	0.52
10:J:24:LEU:HD12	10:J:39:LEU:HD11	1.90	0.52
12:L:39:SER:O	12:L:40:LEU:HB2	2.09	0.52
12:L:41:SER:O	12:L:44:ASP:HB2	2.10	0.52
1:A:262:LEU:HD21	1:A:303:TYR:HE1	1.75	0.52
1:A:591:PHE:HA	1:A:595:THR:CG2	2.37	0.52
1:A:608:ILE:C	1:A:610:GLY:N	2.67	0.52
1:A:655:PHE:O	1:A:658:LEU:HB3	2.09	0.52
1:A:683:ILE:HD13	1:A:801:GLU:CG	2.38	0.52
1:A:884:ASP:HB3	1:A:896:ARG:HH12	1.74	0.52
1:A:899:VAL:HG13	1:A:908:LEU:CD2	2.40	0.52
2:B:744:HIS:HD2	2:B:746:SER:OG	1.93	0.52
3:C:147:LEU:HD12	3:C:151:GLN:O	2.10	0.52
4:D:41:GLN:HB2	4:D:43:GLU:HG3	1.92	0.52
4:D:154:PHE:CD1	4:D:154:PHE:N	2.78	0.52
5:E:55:ARG:O	5:E:57:MET:N	2.43	0.52
5:E:153:HIS:O	5:E:154:ILE:HG13	2.09	0.52
6:F:103:MET:CE	7:G:66:GLY:N	2.63	0.52
6:F:127:GLU:O	6:F:129:LYS:HG3	2.09	0.52
7:G:99:PHE:HZ	7:G:163:ILE:HD13	1.74	0.52
8:H:92:ASP:C	8:H:93:TYR:CD1	2.87	0.52
9:I:82:GLU:HB3	9:I:104:LEU:CD1	2.40	0.52
1:A:172:PRO:HD3	1:A:185:TRP:NE1	2.24	0.52
1:A:567:LYS:HB3	1:A:568:PRO:CD	2.37	0.52
1:A:944:ARG:NE	1:A:1298:TYR:HE1	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001:ARG:O	1:A:1002:GLY:O	2.28	0.52
3:C:235:VAL:HG12	10:J:13:VAL:HG23	1.91	0.52
4:D:54:GLU:O	4:D:58:VAL:HG23	2.10	0.52
7:G:1:MET:HE1	7:G:80:LYS:H	1.73	0.52
9:I:111:THR:CG2	9:I:112:SER:N	2.71	0.52
1:A:130:ASP:C	1:A:132:LYS:H	2.17	0.52
1:A:188:ASP:CB	1:A:191:THR:HB	2.33	0.52
1:A:196:GLU:CB	1:A:197:PRO:HD2	2.36	0.52
1:A:215:SER:HB3	1:A:218:ASP:CG	2.34	0.52
1:A:317:LYS:O	1:A:318:SER:HB3	2.09	0.52
1:A:784:LEU:C	1:A:786:HIS:H	2.17	0.52
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.43	0.52
1:A:1036:ARG:HG2	1:A:1036:ARG:NH1	2.25	0.52
2:B:196:PRO:HG2	2:B:197:PHE:H	1.74	0.52
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.44	0.52
3:C:152:GLU:HG2	3:C:153:LEU:N	2.24	0.52
4:D:56:ARG:NH2	4:D:155:ARG:HA	2.25	0.52
7:G:106:MET:HE3	7:G:108:VAL:HG23	1.92	0.52
8:H:76:THR:O	8:H:77:ARG:HB2	2.09	0.52
9:I:69:PRO:HB2	9:I:85:PHE:CE2	2.45	0.52
1:A:15:LYS:HG3	2:B:1219:ASP:HA	1.92	0.52
1:A:116:ASP:C	1:A:118:HIS:H	2.16	0.52
1:A:350:ARG:HG3	1:A:350:ARG:NH1	2.24	0.52
1:A:384:ASN:O	1:A:385:ILE:C	2.53	0.52
1:A:475:THR:CG2	1:A:476:SER:N	2.72	0.52
1:A:904:THR:O	1:A:904:THR:HG22	2.09	0.52
1:A:973:ILE:O	1:A:973:ILE:HG22	2.09	0.52
1:A:1118:VAL:O	1:A:1305:VAL:HG13	2.09	0.52
1:A:1127:ASP:HB3	1:A:1130:GLN:CB	2.39	0.52
1:A:1156:PRO:HA	1:A:1190:PRO:HB3	1.92	0.52
1:A:1289:ARG:HD2	1:A:1303:GLU:OE2	2.09	0.52
3:C:125:MET:HG3	3:C:127:ARG:NH2	2.25	0.52
5:E:31:THR:HG23	5:E:34:GLU:CB	2.38	0.52
6:F:79:ARG:HH22	6:F:150:GLU:CD	2.17	0.52
1:A:18:GLN:HB2	2:B:1215:ARG:HB2	1.91	0.52
1:A:320:ARG:NH2	15:P:3:U:O2'	2.42	0.52
1:A:456:MET:HE2	1:A:507:VAL:HG13	1.91	0.52
1:A:531:ILE:HD11	1:A:578:LEU:HD11	1.91	0.52
1:A:645:LEU:HG	1:A:649:ILE:HD11	1.91	0.52
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.74	0.52
1:A:896:ARG:HB3	1:A:897:TYR:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:LEU:O	1:A:939:ASP:HB2	2.10	0.52
1:A:1115:SER:O	1:A:1116:LEU:HB2	2.10	0.52
1:A:1265:ASN:C	1:A:1267:MET:N	2.66	0.52
2:B:205:ILE:N	2:B:205:ILE:HD12	2.25	0.52
2:B:806:THR:HB	2:B:809:MET:HG3	1.92	0.52
6:F:130:ILE:HG22	6:F:132:LEU:HG	1.91	0.52
9:I:26:LEU:HD23	9:I:37:GLU:CA	2.36	0.52
1:A:396:PRO:HB3	1:A:402:ALA:O	2.09	0.52
1:A:399:HIS:CB	1:A:400:PRO:CD	2.88	0.52
1:A:537:ARG:HH22	8:H:122:LEU:HG	1.74	0.52
1:A:629:LEU:HD11	1:A:645:LEU:HD21	1.92	0.52
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.92	0.52
1:A:858:ASN:ND2	1:A:860:LEU:H	2.08	0.52
1:A:1152:ILE:HG23	1:A:1193:LEU:HD13	1.92	0.52
2:B:254:LEU:CD1	2:B:273:LEU:HD23	2.40	0.52
2:B:363:HIS:C	2:B:365:THR:H	2.17	0.52
2:B:620:ARG:NH2	9:I:89:GLN:NE2	2.57	0.52
2:B:1084:GLN:N	2:B:1084:GLN:HE21	2.07	0.52
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.35	0.52
3:C:34:ARG:HA	3:C:37:MET:HE3	1.91	0.52
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.92	0.52
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.84	0.52
12:L:28:LYS:HB2	12:L:39:SER:HB2	1.91	0.52
1:A:1162:VAL:HG11	9:I:41:PRO:HG3	1.91	0.51
1:A:1173:HIS:ND1	1:A:1173:HIS:O	2.43	0.51
2:B:113:TYR:HB3	2:B:114:PRO:HD2	1.91	0.51
2:B:192:LEU:O	2:B:193:LYS:HB2	2.09	0.51
2:B:269:ILE:CG2	2:B:282:ILE:HD13	2.40	0.51
2:B:294:ASP:HB2	9:I:12:ASN:HA	1.92	0.51
2:B:521:LEU:HD13	2:B:633:VAL:CG1	2.40	0.51
2:B:558:LEU:C	2:B:560:GLU:N	2.68	0.51
2:B:770:GLN:HG2	2:B:983:ARG:O	2.09	0.51
4:D:53:SER:H	4:D:148:LEU:HD22	1.71	0.51
9:I:62:ILE:O	9:I:62:ILE:HG12	2.10	0.51
11:K:101:LEU:C	11:K:101:LEU:HD23	2.35	0.51
1:A:200:ARG:HG3	1:A:201:VAL:N	2.25	0.51
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.09	0.51
1:A:560:ILE:HD12	8:H:79:TRP:HB3	1.92	0.51
1:A:685:GLU:OE2	1:A:686:ALA:HB2	2.11	0.51
1:A:700:ASN:HB2	9:I:98:VAL:HG21	1.92	0.51
1:A:1074:GLU:C	1:A:1076:ALA:N	2.66	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1151:GLU:OE2	9:I:45:ARG:HD2	2.10	0.51
1:A:1154:TYR:HD1	1:A:1191:TRP:CZ3	2.28	0.51
2:B:68:THR:OG1	2:B:91:SER:CB	2.58	0.51
2:B:102:VAL:HB	2:B:110:HIS:HB3	1.92	0.51
2:B:216:GLU:HB3	2:B:500:THR:CG2	2.37	0.51
2:B:314:LEU:O	2:B:317:CYS:HB3	2.11	0.51
2:B:327:ARG:O	2:B:327:ARG:HG2	2.10	0.51
2:B:806:THR:HG22	2:B:807:ARG:N	2.24	0.51
2:B:1162:ILE:HD11	2:B:1194:ILE:CD1	2.41	0.51
3:C:18:VAL:O	3:C:20:PHE:HD2	1.93	0.51
3:C:176:ILE:HG22	3:C:177:GLU:H	1.74	0.51
5:E:124:VAL:CG1	5:E:132:ILE:HG13	2.39	0.51
7:G:137:ILE:HG21	7:G:143:ILE:HD11	1.93	0.51
1:A:10:PRO:HG2	2:B:1191:ILE:O	2.09	0.51
1:A:12:ARG:CB	2:B:1218:THR:HG22	2.38	0.51
1:A:630:ILE:HG23	1:A:631:HIS:H	1.74	0.51
1:A:672:ASP:OD2	1:A:674:PRO:HG2	2.10	0.51
1:A:942:PHE:HZ	5:E:207:ARG:HG3	1.75	0.51
1:A:1163:ILE:HG22	1:A:1165:GLU:HG2	1.91	0.51
2:B:38:PHE:CD1	2:B:811:TYR:HD2	2.29	0.51
2:B:100:PRO:HD2	2:B:180:TYR:HE1	1.73	0.51
2:B:176:SER:O	2:B:182:SER:HB3	2.10	0.51
2:B:266:ALA:C	2:B:268:THR:H	2.18	0.51
2:B:435:THR:C	2:B:437:GLU:N	2.68	0.51
2:B:547:VAL:HG12	2:B:612:GLU:OE2	2.10	0.51
2:B:558:LEU:O	2:B:560:GLU:N	2.38	0.51
2:B:616:ILE:HD12	2:B:616:ILE:N	2.25	0.51
2:B:871:THR:HG22	2:B:872:GLU:N	2.24	0.51
4:D:51:ASN:O	4:D:52:LEU:O	2.27	0.51
4:D:63:LEU:HD12	4:D:129:LEU:HG	1.92	0.51
4:D:150:ASN:HB3	7:G:142:ARG:HH22	1.75	0.51
7:G:88:ASP:OD2	7:G:88:ASP:N	2.42	0.51
7:G:143:ILE:CG2	7:G:144:ARG:H	2.23	0.51
11:K:12:LEU:H	11:K:12:LEU:CD1	2.18	0.51
12:L:68:GLU:OE1	12:L:68:GLU:N	2.27	0.51
1:A:72:GLU:O	1:A:73:GLY:O	2.29	0.51
1:A:316:GLN:O	1:A:317:LYS:C	2.53	0.51
1:A:332:LYS:HB2	1:A:337:ARG:HH11	1.75	0.51
1:A:816:HIS:HE2	2:B:764:SER:H	1.58	0.51
1:A:830:LYS:HE2	1:A:1081:LEU:HB2	1.91	0.51
2:B:44:VAL:HG23	2:B:48:LEU:HD11	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:GLN:HE22	2:B:496:ARG:CB	2.24	0.51
2:B:210:LYS:HD3	2:B:482:VAL:HG12	1.93	0.51
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.92	0.51
2:B:1067:ARG:NH2	3:C:194:GLU:OE2	2.43	0.51
2:B:1097:HIS:N	2:B:1098:MET:HE2	2.25	0.51
8:H:11:GLN:HA	8:H:53:ASP:O	2.09	0.51
8:H:129:TYR:HA	8:H:131:ASN:HD21	1.75	0.51
11:K:10:PHE:N	11:K:10:PHE:CD2	2.78	0.51
1:A:35:ILE:HG22	1:A:35:ILE:O	2.11	0.51
1:A:443:LEU:HD23	1:A:501:LEU:HD21	1.90	0.51
1:A:592:ASP:N	1:A:595:THR:OG1	2.44	0.51
1:A:844:ALA:HB2	1:A:1389:PHE:CE2	2.46	0.51
1:A:889:SER:HB3	1:A:1297:GLU:CG	2.41	0.51
1:A:1039:LYS:HE3	1:A:1043:ASP:OD2	2.10	0.51
1:A:1191:TRP:CE3	1:A:1191:TRP:HA	2.44	0.51
2:B:214:ALA:HB3	2:B:497:ARG:O	2.10	0.51
2:B:283:VAL:CG2	2:B:317:CYS:O	2.59	0.51
2:B:293:PRO:O	2:B:297:ILE:HG13	2.11	0.51
2:B:376:PHE:CZ	2:B:569:TYR:HB3	2.46	0.51
2:B:547:VAL:N	2:B:612:GLU:OE2	2.41	0.51
2:B:648:HIS:CD2	2:B:649:LYS:H	2.28	0.51
3:C:3:GLU:HG3	11:K:104:ASN:CG	2.35	0.51
4:D:7:THR:HG23	4:D:9:GLN:H	1.75	0.51
4:D:187:THR:HG22	4:D:189:ASP:H	1.75	0.51
5:E:52:ARG:CG	5:E:52:ARG:HH11	2.23	0.51
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.41	0.51
1:A:108:MET:HA	1:A:210:ILE:HG21	1.91	0.51
1:A:108:MET:O	1:A:109:HIS:HB2	2.09	0.51
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.46	0.51
1:A:1166:ASP:O	1:A:1168:GLU:N	2.43	0.51
2:B:65:GLU:OE1	2:B:418:LYS:HE3	2.10	0.51
2:B:244:LEU:HD21	2:B:366:GLN:HE21	1.76	0.51
2:B:778:MET:HE2	2:B:1094:ARG:CD	2.41	0.51
2:B:1081:LEU:O	2:B:1083:ALA:N	2.44	0.51
3:C:260:LEU:O	3:C:264:GLN:HG3	2.10	0.51
4:D:207:LEU:O	4:D:211:LEU:HB2	2.11	0.51
5:E:67:GLU:O	5:E:70:SER:HB3	2.10	0.51
8:H:4:THR:HA	8:H:60:ALA:CB	2.40	0.51
9:I:4:PHE:CE1	9:I:6:PHE:HE2	2.27	0.51
1:A:230:ARG:HG3	1:A:233:TRP:CZ3	2.46	0.51
1:A:265:LYS:O	1:A:265:LYS:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:LEU:HD12	2:B:128:LEU:N	2.25	0.51
2:B:288:ALA:O	2:B:331:LEU:HD11	2.11	0.51
2:B:875:GLU:HG3	2:B:877:PRO:HD3	1.92	0.51
3:C:77:ILE:N	3:C:129:ILE:HD11	2.26	0.51
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.36	0.51
4:D:123:LEU:HG	4:D:149:THR:HG21	1.91	0.51
5:E:116:ILE:O	5:E:121:MET:HE2	2.10	0.51
11:K:68:PHE:CB	11:K:70:ARG:HH11	2.21	0.51
1:A:384:ASN:O	1:A:387:ARG:N	2.43	0.51
1:A:556:TRP:CE3	1:A:558:GLY:HA2	2.46	0.51
1:A:608:ILE:C	1:A:610:GLY:H	2.16	0.51
1:A:899:VAL:CG1	1:A:908:LEU:HD21	2.40	0.51
2:B:541:LEU:HB2	2:B:747:MET:HE3	1.93	0.51
2:B:798:TYR:CZ	3:C:62:PHE:HE2	2.28	0.51
2:B:837:ASP:O	2:B:988:GLY:HA2	2.10	0.51
2:B:975:GLN:HE22	2:B:1100:ASP:CG	2.18	0.51
2:B:1001:PHE:CE2	3:C:34:ARG:NE	2.79	0.51
2:B:1161:HIS:NE2	2:B:1175:LEU:HD21	2.25	0.51
3:C:3:GLU:HG3	11:K:104:ASN:ND2	2.26	0.51
9:I:86:PHE:CE1	9:I:100:PHE:HB2	2.46	0.51
9:I:101:PHE:N	9:I:101:PHE:CD1	2.78	0.51
1:A:146:MET:HB3	1:A:171:GLN:O	2.11	0.51
1:A:208:LEU:HD23	1:A:208:LEU:C	2.36	0.51
1:A:227:VAL:C	1:A:228:PHE:CD2	2.88	0.51
1:A:666:ILE:HG23	2:B:1026:LEU:CB	2.41	0.51
4:D:202:ILE:HD11	4:D:206:GLU:HB3	1.93	0.51
11:K:10:PHE:HA	11:K:37:LYS:HB3	1.92	0.51
1:A:95:PHE:O	1:A:96:ILE:C	2.54	0.51
1:A:817:ALA:O	1:A:820:GLY:N	2.44	0.51
1:A:1166:ASP:O	1:A:1167:GLU:C	2.53	0.51
1:A:1167:GLU:O	1:A:1170:ILE:HG13	2.10	0.51
1:A:1178:ASP:C	1:A:1179:GLU:HG3	2.36	0.51
1:A:1211:GLN:O	1:A:1212:VAL:C	2.54	0.51
1:A:1215:ARG:HG2	1:A:1215:ARG:NH1	2.25	0.51
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.93	0.51
2:B:326:ASP:O	2:B:328:GLU:N	2.43	0.51
2:B:1106:ARG:HD3	2:B:1127:GLY:CA	2.41	0.51
3:C:76:ASP:O	3:C:77:ILE:C	2.54	0.51
5:E:117:THR:HB	5:E:120:ALA:HB2	1.93	0.51
5:E:121:MET:C	5:E:123:LEU:H	2.19	0.51
9:I:78:CYS:SG	9:I:105:SER:HB2	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:CYS:C	1:A:144:THR:H	2.18	0.50
1:A:440:ASP:O	1:A:442:VAL:HG22	2.11	0.50
1:A:699:ALA:CB	9:I:114:GLN:HE21	2.24	0.50
2:B:63:ILE:HD12	2:B:421:PHE:CE2	2.46	0.50
2:B:613:VAL:HG13	2:B:628:THR:HA	1.93	0.50
2:B:944:THR:HG21	2:B:1122:ARG:HH21	1.68	0.50
4:D:53:SER:CB	4:D:152:SER:HB2	2.41	0.50
5:E:149:LEU:N	5:E:149:LEU:HD23	2.26	0.50
6:F:117:PRO:C	6:F:119:ARG:N	2.69	0.50
8:H:84:ALA:HA	8:H:87:ARG:CG	2.41	0.50
8:H:89:LEU:CB	8:H:91:ASP:OD1	2.59	0.50
8:H:101:ALA:HA	8:H:116:TYR:HA	1.92	0.50
12:L:24:THR:O	12:L:25:ALA:HB3	2.11	0.50
1:A:35:ILE:CD1	1:A:241:VAL:HG21	2.41	0.50
1:A:65:LEU:O	1:A:66:LYS:C	2.54	0.50
1:A:149:GLU:HB2	1:A:164:ARG:HH21	1.76	0.50
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.92	0.50
1:A:230:ARG:O	1:A:231:PRO:C	2.54	0.50
1:A:472:LEU:O	1:A:475:THR:CB	2.57	0.50
1:A:640:GLN:O	1:A:641:VAL:C	2.53	0.50
1:A:1273:LEU:HD12	1:A:1273:LEU:N	2.25	0.50
6:F:70:LYS:O	6:F:72:LYS:N	2.35	0.50
15:P:4:C:H2'	15:P:5:C:C6	2.46	0.50
1:A:55:ASP:C	1:A:57:ARG:N	2.55	0.50
1:A:149:GLU:HB2	1:A:164:ARG:NH2	2.27	0.50
1:A:225:ASN:ND2	1:A:228:PHE:N	2.53	0.50
1:A:560:ILE:CG1	8:H:79:TRP:H	2.24	0.50
1:A:698:GLN:NE2	9:I:99:LEU:HD11	2.26	0.50
1:A:803:SER:OG	1:A:806:ARG:HG3	2.12	0.50
1:A:817:ALA:O	1:A:818:MET:C	2.53	0.50
1:A:1118:VAL:HG12	1:A:1327:ILE:HG13	1.92	0.50
2:B:60:GLN:NE2	2:B:94:LYS:HA	2.26	0.50
2:B:67:SER:O	2:B:68:THR:C	2.54	0.50
2:B:707:PRO:O	2:B:708:GLU:C	2.54	0.50
3:C:100:THR:CG2	3:C:102:GLN:NE2	2.75	0.50
4:D:185:CYS:O	4:D:211:LEU:HD22	2.10	0.50
8:H:31:THR:O	8:H:31:THR:HG22	2.10	0.50
8:H:39:THR:O	8:H:123:MET:HG3	2.11	0.50
8:H:131:ASN:C	8:H:133:ASN:H	2.19	0.50
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.45	0.50
1:A:269:ILE:CG1	1:A:299:HIS:HB3	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:919:ILE:HG21	1:A:983:ILE:CD1	2.42	0.50
1:A:1070:GLN:O	1:A:1074:GLU:HB2	2.11	0.50
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.11	0.50
2:B:340:ALA:CB	2:B:343:ILE:HG12	2.24	0.50
2:B:453:ILE:O	2:B:454:THR:C	2.53	0.50
2:B:703:ILE:HG23	2:B:741:CYS:HA	1.92	0.50
2:B:827:ILE:O	2:B:1085:ILE:HG23	2.11	0.50
2:B:880:THR:CB	2:B:934:LYS:HD3	2.38	0.50
4:D:24:ALA:O	4:D:26:THR:N	2.44	0.50
6:F:80:ALA:H	6:F:144:GLU:CD	2.20	0.50
8:H:81:PRO:HB2	8:H:82:PRO:HD3	1.91	0.50
9:I:111:THR:HG21	9:I:113:ASP:HB2	1.93	0.50
1:A:326:ARG:HH22	1:A:1407:GLU:HG2	1.76	0.50
1:A:802:ASN:ND2	2:B:728:ARG:HB2	2.27	0.50
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.92	0.50
1:A:1156:PRO:HA	1:A:1190:PRO:CB	2.42	0.50
2:B:313:MET:CE	2:B:390:LEU:HD11	2.42	0.50
2:B:358:LYS:HA	2:B:366:GLN:HB3	1.92	0.50
2:B:521:LEU:HD13	2:B:633:VAL:CB	2.42	0.50
2:B:1084:GLN:C	2:B:1085:ILE:HD12	2.37	0.50
4:D:26:THR:O	4:D:26:THR:HG22	2.12	0.50
4:D:67:ARG:CA	4:D:133:THR:HG21	2.41	0.50
4:D:185:CYS:HB2	4:D:211:LEU:HD21	1.92	0.50
4:D:191:ALA:CB	4:D:207:LEU:HD21	2.42	0.50
4:D:206:GLU:O	4:D:210:ILE:HG13	2.11	0.50
6:F:73:ALA:HB1	6:F:143:PHE:H	1.76	0.50
7:G:4:ILE:HA	7:G:76:ALA:O	2.12	0.50
8:H:63:LEU:HD13	8:H:64:ASN:H	1.77	0.50
11:K:31:VAL:CG1	11:K:32:VAL:H	2.18	0.50
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.93	0.50
12:L:47:ARG:NH2	12:L:54:ARG:HE	2.09	0.50
1:A:404:TYR:HB2	1:A:433:GLU:HB2	1.94	0.50
1:A:775:ILE:HD12	1:A:818:MET:SD	2.52	0.50
1:A:863:VAL:HG11	1:A:866:PHE:CD2	2.46	0.50
1:A:886:ILE:CG2	1:A:887:GLY:N	2.74	0.50
2:B:179:CYS:SG	2:B:181:LEU:HB2	2.51	0.50
2:B:461:LEU:H	2:B:461:LEU:CD1	2.24	0.50
2:B:579:ARG:CA	2:B:589:VAL:HG22	2.40	0.50
2:B:847:ASP:HB3	3:C:167:HIS:NE2	2.26	0.50
4:D:16:LYS:C	4:D:18:VAL:H	2.19	0.50
11:K:53:ASP:HB3	11:K:56:VAL:CG2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:VAL:HG11	1:A:211:PHE:CE2	2.47	0.50
1:A:113:LEU:O	1:A:114:LEU:HD23	2.12	0.50
1:A:284:ALA:C	1:A:286:HIS:N	2.65	0.50
1:A:343:LYS:HD3	2:B:1155:SER:OG	2.11	0.50
1:A:567:LYS:CD	1:A:568:PRO:HD3	2.41	0.50
1:A:767:GLN:HA	1:A:799:PHE:HA	1.93	0.50
1:A:896:ARG:NH2	1:A:1030:ARG:HH21	2.10	0.50
1:A:1011:GLN:NE2	1:A:1015:VAL:CG2	2.75	0.50
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.11	0.50
1:A:1209:MET:CE	1:A:1236:LEU:HB3	2.42	0.50
2:B:842:ASN:ND2	2:B:845:SER:H	2.10	0.50
2:B:942:ARG:O	2:B:943:SER:C	2.55	0.50
5:E:124:VAL:HG13	5:E:132:ILE:CB	2.42	0.50
5:E:153:HIS:HB3	5:E:196:VAL:HG11	1.94	0.50
1:A:41:MET:CB	1:A:50:ILE:H	2.25	0.50
1:A:95:PHE:CD1	1:A:234:MET:HG2	2.47	0.50
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.93	0.50
1:A:551:TYR:CD2	11:K:62:LYS:HD3	2.47	0.50
1:A:568:PRO:HD2	1:A:569:LYS:H	1.76	0.50
1:A:590:ARG:HG3	1:A:590:ARG:HH11	1.77	0.50
1:A:771:GLU:O	1:A:773:LYS:HG3	2.11	0.50
1:A:1093:LYS:O	1:A:1094:VAL:HG13	2.12	0.50
2:B:67:SER:O	2:B:68:THR:O	2.30	0.50
2:B:370:PHE:HE2	2:B:373:ARG:HH11	1.57	0.50
2:B:563:MET:HE2	2:B:587:HIS:C	2.36	0.50
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.51	0.50
4:D:202:ILE:HG23	4:D:207:LEU:HB2	1.93	0.50
5:E:60:PHE:C	5:E:60:PHE:CD2	2.88	0.50
5:E:94:LYS:HG3	5:E:98:ILE:CD1	2.41	0.50
6:F:74:ILE:HD12	6:F:144:GLU:HG3	1.93	0.50
9:I:99:LEU:C	9:I:100:PHE:CD1	2.90	0.50
1:A:374:LEU:O	1:A:436:ILE:HG12	2.11	0.50
1:A:590:ARG:HB2	1:A:605:MET:HB3	1.94	0.50
1:A:777:PHE:C	1:A:779:PHE:N	2.69	0.50
2:B:96:TYR:N	2:B:129:PHE:O	2.43	0.50
2:B:357:GLN:O	2:B:366:GLN:HA	2.12	0.50
2:B:1087:PHE:C	2:B:1087:PHE:CD2	2.88	0.50
2:B:1189:ILE:HD11	7:G:39:THR:HG23	1.93	0.50
3:C:182:PRO:HG3	3:C:206:ASN:O	2.12	0.50
4:D:168:LYS:HG3	4:D:177:VAL:CG1	2.35	0.50
5:E:45:LYS:HB3	5:E:46:TYR:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:100:THR:O	8:H:117:SER:N	2.45	0.50
10:J:16:ASP:OD1	10:J:17:LYS:HD2	2.11	0.50
11:K:49:GLU:OE2	11:K:97:LYS:HE3	2.12	0.50
1:A:63:ARG:HG3	1:A:63:ARG:O	2.12	0.49
1:A:335:ARG:HD3	2:B:1202:LEU:HD23	1.93	0.49
1:A:700:ASN:ND2	9:I:115:LYS:HD2	2.27	0.49
1:A:781:ASP:O	1:A:790:ASP:N	2.46	0.49
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.27	0.49
2:B:284:ILE:HG12	2:B:324:ILE:HD12	1.94	0.49
2:B:526:GLU:HG2	2:B:526:GLU:O	2.11	0.49
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.47	0.49
2:B:1002:THR:O	2:B:1003:ALA:C	2.55	0.49
3:C:8:VAL:HG12	3:C:9:LYS:N	2.25	0.49
5:E:147:HIS:O	5:E:148:GLU:C	2.55	0.49
8:H:15:VAL:HG13	8:H:26:ILE:CG1	2.37	0.49
8:H:100:THR:HG22	8:H:101:ALA:H	1.76	0.49
8:H:102:TYR:CE2	8:H:115:TYR:HB3	2.47	0.49
1:A:32:VAL:O	1:A:57:ARG:CD	2.61	0.49
1:A:170:THR:HG22	1:A:171:GLN:N	2.25	0.49
1:A:393:ARG:CB	1:A:393:ARG:HH11	2.26	0.49
1:A:596:THR:O	1:A:597:LEU:HB2	2.12	0.49
1:A:676:MET:O	1:A:679:ILE:HB	2.11	0.49
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.27	0.49
2:B:165:VAL:HG12	2:B:166:PHE:N	2.27	0.49
2:B:360:PHE:HD2	2:B:374:LYS:HD3	1.77	0.49
2:B:604:ARG:HG3	2:B:611:PRO:HA	1.93	0.49
2:B:661:LEU:HG	2:B:679:TYR:CD2	2.47	0.49
2:B:1034:VAL:C	2:B:1036:ALA:N	2.71	0.49
2:B:1084:GLN:OE1	3:C:189:THR:CG2	2.60	0.49
7:G:74:TYR:H	7:G:74:TYR:HD2	1.59	0.49
9:I:50:THR:HG22	9:I:52:ILE:H	1.77	0.49
1:A:208:LEU:HD23	1:A:209:ASN:N	2.27	0.49
1:A:243:PRO:CB	1:A:244:PRO:HD2	2.40	0.49
1:A:427:GLN:O	1:A:430:TRP:HB2	2.12	0.49
1:A:492:PRO:O	1:A:493:GLN:NE2	2.45	0.49
1:A:523:ILE:HD11	1:A:649:ILE:HB	1.93	0.49
1:A:546:VAL:HG13	1:A:577:ILE:HG21	1.93	0.49
1:A:590:ARG:HD3	1:A:592:ASP:OD2	2.12	0.49
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.94	0.49
1:A:865:GLN:NE2	1:A:1370:LEU:HA	2.28	0.49
1:A:944:ARG:CZ	1:A:1298:TYR:HE1	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.75	0.49
2:B:213:ILE:HD11	2:B:497:ARG:H	1.77	0.49
2:B:244:LEU:HD11	2:B:366:GLN:NE2	2.21	0.49
2:B:377:PHE:O	2:B:380:TYR:N	2.45	0.49
2:B:707:PRO:HG2	2:B:708:GLU:H	1.77	0.49
2:B:857:ARG:NH2	2:B:942:ARG:NH2	2.60	0.49
2:B:1001:PHE:CD2	3:C:34:ARG:NH2	2.80	0.49
2:B:1002:THR:CG2	2:B:1006:ILE:CG1	2.80	0.49
2:B:1077:THR:HG22	11:K:44:ASN:ND2	2.26	0.49
3:C:258:ILE:O	3:C:262:LEU:HG	2.11	0.49
4:D:29:LEU:HD22	7:G:82:PHE:CE2	2.47	0.49
5:E:186:LEU:N	5:E:186:LEU:HD23	2.27	0.49
7:G:23:LYS:HG3	7:G:56:ILE:HD12	1.95	0.49
1:A:52:GLY:C	1:A:56:PRO:HG2	2.37	0.49
1:A:100:LYS:O	1:A:104:GLU:HG3	2.13	0.49
1:A:331:GLY:O	1:A:332:LYS:O	2.31	0.49
1:A:464:PRO:HG2	1:A:465:TYR:HD1	1.77	0.49
1:A:524:VAL:HG12	1:A:525:GLN:CG	2.41	0.49
1:A:567:LYS:CD	8:H:95:TYR:HA	2.42	0.49
1:A:666:ILE:HD11	2:B:1086:PHE:HE1	1.77	0.49
1:A:946:VAL:C	1:A:947:PHE:HD1	2.20	0.49
1:A:971:PHE:O	1:A:973:ILE:N	2.45	0.49
1:A:1138:ILE:C	1:A:1275:GLY:HA2	2.37	0.49
1:A:1443:VAL:CG1	6:F:132:LEU:HD13	2.42	0.49
2:B:766:ARG:HG3	2:B:1022:THR:CG2	2.42	0.49
2:B:801:LYS:O	10:J:52:THR:CG2	2.59	0.49
2:B:1020:ARG:HH11	2:B:1020:ARG:HG3	1.76	0.49
3:C:58:LEU:N	3:C:58:LEU:CD2	2.73	0.49
5:E:73:PRO:HB2	5:E:74:ASP:OD1	2.11	0.49
5:E:100:ILE:HG23	5:E:105:PHE:CD1	2.47	0.49
5:E:186:LEU:O	5:E:187:TYR:C	2.55	0.49
5:E:202:SER:C	5:E:204:THR:H	2.19	0.49
6:F:99:LEU:O	6:F:99:LEU:HD12	2.13	0.49
8:H:105:GLU:O	8:H:112:ILE:HG23	2.13	0.49
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.94	0.49
15:P:6:A:H2'	15:P:7:G:C8	2.46	0.49
1:A:159:THR:O	1:A:159:THR:HG22	2.12	0.49
1:A:174:ILE:HG22	1:A:175:ARG:H	1.76	0.49
1:A:189:ARG:O	1:A:190:ALA:CB	2.60	0.49
1:A:359:LEU:O	1:A:471:ASN:ND2	2.45	0.49
1:A:964:ILE:O	1:A:967:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1124:HIS:ND1	1:A:1124:HIS:N	2.60	0.49
1:A:1391:ARG:HG3	1:A:1392:SER:N	2.26	0.49
2:B:100:PRO:CG	2:B:180:TYR:HE1	2.25	0.49
2:B:278:GLN:CG	2:B:279:ASP:H	2.25	0.49
2:B:461:LEU:N	2:B:461:LEU:HD12	2.27	0.49
2:B:583:ASN:ND2	2:B:628:THR:HG22	2.28	0.49
8:H:89:LEU:HB3	8:H:91:ASP:OD1	2.13	0.49
10:J:8:PHE:H	10:J:49:MET:CE	2.26	0.49
12:L:47:ARG:HH11	12:L:47:ARG:HG3	1.78	0.49
1:A:202:LEU:HA	1:A:206:GLU:OE1	2.13	0.49
1:A:311:GLN:HB2	1:A:312:PRO:HD3	1.95	0.49
1:A:524:VAL:HG12	1:A:525:GLN:HG3	1.94	0.49
1:A:567:LYS:HZ3	8:H:95:TYR:HB2	1.77	0.49
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.53	0.49
1:A:1430:LEU:HB3	1:A:1432:GLN:HG3	1.95	0.49
2:B:36:ALA:HA	2:B:39:ARG:HD2	1.94	0.49
2:B:901:PRO:O	2:B:949:VAL:HB	2.12	0.49
4:D:195:ILE:HG22	4:D:195:ILE:O	2.12	0.49
5:E:178:ILE:CG2	5:E:212:ARG:HB3	2.43	0.49
5:E:197:LYS:CE	5:E:199:ILE:HD11	2.35	0.49
1:A:39:GLU:OE1	1:A:50:ILE:HD12	2.13	0.49
1:A:262:LEU:CD2	1:A:303:TYR:HE1	2.25	0.49
1:A:332:LYS:O	1:A:333:GLU:CB	2.60	0.49
1:A:537:ARG:NH1	8:H:120:GLY:O	2.46	0.49
1:A:754:SER:O	1:A:755:PHE:C	2.55	0.49
1:A:1280:GLU:O	1:A:1309:ASP:HB3	2.12	0.49
2:B:56:ASP:HB2	2:B:57:TYR:HD1	1.77	0.49
2:B:258:LEU:O	2:B:258:LEU:CG	2.60	0.49
2:B:306:ASN:C	2:B:308:TRP:H	2.21	0.49
2:B:510:LYS:HB2	2:B:511:PRO:HD3	1.94	0.49
2:B:582:VAL:HB	2:B:587:HIS:CD2	2.47	0.49
2:B:616:ILE:HD13	2:B:625:LYS:HB2	1.95	0.49
2:B:1152:MET:C	2:B:1157:ALA:HB2	2.38	0.49
4:D:40:HIS:CB	7:G:73:LYS:HZ2	2.26	0.49
4:D:203:SER:OG	4:D:206:GLU:HB2	2.13	0.49
8:H:64:ASN:ND2	8:H:88:SER:C	2.71	0.49
8:H:118:PHE:CZ	8:H:142:LEU:HD22	2.48	0.49
11:K:1:MET:HA	11:K:1:MET:HE3	1.95	0.49
1:A:54:ASN:C	1:A:56:PRO:HD3	2.38	0.49
1:A:390:GLN:O	1:A:394:ASN:CB	2.53	0.49
1:A:567:LYS:CG	1:A:568:PRO:CD	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:LEU:HD21	1:A:1371:LEU:HD22	1.95	0.49
2:B:23:ALA:N	2:B:654:ARG:HB3	2.25	0.49
2:B:180:TYR:CD1	2:B:180:TYR:N	2.80	0.49
2:B:734:HIS:O	2:B:735:ALA:HB3	2.13	0.49
2:B:737:THR:CG2	9:I:66:PRO:HA	2.42	0.49
2:B:864:LYS:HD2	2:B:872:GLU:OE2	2.13	0.49
2:B:916:THR:HB	2:B:935:ARG:CG	2.43	0.49
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.94	0.49
3:C:82:TYR:CE1	3:C:161:LYS:HG2	2.47	0.49
5:E:16:PHE:O	5:E:19:VAL:N	2.46	0.49
8:H:101:ALA:HB2	8:H:116:TYR:CZ	2.48	0.49
9:I:44:TYR:CD1	9:I:45:ARG:N	2.80	0.49
1:A:9:ALA:CB	2:B:1193:GLN:HB2	2.43	0.49
1:A:32:VAL:O	1:A:57:ARG:HD3	2.13	0.49
1:A:547:LEU:HD22	11:K:58:PHE:HE1	1.73	0.49
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	1.94	0.49
1:A:942:PHE:C	1:A:942:PHE:CD2	2.91	0.49
1:A:1226:VAL:HG22	1:A:1240:CYS:HB3	1.95	0.49
1:A:1316:VAL:O	1:A:1316:VAL:HG12	2.13	0.49
2:B:125:SER:HB3	2:B:171:PRO:HA	1.95	0.49
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.76	0.49
2:B:809:MET:HE2	2:B:814:PHE:CD2	2.48	0.49
2:B:821:GLN:NE2	2:B:851:PHE:HA	2.28	0.49
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.53	0.49
3:C:77:ILE:C	3:C:79:GLN:H	2.21	0.49
3:C:98:VAL:O	3:C:99:LEU:HD23	2.13	0.49
3:C:148:ARG:HG2	3:C:149:LYS:N	2.28	0.49
4:D:40:HIS:HB2	7:G:73:LYS:CE	2.43	0.49
6:F:82:THR:HG22	6:F:84:TYR:N	2.23	0.49
10:J:56:LEU:O	10:J:57:ILE:C	2.54	0.49
1:A:86:LEU:HD13	1:A:90:VAL:HG23	1.95	0.49
1:A:187:LYS:O	1:A:188:ASP:HB2	2.13	0.49
1:A:288:ALA:HA	1:A:291:GLU:OE2	2.12	0.49
1:A:364:VAL:O	1:A:364:VAL:HG13	2.12	0.49
1:A:590:ARG:NH1	1:A:590:ARG:CG	2.74	0.49
1:A:591:PHE:HA	1:A:595:THR:CB	2.43	0.49
1:A:753:GLY:HA2	1:A:757:ASN:ND2	2.28	0.49
1:A:1364:ASN:O	1:A:1365:TYR:C	2.56	0.49
1:A:1377:THR:O	1:A:1378:GLN:C	2.55	0.49
2:B:40:GLU:OE1	2:B:682:SER:HB2	2.13	0.49
2:B:171:PRO:HD2	2:B:457:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:ILE:HG22	2:B:173:MET:N	2.27	0.49
2:B:190:TYR:CE2	10:J:62:ARG:HB3	2.48	0.49
2:B:273:LEU:HD12	2:B:276:ILE:HD12	1.93	0.49
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.35	0.49
2:B:873:THR:CG2	2:B:874:PHE:N	2.75	0.49
3:C:41:ILE:CG2	3:C:172:PRO:HG3	2.43	0.49
7:G:88:ASP:CB	7:G:144:ARG:HA	2.39	0.49
8:H:118:PHE:N	8:H:118:PHE:CD1	2.81	0.49
11:K:55:LYS:HB2	11:K:81:TYR:HE1	1.77	0.49
1:A:594:GLY:N	1:A:603:ASN:ND2	2.60	0.48
1:A:867:ILE:HG22	1:A:872:GLY:N	2.28	0.48
1:A:1239:ARG:HH11	1:A:1239:ARG:HB3	1.78	0.48
2:B:38:PHE:CD1	2:B:811:TYR:CD2	3.01	0.48
2:B:171:PRO:HD2	2:B:457:LEU:HD12	1.94	0.48
2:B:497:ARG:HH22	2:B:775:LYS:CD	2.26	0.48
2:B:525:ALA:O	2:B:768:THR:HG23	2.13	0.48
2:B:635:ARG:HB2	2:B:636:PRO:CD	2.42	0.48
2:B:778:MET:HE1	2:B:853:SER:CB	2.40	0.48
2:B:801:LYS:N	10:J:52:THR:CG2	2.75	0.48
2:B:1002:THR:HG21	2:B:1006:ILE:CG1	2.41	0.48
2:B:1215:ARG:CZ	4:D:15:LEU:HD21	2.43	0.48
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.94	0.48
4:D:14:ARG:O	4:D:16:LYS:HG2	2.13	0.48
4:D:56:ARG:CA	4:D:148:LEU:HD13	2.43	0.48
4:D:214:LEU:O	4:D:218:GLU:HB2	2.13	0.48
5:E:106:GLN:HA	5:E:130:ALA:HB2	1.95	0.48
7:G:132:SER:HB3	7:G:135:ASP:HB2	1.95	0.48
9:I:7:CYS:SG	9:I:8:ARG:O	2.71	0.48
12:L:46:VAL:O	12:L:56:LEU:HD11	2.13	0.48
1:A:186:LYS:O	1:A:187:LYS:CB	2.61	0.48
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.48	0.48
1:A:443:LEU:CD1	1:A:455:MET:HB3	2.42	0.48
1:A:491:VAL:HG12	1:A:492:PRO:O	2.13	0.48
1:A:605:MET:HE2	1:A:607:ILE:CG1	2.43	0.48
1:A:666:ILE:CD1	1:A:667:GLY:N	2.73	0.48
1:A:680:THR:HG23	2:B:729:ILE:CD1	2.43	0.48
1:A:731:ARG:HA	1:A:734:GLU:HB3	1.94	0.48
1:A:858:ASN:C	1:A:858:ASN:ND2	2.72	0.48
1:A:914:GLU:HB2	1:A:979:SER:O	2.13	0.48
2:B:639:ILE:HG22	2:B:641:GLU:HG2	1.95	0.48
2:B:810:GLU:HA	2:B:815:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:918:ILE:HG13	2:B:935:ARG:CZ	2.43	0.48
2:B:1104:HIS:CG	2:B:1122:ARG:HB2	2.48	0.48
3:C:55:THR:O	3:C:56:THR:O	2.31	0.48
3:C:164:ALA:HA	3:C:167:HIS:O	2.13	0.48
4:D:202:ILE:CG2	4:D:207:LEU:HB2	2.43	0.48
6:F:89:GLU:HB3	6:F:134:ILE:HD11	1.95	0.48
6:F:101:ILE:HG23	6:F:107:VAL:HG22	1.94	0.48
7:G:26:LEU:HD12	7:G:56:ILE:HD13	1.95	0.48
12:L:34:CYS:O	12:L:35:SER:C	2.55	0.48
12:L:38:LEU:HD13	12:L:49:LYS:HG2	1.94	0.48
1:A:64:ASN:O	1:A:65:LEU:C	2.55	0.48
1:A:598:LEU:O	1:A:598:LEU:HD23	2.14	0.48
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.96	0.48
1:A:787:PHE:CE1	1:A:796:SER:HA	2.49	0.48
1:A:889:SER:HB3	1:A:1297:GLU:HG2	1.94	0.48
1:A:913:LEU:HD12	1:A:914:GLU:N	2.28	0.48
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.13	0.48
1:A:1436:ILE:O	1:A:1437:GLY:C	2.56	0.48
2:B:388:CYS:C	2:B:390:LEU:H	2.21	0.48
2:B:411:PRO:O	2:B:414:ALA:HB3	2.13	0.48
2:B:418:LYS:HG2	2:B:422:LYS:HE3	1.96	0.48
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.24	0.48
2:B:681:TRP:HA	2:B:684:LEU:HD12	1.95	0.48
2:B:1150:ARG:NH1	2:B:1150:ARG:HB3	2.28	0.48
4:D:54:GLU:OE2	4:D:164:ILE:HD11	2.14	0.48
5:E:64:PRO:HB2	5:E:69:ILE:HD11	1.94	0.48
6:F:148:VAL:HG23	6:F:149:GLU:H	1.78	0.48
7:G:6:ASP:HB3	7:G:73:LYS:NZ	2.28	0.48
1:A:10:PRO:HA	4:D:1:MET:HB2	1.94	0.48
1:A:157:ASP:C	1:A:159:THR:N	2.71	0.48
1:A:492:PRO:HB3	1:A:501:LEU:HD12	1.95	0.48
1:A:1356:ILE:HG21	1:A:1363:VAL:HG21	1.95	0.48
2:B:22:SER:HA	2:B:654:ARG:CB	2.43	0.48
2:B:67:SER:HB2	2:B:92:PHE:CD1	2.48	0.48
2:B:653:VAL:HG13	2:B:657:HIS:CG	2.49	0.48
2:B:821:GLN:NE2	2:B:850:LEU:HD12	2.28	0.48
2:B:1068:GLY:O	2:B:1069:PHE:O	2.31	0.48
4:D:191:ALA:C	4:D:193:THR:H	2.21	0.48
4:D:218:GLU:O	4:D:219:THR:C	2.56	0.48
5:E:177:ARG:C	5:E:212:ARG:HD3	2.38	0.48
12:L:39:SER:O	12:L:40:LEU:CB	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:47:ARG:HG2	12:L:52:GLY:O	2.13	0.48
1:A:963:ILE:HD11	1:A:1048:ASN:HB2	1.95	0.48
1:A:1120:LEU:O	1:A:1323:ASP:N	2.47	0.48
1:A:1142:THR:HB	1:A:1271:ILE:O	2.14	0.48
1:A:1230:GLU:C	1:A:1232:ASN:N	2.71	0.48
1:A:1356:ILE:HG21	1:A:1363:VAL:CG2	2.44	0.48
2:B:169:ARG:CB	2:B:454:THR:HG23	2.43	0.48
3:C:35:ARG:HB3	3:C:35:ARG:HH11	1.78	0.48
3:C:160:LYS:O	3:C:161:LYS:O	2.31	0.48
3:C:259:LEU:HD21	11:K:91:CYS:CB	2.41	0.48
5:E:78:LEU:HD11	5:E:109:ILE:HD11	1.95	0.48
5:E:202:SER:HB3	5:E:205:SER:O	2.13	0.48
6:F:74:ILE:CG2	6:F:75:PRO:HD2	2.42	0.48
6:F:89:GLU:HB3	6:F:134:ILE:CD1	2.44	0.48
8:H:40:LEU:HG	8:H:41:ASP:O	2.13	0.48
8:H:41:ASP:O	8:H:42:ILE:HG13	2.14	0.48
8:H:42:ILE:HG22	8:H:44:VAL:HG22	1.95	0.48
9:I:6:PHE:CD1	9:I:11:ASN:OD1	2.64	0.48
10:J:27:GLU:C	10:J:29:GLU:N	2.71	0.48
11:K:65:HIS:CD2	11:K:67:PHE:N	2.67	0.48
1:A:90:VAL:HG11	1:A:297:GLN:HA	1.96	0.48
1:A:105:CYS:SG	1:A:139:TRP:HA	2.54	0.48
1:A:452:LYS:HG3	2:B:1140:ALA:CB	2.44	0.48
1:A:474:VAL:HG22	1:A:474:VAL:O	2.12	0.48
1:A:833:GLU:HG2	1:A:1102:LYS:HD2	1.94	0.48
1:A:914:GLU:C	1:A:916:GLY:H	2.22	0.48
1:A:960:ILE:HA	1:A:963:ILE:CG2	2.43	0.48
2:B:204:ILE:C	2:B:205:ILE:HD12	2.39	0.48
2:B:1107:ALA:O	2:B:1108:ARG:HB3	2.13	0.48
3:C:123:ASN:C	3:C:125:MET:N	2.69	0.48
5:E:77:SER:O	5:E:105:PHE:HB3	2.13	0.48
5:E:100:ILE:HG23	5:E:105:PHE:CB	2.42	0.48
5:E:173:SER:C	5:E:175:LEU:H	2.21	0.48
7:G:15:PRO:CA	7:G:18:PHE:CD1	2.91	0.48
7:G:79:PHE:CE2	7:G:105:PRO:HD2	2.49	0.48
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.95	0.48
13:T:15:DC:H2'	13:T:16:DT:H71	1.94	0.48
1:A:33:ALA:O	1:A:83:HIS:HD2	1.97	0.48
1:A:381:THR:HG22	1:A:383:TYR:H	1.79	0.48
1:A:658:LEU:HD12	2:B:830:TYR:CD1	2.49	0.48
1:A:744:LYS:CG	1:A:748:MET:HE2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:SER:O	1:A:919:ILE:HG13	2.13	0.48
2:B:181:LEU:CD2	2:B:189:LEU:HD22	2.43	0.48
2:B:213:ILE:HD12	2:B:214:ALA:H	1.78	0.48
2:B:254:LEU:HD11	2:B:273:LEU:HD23	1.96	0.48
2:B:572:HIS:O	2:B:573:GLN:C	2.56	0.48
2:B:600:LEU:O	2:B:609:ILE:HD11	2.14	0.48
2:B:601:ARG:C	2:B:603:LEU:N	2.70	0.48
2:B:1187:ASN:OD1	2:B:1190:ASP:N	2.43	0.48
3:C:73:GLN:HE21	3:C:74:SER:H	1.62	0.48
4:D:192:LYS:HE3	4:D:204:ASP:OD1	2.14	0.48
5:E:2:ASP:O	5:E:3:GLN:HG2	2.14	0.48
5:E:11:ARG:C	5:E:13:TRP:N	2.70	0.48
5:E:100:ILE:HG23	5:E:105:PHE:CG	2.49	0.48
8:H:118:PHE:C	8:H:120:GLY:N	2.72	0.48
9:I:69:PRO:HB2	9:I:85:PHE:HE2	1.77	0.48
11:K:18:LYS:NZ	11:K:37:LYS:O	2.47	0.48
12:L:58:LYS:O	12:L:58:LYS:HG2	2.12	0.48
1:A:224:PHE:CE2	1:A:234:MET:HE2	2.48	0.48
1:A:540:PHE:HA	1:A:572:TRP:O	2.12	0.48
1:A:814:PHE:HE1	2:B:519:TRP:HA	1.77	0.48
1:A:958:VAL:CG2	1:A:1053:PHE:HA	2.44	0.48
1:A:1001:ARG:HD2	6:F:81:THR:O	2.14	0.48
1:A:1341:ILE:C	1:A:1344:GLY:H	2.22	0.48
1:A:1376:THR:O	1:A:1377:THR:C	2.57	0.48
2:B:274:PRO:O	2:B:275:TYR:HB2	2.13	0.48
2:B:299:GLU:CG	2:B:571:PRO:HG3	2.43	0.48
2:B:589:VAL:CG1	2:B:590:HIS:N	2.75	0.48
2:B:635:ARG:O	2:B:692:TYR:HA	2.13	0.48
2:B:653:VAL:HG13	2:B:657:HIS:CD2	2.48	0.48
2:B:687:GLU:O	2:B:688:GLY:C	2.55	0.48
2:B:814:PHE:O	2:B:817:LEU:N	2.47	0.48
2:B:855:PHE:CD2	2:B:972:LYS:HE3	2.48	0.48
2:B:999:MET:HE2	2:B:1011:ILE:CD1	2.43	0.48
3:C:66:ARG:NH2	10:J:2:ILE:CG2	2.76	0.48
4:D:163:VAL:O	4:D:166:LEU:HB3	2.13	0.48
4:D:192:LYS:HZ2	4:D:192:LYS:HB3	1.79	0.48
5:E:90:VAL:O	5:E:90:VAL:HG22	2.13	0.48
5:E:133:GLU:HG2	5:E:135:PHE:HE1	1.79	0.48
5:E:147:HIS:HD2	5:E:149:LEU:H	1.61	0.48
6:F:94:LEU:CD2	6:F:122:MET:HA	2.44	0.48
6:F:130:ILE:O	6:F:148:VAL:CG2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:135:ARG:NH2	6:F:145:ASP:OD2	2.46	0.48
8:H:56:THR:HB	8:H:145:ARG:HG2	1.96	0.48
10:J:7:CYS:SG	10:J:49:MET:CE	3.02	0.48
11:K:42:LEU:HD22	11:K:71:PHE:HZ	1.79	0.48
11:K:85:ASP:O	11:K:88:LYS:HB2	2.14	0.48
1:A:919:ILE:HD13	1:A:983:ILE:CD1	2.44	0.48
1:A:1273:LEU:N	1:A:1273:LEU:CD1	2.76	0.48
2:B:743:ILE:HD13	2:B:743:ILE:N	2.28	0.48
2:B:865:LYS:CD	2:B:961:LEU:HD21	2.43	0.48
2:B:1187:ASN:O	2:B:1188:LYS:CB	2.62	0.48
3:C:3:GLU:HB3	11:K:104:ASN:HD21	1.78	0.48
3:C:29:MET:O	3:C:32:SER:HB2	2.14	0.48
3:C:179:GLU:HG2	3:C:180:TYR:N	2.28	0.48
8:H:43:ASN:HB3	8:H:95:TYR:OH	2.13	0.48
8:H:107:VAL:HG21	8:H:124:ARG:NH2	2.29	0.48
12:L:38:LEU:HD11	12:L:49:LYS:HE2	1.96	0.48
1:A:308:ILE:HG22	1:A:309:ALA:N	2.19	0.48
1:A:325:ILE:HG22	2:B:1210:MET:HE2	1.95	0.48
1:A:345:VAL:HG23	1:A:346:ASP:O	2.13	0.48
1:A:958:VAL:HG11	1:A:1049:ILE:HG23	1.95	0.48
1:A:1164:PRO:C	1:A:1166:ASP:N	2.71	0.48
1:A:1209:MET:O	1:A:1210:GLY:C	2.56	0.48
1:A:1348:LEU:HD21	1:A:1375:MET:SD	2.54	0.48
1:A:1404:GLU:HB3	1:A:1408:ILE:HG13	1.96	0.48
2:B:67:SER:HB2	2:B:92:PHE:HD1	1.79	0.48
2:B:126:SER:CB	2:B:172:ILE:HD11	2.43	0.48
2:B:361:LEU:N	2:B:362:PRO:CD	2.77	0.48
2:B:542:MET:CG	2:B:747:MET:HE2	2.43	0.48
2:B:1156:ASP:O	2:B:1157:ALA:HB3	2.14	0.48
3:C:209:TYR:N	3:C:209:TYR:CD1	2.82	0.48
4:D:40:HIS:HB3	7:G:73:LYS:NZ	2.28	0.48
8:H:42:ILE:O	8:H:44:VAL:HG23	2.13	0.48
9:I:19:ASP:OD1	9:I:22:ASN:HB2	2.13	0.48
1:A:500:GLU:CD	2:B:1145:SER:HB2	2.39	0.47
1:A:853:ASP:OD1	1:A:855:THR:CG2	2.62	0.47
1:A:942:PHE:C	1:A:942:PHE:HD2	2.22	0.47
1:A:1035:TYR:O	1:A:1037:LEU:N	2.46	0.47
2:B:843:GLN:N	2:B:994:TYR:O	2.31	0.47
2:B:973:ILE:CG2	2:B:974:PRO:HD2	2.44	0.47
2:B:1017:ILE:CB	2:B:1018:PRO:HD3	2.41	0.47
3:C:190:ASP:O	3:C:191:TYR:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:195:GLN:HB3	3:C:196:ASP:H	1.51	0.47
4:D:137:ASN:H	4:D:137:ASN:HD22	1.51	0.47
8:H:100:THR:N	8:H:117:SER:O	2.41	0.47
1:A:6:TYR:CD1	1:A:7:SER:N	2.82	0.47
1:A:323:LYS:H	1:A:323:LYS:CD	2.24	0.47
1:A:332:LYS:C	1:A:334:GLY:H	2.22	0.47
1:A:347:PHE:HB3	1:A:491:VAL:HB	1.96	0.47
1:A:361:LEU:HA	1:A:471:ASN:ND2	2.29	0.47
1:A:444:PHE:CB	1:A:458:HIS:HD2	2.27	0.47
1:A:500:GLU:O	1:A:504:LEU:HD13	2.14	0.47
1:A:886:ILE:CG2	1:A:952:ALA:HB2	2.44	0.47
1:A:971:PHE:C	1:A:973:ILE:N	2.72	0.47
2:B:466:TRP:N	2:B:475:SER:HB2	2.29	0.47
2:B:593:PRO:O	2:B:596:LEU:N	2.47	0.47
2:B:616:ILE:HD12	2:B:616:ILE:H	1.79	0.47
2:B:807:ARG:NH1	2:B:807:ARG:HB3	2.28	0.47
2:B:882:THR:HG22	2:B:884:ARG:N	2.29	0.47
6:F:138:LEU:CD2	6:F:139:PRO:HD2	2.43	0.47
7:G:96:GLN:HA	7:G:121:PHE:CZ	2.50	0.47
11:K:24:ASP:H	11:K:31:VAL:HA	1.79	0.47
13:T:15:DC:H2"	13:T:16:DT:OP2	2.14	0.47
1:A:474:VAL:C	1:A:477:PRO:HD2	2.39	0.47
1:A:939:ASP:O	1:A:940:ARG:C	2.57	0.47
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.96	0.47
2:B:745:PRO:C	2:B:747:MET:N	2.72	0.47
2:B:814:PHE:O	2:B:816:GLU:N	2.47	0.47
2:B:826:ALA:CB	2:B:1008:PRO:HB3	2.42	0.47
2:B:880:THR:HG22	2:B:880:THR:O	2.14	0.47
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.96	0.47
3:C:31:ASN:O	3:C:32:SER:C	2.58	0.47
3:C:105:GLY:O	3:C:149:LYS:O	2.31	0.47
3:C:124:LEU:HD23	3:C:124:LEU:HA	1.72	0.47
4:D:23:ASN:O	7:G:83:LYS:HD2	2.14	0.47
4:D:118:THR:HB	4:D:121:LYS:HB2	1.96	0.47
4:D:192:LYS:HZ2	4:D:192:LYS:CB	2.27	0.47
5:E:7:ARG:HD2	5:E:7:ARG:C	2.38	0.47
6:F:119:ARG:O	6:F:122:MET:HB2	2.14	0.47
9:I:111:THR:CG2	9:I:113:ASP:HB2	2.45	0.47
11:K:55:LYS:CB	11:K:81:TYR:CE1	2.97	0.47
12:L:31:CYS:HB2	12:L:48:CYS:SG	2.53	0.47
12:L:55:ILE:HG12	12:L:56:LEU:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:T:11:DA:H2''	13:T:12:DG:O5'	2.15	0.47
1:A:7:SER:HB2	2:B:1175:LEU:HD22	1.94	0.47
1:A:123:ARG:O	1:A:124:GLN:C	2.57	0.47
1:A:228:PHE:CD2	1:A:228:PHE:N	2.83	0.47
1:A:311:GLN:HB2	1:A:312:PRO:CD	2.44	0.47
1:A:350:ARG:HB2	1:A:488:ASN:OD1	2.15	0.47
1:A:730:GLY:O	1:A:731:ARG:C	2.56	0.47
1:A:774:ARG:CZ	1:A:797:LYS:CB	2.92	0.47
1:A:811:GLN:O	1:A:812:GLU:C	2.57	0.47
1:A:1114:PRO:O	1:A:1115:SER:O	2.31	0.47
2:B:286:PHE:HA	2:B:289:LEU:HD12	1.96	0.47
2:B:840:ILE:CG2	2:B:994:TYR:HD1	2.26	0.47
2:B:888:GLY:O	2:B:889:THR:C	2.56	0.47
2:B:1065:GLN:HB3	2:B:1069:PHE:O	2.14	0.47
2:B:1165:ILE:HG22	4:D:15:LEU:HA	1.97	0.47
5:E:136:ASN:OD1	5:E:137:GLU:N	2.47	0.47
7:G:119:LEU:CD1	7:G:132:SER:HB2	2.44	0.47
7:G:164:LYS:O	7:G:164:LYS:HG2	2.13	0.47
8:H:63:LEU:HD13	8:H:64:ASN:N	2.29	0.47
10:J:25:LEU:O	10:J:29:GLU:HA	2.15	0.47
11:K:55:LYS:HD2	11:K:81:TYR:HD1	1.78	0.47
12:L:26:THR:CG2	12:L:62:LYS:HZ1	2.25	0.47
1:A:134:ARG:C	1:A:136:ALA:H	2.23	0.47
1:A:265:LYS:O	1:A:269:ILE:HG13	2.14	0.47
1:A:442:VAL:HG11	1:A:489:LEU:HD11	1.97	0.47
1:A:692:ASP:C	1:A:694:THR:H	2.21	0.47
1:A:707:GLY:O	1:A:708:MET:HG3	2.14	0.47
1:A:870:GLU:HG2	5:E:208:TYR:CD2	2.49	0.47
1:A:1242:VAL:CG1	1:A:1243:VAL:H	2.14	0.47
2:B:99:LYS:HB3	2:B:100:PRO:HD2	1.96	0.47
2:B:332:ASP:C	2:B:334:ILE:H	2.22	0.47
2:B:455:SER:O	2:B:458:LYS:HB2	2.13	0.47
2:B:654:ARG:C	2:B:656:GLY:N	2.71	0.47
3:C:176:ILE:CG2	3:C:177:GLU:N	2.78	0.47
5:E:89:GLY:C	5:E:91:LYS:H	2.21	0.47
6:F:109:VAL:HG11	6:F:123:LYS:CD	2.44	0.47
8:H:86:ASP:O	8:H:87:ARG:O	2.32	0.47
10:J:57:ILE:CA	10:J:60:PHE:HD2	2.24	0.47
1:A:84:ILE:O	1:A:84:ILE:CG2	2.61	0.47
1:A:265:LYS:HD3	1:A:303:TYR:CA	2.44	0.47
1:A:326:ARG:NH2	1:A:1407:GLU:HG2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:LYS:O	1:A:706:HIS:C	2.57	0.47
1:A:709:THR:HG23	9:I:94:ASP:HA	1.97	0.47
1:A:733:ALA:O	1:A:737:LEU:HG	2.14	0.47
1:A:1121:GLU:HB3	1:A:1124:HIS:CD2	2.49	0.47
1:A:1135:ARG:C	1:A:1137:ALA:H	2.22	0.47
1:A:1423:GLY:H	1:A:1426:GLU:HG3	1.80	0.47
2:B:276:ILE:O	2:B:278:GLN:N	2.40	0.47
2:B:451:LYS:O	2:B:455:SER:OG	2.32	0.47
2:B:891:ASP:O	2:B:893:LEU:N	2.47	0.47
2:B:1034:VAL:HG21	2:B:1055:ILE:HG23	1.97	0.47
2:B:1047:PHE:CD1	2:B:1047:PHE:N	2.82	0.47
2:B:1065:GLN:NE2	2:B:1067:ARG:H	2.06	0.47
2:B:1072:MET:HE3	2:B:1085:ILE:CB	2.36	0.47
2:B:1112:GLN:HG2	2:B:1113:VAL:N	2.29	0.47
4:D:22:GLU:OE1	4:D:22:GLU:N	2.37	0.47
6:F:71:GLU:O	6:F:72:LYS:C	2.57	0.47
6:F:134:ILE:O	6:F:134:ILE:HG22	2.12	0.47
8:H:58:THR:C	8:H:59:ILE:HG13	2.40	0.47
9:I:85:PHE:HD2	9:I:85:PHE:H	1.50	0.47
1:A:116:ASP:OD2	1:A:164:ARG:HD2	2.15	0.47
1:A:170:THR:CG2	1:A:171:GLN:N	2.76	0.47
1:A:174:ILE:CG2	1:A:175:ARG:N	2.78	0.47
1:A:224:PHE:CZ	1:A:234:MET:HE2	2.50	0.47
1:A:398:GLU:O	1:A:399:HIS:C	2.57	0.47
1:A:444:PHE:HD1	1:A:489:LEU:HB2	1.80	0.47
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.95	0.47
1:A:456:MET:HE1	1:A:521:MET:HE3	1.96	0.47
1:A:477:PRO:HG3	1:A:520:CYS:O	2.15	0.47
1:A:515:GLN:HA	1:A:1367:HIS:NE2	2.30	0.47
1:A:567:LYS:HZ3	8:H:95:TYR:CB	2.28	0.47
1:A:834:THR:HG21	1:A:1077:THR:CB	2.45	0.47
1:A:940:ARG:HG2	1:A:940:ARG:HH11	1.80	0.47
1:A:1081:LEU:HD11	1:A:1098:VAL:N	2.25	0.47
1:A:1115:SER:O	1:A:1311:VAL:HG22	2.15	0.47
1:A:1121:GLU:O	1:A:1122:PRO:C	2.57	0.47
1:A:1129:GLU:O	1:A:1130:GLN:C	2.57	0.47
1:A:1214:GLU:O	1:A:1218:GLN:HG2	2.15	0.47
1:A:1360:GLY:O	1:A:1361:SER:O	2.32	0.47
2:B:205:ILE:O	2:B:206:ASN:C	2.57	0.47
2:B:247:GLY:C	2:B:249:ARG:H	2.23	0.47
2:B:352:ALA:HA	2:B:355:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:HIS:O	2:B:364:ILE:CB	2.63	0.47
2:B:449:ASN:C	2:B:451:LYS:N	2.70	0.47
2:B:1057:LYS:O	2:B:1061:GLU:HG3	2.14	0.47
3:C:43:THR:O	3:C:44:LEU:HB2	2.14	0.47
3:C:167:HIS:HE1	12:L:70:ARG:HA	1.80	0.47
3:C:233:GLU:HB3	3:C:234:SER:H	1.53	0.47
4:D:29:LEU:HB3	7:G:82:PHE:CE2	2.50	0.47
4:D:67:ARG:HA	4:D:133:THR:CG2	2.45	0.47
4:D:208:GLU:O	4:D:209:ARG:C	2.58	0.47
5:E:52:ARG:HH11	5:E:52:ARG:HG3	1.78	0.47
5:E:79:TRP:HE1	5:E:81:GLU:HB2	1.79	0.47
6:F:73:ALA:HB2	6:F:143:PHE:CD2	2.50	0.47
6:F:75:PRO:C	6:F:77:ASP:N	2.70	0.47
6:F:150:GLU:O	6:F:151:LEU:C	2.57	0.47
7:G:44:TYR:CD2	7:G:105:PRO:HB2	2.49	0.47
7:G:112:LYS:O	7:G:115:MET:HG2	2.14	0.47
8:H:103:LYS:HG2	8:H:104:PHE:N	2.30	0.47
9:I:98:VAL:HG12	9:I:99:LEU:N	2.28	0.47
1:A:203:SER:OG	1:A:206:GLU:HB2	2.15	0.47
1:A:244:PRO:CB	1:A:245:PRO:HD3	2.45	0.47
1:A:469:ARG:HB3	1:A:469:ARG:HH11	1.80	0.47
1:A:511:ILE:CG2	1:A:634:THR:HG21	2.44	0.47
1:A:552:TRP:CE3	1:A:651:LYS:HB3	2.50	0.47
1:A:600:PRO:HG2	1:A:601:LYS:N	2.18	0.47
1:A:626:ASN:C	1:A:628:GLY:H	2.21	0.47
1:A:726:ARG:HD2	1:A:765:VAL:O	2.15	0.47
1:A:883:LEU:O	1:A:886:ILE:HG22	2.15	0.47
1:A:1164:PRO:C	1:A:1166:ASP:H	2.23	0.47
1:A:1445:ILE:HD13	7:G:70:PHE:CZ	2.50	0.47
2:B:29:ASP:CB	2:B:658:ILE:HD13	2.44	0.47
2:B:46:GLN:NE2	2:B:496:ARG:HB3	2.30	0.47
2:B:227:LYS:H	2:B:395:GLN:CD	2.23	0.47
3:C:35:ARG:HD3	11:K:41:THR:HA	1.96	0.47
4:D:119:ARG:HD3	4:D:221:TYR:CD2	2.50	0.47
5:E:22:MET:HE3	5:E:26:ARG:HH11	1.75	0.47
7:G:51:TYR:C	7:G:51:TYR:CD2	2.93	0.47
7:G:111:THR:O	7:G:112:LYS:C	2.57	0.47
8:H:12:VAL:HG13	8:H:26:ILE:HG21	1.96	0.47
11:K:49:GLU:HA	11:K:52:ASN:ND2	2.30	0.47
11:K:79:GLU:C	11:K:81:TYR:H	2.23	0.47
13:T:15:DC:C2'	13:T:16:DT:C7	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:MET:H	1:A:41:MET:HE3	1.80	0.47
1:A:154:SER:OG	1:A:162:VAL:HG23	2.15	0.47
1:A:541:ILE:HD11	1:A:656:TRP:NE1	2.28	0.47
1:A:1327:ILE:HG23	5:E:147:HIS:HE1	1.80	0.47
2:B:199:MET:HE2	2:B:492:LEU:CD2	2.45	0.47
2:B:269:ILE:HG21	2:B:282:ILE:HD13	1.96	0.47
2:B:957:ASN:O	2:B:959:ASP:N	2.48	0.47
2:B:1223:ASP:HB3	2:B:1224:PHE:H	1.50	0.47
3:C:77:ILE:HG22	3:C:78:GLU:N	2.29	0.47
4:D:137:ASN:C	4:D:139:LYS:H	2.23	0.47
5:E:212:ARG:HH11	5:E:212:ARG:HG3	1.79	0.47
6:F:70:LYS:C	6:F:72:LYS:N	2.72	0.47
6:F:72:LYS:HE3	6:F:72:LYS:CA	2.44	0.47
7:G:29:LYS:O	7:G:30:LEU:C	2.58	0.47
7:G:88:ASP:HB2	7:G:143:ILE:O	2.15	0.47
7:G:91:VAL:HB	7:G:139:ILE:O	2.13	0.47
8:H:43:ASN:OD1	8:H:46:LEU:N	2.48	0.47
1:A:299:HIS:C	1:A:301:ALA:N	2.71	0.47
1:A:332:LYS:C	1:A:333:GLU:HG2	2.40	0.47
1:A:552:TRP:NE1	11:K:62:LYS:HB2	2.30	0.47
1:A:852:TYR:CD2	1:A:1060:PRO:CB	2.96	0.47
1:A:1058:VAL:O	1:A:1060:PRO:HD3	2.15	0.47
1:A:1284:MET:HA	1:A:1306:LEU:HD23	1.97	0.47
2:B:54:PHE:CZ	2:B:59:LEU:HD13	2.50	0.47
2:B:195:CYS:HB2	2:B:784:ASN:HB3	1.97	0.47
2:B:449:ASN:O	2:B:450:ALA:C	2.58	0.47
2:B:687:GLU:O	2:B:689:LEU:N	2.48	0.47
2:B:745:PRO:O	2:B:747:MET:N	2.48	0.47
2:B:746:SER:HB3	2:B:1046:PRO:CB	2.45	0.47
3:C:221:TYR:CE1	3:C:222:LYS:HG3	2.50	0.47
8:H:116:TYR:HE2	8:H:140:ALA:CB	2.27	0.47
9:I:80:SER:OG	9:I:105:SER:HB2	2.15	0.47
10:J:7:CYS:CB	10:J:49:MET:HE3	2.44	0.47
1:A:226:GLU:O	1:A:226:GLU:HG2	2.15	0.46
1:A:299:HIS:O	1:A:301:ALA:N	2.48	0.46
1:A:317:LYS:HG2	2:B:471:LYS:NZ	2.29	0.46
1:A:567:LYS:CB	8:H:96:VAL:H	2.18	0.46
1:A:701:LEU:O	1:A:702:LEU:HG	2.14	0.46
1:A:821:ARG:HB2	1:A:821:ARG:NH1	2.30	0.46
1:A:921:GLY:O	1:A:923:LEU:N	2.48	0.46
2:B:170:LEU:O	2:B:172:ILE:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:MET:HE2	2:B:492:LEU:HD21	1.97	0.46
2:B:289:LEU:HD22	2:B:375:ALA:HB2	1.97	0.46
2:B:487:THR:O	2:B:490:SER:HB3	2.15	0.46
2:B:492:LEU:O	2:B:495:LEU:N	2.48	0.46
2:B:687:GLU:CB	2:B:689:LEU:HG	2.44	0.46
2:B:693:ILE:HD13	2:B:701:ILE:HD13	1.97	0.46
2:B:1023:VAL:O	2:B:1026:LEU:N	2.48	0.46
3:C:88:CYS:SG	3:C:91:HIS:CA	3.03	0.46
9:I:7:CYS:C	9:I:8:ARG:O	2.56	0.46
9:I:53:GLY:O	9:I:89:GLN:HB2	2.15	0.46
9:I:61:ASP:C	9:I:63:GLY:H	2.23	0.46
11:K:44:ASN:N	11:K:61:TYR:CE1	2.83	0.46
1:A:168:GLY:O	1:A:169:ASN:C	2.58	0.46
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.30	0.46
1:A:482:PHE:CD2	1:A:482:PHE:N	2.80	0.46
1:A:675:THR:HG21	1:A:736:ASN:CG	2.41	0.46
1:A:1017:LEU:HD23	5:E:204:THR:C	2.40	0.46
1:A:1081:LEU:HD12	1:A:1098:VAL:HG23	1.97	0.46
1:A:1237:ILE:HG22	1:A:1238:ILE:H	1.78	0.46
1:A:1314:SER:C	1:A:1315:GLU:HG3	2.40	0.46
2:B:26:THR:O	2:B:29:ASP:HB2	2.15	0.46
2:B:789:MET:HE2	2:B:953:LEU:CD2	2.46	0.46
3:C:16:ASP:O	3:C:17:ASN:CG	2.59	0.46
3:C:169:LYS:HE3	3:C:170:TRP:CZ2	2.50	0.46
5:E:147:HIS:CD2	5:E:149:LEU:H	2.33	0.46
7:G:106:MET:CG	7:G:107:LYS:N	2.78	0.46
8:H:40:LEU:CD1	8:H:123:MET:HB2	2.45	0.46
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.49	0.46
8:H:110:ASP:O	8:H:128:ASN:HB2	2.15	0.46
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.49	0.46
11:K:78:THR:O	11:K:81:TYR:HB3	2.14	0.46
1:A:293:GLU:C	1:A:295:LEU:N	2.73	0.46
1:A:334:GLY:O	1:A:335:ARG:C	2.58	0.46
1:A:693:VAL:O	1:A:693:VAL:HG12	2.15	0.46
1:A:709:THR:HB	1:A:712:GLU:HG3	1.96	0.46
1:A:847:ASP:O	1:A:858:ASN:HA	2.16	0.46
1:A:873:MET:HG3	1:A:1056:SER:O	2.15	0.46
1:A:1002:GLY:CA	1:A:1007:ILE:HG21	2.29	0.46
1:A:1444:MET:O	6:F:132:LEU:HA	2.15	0.46
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.44	0.46
2:B:118:ARG:CG	2:B:204:ILE:HD13	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:ARG:NH1	12:L:54:ARG:HH11	2.13	0.46
2:B:312:GLU:O	2:B:315:LYS:HB2	2.15	0.46
2:B:792:MET:HG2	2:B:855:PHE:HE1	1.79	0.46
2:B:896:ASP:OD1	2:B:898:LEU:HB2	2.16	0.46
3:C:11:ARG:NH2	3:C:206:ASN:OD1	2.47	0.46
4:D:118:THR:O	4:D:120:GLU:N	2.47	0.46
6:F:96:THR:O	6:F:100:GLN:HG3	2.16	0.46
7:G:88:ASP:HB3	7:G:144:ARG:HB2	1.97	0.46
7:G:96:GLN:HA	7:G:121:PHE:CE2	2.50	0.46
8:H:80:ARG:HH12	11:K:57:LEU:HD11	1.80	0.46
9:I:2:THR:O	9:I:3:THR:C	2.58	0.46
12:L:26:THR:CG2	12:L:27:LEU:N	2.79	0.46
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.96	0.46
1:A:269:ILE:HG23	1:A:300:VAL:CG2	2.46	0.46
1:A:332:LYS:HB2	1:A:337:ARG:HD2	1.96	0.46
1:A:402:ALA:HB1	1:A:433:GLU:O	2.16	0.46
1:A:834:THR:HG21	1:A:1077:THR:CA	2.46	0.46
1:A:1067:LEU:O	1:A:1069:ALA:N	2.48	0.46
1:A:1345:ARG:NH1	1:A:1373:ASP:OD1	2.48	0.46
1:A:1423:GLY:CA	1:A:1426:GLU:HG2	2.46	0.46
2:B:610:ASN:C	2:B:612:GLU:H	2.23	0.46
2:B:768:THR:O	2:B:771:SER:HB2	2.16	0.46
2:B:847:ASP:O	2:B:849:GLY:N	2.49	0.46
2:B:1064:TYR:O	2:B:1065:GLN:C	2.59	0.46
3:C:5:GLY:O	3:C:7:GLN:N	2.48	0.46
4:D:68:ARG:C	4:D:70:PHE:H	2.22	0.46
5:E:129:PRO:O	5:E:130:ALA:O	2.33	0.46
10:J:8:PHE:H	10:J:49:MET:HE1	1.80	0.46
11:K:42:LEU:HD21	11:K:46:ILE:HD12	1.97	0.46
12:L:55:ILE:CG1	12:L:56:LEU:H	2.29	0.46
14:N:5:DC:H2'	14:N:6:DT:H72	1.98	0.46
15:P:6:A:H2'	15:P:7:G:H8	1.80	0.46
1:A:23:SER:O	1:A:25:GLU:N	2.49	0.46
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.98	0.46
1:A:537:ARG:O	1:A:540:PHE:CE1	2.68	0.46
1:A:542:GLU:O	1:A:546:VAL:HG23	2.16	0.46
1:A:725:ALA:HA	1:A:728:LYS:HE2	1.96	0.46
1:A:840:ARG:HH12	1:A:1102:LYS:HE3	1.81	0.46
1:A:901:LEU:HD11	1:A:983:ILE:HD13	1.97	0.46
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	3.03	0.46
1:A:1152:ILE:HG22	1:A:1193:LEU:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1213:GLY:O	1:A:1216:ILE:N	2.49	0.46
1:A:1371:LEU:O	1:A:1375:MET:HG3	2.14	0.46
2:B:116:GLU:C	2:B:118:ARG:N	2.71	0.46
2:B:388:CYS:O	2:B:390:LEU:N	2.48	0.46
2:B:496:ARG:HD2	2:B:751:VAL:CG2	2.45	0.46
2:B:653:VAL:HA	2:B:657:HIS:CD2	2.50	0.46
2:B:831:SER:HB3	2:B:994:TYR:OH	2.15	0.46
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.50	0.46
2:B:1077:THR:HG22	11:K:44:ASN:HD21	1.81	0.46
2:B:1166:CYS:SG	2:B:1166:CYS:O	2.73	0.46
3:C:17:ASN:OD1	3:C:233:GLU:HG2	2.15	0.46
3:C:31:ASN:OD1	3:C:34:ARG:HD3	2.16	0.46
3:C:115:SER:O	3:C:118:LEU:HG	2.15	0.46
5:E:23:VAL:O	5:E:28:TYR:HD1	1.98	0.46
5:E:98:ILE:HG22	5:E:102:GLU:CD	2.41	0.46
8:H:145:ARG:O	8:H:146:ARG:HB2	2.15	0.46
1:A:42:ASP:OD1	1:A:47:ARG:HA	2.15	0.46
1:A:675:THR:HG21	1:A:736:ASN:ND2	2.30	0.46
1:A:829:VAL:O	1:A:832:ALA:N	2.49	0.46
1:A:853:ASP:OD1	1:A:855:THR:N	2.49	0.46
1:A:1035:TYR:O	1:A:1036:ARG:C	2.58	0.46
1:A:1215:ARG:O	1:A:1218:GLN:HG3	2.16	0.46
1:A:1289:ARG:HH12	1:A:1326:ARG:NH1	2.13	0.46
1:A:1389:PHE:CD1	1:A:1390:ASN:N	2.83	0.46
1:A:1404:GLU:HB2	1:A:1408:ILE:CG1	2.46	0.46
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.45	0.46
2:B:762:ASN:OD1	2:B:1022:THR:HA	2.16	0.46
2:B:785:TYR:HE2	10:J:60:PHE:CE1	2.33	0.46
2:B:891:ASP:C	2:B:893:LEU:N	2.72	0.46
2:B:955:THR:HG22	2:B:956:THR:N	2.29	0.46
2:B:1069:PHE:CD1	2:B:1069:PHE:N	2.82	0.46
2:B:1183:LYS:C	2:B:1185:CYS:N	2.73	0.46
3:C:69:LEU:N	3:C:69:LEU:HD12	2.31	0.46
3:C:76:ASP:OD2	3:C:128:ASN:N	2.47	0.46
3:C:167:HIS:CD2	3:C:168:ALA:H	2.32	0.46
4:D:140:ASP:O	4:D:143:ASN:N	2.49	0.46
4:D:154:PHE:HA	4:D:219:THR:HB	1.98	0.46
4:D:187:THR:HG22	4:D:188:ALA:N	2.31	0.46
5:E:116:ILE:HG22	5:E:117:THR:N	2.31	0.46
6:F:113:GLY:O	6:F:115:THR:HG23	2.15	0.46
8:H:22:LYS:HD3	8:H:45:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:82:PRO:HG3	11:K:54:ARG:CD	2.45	0.46
11:K:20:LYS:HB3	11:K:34:THR:HB	1.97	0.46
1:A:218:ASP:O	1:A:219:PHE:C	2.59	0.46
1:A:332:LYS:HB2	1:A:337:ARG:NH1	2.30	0.46
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.97	0.46
1:A:830:LYS:HG3	1:A:1098:VAL:HG11	1.98	0.46
1:A:930:ASP:O	1:A:931:GLU:C	2.58	0.46
2:B:69:LEU:HB3	2:B:70:ILE:H	1.63	0.46
2:B:213:ILE:HG12	2:B:497:ARG:HB3	1.98	0.46
2:B:855:PHE:HD2	2:B:972:LYS:HE3	1.79	0.46
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.46	0.46
2:B:957:ASN:O	2:B:958:GLN:C	2.58	0.46
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.14	0.46
2:B:1085:ILE:N	2:B:1085:ILE:CD1	2.74	0.46
2:B:1130:PHE:CE1	2:B:1134:GLU:HB3	2.51	0.46
3:C:82:TYR:CE2	3:C:161:LYS:HG2	2.51	0.46
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.30	0.46
3:C:154:LYS:O	3:C:155:LEU:HD23	2.15	0.46
4:D:142:LYS:O	4:D:146:GLN:HG3	2.15	0.46
7:G:137:ILE:CG2	7:G:143:ILE:HD11	2.45	0.46
8:H:113:ALA:HB1	8:H:125:LEU:O	2.16	0.46
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.97	0.46
10:J:24:LEU:O	10:J:30:LEU:HB2	2.16	0.46
12:L:53:HIS:C	12:L:55:ILE:HD13	2.41	0.46
1:A:52:GLY:N	1:A:56:PRO:HG3	2.31	0.46
1:A:367:PRO:HG2	1:A:370:ILE:HD12	1.96	0.46
1:A:432:VAL:O	1:A:432:VAL:HG12	2.15	0.46
1:A:439:ASN:N	1:A:460:VAL:O	2.46	0.46
1:A:553:VAL:HG22	1:A:652:VAL:CG2	2.46	0.46
1:A:874:ASP:C	1:A:874:ASP:OD1	2.59	0.46
1:A:877:HIS:CG	1:A:1056:SER:HA	2.51	0.46
1:A:949:ASP:HB3	1:A:951:GLU:H	1.80	0.46
1:A:1042:PHE:HE2	1:A:1046:LEU:HD11	1.78	0.46
1:A:1325:THR:CG2	1:A:1326:ARG:HG3	2.46	0.46
1:A:1446:ASP:O	1:A:1447:GLU:C	2.58	0.46
2:B:251:ILE:O	2:B:251:ILE:HG22	2.16	0.46
2:B:746:SER:HB3	2:B:1046:PRO:HB2	1.98	0.46
2:B:895:ASP:C	2:B:897:GLY:N	2.73	0.46
2:B:1072:MET:CE	2:B:1087:PHE:HB2	2.45	0.46
2:B:1181:GLU:N	2:B:1188:LYS:HG3	2.31	0.46
3:C:173:ALA:O	3:C:174:ALA:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:100:ILE:O	5:E:100:ILE:CG2	2.63	0.46
5:E:163:GLU:OE2	5:E:167:ARG:HG2	2.15	0.46
6:F:90:ARG:HG3	6:F:91:ALA:H	1.79	0.46
8:H:112:ILE:CG2	8:H:113:ALA:N	2.79	0.46
9:I:50:THR:CG2	9:I:51:ASN:N	2.79	0.46
11:K:98:LEU:O	11:K:99:GLY:C	2.59	0.46
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.96	0.46
1:A:127:ALA:O	1:A:129:LYS:N	2.49	0.46
1:A:377:PRO:CD	1:A:493:GLN:OE1	2.64	0.46
1:A:575:LYS:HB3	1:A:612:ILE:CG2	2.45	0.46
1:A:618:GLU:O	1:A:620:LYS:N	2.49	0.46
1:A:667:GLY:HA3	3:C:192:TRP:CH2	2.50	0.46
1:A:726:ARG:HD3	1:A:766:GLY:HA2	1.98	0.46
1:A:786:HIS:CE1	2:B:519:TRP:CZ2	3.02	0.46
1:A:883:LEU:HD11	1:A:1017:LEU:HD11	1.98	0.46
1:A:1004:ASN:ND2	1:A:1007:ILE:HG12	2.31	0.46
1:A:1041:ALA:O	1:A:1044:TRP:HB3	2.15	0.46
1:A:1126:ALA:O	1:A:1128:GLN:N	2.49	0.46
1:A:1187:GLN:HA	1:A:1244:ARG:CD	2.45	0.46
2:B:120:ARG:NH1	12:L:54:ARG:NH1	2.64	0.46
2:B:215:GLN:HA	2:B:215:GLN:NE2	2.31	0.46
2:B:515:HIS:O	2:B:518:HIS:HB2	2.16	0.46
2:B:591:ARG:O	2:B:593:PRO:CD	2.64	0.46
2:B:656:GLY:O	2:B:657:HIS:C	2.59	0.46
2:B:773:MET:SD	2:B:987:LYS:HE3	2.55	0.46
2:B:794:ASN:O	2:B:795:ILE:HD12	2.15	0.46
2:B:830:TYR:HE2	2:B:1000:PRO:CD	2.22	0.46
2:B:860:MET:HG2	2:B:861:ASP:H	1.78	0.46
3:C:27:LEU:HD11	3:C:178:PHE:HE2	1.80	0.46
5:E:159:ASP:O	5:E:160:GLU:C	2.59	0.46
8:H:80:ARG:NH1	11:K:57:LEU:HD11	2.31	0.46
9:I:6:PHE:HA	9:I:14:LEU:HG	1.98	0.46
9:I:55:THR:O	9:I:56:ALA:C	2.58	0.46
1:A:255:SER:OG	2:B:918:ILE:HG23	2.14	0.46
1:A:332:LYS:HA	1:A:337:ARG:HB3	1.98	0.46
1:A:353:ILE:HD11	1:A:480:ALA:HB1	1.97	0.46
1:A:360:GLU:C	1:A:471:ASN:HD22	2.24	0.46
1:A:470:LEU:HD13	1:A:487:MET:CE	2.40	0.46
1:A:596:THR:C	1:A:597:LEU:HD12	2.41	0.46
1:A:700:ASN:HB2	9:I:98:VAL:CG2	2.46	0.46
1:A:725:ALA:O	1:A:728:LYS:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:921:GLY:O	1:A:922:ASP:C	2.58	0.46
1:A:1230:GLU:C	1:A:1232:ASN:H	2.23	0.46
1:A:1308:THR:CG2	1:A:1310:GLY:O	2.63	0.46
1:A:1342:GLU:CD	5:E:198:ILE:HG21	2.41	0.46
2:B:25:ILE:HG23	2:B:658:ILE:CD1	2.44	0.46
2:B:244:LEU:HB2	2:B:249:ARG:HA	1.98	0.46
2:B:390:LEU:O	2:B:392:ARG:N	2.48	0.46
2:B:857:ARG:O	2:B:967:ARG:HA	2.16	0.46
2:B:859:TYR:H	2:B:859:TYR:HD1	1.62	0.46
2:B:969:ARG:HG2	2:B:970:THR:N	2.31	0.46
2:B:1050:ILE:N	2:B:1050:ILE:CD1	2.79	0.46
3:C:118:LEU:HD12	3:C:132:PRO:HG3	1.98	0.46
3:C:138:GLU:HB2	3:C:140:ASN:ND2	2.31	0.46
3:C:176:ILE:HG22	3:C:177:GLU:O	2.16	0.46
4:D:63:LEU:O	4:D:63:LEU:HD13	2.16	0.46
6:F:138:LEU:HD23	6:F:138:LEU:HA	1.73	0.46
8:H:40:LEU:HD13	8:H:123:MET:SD	2.56	0.46
1:A:280:GLU:O	1:A:282:ASN:N	2.48	0.45
1:A:319:GLY:O	1:A:320:ARG:C	2.60	0.45
1:A:513:SER:OG	1:A:515:GLN:HG2	2.15	0.45
1:A:626:ASN:O	1:A:631:HIS:CD2	2.70	0.45
1:A:666:ILE:CD1	1:A:667:GLY:H	2.13	0.45
1:A:761:MET:HA	1:A:804:TYR:HB2	1.97	0.45
1:A:774:ARG:CZ	1:A:797:LYS:HG3	2.45	0.45
1:A:803:SER:HG	1:A:806:ARG:HG3	1.81	0.45
1:A:833:GLU:HG3	1:A:1102:LYS:NZ	2.31	0.45
1:A:1094:VAL:O	1:A:1095:THR:C	2.60	0.45
1:A:1389:PHE:CG	1:A:1390:ASN:N	2.83	0.45
2:B:101:MET:HB3	2:B:109:THR:CG2	2.46	0.45
2:B:435:THR:O	2:B:437:GLU:N	2.49	0.45
2:B:686:ASN:C	2:B:688:GLY:N	2.74	0.45
2:B:689:LEU:O	2:B:690:VAL:HG23	2.15	0.45
2:B:789:MET:CE	2:B:965:LYS:HB3	2.47	0.45
2:B:879:ARG:HD3	2:B:879:ARG:HA	1.51	0.45
2:B:889:THR:HG23	2:B:891:ASP:OD2	2.16	0.45
2:B:1041:GLU:O	2:B:1042:GLY:C	2.59	0.45
3:C:100:THR:HG22	3:C:102:GLN:NE2	2.31	0.45
3:C:147:LEU:HB2	3:C:151:GLN:CB	2.42	0.45
3:C:232:VAL:HG11	3:C:244:VAL:CG2	2.46	0.45
4:D:31:GLN:C	4:D:33:PHE:H	2.23	0.45
4:D:128:VAL:O	4:D:132:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:19:ASP:HB2	9:I:24:ARG:HG3	1.98	0.45
9:I:72:ASP:HB2	9:I:81:ARG:HB3	1.98	0.45
11:K:40:HIS:O	11:K:41:THR:C	2.59	0.45
1:A:309:ALA:C	1:A:311:GLN:H	2.24	0.45
1:A:606:LEU:HD11	1:A:608:ILE:HG13	1.99	0.45
1:A:689:LYS:HE2	1:A:721:PHE:CE2	2.51	0.45
1:A:768:GLN:NE2	1:A:816:HIS:ND1	2.65	0.45
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.51	0.45
1:A:857:ARG:NH1	6:F:139:PRO:HB2	2.32	0.45
1:A:899:VAL:HG22	1:A:908:LEU:HD21	1.98	0.45
1:A:1139:GLU:O	1:A:1140:HIS:C	2.60	0.45
1:A:1445:ILE:HD12	7:G:59:GLY:O	2.17	0.45
2:B:57:TYR:HD1	2:B:57:TYR:N	2.09	0.45
2:B:102:VAL:N	2:B:110:HIS:O	2.44	0.45
2:B:193:LYS:HZ1	12:L:32:ALA:HB1	1.78	0.45
2:B:221:ASN:OD1	2:B:242:SER:HA	2.16	0.45
2:B:261:ARG:HH11	2:B:261:ARG:HG3	1.81	0.45
2:B:265:SER:O	2:B:266:ALA:HB3	2.16	0.45
2:B:306:ASN:C	2:B:308:TRP:N	2.74	0.45
2:B:324:ILE:HG12	2:B:329:THR:HG22	1.98	0.45
2:B:680:THR:OG1	2:B:681:TRP:N	2.48	0.45
2:B:762:ASN:HD21	2:B:1024:ALA:HB3	1.82	0.45
2:B:912:ILE:O	2:B:938:SER:HA	2.16	0.45
2:B:942:ARG:O	2:B:944:THR:N	2.50	0.45
2:B:1169:MET:O	2:B:1170:THR:C	2.58	0.45
5:E:205:SER:O	5:E:206:GLY:C	2.59	0.45
6:F:75:PRO:C	6:F:77:ASP:H	2.24	0.45
6:F:113:GLY:O	6:F:114:GLU:C	2.59	0.45
11:K:43:GLY:HA3	11:K:61:TYR:CE1	2.51	0.45
12:L:55:ILE:HG12	12:L:56:LEU:H	1.82	0.45
1:A:44:THR:O	1:A:45:GLN:HB2	2.17	0.45
1:A:52:GLY:H	1:A:56:PRO:HG3	1.80	0.45
1:A:134:ARG:C	1:A:136:ALA:N	2.73	0.45
1:A:146:MET:O	1:A:170:THR:HG23	2.15	0.45
1:A:230:ARG:O	1:A:232:GLU:N	2.49	0.45
1:A:283:GLY:O	1:A:285:PRO:HD3	2.16	0.45
1:A:574:GLY:O	1:A:575:LYS:C	2.59	0.45
1:A:1004:ASN:ND2	5:E:167:ARG:CD	2.74	0.45
2:B:43:LEU:HA	2:B:43:LEU:HD23	1.78	0.45
2:B:97:VAL:HG22	2:B:128:LEU:HG	1.97	0.45
2:B:240:ILE:HG23	2:B:240:ILE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:THR:CG2	2:B:254:LEU:N	2.80	0.45
2:B:261:ARG:HG3	2:B:261:ARG:NH1	2.31	0.45
2:B:383:ASN:O	2:B:387:LEU:HD13	2.16	0.45
2:B:779:GLY:O	2:B:795:ILE:HA	2.16	0.45
2:B:858:SER:HA	2:B:966:VAL:O	2.16	0.45
2:B:1159:ARG:CD	2:B:1193:GLN:HE21	2.28	0.45
2:B:1166:CYS:O	2:B:1168:LEU:N	2.41	0.45
3:C:11:ARG:HD3	3:C:209:TYR:OH	2.16	0.45
3:C:77:ILE:O	3:C:79:GLN:N	2.50	0.45
3:C:238:ILE:CD1	3:C:246:ARG:NH1	2.78	0.45
4:D:119:ARG:HD3	4:D:221:TYR:CE2	2.52	0.45
7:G:96:GLN:O	7:G:112:LYS:CD	2.63	0.45
1:A:639:PRO:CD	1:A:640:GLN:H	2.28	0.45
1:A:1120:LEU:H	1:A:1120:LEU:CD1	2.20	0.45
1:A:1127:ASP:HB3	1:A:1130:GLN:HB2	1.99	0.45
1:A:1144:LYS:HD2	1:A:1268:LEU:O	2.17	0.45
1:A:1317:MET:C	1:A:1319:VAL:H	2.24	0.45
1:A:1341:ILE:HG23	1:A:1342:GLU:H	1.82	0.45
2:B:344:LYS:O	2:B:345:LYS:C	2.59	0.45
2:B:345:LYS:C	2:B:348:ARG:HG2	2.42	0.45
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.46	0.45
2:B:605:ARG:HB3	2:B:688:GLY:HA2	1.99	0.45
2:B:620:ARG:NH2	9:I:89:GLN:HE22	2.15	0.45
2:B:661:LEU:HD11	2:B:684:LEU:CD1	2.43	0.45
2:B:661:LEU:CD1	2:B:684:LEU:HD11	2.42	0.45
2:B:806:THR:HG21	2:B:808:ALA:HB3	1.98	0.45
2:B:815:ARG:O	10:J:54:VAL:HG21	2.16	0.45
3:C:15:LYS:O	3:C:240:VAL:CG2	2.65	0.45
3:C:17:ASN:N	3:C:240:VAL:HG11	2.32	0.45
4:D:117:GLU:OE2	4:D:155:ARG:O	2.33	0.45
4:D:191:ALA:HB3	4:D:207:LEU:HD21	1.99	0.45
5:E:78:LEU:HD21	5:E:109:ILE:HD12	1.99	0.45
8:H:83:GLN:O	8:H:85:GLY:N	2.49	0.45
9:I:33:SER:O	9:I:35:VAL:HG23	2.16	0.45
14:N:4:DA:H2''	14:N:5:DC:H6	1.81	0.45
1:A:38:PRO:CA	1:A:270:LEU:HD23	2.44	0.45
1:A:262:LEU:HD12	1:A:328:ARG:NH2	2.32	0.45
1:A:300:VAL:O	1:A:300:VAL:HG12	2.16	0.45
1:A:332:LYS:CA	1:A:337:ARG:HB3	2.46	0.45
1:A:560:ILE:CD1	8:H:79:TRP:HB3	2.46	0.45
1:A:836:TYR:HB2	13:T:18:DA:H5'	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:LEU:HD23	1:A:983:ILE:HG21	1.99	0.45
1:A:939:ASP:O	1:A:942:PHE:N	2.46	0.45
1:A:953:ASN:C	1:A:954:TRP:CD1	2.95	0.45
2:B:63:ILE:O	2:B:67:SER:HB3	2.16	0.45
2:B:116:GLU:C	2:B:118:ARG:H	2.24	0.45
2:B:287:ARG:NH1	2:B:324:ILE:O	2.49	0.45
2:B:343:ILE:CG2	2:B:347:LYS:HG3	2.47	0.45
2:B:529:GLU:OE2	2:B:769:TYR:CD1	2.70	0.45
2:B:751:VAL:HG13	2:B:812:LEU:HD22	1.99	0.45
2:B:766:ARG:HH21	15:P:11:U:H3	1.65	0.45
2:B:814:PHE:C	2:B:816:GLU:N	2.75	0.45
2:B:911:ILE:O	2:B:911:ILE:HG22	2.16	0.45
2:B:1146:PHE:O	2:B:1147:LEU:C	2.60	0.45
2:B:1161:HIS:CE1	2:B:1175:LEU:HD21	2.52	0.45
3:C:49:VAL:HG21	3:C:64:ALA:HA	1.98	0.45
3:C:168:ALA:O	3:C:171:GLY:N	2.47	0.45
4:D:51:ASN:OD1	4:D:54:GLU:CB	2.65	0.45
5:E:172:GLU:HG3	5:E:213:ILE:CD1	2.47	0.45
7:G:119:LEU:HA	7:G:131:GLN:O	2.16	0.45
8:H:9:ILE:HG12	8:H:56:THR:HA	1.98	0.45
8:H:59:ILE:HG12	8:H:142:LEU:HD12	1.96	0.45
10:J:53:HIS:CE1	10:J:55:ASP:HA	2.51	0.45
12:L:32:ALA:H	12:L:55:ILE:HG13	1.82	0.45
1:A:73:GLY:O	1:A:74:MET:C	2.60	0.45
1:A:347:PHE:N	1:A:347:PHE:CD1	2.85	0.45
1:A:672:ASP:O	1:A:673:GLY:C	2.59	0.45
1:A:783:THR:O	1:A:784:LEU:HD23	2.16	0.45
1:A:1017:LEU:HD12	1:A:1017:LEU:O	2.16	0.45
1:A:1259:MET:HG3	1:A:1262:LYS:NZ	2.28	0.45
1:A:1341:ILE:HD12	1:A:1379:GLY:O	2.17	0.45
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.98	0.45
2:B:120:ARG:NE	2:B:955:THR:CG2	2.74	0.45
2:B:282:ILE:HD11	2:B:317:CYS:SG	2.56	0.45
2:B:365:THR:HG23	2:B:367:LEU:N	2.30	0.45
2:B:516:ASN:C	2:B:518:HIS:H	2.24	0.45
2:B:766:ARG:HA	2:B:766:ARG:HD3	1.80	0.45
2:B:801:LYS:O	2:B:822:ASN:ND2	2.50	0.45
2:B:936:ASP:OD1	2:B:937:ALA:N	2.49	0.45
3:C:178:PHE:CE1	3:C:230:MET:HE2	2.49	0.45
3:C:183:TRP:O	3:C:184:ASN:C	2.59	0.45
5:E:42:PHE:HZ	5:E:58:MET:CE	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:138:THR:CG2	7:G:139:ILE:N	2.60	0.45
8:H:130:ARG:N	8:H:130:ARG:CD	2.74	0.45
9:I:7:CYS:O	9:I:8:ARG:O	2.34	0.45
10:J:56:LEU:O	10:J:59:LYS:N	2.50	0.45
11:K:55:LYS:HB3	11:K:81:TYR:CE1	2.51	0.45
1:A:49:LYS:NZ	1:A:61:ILE:CG1	2.78	0.45
1:A:77:CYS:C	1:A:78:PRO:O	2.59	0.45
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.63	0.45
1:A:95:PHE:HD1	1:A:234:MET:HA	1.82	0.45
1:A:134:ARG:HG2	1:A:138:ILE:HD11	1.99	0.45
1:A:452:LYS:HE3	2:B:1141:HIS:ND1	2.32	0.45
1:A:562:THR:HA	1:A:563:PRO:HD3	1.79	0.45
1:A:971:PHE:HE2	1:A:1040:GLN:HG2	1.82	0.45
1:A:1123:GLY:O	1:A:1125:ALA:N	2.49	0.45
1:A:1213:GLY:C	1:A:1215:ARG:N	2.75	0.45
1:A:1431:GLY:HA3	2:B:1152:MET:SD	2.56	0.45
2:B:58:THR:O	2:B:62:ILE:HG13	2.17	0.45
2:B:100:PRO:CD	2:B:180:TYR:HE1	2.29	0.45
2:B:293:PRO:C	2:B:294:ASP:O	2.58	0.45
2:B:294:ASP:C	2:B:296:GLU:N	2.72	0.45
2:B:582:VAL:HG22	2:B:626:ILE:HG21	1.99	0.45
2:B:616:ILE:HG13	2:B:697:GLU:HA	1.98	0.45
2:B:640:VAL:HG23	2:B:740:HIS:HA	1.99	0.45
2:B:658:ILE:HG22	2:B:659:ALA:N	2.32	0.45
3:C:114:TYR:HB3	3:C:140:ASN:O	2.17	0.45
4:D:130:LEU:HD13	4:D:142:LYS:HG3	1.98	0.45
5:E:46:TYR:CE2	5:E:58:MET:HA	2.51	0.45
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.97	0.45
7:G:20:PRO:HG2	7:G:21:ARG:H	1.81	0.45
11:K:28:PRO:O	11:K:29:ASN:C	2.58	0.45
1:A:12:ARG:HD2	2:B:1218:THR:CB	2.43	0.45
1:A:417:TYR:O	1:A:418:SER:C	2.60	0.45
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.99	0.45
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.99	0.45
1:A:834:THR:HG21	1:A:1077:THR:CG2	2.46	0.45
1:A:850:VAL:HG21	1:A:1058:VAL:HG11	1.99	0.45
1:A:883:LEU:CD2	1:A:1021:LEU:HB2	2.46	0.45
1:A:902:LEU:HD11	1:A:923:LEU:CD2	2.44	0.45
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.99	0.45
1:A:1277:GLU:C	1:A:1279:ILE:H	2.25	0.45
2:B:211:VAL:O	2:B:211:VAL:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:ILE:CG2	2:B:235:SER:N	2.79	0.45
2:B:467:GLY:O	2:B:468:GLU:C	2.59	0.45
2:B:515:HIS:CD2	2:B:516:ASN:H	2.34	0.45
2:B:611:PRO:HB3	2:B:685:LEU:CD1	2.47	0.45
2:B:638:PHE:CA	2:B:690:VAL:HG22	2.23	0.45
2:B:755:ILE:O	2:B:755:ILE:HG22	2.17	0.45
2:B:995:ARG:HH12	3:C:165:LYS:HG2	1.82	0.45
2:B:1112:GLN:HG2	2:B:1113:VAL:H	1.81	0.45
2:B:1171:VAL:HA	2:B:1182:CYS:HB2	1.99	0.45
2:B:1197:PRO:C	2:B:1199:ALA:N	2.74	0.45
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.98	0.45
4:D:8:PHE:CD2	7:G:6:ASP:O	2.70	0.45
5:E:73:PRO:HB2	5:E:74:ASP:H	1.61	0.45
5:E:153:HIS:C	5:E:154:ILE:HG13	2.42	0.45
5:E:173:SER:C	5:E:175:LEU:N	2.75	0.45
8:H:26:ILE:C	8:H:27:GLU:HG3	2.42	0.45
8:H:64:ASN:CB	8:H:88:SER:HB2	2.34	0.45
11:K:47:ARG:C	11:K:47:ARG:HD2	2.41	0.45
1:A:76:GLU:O	1:A:78:PRO:CD	2.65	0.45
1:A:270:LEU:O	1:A:273:ASN:HB3	2.17	0.45
1:A:332:LYS:CG	1:A:333:GLU:HG2	2.46	0.45
1:A:600:PRO:HA	8:H:25:ARG:NH2	2.31	0.45
1:A:722:LEU:H	1:A:722:LEU:HD12	1.82	0.45
1:A:734:GLU:C	1:A:736:ASN:N	2.74	0.45
1:A:767:GLN:NE2	1:A:774:ARG:HB2	2.32	0.45
1:A:992:ASP:O	1:A:993:LEU:C	2.59	0.45
1:A:1067:LEU:C	1:A:1067:LEU:CD1	2.90	0.45
1:A:1259:MET:HA	1:A:1262:LYS:HG3	1.98	0.45
2:B:48:LEU:O	2:B:49:ASP:C	2.59	0.45
2:B:128:LEU:HB2	2:B:167:ILE:O	2.17	0.45
2:B:653:VAL:HG22	2:B:689:LEU:HD22	1.99	0.45
2:B:899:ILE:HG23	2:B:903:VAL:HG21	1.97	0.45
2:B:999:MET:HE2	2:B:1000:PRO:HD3	1.99	0.45
3:C:65:HIS:O	3:C:69:LEU:HD13	2.17	0.45
4:D:7:THR:HB	7:G:42:PHE:CE2	2.52	0.45
4:D:41:GLN:OE1	4:D:41:GLN:HA	2.17	0.45
4:D:55:ALA:HB3	4:D:148:LEU:HD11	1.98	0.45
4:D:119:ARG:CG	4:D:221:TYR:HE2	2.29	0.45
7:G:115:MET:SD	7:G:119:LEU:HD23	2.56	0.45
8:H:5:LEU:CD1	8:H:135:LEU:HD12	2.47	0.45
13:T:20:DG:H2''	13:T:21:DC:H5'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:HG12	1:A:107:CYS:N	2.32	0.45
1:A:162:VAL:HG12	1:A:163:SER:N	2.32	0.45
1:A:225:ASN:HD22	1:A:228:PHE:H	1.56	0.45
1:A:507:VAL:N	1:A:508:PRO:CD	2.79	0.45
1:A:567:LYS:HE2	8:H:46:LEU:O	2.17	0.45
1:A:880:LYS:HA	1:A:954:TRP:O	2.17	0.45
1:A:889:SER:C	1:A:891:ALA:N	2.74	0.45
1:A:896:ARG:HH21	1:A:1030:ARG:CZ	2.29	0.45
1:A:1040:GLN:O	1:A:1041:ALA:C	2.60	0.45
1:A:1100:ARG:O	1:A:1104:ILE:HG13	2.17	0.45
1:A:1237:ILE:CG2	1:A:1238:ILE:H	2.30	0.45
1:A:1293:SER:HB2	1:A:1299:VAL:CG2	2.47	0.45
1:A:1395:GLY:HA3	1:A:1419:ASP:OD2	2.16	0.45
2:B:890:TYR:O	2:B:891:ASP:C	2.59	0.45
2:B:953:LEU:HD23	2:B:953:LEU:H	1.81	0.45
3:C:239:PRO:O	3:C:241:ASP:N	2.50	0.45
4:D:3:VAL:O	4:D:4:SER:C	2.60	0.45
5:E:90:VAL:O	5:E:93:MET:HB3	2.17	0.45
6:F:99:LEU:HD21	7:G:64:THR:O	2.16	0.45
8:H:138:GLU:O	8:H:139:ASN:C	2.58	0.45
11:K:78:THR:O	11:K:79:GLU:O	2.35	0.45
12:L:52:GLY:O	12:L:54:ARG:N	2.50	0.45
1:A:153:PRO:HA	1:A:161:LEU:HA	1.99	0.44
1:A:326:ARG:CG	1:A:327:ALA:N	2.78	0.44
1:A:349:ALA:C	2:B:1128:LEU:HD11	2.41	0.44
1:A:403:LYS:C	1:A:415:LEU:HB2	2.42	0.44
1:A:464:PRO:HG2	1:A:465:TYR:CD1	2.52	0.44
1:A:556:TRP:C	1:A:558:GLY:N	2.74	0.44
1:A:755:PHE:HA	1:A:758:ILE:HD12	1.98	0.44
1:A:771:GLU:C	1:A:773:LYS:H	2.25	0.44
1:A:932:GLU:O	1:A:936:LEU:HG	2.17	0.44
1:A:972:HIS:O	1:A:973:ILE:C	2.58	0.44
1:A:1152:ILE:CG2	1:A:1193:LEU:HD13	2.46	0.44
1:A:1325:THR:OG1	5:E:146:HIS:O	2.33	0.44
1:A:1339:LEU:O	5:E:183:PRO:HB2	2.16	0.44
1:A:1349:TYR:CD2	1:A:1349:TYR:C	2.94	0.44
2:B:313:MET:CE	2:B:386:LEU:HD22	2.47	0.44
2:B:344:LYS:O	2:B:345:LYS:O	2.34	0.44
2:B:461:LEU:CD1	2:B:461:LEU:N	2.80	0.44
2:B:1150:ARG:HG3	2:B:1150:ARG:NH1	2.18	0.44
3:C:9:LYS:O	3:C:10:ILE:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:ILE:H	3:C:38:ILE:HG13	1.44	0.44
5:E:16:PHE:CD1	5:E:58:MET:HE2	2.52	0.44
5:E:23:VAL:HB	5:E:30:ILE:HD11	1.99	0.44
5:E:78:LEU:HD21	5:E:80:VAL:HG23	1.98	0.44
5:E:122:LYS:C	5:E:123:LEU:HG	2.42	0.44
7:G:154:VAL:HG12	7:G:155:SER:N	2.32	0.44
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.99	0.44
8:H:64:ASN:HA	8:H:90:ALA:HB2	1.99	0.44
1:A:18:GLN:CB	2:B:1215:ARG:HB2	2.47	0.44
1:A:75:ASN:O	1:A:76:GLU:HB2	2.17	0.44
1:A:202:LEU:HD13	1:A:207:ILE:HD11	1.99	0.44
1:A:341:MET:CE	2:B:1135:ARG:NH1	2.80	0.44
1:A:829:VAL:C	1:A:831:THR:N	2.74	0.44
1:A:894:GLU:C	1:A:896:ARG:N	2.75	0.44
1:A:1067:LEU:C	1:A:1067:LEU:HD13	2.40	0.44
1:A:1157:ASP:C	1:A:1159:ARG:H	2.24	0.44
1:A:1161:THR:CG2	1:A:1163:ILE:HG13	2.45	0.44
2:B:460:ALA:HB1	2:B:466:TRP:CE3	2.53	0.44
2:B:649:LYS:HD3	2:B:736:THR:O	2.16	0.44
2:B:846:ILE:CG2	2:B:974:PRO:HG2	2.47	0.44
2:B:1023:VAL:C	2:B:1025:HIS:N	2.73	0.44
3:C:99:LEU:HD23	3:C:99:LEU:N	2.31	0.44
4:D:39:ASN:HD22	4:D:41:GLN:HB2	1.82	0.44
6:F:79:ARG:HH11	6:F:79:ARG:CG	2.28	0.44
7:G:145:VAL:HG12	7:G:146:LYS:H	1.81	0.44
8:H:100:THR:CB	8:H:138:GLU:HG3	2.47	0.44
9:I:55:THR:HG23	9:I:86:PHE:CZ	2.52	0.44
10:J:16:ASP:CG	10:J:17:LYS:HD2	2.42	0.44
11:K:90:ALA:O	11:K:93:SER:HB3	2.17	0.44
1:A:156:ASP:O	1:A:157:ASP:C	2.60	0.44
1:A:332:LYS:CB	1:A:337:ARG:HD2	2.47	0.44
1:A:361:LEU:HA	1:A:471:ASN:CG	2.42	0.44
1:A:478:TYR:O	1:A:479:ASN:CB	2.65	0.44
1:A:630:ILE:CD1	1:A:646:PHE:CZ	2.99	0.44
1:A:637:LYS:HG3	1:A:641:VAL:HG11	1.98	0.44
1:A:714:PHE:O	1:A:715:GLU:C	2.61	0.44
1:A:874:ASP:O	1:A:876:ALA:N	2.51	0.44
1:A:1269:GLU:C	1:A:1271:ILE:H	2.25	0.44
2:B:578:THR:O	2:B:579:ARG:C	2.61	0.44
2:B:830:TYR:CE2	2:B:1000:PRO:CD	2.97	0.44
2:B:1096:ARG:HA	2:B:1098:MET:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:112:ASN:HB3	3:C:114:TYR:CE1	2.52	0.44
3:C:138:GLU:OE1	3:C:138:GLU:N	2.50	0.44
5:E:10:SER:O	5:E:13:TRP:HB3	2.17	0.44
8:H:106:GLU:O	8:H:108:SER:N	2.50	0.44
9:I:4:PHE:HD1	9:I:5:ARG:N	2.15	0.44
10:J:9:SER:CB	10:J:45:CYS:HB2	2.47	0.44
13:T:8:DT:H2''	13:T:9:DC:OP2	2.17	0.44
1:A:293:GLU:O	1:A:296:LEU:N	2.48	0.44
1:A:326:ARG:HG3	1:A:327:ALA:N	2.24	0.44
1:A:418:SER:C	1:A:420:ARG:N	2.72	0.44
1:A:516:SER:O	1:A:517:ASN:C	2.60	0.44
1:A:682:THR:HG23	1:A:728:LYS:HE3	1.98	0.44
1:A:784:LEU:HB3	1:A:785:PRO:HD2	1.99	0.44
1:A:1072:ILE:HG23	1:A:1356:ILE:HD11	1.99	0.44
1:A:1095:THR:HG22	1:A:1100:ARG:HB2	2.00	0.44
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.99	0.44
1:A:1239:ARG:HB3	1:A:1239:ARG:NH1	2.32	0.44
1:A:1244:ARG:CB	1:A:1245:PRO:CA	2.86	0.44
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.97	0.44
2:B:834:ASN:HA	2:B:839:MET:HA	1.98	0.44
2:B:953:LEU:HD23	2:B:953:LEU:N	2.33	0.44
2:B:1045:SER:O	2:B:1046:PRO:O	2.36	0.44
2:B:1081:LEU:C	2:B:1083:ALA:H	2.23	0.44
4:D:7:THR:HB	7:G:42:PHE:HE2	1.83	0.44
9:I:86:PHE:CD1	9:I:86:PHE:C	2.96	0.44
14:N:3:DT:H3'	14:N:3:DT:OP2	2.17	0.44
1:A:22:PHE:CE1	2:B:1213:THR:HG22	2.52	0.44
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.98	0.44
1:A:278:THR:O	1:A:278:THR:HG22	2.17	0.44
1:A:630:ILE:CG2	1:A:631:HIS:N	2.80	0.44
1:A:645:LEU:CG	1:A:649:ILE:HD11	2.48	0.44
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.16	0.44
1:A:1159:ARG:O	1:A:1160:SER:HB3	2.17	0.44
1:A:1278:ASN:HD22	1:A:1312:ASN:HB2	1.81	0.44
1:A:1289:ARG:NH1	1:A:1326:ARG:NH1	2.65	0.44
1:A:1447:GLU:O	1:A:1448:GLU:C	2.61	0.44
1:A:1449:SER:C	1:A:1451:VAL:H	2.25	0.44
2:B:170:LEU:C	2:B:170:LEU:HD12	2.42	0.44
2:B:519:TRP:CD1	2:B:519:TRP:C	2.95	0.44
2:B:797:TYR:CE1	2:B:971:THR:HG23	2.53	0.44
2:B:801:LYS:HD2	2:B:815:ARG:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:877:PRO:HB2	2:B:934:LYS:HD2	2.00	0.44
2:B:893:LEU:C	2:B:894:ASP:O	2.58	0.44
2:B:997:GLU:HB3	3:C:35:ARG:NH1	2.32	0.44
2:B:1050:ILE:HG22	2:B:1051:THR:N	2.33	0.44
2:B:1115:THR:CG2	2:B:1117:GLN:HG3	2.42	0.44
3:C:20:PHE:CZ	3:C:230:MET:HB2	2.53	0.44
3:C:172:PRO:CD	3:C:173:ALA:H	2.31	0.44
4:D:18:VAL:O	4:D:19:GLU:CB	2.58	0.44
4:D:60:LYS:HE3	4:D:126:ILE:HD11	1.99	0.44
4:D:145:MET:O	4:D:149:THR:N	2.50	0.44
4:D:166:LEU:HD11	4:D:210:ILE:HG23	1.99	0.44
6:F:110:ASP:O	6:F:111:LEU:C	2.60	0.44
9:I:61:ASP:C	9:I:63:GLY:N	2.75	0.44
13:T:11:DA:C2	13:T:12:DG:C4	3.06	0.44
1:A:275:SER:O	1:A:279:LEU:HG	2.17	0.44
1:A:623:GLY:C	1:A:625:SER:H	2.26	0.44
1:A:1259:MET:HG3	1:A:1262:LYS:CE	2.48	0.44
1:A:1398:MET:O	1:A:1400:CYS:N	2.50	0.44
2:B:496:ARG:HD2	2:B:751:VAL:HG23	2.00	0.44
2:B:684:LEU:HD23	2:B:689:LEU:HD12	1.99	0.44
2:B:705:MET:CE	2:B:742:GLU:HG2	2.48	0.44
3:C:235:VAL:HG11	10:J:6:ARG:NH2	2.32	0.44
9:I:105:SER:O	9:I:106:CYS:CB	2.59	0.44
13:T:25:DG:H2''	13:T:26:DT:H5'	1.99	0.44
1:A:54:ASN:CB	1:A:247:ARG:HH22	2.31	0.44
1:A:72:GLU:HB3	1:A:76:GLU:CG	2.45	0.44
1:A:101:LYS:HA	1:A:104:GLU:OE1	2.17	0.44
1:A:103:CYS:C	1:A:105:CYS:N	2.75	0.44
1:A:230:ARG:O	1:A:233:TRP:N	2.51	0.44
1:A:360:GLU:O	1:A:361:LEU:C	2.59	0.44
1:A:442:VAL:CG2	1:A:460:VAL:HG23	2.48	0.44
1:A:605:MET:HE2	1:A:607:ILE:HG12	1.99	0.44
1:A:682:THR:HG22	1:A:728:LYS:HE3	1.98	0.44
1:A:1127:ASP:CB	1:A:1130:GLN:HB2	2.47	0.44
1:A:1271:ILE:O	1:A:1271:ILE:HG22	2.16	0.44
1:A:1272:THR:HG22	1:A:1273:LEU:N	2.32	0.44
2:B:189:LEU:O	2:B:192:LEU:N	2.50	0.44
2:B:213:ILE:HD11	2:B:497:ARG:CA	2.48	0.44
2:B:348:ARG:O	2:B:351:TYR:HB3	2.18	0.44
2:B:357:GLN:HG2	2:B:366:GLN:O	2.17	0.44
2:B:616:ILE:HD12	2:B:625:LYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:659:ALA:HA	2:B:662:MET:HE3	2.00	0.44
2:B:870:ILE:CG2	2:B:917:PRO:HG2	2.48	0.44
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.47	0.44
5:E:154:ILE:HG22	5:E:155:ARG:O	2.17	0.44
7:G:17:PHE:O	7:G:19:GLY:N	2.44	0.44
9:I:69:PRO:HG2	9:I:85:PHE:CE2	2.52	0.44
1:A:208:LEU:HD21	1:A:212:LYS:HE3	1.99	0.44
1:A:407:ARG:HB3	1:A:430:TRP:CZ2	2.53	0.44
1:A:605:MET:HE2	1:A:607:ILE:HD11	1.99	0.44
1:A:1115:SER:O	1:A:1116:LEU:CB	2.65	0.44
1:A:1170:ILE:HG13	1:A:1170:ILE:H	1.62	0.44
1:A:1291:VAL:HG13	1:A:1292:PRO:N	2.33	0.44
1:A:1384:VAL:C	1:A:1385:THR:HG23	2.42	0.44
1:A:1398:MET:C	1:A:1400:CYS:N	2.74	0.44
2:B:305:VAL:O	2:B:305:VAL:HG12	2.18	0.44
2:B:803:LEU:CD1	2:B:1032:SER:HB3	2.48	0.44
2:B:1004:GLU:HB2	2:B:1006:ILE:HG12	1.98	0.44
3:C:67:LEU:HD23	3:C:70:ILE:CD1	2.47	0.44
3:C:87:PHE:N	3:C:87:PHE:CD1	2.85	0.44
5:E:95:THR:O	5:E:99:HIS:HB2	2.17	0.44
5:E:121:MET:O	5:E:124:VAL:HG23	2.18	0.44
6:F:84:TYR:CD2	6:F:152:ILE:HB	2.52	0.44
6:F:114:GLU:HA	6:F:114:GLU:OE2	2.18	0.44
6:F:116:ASP:HB3	6:F:119:ARG:HB2	2.00	0.44
7:G:27:LYS:O	7:G:31:LEU:HG	2.17	0.44
8:H:84:ALA:HA	8:H:87:ARG:HG3	2.00	0.44
8:H:100:THR:CG2	8:H:101:ALA:N	2.80	0.44
11:K:1:MET:HG3	11:K:2:ASN:N	2.33	0.44
12:L:38:LEU:O	12:L:39:SER:HB3	2.18	0.44
12:L:52:GLY:O	12:L:53:HIS:C	2.60	0.44
1:A:23:SER:HA	1:A:233:TRP:CD1	2.53	0.44
1:A:68:GLN:C	1:A:70:CYS:N	2.72	0.44
1:A:552:TRP:HE1	11:K:62:LYS:HB2	1.83	0.44
1:A:577:ILE:HA	1:A:580:VAL:HG23	1.99	0.44
1:A:767:GLN:HE21	1:A:774:ARG:CB	2.31	0.44
1:A:853:ASP:OD1	1:A:855:THR:CB	2.66	0.44
1:A:1021:LEU:O	1:A:1024:SER:HB3	2.18	0.44
2:B:186:GLU:HA	2:B:186:GLU:OE2	2.17	0.44
2:B:361:LEU:O	2:B:363:HIS:O	2.36	0.44
2:B:565:PRO:C	2:B:567:GLU:N	2.75	0.44
2:B:737:THR:HG22	9:I:66:PRO:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:751:VAL:O	2:B:752:ALA:C	2.61	0.44
3:C:184:ASN:HD21	3:C:187:LYS:HA	1.79	0.44
3:C:215:GLU:O	3:C:217:ASP:N	2.50	0.44
4:D:155:ARG:HH11	4:D:155:ARG:CG	2.28	0.44
6:F:94:LEU:HD21	6:F:122:MET:HA	2.00	0.44
10:J:37:SER:OG	10:J:47:ARG:NH2	2.49	0.44
12:L:61:THR:HG22	12:L:62:LYS:N	2.33	0.44
1:A:7:SER:C	1:A:9:ALA:N	2.76	0.43
1:A:22:PHE:HE2	1:A:30:ILE:CD1	2.31	0.43
1:A:339:ASN:O	1:A:343:LYS:HG2	2.17	0.43
1:A:456:MET:HB2	1:A:478:TYR:OH	2.17	0.43
1:A:470:LEU:CD1	1:A:487:MET:HE1	2.39	0.43
1:A:606:LEU:CG	1:A:613:ILE:HD12	2.47	0.43
1:A:817:ALA:O	1:A:819:GLY:N	2.50	0.43
1:A:1220:PHE:O	1:A:1221:LYS:CB	2.65	0.43
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.53	0.43
2:B:843:GLN:HB3	2:B:995:ARG:HG3	2.00	0.43
2:B:854:LEU:HB3	2:B:855:PHE:H	1.70	0.43
2:B:867:GLY:C	2:B:869:SER:H	2.26	0.43
2:B:999:MET:CG	2:B:1000:PRO:HD2	2.24	0.43
4:D:176:GLU:C	4:D:178:ALA:N	2.76	0.43
6:F:72:LYS:HB3	6:F:73:ALA:H	1.53	0.43
7:G:115:MET:HB2	7:G:116:PRO:CD	2.43	0.43
8:H:42:ILE:HG22	8:H:44:VAL:CG2	2.48	0.43
8:H:64:ASN:OD1	8:H:90:ALA:N	2.35	0.43
9:I:86:PHE:C	9:I:86:PHE:HD1	2.26	0.43
1:A:133:LYS:O	1:A:136:ALA:HB3	2.18	0.43
1:A:332:LYS:O	1:A:333:GLU:HB2	2.17	0.43
1:A:899:VAL:CG2	1:A:908:LEU:HD21	2.48	0.43
1:A:1164:PRO:O	1:A:1166:ASP:N	2.51	0.43
2:B:39:ARG:CZ	2:B:665:GLU:HG2	2.49	0.43
2:B:68:THR:HG22	2:B:69:LEU:N	2.32	0.43
2:B:258:LEU:HB2	2:B:385:LEU:HD21	2.00	0.43
2:B:270:LYS:HG2	2:B:281:PRO:HA	2.00	0.43
2:B:416:LEU:HD11	2:B:466:TRP:CE2	2.53	0.43
2:B:436:VAL:O	2:B:436:VAL:HG12	2.17	0.43
2:B:591:ARG:O	2:B:592:ASN:C	2.61	0.43
2:B:1084:GLN:NE2	2:B:1084:GLN:H	2.13	0.43
3:C:29:MET:HE3	11:K:98:LEU:HD23	1.99	0.43
3:C:58:LEU:HD22	3:C:58:LEU:H	1.78	0.43
3:C:123:ASN:ND2	3:C:125:MET:HA	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:220:ASP:OD1	3:C:223:ALA:N	2.51	0.43
4:D:39:ASN:O	4:D:42:GLY:N	2.50	0.43
7:G:104:GLY:C	7:G:106:MET:H	2.26	0.43
7:G:127:PRO:HB3	7:G:139:ILE:HD11	2.00	0.43
11:K:88:LYS:O	11:K:91:CYS:HB2	2.18	0.43
1:A:179:LEU:HD13	1:A:297:GLN:HG3	2.00	0.43
1:A:184:SER:HB3	1:A:199:LEU:CD2	2.47	0.43
1:A:239:LEU:HA	1:A:240:PRO:HD2	1.86	0.43
1:A:402:ALA:CB	1:A:434:ARG:HA	2.49	0.43
1:A:445:ASN:HB2	1:A:454:SER:O	2.19	0.43
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.53	0.43
1:A:682:THR:HG22	1:A:682:THR:O	2.18	0.43
1:A:947:PHE:HE2	1:A:954:TRP:CD1	2.36	0.43
1:A:1044:TRP:O	1:A:1045:VAL:C	2.60	0.43
1:A:1389:PHE:C	1:A:1391:ARG:H	2.26	0.43
1:A:1430:LEU:CB	1:A:1432:GLN:HG3	2.48	0.43
1:A:1451:VAL:C	1:A:1453:TYR:N	2.76	0.43
2:B:370:PHE:HE2	2:B:373:ARG:NH1	2.16	0.43
2:B:766:ARG:HA	2:B:769:TYR:HD2	1.82	0.43
2:B:1102:LYS:O	2:B:1103:ILE:C	2.61	0.43
4:D:37:GLN:OE1	7:G:5:LYS:HD2	2.18	0.43
5:E:178:ILE:HG22	5:E:212:ARG:HB3	2.01	0.43
7:G:13:LEU:HD22	7:G:14:HIS:O	2.17	0.43
10:J:31:ASP:O	10:J:32:GLU:C	2.60	0.43
11:K:78:THR:O	11:K:79:GLU:C	2.61	0.43
1:A:55:ASP:N	1:A:56:PRO:CD	2.80	0.43
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.58	0.43
1:A:295:LEU:O	1:A:298:PHE:HB3	2.18	0.43
1:A:539:THR:C	1:A:540:PHE:CD1	2.97	0.43
1:A:714:PHE:HB2	9:I:97:MET:HE1	2.00	0.43
1:A:727:ASP:O	1:A:730:GLY:N	2.51	0.43
1:A:941:LYS:O	1:A:945:GLU:HB2	2.18	0.43
1:A:1130:GLN:HE21	1:A:1134:ILE:HD11	1.83	0.43
2:B:310:MET:HE1	2:B:387:LEU:CD1	2.48	0.43
2:B:510:LYS:CB	2:B:511:PRO:CD	2.96	0.43
2:B:889:THR:HG22	2:B:891:ASP:HB2	2.01	0.43
2:B:1002:THR:O	2:B:1004:GLU:N	2.52	0.43
2:B:1099:VAL:O	2:B:1101:ASP:N	2.52	0.43
3:C:22:LEU:HD23	3:C:23:SER:N	2.34	0.43
3:C:46:ILE:HD12	3:C:67:LEU:O	2.17	0.43
4:D:56:ARG:HH21	4:D:155:ARG:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:170:THR:HG22	4:D:172:LEU:HG	2.00	0.43
7:G:22:MET:O	7:G:23:LYS:C	2.61	0.43
10:J:32:GLU:O	10:J:33:GLY:C	2.61	0.43
13:T:11:DA:C2	13:T:12:DG:C5	3.06	0.43
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.43	0.43
1:A:298:PHE:HZ	1:A:314:ALA:HB2	1.82	0.43
1:A:492:PRO:HB3	1:A:501:LEU:CD1	2.49	0.43
1:A:515:GLN:HB2	1:A:1071:SER:HB3	2.00	0.43
1:A:645:LEU:HG	1:A:649:ILE:CD1	2.48	0.43
1:A:664:THR:CG2	1:A:665:GLY:N	2.81	0.43
1:A:728:LYS:O	1:A:732:LEU:HG	2.19	0.43
1:A:757:ASN:O	1:A:758:ILE:C	2.62	0.43
1:A:826:ASP:O	1:A:827:THR:C	2.60	0.43
1:A:853:ASP:OD1	1:A:855:THR:HB	2.18	0.43
1:A:994:GLN:C	1:A:996:ASN:H	2.26	0.43
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.27	0.43
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.19	0.43
2:B:44:VAL:CG2	2:B:48:LEU:HD11	2.49	0.43
2:B:49:ASP:HA	2:B:52:ASN:HD22	1.84	0.43
2:B:401:PHE:HA	2:B:404:LYS:HG3	2.00	0.43
2:B:516:ASN:C	2:B:518:HIS:N	2.76	0.43
2:B:811:TYR:N	2:B:811:TYR:HD1	2.13	0.43
2:B:830:TYR:CZ	2:B:1000:PRO:HB3	2.53	0.43
2:B:854:LEU:O	2:B:855:PHE:CB	2.63	0.43
2:B:950:ASP:O	2:B:951:GLN:CB	2.66	0.43
3:C:27:LEU:HD11	3:C:178:PHE:CE2	2.54	0.43
3:C:212:PRO:CB	3:C:213:PRO:HD2	2.48	0.43
4:D:39:ASN:ND2	4:D:41:GLN:HB2	2.34	0.43
4:D:120:GLU:HA	4:D:123:LEU:HD12	2.00	0.43
5:E:151:PRO:HB3	5:E:200:ARG:HB3	2.00	0.43
5:E:196:VAL:HG12	5:E:197:LYS:N	2.33	0.43
6:F:81:THR:HB	6:F:136:ARG:HH11	1.84	0.43
6:F:105:ALA:HB1	6:F:106:PRO:CD	2.49	0.43
8:H:40:LEU:HD13	8:H:123:MET:CE	2.48	0.43
8:H:127:GLY:O	8:H:128:ASN:CB	2.66	0.43
9:I:74:GLU:O	9:I:74:GLU:HG3	2.18	0.43
12:L:32:ALA:H	12:L:55:ILE:CG1	2.32	0.43
13:T:12:DG:N2	14:N:6:DT:C2	2.87	0.43
13:T:15:DC:H2"	13:T:16:DT:C6	2.53	0.43
1:A:206:GLU:O	1:A:210:ILE:HG13	2.19	0.43
1:A:262:LEU:CD2	1:A:303:TYR:CE1	3.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.48	0.43
1:A:744:LYS:HG2	1:A:748:MET:SD	2.58	0.43
1:A:817:ALA:C	1:A:819:GLY:N	2.76	0.43
1:A:1213:GLY:HA2	1:A:1216:ILE:HD12	2.01	0.43
1:A:1369:ALA:O	1:A:1370:LEU:C	2.61	0.43
1:A:1369:ALA:C	1:A:1372:VAL:HG12	2.39	0.43
2:B:69:LEU:HD11	2:B:425:THR:HG22	2.00	0.43
2:B:195:CYS:HB2	2:B:784:ASN:CG	2.43	0.43
2:B:502:ILE:HG22	2:B:507:LYS:HB2	2.01	0.43
2:B:558:LEU:HD21	2:B:600:LEU:HD11	2.00	0.43
2:B:639:ILE:CD1	2:B:691:GLU:HG3	2.41	0.43
2:B:762:ASN:ND2	2:B:1024:ALA:HB3	2.34	0.43
2:B:876:LYS:HD2	2:B:893:LEU:O	2.17	0.43
3:C:269:LYS:O	3:C:270:VAL:HG22	2.18	0.43
4:D:170:THR:C	4:D:172:LEU:H	2.27	0.43
4:D:207:LEU:HA	4:D:210:ILE:HD12	2.01	0.43
9:I:13:MET:HG3	9:I:14:LEU:N	2.33	0.43
9:I:68:LEU:HB3	9:I:84:VAL:HG23	2.00	0.43
12:L:38:LEU:HD11	12:L:49:LYS:HG2	2.01	0.43
12:L:44:ASP:O	12:L:45:ALA:HB3	2.18	0.43
1:A:125:ALA:C	1:A:127:ALA:N	2.76	0.43
1:A:567:LYS:HZ2	8:H:94:ASP:C	2.27	0.43
1:A:628:GLY:O	1:A:629:LEU:C	2.62	0.43
1:A:1013:ASP:HB3	5:E:207:ARG:O	2.19	0.43
1:A:1168:GLU:O	1:A:1172:LEU:HG	2.19	0.43
1:A:1402:PHE:CD1	1:A:1403:GLU:HG3	2.53	0.43
2:B:68:THR:CG2	2:B:69:LEU:N	2.82	0.43
2:B:335:GLY:O	2:B:339:THR:HG21	2.19	0.43
2:B:661:LEU:C	2:B:663:ALA:N	2.77	0.43
2:B:745:PRO:C	2:B:747:MET:H	2.25	0.43
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.99	0.43
3:C:239:PRO:O	3:C:240:VAL:C	2.62	0.43
5:E:11:ARG:C	5:E:13:TRP:H	2.27	0.43
5:E:46:TYR:CD2	5:E:58:MET:HG2	2.54	0.43
5:E:198:ILE:HD12	5:E:198:ILE:H	1.83	0.43
7:G:35:GLU:OE2	7:G:48:VAL:HG23	2.19	0.43
8:H:5:LEU:O	8:H:133:ASN:HB3	2.19	0.43
8:H:82:PRO:CG	11:K:54:ARG:HD2	2.46	0.43
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.53	0.43
10:J:14:VAL:CG1	10:J:50:ILE:HD11	2.49	0.43
1:A:69:THR:O	1:A:70:CYS:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:PRO:CG	1:A:245:PRO:HD3	2.48	0.43
1:A:334:GLY:C	1:A:336:ILE:N	2.76	0.43
1:A:452:LYS:HG3	2:B:1140:ALA:HB1	1.99	0.43
1:A:489:LEU:HD12	1:A:490:HIS:N	2.33	0.43
1:A:525:GLN:OE1	2:B:836:GLU:HG2	2.19	0.43
1:A:784:LEU:C	1:A:786:HIS:N	2.76	0.43
1:A:784:LEU:HD11	1:A:815:PHE:CE2	2.54	0.43
1:A:1116:LEU:HA	1:A:1329:THR:HA	2.01	0.43
1:A:1120:LEU:HD12	1:A:1120:LEU:N	2.28	0.43
1:A:1213:GLY:HA2	1:A:1216:ILE:CD1	2.48	0.43
1:A:1423:GLY:O	1:A:1424:VAL:C	2.61	0.43
1:A:1434:ALA:HA	1:A:1435:PRO:HD3	1.89	0.43
2:B:378:LEU:CD1	2:B:382:ILE:HD11	2.49	0.43
2:B:483:LEU:HD11	2:B:491:THR:CG2	2.49	0.43
2:B:502:ILE:HG22	2:B:507:LYS:HG3	2.01	0.43
2:B:560:GLU:O	2:B:561:TRP:CD1	2.72	0.43
2:B:882:THR:C	2:B:884:ARG:N	2.75	0.43
2:B:1174:LYS:O	2:B:1175:LEU:C	2.60	0.43
4:D:16:LYS:C	4:D:18:VAL:N	2.76	0.43
4:D:60:LYS:NZ	4:D:122:GLU:OE2	2.52	0.43
5:E:168:TYR:O	5:E:169:ARG:C	2.62	0.43
6:F:82:THR:HA	6:F:83:PRO:HD3	1.66	0.43
6:F:93:ILE:HG23	6:F:132:LEU:HD12	2.00	0.43
6:F:108:PHE:CD2	6:F:108:PHE:N	2.85	0.43
9:I:98:VAL:HG12	9:I:99:LEU:H	1.84	0.43
11:K:43:GLY:HA3	11:K:61:TYR:HE1	1.84	0.43
14:N:8:DG:H2"	14:N:9:DA:OP2	2.18	0.43
1:A:57:ARG:O	1:A:68:GLN:HG3	2.19	0.43
1:A:153:PRO:HB3	1:A:161:LEU:CD2	2.49	0.43
1:A:254:GLU:O	1:A:255:SER:OG	2.29	0.43
1:A:293:GLU:C	1:A:295:LEU:H	2.27	0.43
1:A:483:ASP:HB2	2:B:987:LYS:CB	2.49	0.43
1:A:590:ARG:HG2	1:A:591:PHE:N	2.32	0.43
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	2.01	0.43
1:A:1094:VAL:HG12	1:A:1113:THR:HG21	1.99	0.43
1:A:1142:THR:O	1:A:1143:LEU:C	2.62	0.43
1:A:1348:LEU:HD23	1:A:1372:VAL:HG23	2.00	0.43
1:A:1406:VAL:O	1:A:1407:GLU:C	2.61	0.43
1:A:1443:VAL:C	1:A:1444:MET:CG	2.92	0.43
2:B:210:LYS:HG3	2:B:461:LEU:O	2.18	0.43
2:B:273:LEU:O	2:B:276:ILE:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.45	0.43
2:B:464:GLY:C	2:B:465:ASN:HD22	2.26	0.43
2:B:566:LEU:HD22	2:B:586:TRP:O	2.19	0.43
2:B:864:LYS:HG3	2:B:872:GLU:OE1	2.18	0.43
2:B:1181:GLU:H	2:B:1188:LYS:HG3	1.83	0.43
3:C:229:TYR:CD1	3:C:229:TYR:N	2.87	0.43
4:D:9:GLN:HE22	4:D:31:GLN:HB3	1.84	0.43
5:E:90:VAL:HG23	5:E:120:ALA:HA	2.01	0.43
5:E:155:ARG:O	5:E:156:LEU:HD23	2.19	0.43
6:F:74:ILE:HG22	6:F:75:PRO:N	2.33	0.43
6:F:138:LEU:HD22	6:F:139:PRO:HD2	2.00	0.43
9:I:55:THR:O	9:I:58:VAL:HG23	2.19	0.43
10:J:36:LEU:HD22	10:J:41:LEU:HD12	2.01	0.43
1:A:506:ALA:CB	1:A:508:PRO:HD2	2.49	0.43
1:A:531:ILE:N	1:A:653:VAL:HG11	2.34	0.43
1:A:540:PHE:CD1	1:A:540:PHE:N	2.87	0.43
1:A:586:ILE:HD11	1:A:633:VAL:HA	2.00	0.43
1:A:699:ALA:HB1	9:I:114:GLN:NE2	2.34	0.43
1:A:867:ILE:HD12	1:A:867:ILE:N	2.33	0.43
1:A:886:ILE:HG23	1:A:887:GLY:H	1.80	0.43
1:A:1259:MET:HE2	1:A:1262:LYS:NZ	2.34	0.43
1:A:1313:LEU:C	1:A:1315:GLU:N	2.77	0.43
1:A:1341:ILE:CG2	1:A:1342:GLU:H	2.32	0.43
1:A:1398:MET:O	1:A:1399:ARG:C	2.62	0.43
2:B:603:LEU:HB3	2:B:609:ILE:CD1	2.29	0.43
2:B:700:SER:O	2:B:701:ILE:HG22	2.18	0.43
2:B:816:GLU:N	2:B:816:GLU:OE1	2.49	0.43
3:C:77:ILE:HA	3:C:129:ILE:HD11	2.01	0.43
3:C:174:ALA:O	3:C:175:ALA:CB	2.67	0.43
4:D:214:LEU:O	4:D:218:GLU:N	2.50	0.43
5:E:116:ILE:C	5:E:121:MET:HE2	2.44	0.43
7:G:114:LEU:HD12	7:G:114:LEU:HA	1.90	0.43
9:I:88:SER:HB3	9:I:95:THR:HG21	2.01	0.43
11:K:12:LEU:HD23	11:K:16:GLU:O	2.19	0.43
1:A:179:LEU:CD1	1:A:297:GLN:HG3	2.49	0.42
1:A:325:ILE:O	1:A:326:ARG:C	2.62	0.42
1:A:380:VAL:HG13	1:A:385:ILE:CD1	2.48	0.42
1:A:477:PRO:HG2	1:A:521:MET:HG2	2.00	0.42
1:A:614:PHE:CD1	1:A:614:PHE:C	2.97	0.42
1:A:1067:LEU:C	1:A:1069:ALA:N	2.77	0.42
1:A:1453:TYR:O	1:A:1454:MET:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:SER:HA	2:B:811:TYR:HE2	1.84	0.42
2:B:459:TYR:CE1	2:B:469:GLN:HB3	2.54	0.42
2:B:469:GLN:CG	2:B:470:LYS:N	2.80	0.42
2:B:498:THR:N	2:B:537:LYS:O	2.52	0.42
2:B:727:LYS:HE2	2:B:1049:ASP:OD1	2.20	0.42
2:B:731:VAL:HG12	2:B:732:SER:N	2.33	0.42
2:B:758:PHE:HZ	2:B:1031:LEU:HD22	1.84	0.42
2:B:797:TYR:O	10:J:1:MET:HG2	2.19	0.42
2:B:1070:GLU:OE1	10:J:44:TYR:OH	2.36	0.42
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.33	0.42
3:C:24:ASN:CA	3:C:226:ASP:HB3	2.47	0.42
3:C:55:THR:O	3:C:55:THR:HG22	2.19	0.42
3:C:124:LEU:C	3:C:126:GLY:N	2.77	0.42
3:C:124:LEU:CD2	3:C:129:ILE:O	2.68	0.42
4:D:39:ASN:ND2	4:D:41:GLN:CG	2.82	0.42
4:D:153:ARG:NH2	4:D:184:ALA:HA	2.34	0.42
4:D:187:THR:C	4:D:189:ASP:N	2.75	0.42
4:D:219:THR:HG22	4:D:220:LEU:O	2.19	0.42
5:E:136:ASN:OD1	5:E:138:ALA:N	2.52	0.42
7:G:38:CYS:HA	7:G:43:GLY:O	2.19	0.42
7:G:62:LEU:CB	7:G:63:PRO:CD	2.91	0.42
8:H:10:PHE:CD1	8:H:10:PHE:N	2.87	0.42
11:K:42:LEU:C	11:K:42:LEU:CD2	2.90	0.42
1:A:53:LEU:HD23	1:A:54:ASN:CB	2.46	0.42
1:A:293:GLU:O	1:A:295:LEU:N	2.52	0.42
1:A:335:ARG:HA	1:A:339:ASN:ND2	2.32	0.42
1:A:353:ILE:O	1:A:353:ILE:HG13	2.19	0.42
1:A:373:THR:HG21	2:B:1105:ALA:HB3	2.00	0.42
1:A:751:SER:O	1:A:752:LYS:CG	2.65	0.42
1:A:864:ILE:HG21	1:A:1374:VAL:HG22	2.02	0.42
1:A:1100:ARG:O	1:A:1100:ARG:HD2	2.19	0.42
1:A:1140:HIS:CA	1:A:1275:GLY:HA3	2.49	0.42
1:A:1155:ASP:CG	1:A:1161:THR:HA	2.43	0.42
1:A:1166:ASP:OD2	1:A:1239:ARG:NE	2.45	0.42
1:A:1376:THR:HG23	1:A:1377:THR:H	1.85	0.42
2:B:351:TYR:CD1	2:B:355:ILE:HD11	2.54	0.42
2:B:458:LYS:O	2:B:459:TYR:C	2.61	0.42
2:B:882:THR:HG21	2:B:935:ARG:CA	2.40	0.42
2:B:1098:MET:O	2:B:1099:VAL:C	2.61	0.42
3:C:24:ASN:O	3:C:24:ASN:CG	2.62	0.42
3:C:58:LEU:HD12	3:C:62:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:119:ARG:HG3	4:D:221:TYR:HE2	1.84	0.42
5:E:31:THR:OG1	5:E:34:GLU:N	2.35	0.42
5:E:154:ILE:O	5:E:196:VAL:HA	2.20	0.42
6:F:116:ASP:OD1	6:F:118:LEU:N	2.52	0.42
7:G:111:THR:HG22	7:G:113:HIS:H	1.84	0.42
7:G:125:SER:C	7:G:126:ASN:HD22	2.27	0.42
8:H:143:LEU:HD12	8:H:143:LEU:N	2.34	0.42
9:I:19:ASP:CG	9:I:22:ASN:HB2	2.44	0.42
9:I:55:THR:HG22	9:I:55:THR:O	2.20	0.42
9:I:86:PHE:HE1	9:I:100:PHE:HB2	1.84	0.42
10:J:12:LYS:O	10:J:13:VAL:C	2.62	0.42
1:A:12:ARG:HD2	2:B:1218:THR:CG2	2.48	0.42
1:A:25:GLU:O	1:A:28:ARG:N	2.52	0.42
1:A:79:GLY:C	1:A:243:PRO:HG3	2.45	0.42
1:A:722:LEU:HD12	1:A:722:LEU:N	2.33	0.42
1:A:781:ASP:HB3	1:A:790:ASP:H	1.83	0.42
1:A:814:PHE:O	1:A:817:ALA:HB3	2.20	0.42
1:A:873:MET:C	1:A:1058:VAL:CG2	2.89	0.42
1:A:1400:CYS:O	1:A:1405:THR:HA	2.19	0.42
1:A:1409:LEU:O	1:A:1412:ALA:HB3	2.19	0.42
2:B:420:LEU:O	2:B:423:LYS:N	2.48	0.42
2:B:492:LEU:O	2:B:493:SER:C	2.61	0.42
2:B:824:ILE:HG12	10:J:48:ARG:HH12	1.84	0.42
2:B:893:LEU:HD22	2:B:897:GLY:O	2.20	0.42
2:B:999:MET:HE3	2:B:999:MET:CA	2.32	0.42
2:B:1065:GLN:HG3	2:B:1067:ARG:N	2.31	0.42
3:C:69:LEU:N	3:C:69:LEU:CD1	2.81	0.42
3:C:86:CYS:SG	3:C:87:PHE:N	2.92	0.42
3:C:131:HIS:HA	3:C:132:PRO:HD3	1.76	0.42
3:C:136:ASP:CB	3:C:141:GLY:H	2.32	0.42
4:D:58:VAL:O	4:D:59:ILE:C	2.62	0.42
6:F:74:ILE:HG22	6:F:75:PRO:O	2.19	0.42
6:F:82:THR:HG23	6:F:83:PRO:HD2	2.01	0.42
7:G:145:VAL:CG1	7:G:146:LYS:N	2.81	0.42
12:L:36:SER:O	12:L:37:LYS:O	2.37	0.42
12:L:58:LYS:O	12:L:59:ALA:O	2.37	0.42
13:T:16:DT:H2''	13:T:17:DT:C5'	2.37	0.42
1:A:38:PRO:CD	1:A:39:GLU:H	2.32	0.42
1:A:40:THR:C	1:A:41:MET:HG3	2.43	0.42
1:A:90:VAL:HG13	1:A:297:GLN:HA	2.01	0.42
1:A:116:ASP:O	1:A:118:HIS:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:CG	8:H:94:ASP:O	2.64	0.42
1:A:578:LEU:HD23	1:A:612:ILE:CD1	2.50	0.42
1:A:709:THR:HG22	1:A:710:LEU:H	1.84	0.42
1:A:1018:PHE:O	1:A:1019:CYS:C	2.60	0.42
1:A:1243:VAL:HG22	1:A:1244:ARG:N	2.34	0.42
1:A:1369:ALA:HA	1:A:1372:VAL:HG12	2.01	0.42
1:A:1385:THR:O	1:A:1386:ARG:C	2.62	0.42
1:A:1450:LEU:HD11	7:G:18:PHE:O	2.18	0.42
2:B:298:LEU:N	2:B:298:LEU:CD2	2.82	0.42
2:B:700:SER:O	2:B:701:ILE:CG2	2.68	0.42
2:B:766:ARG:NH2	15:P:11:U:H3	2.17	0.42
2:B:828:ALA:HB2	2:B:1085:ILE:HG23	2.02	0.42
2:B:880:THR:O	2:B:881:ASN:HB2	2.20	0.42
2:B:955:THR:HG23	2:B:956:THR:N	2.33	0.42
2:B:975:GLN:HG2	2:B:976:ILE:H	1.84	0.42
6:F:108:PHE:CE1	6:F:131:PRO:HG3	2.54	0.42
7:G:1:MET:O	7:G:2:PHE:O	2.36	0.42
7:G:45:ILE:HD13	7:G:78:VAL:HG11	2.01	0.42
8:H:40:LEU:C	8:H:41:ASP:O	2.60	0.42
10:J:34:THR:O	10:J:35:ALA:C	2.62	0.42
11:K:17:SER:O	11:K:18:LYS:C	2.63	0.42
14:N:4:DA:H2"	14:N:5:DC:C5	2.54	0.42
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.45	0.42
1:A:96:ILE:HG22	1:A:97:ALA:N	2.34	0.42
1:A:222:LEU:HB3	1:A:223:GLY:H	1.72	0.42
1:A:456:MET:HE3	1:A:510:GLN:HB2	2.01	0.42
1:A:842:VAL:C	1:A:844:ALA:N	2.76	0.42
1:A:862:ASN:HA	5:E:174:GLN:HB3	2.01	0.42
1:A:892:ALA:O	1:A:893:PHE:C	2.59	0.42
1:A:1019:CYS:HA	1:A:1022:LEU:HB3	2.02	0.42
1:A:1054:LEU:HD13	6:F:84:TYR:OH	2.19	0.42
1:A:1202:MET:SD	1:A:1207:LEU:HD12	2.60	0.42
2:B:510:LYS:HD2	2:B:511:PRO:HD3	2.00	0.42
2:B:593:PRO:CA	2:B:596:LEU:HB3	2.49	0.42
2:B:653:VAL:HG22	2:B:689:LEU:HD13	2.02	0.42
2:B:806:THR:O	2:B:809:MET:HG3	2.20	0.42
2:B:821:GLN:HE22	2:B:851:PHE:CA	2.32	0.42
2:B:955:THR:HG23	2:B:956:THR:H	1.84	0.42
2:B:1096:ARG:CA	2:B:1098:MET:HE2	2.49	0.42
2:B:1138:MET:HE2	2:B:1146:PHE:HD2	1.84	0.42
2:B:1163:CYS:C	2:B:1165:ILE:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:238:ILE:HG12	3:C:246:ARG:NH1	2.35	0.42
4:D:53:SER:HB3	4:D:153:ARG:H	1.84	0.42
4:D:156:ASP:O	4:D:160:VAL:HG23	2.20	0.42
4:D:210:ILE:O	4:D:213:GLU:HB2	2.19	0.42
6:F:123:LYS:O	6:F:124:GLU:C	2.63	0.42
7:G:21:ARG:HG2	7:G:24:GLN:HG2	2.02	0.42
7:G:99:PHE:O	7:G:99:PHE:CD1	2.73	0.42
7:G:153:GLN:HG2	7:G:154:VAL:N	2.34	0.42
8:H:3:ASN:O	8:H:60:ALA:HB1	2.20	0.42
8:H:11:GLN:O	8:H:28:ALA:CB	2.67	0.42
8:H:139:ASN:O	8:H:140:ALA:CB	2.67	0.42
10:J:16:ASP:O	10:J:18:TRP:N	2.52	0.42
10:J:48:ARG:HH21	10:J:49:MET:HE1	1.83	0.42
12:L:28:LYS:HD2	12:L:39:SER:OG	2.18	0.42
1:A:464:PRO:O	1:A:465:TYR:HB2	2.20	0.42
1:A:637:LYS:HB3	1:A:641:VAL:CG2	2.33	0.42
1:A:849:MET:HE1	1:A:1061:GLY:HA2	1.98	0.42
1:A:857:ARG:CD	1:A:861:GLY:O	2.60	0.42
1:A:859:SER:HB2	1:A:1422:ARG:HB2	2.01	0.42
1:A:867:ILE:HG12	1:A:1000:LEU:HD11	2.01	0.42
1:A:878:ILE:C	1:A:879:GLU:HG3	2.45	0.42
1:A:946:VAL:HG22	5:E:201:LYS:HD2	2.02	0.42
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.35	0.42
1:A:1152:ILE:HD11	9:I:44:TYR:CD2	2.47	0.42
1:A:1189:SER:OG	1:A:1256:GLU:OE1	2.32	0.42
2:B:46:GLN:NE2	2:B:496:ARG:CB	2.82	0.42
2:B:258:LEU:O	2:B:259:TYR:C	2.62	0.42
2:B:386:LEU:C	2:B:388:CYS:N	2.76	0.42
2:B:459:TYR:CZ	2:B:469:GLN:HB3	2.55	0.42
2:B:578:THR:C	2:B:589:VAL:HG13	2.45	0.42
2:B:806:THR:CG2	2:B:1046:PRO:HD3	2.47	0.42
2:B:866:TYR:O	2:B:867:GLY:C	2.63	0.42
2:B:992:ILE:CD1	11:K:66:PRO:HB2	2.49	0.42
2:B:1110:PRO:HG3	2:B:1125:ASP:HB3	2.01	0.42
2:B:1134:GLU:O	2:B:1135:ARG:C	2.61	0.42
3:C:100:THR:HG21	3:C:102:GLN:NE2	2.35	0.42
3:C:166:GLU:HG3	11:K:10:PHE:HZ	1.84	0.42
4:D:52:LEU:O	4:D:53:SER:OG	2.36	0.42
4:D:119:ARG:HB2	4:D:221:TYR:CE2	2.53	0.42
5:E:78:LEU:CA	5:E:107:THR:HB	2.41	0.42
5:E:168:TYR:C	5:E:169:ARG:HG2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:53:ASN:N	7:G:53:ASN:HD22	2.17	0.42
8:H:5:LEU:HD13	8:H:135:LEU:HD12	2.01	0.42
8:H:129:TYR:H	8:H:130:ARG:NH1	2.14	0.42
9:I:50:THR:HG23	9:I:52:ILE:HG12	2.02	0.42
10:J:35:ALA:O	10:J:38:ARG:HB3	2.19	0.42
10:J:42:LYS:HE2	10:J:43:ARG:H	1.85	0.42
11:K:79:GLU:CG	11:K:80:GLY:N	2.82	0.42
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.84	0.42
1:A:92:HIS:O	1:A:93:VAL:C	2.62	0.42
1:A:443:LEU:HD22	1:A:443:LEU:HA	1.87	0.42
1:A:640:GLN:HA	1:A:640:GLN:OE1	2.19	0.42
1:A:680:THR:HG23	2:B:729:ILE:HD11	2.01	0.42
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.19	0.42
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.26	0.42
1:A:1074:GLU:H	1:A:1075:PRO:HD2	1.85	0.42
1:A:1119:TYR:O	1:A:1120:LEU:O	2.38	0.42
1:A:1161:THR:O	1:A:1163:ILE:N	2.53	0.42
2:B:20:ASP:C	2:B:22:SER:N	2.68	0.42
2:B:122:LEU:O	2:B:206:ASN:N	2.53	0.42
2:B:257:LYS:N	2:B:270:LYS:O	2.53	0.42
2:B:466:TRP:C	2:B:475:SER:HB3	2.45	0.42
2:B:469:GLN:HG3	2:B:470:LYS:N	2.23	0.42
2:B:653:VAL:HG22	2:B:689:LEU:HB3	2.02	0.42
2:B:831:SER:CB	2:B:994:TYR:OH	2.68	0.42
2:B:969:ARG:HD3	3:C:61:GLU:OE2	2.20	0.42
2:B:1116:ARG:HD2	2:B:1198:TYR:CD1	2.55	0.42
3:C:3:GLU:HG3	11:K:104:ASN:HD21	1.85	0.42
3:C:26:ASP:O	3:C:29:MET:HB3	2.20	0.42
3:C:82:TYR:O	3:C:83:SER:C	2.61	0.42
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.55	0.42
5:E:96:PHE:O	5:E:99:HIS:HB3	2.18	0.42
6:F:77:ASP:O	6:F:78:GLN:CB	2.65	0.42
6:F:95:GLY:O	6:F:96:THR:C	2.62	0.42
9:I:76:PRO:HD3	9:I:110:PHE:CD2	2.54	0.42
9:I:80:SER:OG	9:I:105:SER:CB	2.68	0.42
1:A:116:ASP:O	1:A:117:GLU:C	2.62	0.42
1:A:179:LEU:C	1:A:180:LYS:HG3	2.44	0.42
1:A:351:THR:HG21	2:B:1103:ILE:HG13	2.01	0.42
1:A:370:ILE:CG2	1:A:374:LEU:HG	2.50	0.42
1:A:531:ILE:HD13	1:A:653:VAL:HG21	1.98	0.42
1:A:596:THR:C	1:A:598:LEU:N	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:ARG:C	1:A:679:ILE:N	2.76	0.42
1:A:785:PRO:HG2	1:A:786:HIS:CD2	2.54	0.42
1:A:867:ILE:CG1	1:A:1000:LEU:HD11	2.50	0.42
1:A:950:GLY:O	1:A:951:GLU:C	2.62	0.42
1:A:1114:PRO:O	1:A:1330:ASN:ND2	2.53	0.42
1:A:1115:SER:OG	1:A:1116:LEU:N	2.51	0.42
1:A:1201:ALA:C	1:A:1203:ASN:N	2.74	0.42
1:A:1293:SER:HB3	1:A:1297:GLU:O	2.20	0.42
1:A:1336:MET:HE3	1:A:1381:LEU:HG	2.00	0.42
1:A:1438:THR:O	6:F:92:ARG:NH1	2.52	0.42
1:A:1450:LEU:O	1:A:1450:LEU:HG	2.19	0.42
2:B:53:GLN:CG	2:B:547:VAL:CG2	2.96	0.42
2:B:281:PRO:O	2:B:282:ILE:C	2.63	0.42
2:B:281:PRO:HB3	2:B:320:ASP:OD2	2.18	0.42
2:B:642:ASP:CA	2:B:649:LYS:HA	2.27	0.42
2:B:800:GLN:CB	10:J:52:THR:CG2	2.96	0.42
2:B:1034:VAL:O	2:B:1036:ALA:N	2.52	0.42
2:B:1055:ILE:C	2:B:1057:LYS:H	2.28	0.42
2:B:1065:GLN:NE2	2:B:1066:SER:N	2.67	0.42
2:B:1098:MET:H	2:B:1098:MET:CE	2.29	0.42
3:C:213:PRO:O	3:C:214:ASN:HB3	2.19	0.42
4:D:64:VAL:HG22	4:D:129:LEU:CD2	2.49	0.42
5:E:31:THR:HG1	5:E:34:GLU:H	1.63	0.42
5:E:83:CYS:C	5:E:85:GLU:N	2.77	0.42
6:F:102:SER:C	6:F:104:ASN:H	2.25	0.42
8:H:128:ASN:O	8:H:128:ASN:CG	2.62	0.42
9:I:53:GLY:HA2	9:I:56:ALA:HB2	2.02	0.42
1:A:115:LEU:CD1	1:A:142:CYS:HB3	2.50	0.42
1:A:434:ARG:HE	1:A:437:MET:HE2	1.84	0.42
1:A:444:PHE:HB3	1:A:458:HIS:CD2	2.55	0.42
1:A:528:LEU:HD23	1:A:751:SER:CB	2.45	0.42
1:A:537:ARG:HH22	8:H:122:LEU:CG	2.32	0.42
1:A:896:ARG:HB3	1:A:897:TYR:HD1	1.85	0.42
1:A:1402:PHE:O	1:A:1403:GLU:CB	2.68	0.42
2:B:526:GLU:CD	2:B:752:ALA:CB	2.93	0.42
2:B:563:MET:HE3	2:B:580:VAL:HB	1.99	0.42
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.92	0.42
2:B:1023:VAL:C	2:B:1025:HIS:H	2.27	0.42
3:C:31:ASN:O	3:C:34:ARG:HB3	2.20	0.42
3:C:91:HIS:C	3:C:91:HIS:CD2	2.96	0.42
4:D:67:ARG:HA	4:D:133:THR:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:156:LEU:HD12	5:E:195:VAL:CG1	2.50	0.42
8:H:4:THR:HG22	8:H:5:LEU:N	2.35	0.42
8:H:98:TYR:HE1	8:H:139:ASN:HA	1.85	0.42
12:L:49:LYS:O	12:L:50:ASP:CB	2.66	0.42
1:A:62:ASP:O	1:A:62:ASP:OD1	2.38	0.42
1:A:362:ASP:O	1:A:458:HIS:HA	2.20	0.42
1:A:391:LEU:O	1:A:394:ASN:HB3	2.20	0.42
1:A:440:ASP:O	1:A:460:VAL:HG23	2.20	0.42
1:A:521:MET:O	1:A:624:SER:HB3	2.20	0.42
1:A:528:LEU:HD11	1:A:619:LYS:H	1.85	0.42
1:A:616:VAL:HG12	1:A:617:VAL:N	2.34	0.42
1:A:742:ASN:O	1:A:743:VAL:C	2.63	0.42
1:A:765:VAL:HG23	1:A:802:ASN:O	2.20	0.42
1:A:879:GLU:OE2	1:A:959:ASN:HB2	2.20	0.42
1:A:885:THR:HG23	1:A:893:PHE:HE1	1.85	0.42
1:A:1019:CYS:O	1:A:1020:CYS:C	2.61	0.42
1:A:1277:GLU:O	1:A:1279:ILE:HD12	2.20	0.42
2:B:906:SER:O	2:B:907:GLY:O	2.38	0.42
2:B:956:THR:HG22	2:B:957:ASN:N	2.34	0.42
2:B:1102:LYS:C	2:B:1122:ARG:NH1	2.78	0.42
5:E:13:TRP:O	5:E:16:PHE:N	2.53	0.42
5:E:134:THR:O	5:E:135:PHE:CD1	2.73	0.42
5:E:207:ARG:HB3	5:E:207:ARG:NH1	2.34	0.42
7:G:1:MET:HG2	7:G:85:GLU:CD	2.45	0.42
7:G:15:PRO:O	7:G:16:SER:C	2.62	0.42
7:G:153:GLN:CG	7:G:154:VAL:HG23	2.43	0.42
8:H:12:VAL:HG13	8:H:26:ILE:CG2	2.50	0.42
8:H:26:ILE:CG2	8:H:27:GLU:H	2.24	0.42
8:H:84:ALA:HA	8:H:87:ARG:HB2	2.01	0.42
9:I:19:ASP:CB	9:I:24:ARG:HG3	2.50	0.42
1:A:231:PRO:C	1:A:233:TRP:N	2.78	0.41
1:A:282:ASN:O	1:A:283:GLY:C	2.63	0.41
1:A:315:LEU:CD1	2:B:471:LYS:HB3	2.45	0.41
1:A:381:THR:C	1:A:383:TYR:N	2.77	0.41
1:A:562:THR:HB	8:H:98:TYR:CE2	2.55	0.41
1:A:677:ARG:C	1:A:677:ARG:HD2	2.45	0.41
1:A:779:PHE:HD1	1:A:784:LEU:HA	1.85	0.41
1:A:800:VAL:HG11	1:A:808:LEU:HD11	2.02	0.41
1:A:840:ARG:HH22	1:A:1106:ASN:HD21	1.67	0.41
1:A:885:THR:O	1:A:885:THR:CG2	2.67	0.41
1:A:898:ARG:HA	1:A:933:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1010:ALA:HA	1:A:1013:ASP:OD2	2.20	0.41
1:A:1033:GLN:O	1:A:1036:ARG:NH1	2.53	0.41
1:A:1131:ALA:O	1:A:1132:LYS:C	2.63	0.41
1:A:1191:TRP:HD1	1:A:1256:GLU:CB	2.32	0.41
1:A:1392:SER:C	1:A:1394:THR:H	2.28	0.41
2:B:44:VAL:HG23	2:B:48:LEU:CD1	2.50	0.41
2:B:235:SER:HB3	2:B:258:LEU:HG	2.02	0.41
2:B:980:PHE:HE2	2:B:1094:ARG:CB	2.29	0.41
2:B:1100:ASP:OD2	11:K:1:MET:HB2	2.20	0.41
2:B:1177:HIS:O	2:B:1178:ASN:HB2	2.18	0.41
3:C:67:LEU:HD23	3:C:70:ILE:HD11	2.02	0.41
4:D:51:ASN:C	4:D:52:LEU:O	2.63	0.41
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.76	0.41
6:F:85:MET:HG2	6:F:89:GLU:HB2	2.02	0.41
8:H:108:SER:O	8:H:110:ASP:N	2.53	0.41
1:A:481:ASP:OD2	1:A:481:ASP:N	2.53	0.41
1:A:537:ARG:NH1	8:H:122:LEU:HG	2.34	0.41
1:A:636:GLU:OE2	1:A:962:ARG:NH1	2.53	0.41
1:A:692:ASP:C	1:A:694:THR:N	2.79	0.41
1:A:838:GLN:O	1:A:841:LEU:HB2	2.20	0.41
2:B:23:ALA:O	2:B:654:ARG:HB3	2.20	0.41
2:B:27:ALA:O	2:B:28:GLU:C	2.62	0.41
2:B:664:THR:CG2	2:B:678:GLU:N	2.83	0.41
2:B:687:GLU:C	2:B:689:LEU:N	2.79	0.41
2:B:781:PHE:O	2:B:782:LEU:HG	2.20	0.41
2:B:1011:ILE:O	2:B:1011:ILE:HG22	2.19	0.41
2:B:1047:PHE:O	2:B:1048:THR:HG23	2.20	0.41
2:B:1087:PHE:C	2:B:1087:PHE:HD2	2.27	0.41
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	2.02	0.41
3:C:124:LEU:HD21	3:C:129:ILE:O	2.20	0.41
3:C:213:PRO:O	3:C:214:ASN:CB	2.68	0.41
3:C:269:LYS:HD3	3:C:270:VAL:HG13	2.01	0.41
10:J:6:ARG:HB3	10:J:11:GLY:O	2.20	0.41
11:K:13:GLY:O	11:K:14:GLU:O	2.38	0.41
13:T:12:DG:H2''	13:T:13:DT:O5'	2.20	0.41
1:A:767:GLN:NE2	1:A:797:LYS:O	2.53	0.41
1:A:846:GLU:OE1	1:A:1425:SER:OG	2.38	0.41
1:A:894:GLU:HG2	1:A:933:TYR:OH	2.21	0.41
1:A:910:PRO:HB3	1:A:917:SER:N	2.29	0.41
1:A:946:VAL:HG13	5:E:201:LYS:CB	2.38	0.41
1:A:1107:VAL:HG21	1:A:1383:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1133:LEU:O	1:A:1134:ILE:C	2.63	0.41
1:A:1330:ASN:O	1:A:1332:PHE:N	2.53	0.41
2:B:26:THR:HA	2:B:708:GLU:OE1	2.20	0.41
2:B:597:MET:HE3	2:B:600:LEU:HD12	2.02	0.41
2:B:886:LYS:HB3	2:B:887:HIS:H	1.73	0.41
2:B:982:SER:HB3	2:B:1092:TYR:CE2	2.55	0.41
2:B:1001:PHE:HD2	3:C:34:ARG:HH21	1.64	0.41
5:E:52:ARG:CG	5:E:52:ARG:NH1	2.81	0.41
5:E:89:GLY:HA2	5:E:117:THR:OG1	2.19	0.41
6:F:116:ASP:OD1	6:F:119:ARG:N	2.54	0.41
6:F:147:SER:O	6:F:148:VAL:C	2.63	0.41
7:G:1:MET:O	7:G:2:PHE:C	2.62	0.41
7:G:106:MET:HE2	7:G:106:MET:HB3	1.96	0.41
8:H:24:CYS:HB2	8:H:44:VAL:CG2	2.48	0.41
1:A:92:HIS:O	1:A:94:GLY:N	2.53	0.41
1:A:289:ILE:O	1:A:290:GLU:C	2.63	0.41
1:A:343:LYS:HB3	2:B:1117:GLN:OE1	2.21	0.41
1:A:377:PRO:HD2	1:A:493:GLN:OE1	2.20	0.41
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.21	0.41
1:A:516:SER:O	1:A:518:LYS:HB3	2.20	0.41
1:A:543:LEU:HD12	1:A:547:LEU:HG	2.03	0.41
1:A:1037:LEU:HD13	1:A:1041:ALA:CB	2.50	0.41
1:A:1276:VAL:CG1	1:A:1277:GLU:H	2.29	0.41
1:A:1444:MET:O	6:F:133:VAL:N	2.53	0.41
2:B:355:ILE:HG13	2:B:355:ILE:H	1.71	0.41
2:B:593:PRO:CG	2:B:617:ARG:NH2	2.83	0.41
2:B:619:ILE:CG2	9:I:61:ASP:HB2	2.51	0.41
2:B:654:ARG:C	2:B:656:GLY:H	2.28	0.41
2:B:839:MET:CE	2:B:1010:LEU:HD11	2.50	0.41
2:B:868:MET:O	2:B:870:ILE:HG13	2.19	0.41
4:D:2:ASN:O	4:D:4:SER:N	2.44	0.41
4:D:155:ARG:CG	4:D:155:ARG:NH1	2.84	0.41
6:F:90:ARG:HG2	6:F:155:LEU:HD13	2.02	0.41
7:G:20:PRO:CG	7:G:21:ARG:H	2.33	0.41
8:H:63:LEU:CD1	8:H:64:ASN:N	2.84	0.41
12:L:27:LEU:HB2	12:L:28:LYS:H	1.78	0.41
1:A:188:ASP:O	1:A:195:ASP:HA	2.20	0.41
1:A:258:GLY:O	1:A:259:GLU:C	2.63	0.41
1:A:483:ASP:HB2	2:B:987:LYS:HB3	2.01	0.41
1:A:614:PHE:CB	8:H:122:LEU:HD21	2.50	0.41
1:A:865:GLN:OE1	1:A:869:GLY:N	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1365:TYR:O	1:A:1366:ARG:C	2.63	0.41
1:A:1431:GLY:HA3	2:B:1197:PRO:HD3	2.02	0.41
2:B:119:LEU:HD22	2:B:789:MET:HB2	2.02	0.41
2:B:343:ILE:HG23	2:B:347:LYS:HE2	2.01	0.41
2:B:685:LEU:HG	2:B:686:ASN:N	2.33	0.41
2:B:744:HIS:CG	2:B:745:PRO:HD2	2.55	0.41
2:B:795:ILE:HD12	2:B:795:ILE:N	2.36	0.41
2:B:880:THR:HB	2:B:934:LYS:CD	2.39	0.41
2:B:1074:ASN:O	2:B:1076:HIS:N	2.53	0.41
3:C:209:TYR:H	3:C:209:TYR:HD1	1.69	0.41
6:F:73:ALA:CB	6:F:143:PHE:H	2.34	0.41
6:F:118:LEU:O	6:F:122:MET:CG	2.68	0.41
8:H:83:GLN:C	8:H:85:GLY:N	2.78	0.41
1:A:16:GLU:CG	2:B:1220:ARG:HA	2.51	0.41
1:A:58:LEU:O	1:A:59:GLY:O	2.39	0.41
1:A:441:PRO:HG3	1:A:498:ARG:HB2	2.02	0.41
1:A:523:ILE:CD1	1:A:649:ILE:HG21	2.51	0.41
1:A:552:TRP:HE3	1:A:651:LYS:HB3	1.85	0.41
1:A:622:VAL:O	1:A:622:VAL:HG22	2.20	0.41
1:A:870:GLU:O	1:A:871:ASP:HB3	2.19	0.41
1:A:1303:GLU:O	1:A:1303:GLU:HG3	2.19	0.41
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	2.01	0.41
1:A:1420:ASP:O	1:A:1421:CYS:CB	2.64	0.41
2:B:255:GLN:O	2:B:271:ALA:HB1	2.20	0.41
2:B:278:GLN:HG2	2:B:279:ASP:N	2.35	0.41
2:B:303:TYR:HH	2:B:586:TRP:HH2	1.65	0.41
2:B:318:VAL:C	2:B:320:ASP:N	2.76	0.41
2:B:1003:ALA:O	3:C:177:GLU:HG2	2.21	0.41
2:B:1068:GLY:O	2:B:1069:PHE:C	2.64	0.41
4:D:153:ARG:HD3	4:D:154:PHE:CE1	2.54	0.41
5:E:28:TYR:C	5:E:65:THR:HG23	2.45	0.41
6:F:106:PRO:HG2	7:G:18:PHE:C	2.46	0.41
7:G:117:GLN:C	7:G:119:LEU:N	2.77	0.41
8:H:77:ARG:O	8:H:78:SER:O	2.38	0.41
9:I:35:VAL:CG1	9:I:36:GLU:N	2.79	0.41
1:A:90:VAL:CG1	1:A:297:GLN:CD	2.94	0.41
1:A:515:GLN:HB2	1:A:1071:SER:CB	2.51	0.41
1:A:567:LYS:HG2	1:A:568:PRO:CD	2.51	0.41
1:A:648:ASN:O	1:A:649:ILE:C	2.63	0.41
1:A:874:ASP:N	1:A:1058:VAL:HG23	2.36	0.41
1:A:891:ALA:O	1:A:892:ALA:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:967:ALA:HA	1:A:1044:TRP:CZ3	2.56	0.41
1:A:1118:VAL:O	1:A:1118:VAL:HG23	2.20	0.41
1:A:1135:ARG:HB2	1:A:1306:LEU:HD11	2.02	0.41
1:A:1434:ALA:O	1:A:1436:ILE:N	2.53	0.41
2:B:51:PHE:O	2:B:54:PHE:HB3	2.21	0.41
2:B:224:GLN:O	2:B:238:ALA:HA	2.20	0.41
2:B:467:GLY:N	2:B:475:SER:HB3	2.35	0.41
2:B:582:VAL:O	2:B:582:VAL:HG12	2.21	0.41
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.55	0.41
2:B:766:ARG:HH11	2:B:766:ARG:CG	2.31	0.41
2:B:797:TYR:O	10:J:1:MET:CG	2.69	0.41
3:C:43:THR:CG2	3:C:44:LEU:N	2.60	0.41
3:C:99:LEU:HA	3:C:119:VAL:O	2.20	0.41
4:D:176:GLU:HG2	4:D:197:SER:OG	2.20	0.41
5:E:14:ARG:HB3	5:E:141:VAL:O	2.19	0.41
5:E:112:TYR:CZ	5:E:136:ASN:HB2	2.55	0.41
5:E:112:TYR:HE1	5:E:136:ASN:HD22	1.68	0.41
5:E:164:LEU:HD11	5:E:211:TYR:CE1	2.56	0.41
5:E:165:LEU:HD21	5:E:175:LEU:HD11	2.03	0.41
5:E:172:GLU:O	5:E:175:LEU:HB2	2.21	0.41
5:E:190:LEU:HA	5:E:190:LEU:HD22	1.84	0.41
6:F:89:GLU:OE2	6:F:134:ILE:HG21	2.20	0.41
6:F:109:VAL:CG2	6:F:124:GLU:HG2	2.50	0.41
8:H:89:LEU:HB2	8:H:91:ASP:OD1	2.21	0.41
8:H:128:ASN:O	8:H:128:ASN:OD1	2.38	0.41
9:I:61:ASP:O	9:I:63:GLY:N	2.54	0.41
9:I:78:CYS:O	9:I:79:HIS:C	2.62	0.41
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.65	0.41
1:A:565:ILE:HD13	8:H:46:LEU:HD12	2.03	0.41
1:A:635:ARG:HH21	1:A:877:HIS:HA	1.84	0.41
1:A:913:LEU:HD21	1:A:915:SER:OG	2.20	0.41
1:A:1051:ALA:O	1:A:1052:GLN:C	2.63	0.41
1:A:1301:GLU:O	1:A:1302:PRO:O	2.39	0.41
2:B:120:ARG:CD	2:B:955:THR:HG21	2.50	0.41
2:B:266:ALA:C	2:B:268:THR:N	2.78	0.41
2:B:291:ILE:C	2:B:293:PRO:HD2	2.46	0.41
2:B:773:MET:C	2:B:775:LYS:N	2.77	0.41
2:B:840:ILE:HB	2:B:1011:ILE:HB	2.02	0.41
2:B:1020:ARG:HG3	2:B:1020:ARG:NH1	2.34	0.41
3:C:20:PHE:HE2	3:C:232:VAL:HG23	1.86	0.41
3:C:27:LEU:O	3:C:28:ALA:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:79:GLN:HG3	3:C:127:ARG:HD2	2.03	0.41
3:C:221:TYR:CD1	3:C:222:LYS:HG3	2.55	0.41
4:D:40:HIS:C	4:D:42:GLY:H	2.27	0.41
4:D:53:SER:OG	4:D:54:GLU:N	2.52	0.41
4:D:71:LYS:HA	4:D:74:GLN:HB2	2.02	0.41
4:D:130:LEU:CD1	4:D:142:LYS:HG3	2.51	0.41
5:E:38:PRO:HG2	5:E:41:ASP:OD2	2.21	0.41
5:E:94:LYS:HE2	5:E:98:ILE:HD11	2.02	0.41
6:F:96:THR:O	6:F:99:LEU:HB3	2.21	0.41
9:I:29:CYS:SG	9:I:31:THR:HB	2.61	0.41
9:I:111:THR:CG2	9:I:112:SER:H	2.33	0.41
10:J:14:VAL:O	10:J:14:VAL:CG1	2.68	0.41
10:J:44:TYR:HD2	10:J:44:TYR:N	2.03	0.41
10:J:56:LEU:HB3	10:J:60:PHE:CE2	2.55	0.41
1:A:298:PHE:O	1:A:301:ALA:HB3	2.21	0.41
1:A:351:THR:CG2	2:B:1103:ILE:HG13	2.51	0.41
1:A:371:ALA:HB2	1:A:462:VAL:HG13	2.03	0.41
1:A:383:TYR:N	1:A:383:TYR:HD2	2.15	0.41
1:A:409:SER:O	1:A:410:GLY:C	2.63	0.41
1:A:427:GLN:HB2	1:A:430:TRP:NE1	2.35	0.41
1:A:434:ARG:HG2	1:A:434:ARG:NH1	2.33	0.41
1:A:535:THR:HG23	1:A:575:LYS:HG2	2.02	0.41
1:A:544:ASP:CG	1:A:545:GLN:N	2.79	0.41
1:A:600:PRO:HG2	1:A:601:LYS:HG3	2.03	0.41
1:A:614:PHE:HB2	8:H:122:LEU:HD21	2.02	0.41
1:A:741:ASN:HD22	1:A:744:LYS:N	2.14	0.41
1:A:886:ILE:CG2	1:A:887:GLY:H	2.34	0.41
1:A:897:TYR:HD1	1:A:897:TYR:H	1.67	0.41
1:A:919:ILE:HD13	1:A:983:ILE:HD12	2.03	0.41
1:A:944:ARG:CZ	1:A:1298:TYR:CE1	3.04	0.41
1:A:1006:ILE:HD12	5:E:167:ARG:HB2	2.03	0.41
1:A:1026:LEU:HD23	1:A:1026:LEU:HA	1.72	0.41
1:A:1224:LEU:HD12	1:A:1241:ARG:O	2.21	0.41
1:A:1276:VAL:CG1	1:A:1277:GLU:N	2.82	0.41
2:B:114:PRO:O	2:B:116:GLU:N	2.54	0.41
2:B:221:ASN:HA	2:B:241:ARG:O	2.21	0.41
2:B:223:VAL:C	2:B:224:GLN:HG3	2.45	0.41
2:B:311:LEU:O	2:B:314:LEU:N	2.54	0.41
2:B:323:VAL:O	2:B:323:VAL:HG12	2.20	0.41
2:B:326:ASP:OD1	2:B:329:THR:N	2.47	0.41
2:B:332:ASP:OD1	2:B:348:ARG:CZ	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:334:ILE:HB	2:B:352:ALA:HB2	2.02	0.41
2:B:378:LEU:HD12	2:B:378:LEU:C	2.46	0.41
2:B:556:THR:O	2:B:557:PHE:C	2.64	0.41
2:B:571:PRO:HG2	2:B:572:HIS:CE1	2.56	0.41
2:B:619:ILE:HD13	9:I:64:SER:OG	2.21	0.41
2:B:620:ARG:NH2	9:I:86:PHE:CD2	2.89	0.41
2:B:752:ALA:O	2:B:753:ALA:C	2.63	0.41
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.21	0.41
2:B:918:ILE:HD12	2:B:935:ARG:NH1	2.35	0.41
2:B:999:MET:HG2	2:B:1007:VAL:CG2	2.50	0.41
2:B:999:MET:HB3	2:B:1007:VAL:HG21	2.03	0.41
2:B:1040:ASN:O	2:B:1041:GLU:C	2.64	0.41
3:C:101:LEU:HD13	3:C:118:LEU:CD2	2.31	0.41
3:C:106:GLU:O	3:C:107:SER:C	2.63	0.41
4:D:41:GLN:C	4:D:43:GLU:H	2.29	0.41
5:E:33:GLU:C	5:E:35:VAL:N	2.79	0.41
5:E:74:ASP:OD1	5:E:74:ASP:N	2.50	0.41
6:F:85:MET:HB3	6:F:155:LEU:HD11	2.02	0.41
6:F:90:ARG:CG	6:F:91:ALA:N	2.81	0.41
6:F:98:ALA:O	6:F:99:LEU:C	2.64	0.41
7:G:20:PRO:HG2	7:G:21:ARG:N	2.36	0.41
7:G:114:LEU:HD23	7:G:161:GLY:O	2.20	0.41
8:H:32:THR:CG2	8:H:33:GLN:N	2.80	0.41
8:H:91:ASP:C	8:H:93:TYR:N	2.78	0.41
9:I:82:GLU:HB3	9:I:104:LEU:CG	2.50	0.41
9:I:94:ASP:O	9:I:95:THR:O	2.38	0.41
10:J:2:ILE:HG23	10:J:3:VAL:H	1.85	0.41
11:K:51:LEU:HD13	11:K:59:ALA:HB3	2.03	0.41
12:L:29:TYR:HA	12:L:57:LEU:O	2.20	0.41
12:L:51:CYS:C	12:L:53:HIS:N	2.78	0.41
1:A:112:LYS:HG2	1:A:113:LEU:N	2.36	0.41
1:A:227:VAL:O	1:A:228:PHE:HD2	2.04	0.41
1:A:355:GLY:HA3	1:A:482:PHE:CZ	2.56	0.41
1:A:416:ARG:NH1	1:A:417:TYR:HE2	2.19	0.41
1:A:540:PHE:C	1:A:541:ILE:HG13	2.46	0.41
1:A:567:LYS:HG3	8:H:94:ASP:C	2.46	0.41
1:A:783:THR:HG21	1:A:815:PHE:CE2	2.56	0.41
1:A:818:MET:N	2:B:514:LEU:HD23	2.35	0.41
1:A:825:ILE:HD13	2:B:512:ARG:HB3	2.00	0.41
1:A:1224:LEU:HG	1:A:1226:VAL:HG23	2.02	0.41
1:A:1225:PHE:HZ	1:A:1227:ILE:HD11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1332:PHE:O	1:A:1333:ILE:C	2.64	0.41
1:A:1444:MET:HE1	6:F:135:ARG:NH2	2.35	0.41
2:B:98:THR:O	2:B:126:SER:CB	2.69	0.41
2:B:342:GLY:O	2:B:343:ILE:C	2.64	0.41
2:B:629:ASP:CG	2:B:630:ALA:N	2.79	0.41
2:B:662:MET:HA	2:B:665:GLU:HB2	2.03	0.41
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.87	0.41
2:B:778:MET:CE	2:B:853:SER:HB3	2.41	0.41
2:B:785:TYR:CE2	10:J:60:PHE:CE1	3.08	0.41
2:B:843:GLN:NE2	2:B:847:ASP:OD1	2.52	0.41
2:B:911:ILE:HG23	2:B:966:VAL:HG11	2.02	0.41
2:B:1060:ARG:NE	3:C:202:PRO:HG3	2.36	0.41
4:D:53:SER:O	4:D:57:LEU:HG	2.21	0.41
4:D:64:VAL:C	4:D:66:ARG:N	2.79	0.41
4:D:189:ASP:O	4:D:193:THR:CB	2.69	0.41
6:F:118:LEU:O	6:F:122:MET:HG3	2.20	0.41
8:H:82:PRO:HG2	8:H:83:GLN:H	1.86	0.41
10:J:45:CYS:O	10:J:48:ARG:NE	2.54	0.41
11:K:7:PHE:HA	11:K:10:PHE:HE2	1.86	0.41
11:K:83:PRO:O	11:K:84:LYS:C	2.61	0.41
1:A:25:GLU:O	1:A:26:GLU:C	2.63	0.40
1:A:130:ASP:O	1:A:132:LYS:N	2.54	0.40
1:A:317:LYS:HG2	2:B:471:LYS:HZ1	1.85	0.40
1:A:497:THR:O	1:A:500:GLU:HB2	2.21	0.40
1:A:584:ASN:HA	1:A:609:ASP:O	2.22	0.40
1:A:630:ILE:CD1	1:A:646:PHE:HZ	2.31	0.40
1:A:690:VAL:O	1:A:691:LEU:C	2.64	0.40
1:A:722:LEU:O	1:A:723:ASN:C	2.64	0.40
1:A:1191:TRP:HD1	1:A:1256:GLU:HB3	1.86	0.40
2:B:56:ASP:HB2	2:B:57:TYR:CD1	2.56	0.40
2:B:283:VAL:O	2:B:284:ILE:C	2.64	0.40
2:B:684:LEU:O	2:B:689:LEU:HB2	2.21	0.40
2:B:820:GLY:C	2:B:1091:TYR:CE1	3.00	0.40
2:B:863:GLU:O	2:B:961:LEU:HD22	2.21	0.40
2:B:1102:LYS:CA	2:B:1122:ARG:NH1	2.84	0.40
3:C:3:GLU:CG	11:K:104:ASN:HD21	2.33	0.40
4:D:57:LEU:CD1	4:D:160:VAL:HG21	2.44	0.40
4:D:123:LEU:HG	4:D:149:THR:CG2	2.51	0.40
6:F:117:PRO:HG2	6:F:118:LEU:H	1.86	0.40
11:K:68:PHE:N	11:K:68:PHE:CD2	2.89	0.40
1:A:51:GLY:HA2	1:A:56:PRO:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ILE:O	1:A:129:LYS:C	2.65	0.40
1:A:335:ARG:HA	1:A:335:ARG:HE	1.85	0.40
1:A:335:ARG:NH1	2:B:1202:LEU:CD2	2.79	0.40
1:A:573:SER:O	1:A:574:GLY:C	2.64	0.40
1:A:605:MET:HG2	1:A:621:THR:CG2	2.51	0.40
1:A:814:PHE:CD1	2:B:519:TRP:HE3	2.39	0.40
1:A:1050:GLU:HG3	1:A:1051:ALA:N	2.35	0.40
1:A:1127:ASP:OD1	1:A:1130:GLN:HB2	2.20	0.40
1:A:1170:ILE:HG22	1:A:1174:PHE:CE1	2.57	0.40
1:A:1375:MET:HE3	1:A:1384:VAL:CG2	2.51	0.40
2:B:258:LEU:O	2:B:259:TYR:O	2.39	0.40
2:B:782:LEU:HD12	2:B:788:ARG:HH11	1.86	0.40
2:B:814:PHE:C	2:B:816:GLU:H	2.29	0.40
2:B:847:ASP:CG	3:C:167:HIS:HD2	2.29	0.40
2:B:901:PRO:HA	2:B:949:VAL:HG12	2.03	0.40
3:C:20:PHE:CD1	3:C:20:PHE:C	2.98	0.40
3:C:114:TYR:HE2	10:J:19:GLU:OE2	2.05	0.40
5:E:207:ARG:NH1	5:E:207:ARG:CB	2.84	0.40
8:H:135:LEU:HD13	8:H:137:GLN:HE21	1.81	0.40
9:I:7:CYS:CB	9:I:14:LEU:HD21	2.31	0.40
12:L:32:ALA:HB2	12:L:55:ILE:CG1	2.32	0.40
1:A:33:ALA:O	1:A:83:HIS:CD2	2.74	0.40
1:A:91:PHE:HB3	1:A:96:ILE:CG1	2.51	0.40
1:A:320:ARG:HA	1:A:321:PRO:HD3	1.94	0.40
1:A:873:MET:HE3	1:A:957:PRO:HG3	2.03	0.40
1:A:1125:ALA:C	1:A:1127:ASP:H	2.29	0.40
1:A:1192:LEU:HD13	1:A:1239:ARG:NH1	2.36	0.40
1:A:1425:SER:O	1:A:1426:GLU:C	2.64	0.40
2:B:50:SER:OG	2:B:411:PRO:HD3	2.21	0.40
2:B:497:ARG:HH12	2:B:775:LYS:HE2	1.86	0.40
2:B:640:VAL:HG12	2:B:640:VAL:O	2.21	0.40
2:B:749:LEU:HB3	2:B:753:ALA:HB3	2.02	0.40
2:B:785:TYR:N	2:B:785:TYR:CD2	2.89	0.40
2:B:944:THR:HG21	2:B:1122:ARG:CZ	2.48	0.40
3:C:54:ASN:HB2	3:C:153:LEU:HD12	2.02	0.40
3:C:112:ASN:N	3:C:112:ASN:HD22	2.19	0.40
4:D:40:HIS:CE1	4:D:41:GLN:CD	3.00	0.40
4:D:56:ARG:HA	4:D:148:LEU:HD13	2.02	0.40
4:D:75:LYS:HE2	4:D:75:LYS:HB3	1.92	0.40
4:D:189:ASP:O	4:D:193:THR:HB	2.20	0.40
5:E:32:GLN:HG3	5:E:36:GLU:OE2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:42:PHE:O	5:E:43:LYS:C	2.64	0.40
5:E:161:LYS:O	5:E:164:LEU:N	2.54	0.40
5:E:190:LEU:HD13	5:E:191:LYS:H	1.87	0.40
7:G:127:PRO:CB	7:G:139:ILE:HD11	2.51	0.40
8:H:40:LEU:CB	8:H:123:MET:HE3	2.48	0.40
9:I:68:LEU:HB3	9:I:84:VAL:CG2	2.52	0.40
11:K:6:ARG:HA	11:K:6:ARG:HD3	1.90	0.40
1:A:72:GLU:CB	1:A:76:GLU:HG2	2.48	0.40
1:A:78:PRO:CB	2:B:1201:LYS:HE3	2.49	0.40
1:A:230:ARG:N	1:A:233:TRP:HE3	2.11	0.40
1:A:269:ILE:CG2	1:A:300:VAL:HG22	2.51	0.40
1:A:284:ALA:O	1:A:286:HIS:N	2.47	0.40
1:A:334:GLY:O	1:A:336:ILE:N	2.55	0.40
1:A:356:ASP:OD2	11:K:65:HIS:CE1	2.70	0.40
1:A:438:ASP:O	1:A:439:ASN:CB	2.64	0.40
1:A:473:SER:OG	1:A:646:PHE:HD2	2.04	0.40
1:A:514:PRO:HB2	1:A:875:ALA:HB3	2.04	0.40
1:A:546:VAL:HG21	1:A:572:TRP:CE3	2.57	0.40
1:A:593:GLU:C	1:A:595:THR:H	2.29	0.40
1:A:608:ILE:CB	1:A:613:ILE:HD11	2.48	0.40
1:A:688:LYS:HA	1:A:691:LEU:HB3	2.03	0.40
1:A:1051:ALA:C	1:A:1053:PHE:N	2.76	0.40
1:A:1067:LEU:HD12	1:A:1367:HIS:CE1	2.57	0.40
1:A:1142:THR:O	1:A:1145:SER:OG	2.39	0.40
1:A:1173:HIS:C	1:A:1174:PHE:HD1	2.29	0.40
2:B:276:ILE:HG22	2:B:278:GLN:O	2.21	0.40
2:B:349:ILE:O	2:B:353:LYS:HG3	2.22	0.40
2:B:582:VAL:CG2	2:B:626:ILE:HB	2.51	0.40
2:B:700:SER:C	2:B:701:ILE:CG2	2.93	0.40
2:B:1135:ARG:HG3	2:B:1147:LEU:HD11	2.03	0.40
2:B:1180:PHE:O	2:B:1181:GLU:C	2.62	0.40
3:C:187:LYS:C	3:C:189:THR:H	2.29	0.40
3:C:233:GLU:O	3:C:240:VAL:HG13	2.22	0.40
3:C:241:ASP:CG	3:C:242:GLN:N	2.79	0.40
3:C:242:GLN:O	3:C:244:VAL:N	2.54	0.40
4:D:7:THR:HG21	4:D:32:GLU:OE2	2.20	0.40
6:F:69:LEU:C	6:F:71:GLU:H	2.28	0.40
11:K:3:ALA:C	11:K:4:PRO:O	2.64	0.40
12:L:47:ARG:HG3	12:L:47:ARG:NH1	2.36	0.40
1:A:456:MET:HE1	1:A:521:MET:HE1	2.02	0.40
1:A:481:ASP:OD1	1:A:483:ASP:OD1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:GLN:O	1:A:526:ASP:C	2.63	0.40
1:A:577:ILE:O	1:A:578:LEU:C	2.65	0.40
1:A:590:ARG:HD2	1:A:605:MET:HB2	2.04	0.40
1:A:720:ARG:NH1	1:A:720:ARG:HB2	2.36	0.40
1:A:977:LYS:HB3	1:A:978:PRO:HD2	2.03	0.40
1:A:982:THR:C	1:A:984:LYS:N	2.75	0.40
1:A:1342:GLU:OE2	5:E:212:ARG:NH1	2.55	0.40
2:B:95:ILE:HA	2:B:129:PHE:O	2.22	0.40
2:B:167:ILE:N	2:B:167:ILE:CD1	2.82	0.40
2:B:167:ILE:CG2	2:B:453:ILE:HD12	2.40	0.40
2:B:170:LEU:HD12	2:B:171:PRO:N	2.37	0.40
2:B:195:CYS:HB2	2:B:784:ASN:OD1	2.22	0.40
2:B:253:THR:CG2	2:B:254:LEU:H	2.28	0.40
2:B:410:GLY:O	2:B:411:PRO:C	2.64	0.40
2:B:705:MET:HB3	2:B:706:GLN:H	1.70	0.40
2:B:791:THR:HG22	2:B:858:SER:HB2	2.04	0.40
2:B:797:TYR:HE1	2:B:971:THR:HG23	1.87	0.40
2:B:834:ASN:HB3	2:B:840:ILE:HG13	2.03	0.40
2:B:995:ARG:NH1	3:C:165:LYS:HG2	2.37	0.40
2:B:1006:ILE:HD13	10:J:44:TYR:CZ	2.56	0.40
3:C:111:THR:C	3:C:112:ASN:HD22	2.30	0.40
3:C:131:HIS:O	3:C:133:ILE:N	2.54	0.40
4:D:39:ASN:HD21	4:D:41:GLN:CG	2.33	0.40
4:D:130:LEU:HA	4:D:134:THR:OG1	2.22	0.40
11:K:89:ASN:O	11:K:90:ALA:C	2.64	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	1421/1733 (82%)	929 (65%)	311 (22%)	181 (13%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1111/1224 (91%)	712 (64%)	251 (23%)	148 (13%)	0	3
3	C	268/324 (83%)	165 (62%)	69 (26%)	34 (13%)	0	4
4	D	178/221 (80%)	125 (70%)	29 (16%)	24 (14%)	0	3
5	E	212/215 (99%)	145 (68%)	42 (20%)	25 (12%)	0	5
6	F	86/155 (56%)	60 (70%)	21 (24%)	5 (6%)	1	16
7	G	169/171 (99%)	133 (79%)	25 (15%)	11 (6%)	1	15
8	H	133/146 (91%)	78 (59%)	26 (20%)	29 (22%)	0	1
9	I	115/122 (94%)	72 (63%)	29 (25%)	14 (12%)	0	4
10	J	63/70 (90%)	35 (56%)	14 (22%)	14 (22%)	0	1
11	K	114/120 (95%)	80 (70%)	31 (27%)	3 (3%)	4	28
12	L	45/70 (64%)	18 (40%)	13 (29%)	14 (31%)	0	0
All	All	3915/4571 (86%)	2552 (65%)	861 (22%)	502 (13%)	0	4

All (502) 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	58	LEU
1	A	67	CYS
1	A	69	THR
1	A	73	GLY
1	A	76	GLU
1	A	84	ILE
1	A	130	ASP
1	A	154	SER
1	A	167	CYS
1	A	187	LYS
1	A	193	ASP
1	A	259	GLU
1	A	311	GLN
1	A	312	PRO
1	A	317	LYS
1	A	318	SER
1	A	385	ILE

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Mol	Chain	Res	Type
1	A	410	GLY
1	A	439	ASN
1	A	536	LEU
1	A	567	LYS
1	A	583	PRO
1	A	603	ASN
1	A	641	VAL
1	A	666	ILE
1	A	775	ILE
1	A	846	GLU
1	A	852	TYR
1	A	875	ALA
1	A	916	GLY
1	A	968	GLN
1	A	973	ILE
1	A	1002	GLY
1	A	1016	THR
1	A	1036	ARG
1	A	1114	PRO
1	A	1115	SER
1	A	1116	LEU
1	A	1120	LEU
1	A	1122	PRO
1	A	1167	GLU
1	A	1176	LEU
1	A	1177	LEU
1	A	1178	ASP
1	A	1202	MET
1	A	1212	VAL
1	A	1223	ASP
1	A	1233	ASP
1	A	1244	ARG
1	A	1255	GLU
1	A	1314	SER
1	A	1341	ILE
1	A	1361	SER
1	A	1365	TYR
1	A	1378	GLN
2	B	46	GLN
2	B	68	THR
2	B	108	VAL
2	B	124	TYR

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Mol	Chain	Res	Type
2	B	186	GLU
2	B	229	ALA
2	B	282	ILE
2	B	344	LYS
2	B	345	LYS
2	B	346	GLU
2	B	365	THR
2	B	367	LEU
2	B	391	ASP
2	B	468	GLU
2	B	469	GLN
2	B	509	ALA
2	B	511	PRO
2	B	543	SER
2	B	566	LEU
2	B	575	PRO
2	B	629	ASP
2	B	705	MET
2	B	707	PRO
2	B	708	GLU
2	B	712	PRO
2	B	723	VAL
2	B	751	VAL
2	B	855	PHE
2	B	867	GLY
2	B	879	ARG
2	B	882	THR
2	B	907	GLY
2	B	958	GLN
2	B	1041	GLU
2	B	1045	SER
2	B	1046	PRO
2	B	1069	PHE
2	B	1097	HIS
2	B	1156	ASP
2	B	1171	VAL
2	B	1175	LEU
2	B	1181	GLU
2	B	1183	LYS
3	C	6	PRO
3	C	56	THR
3	C	60	ASP

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Mol	Chain	Res	Type
3	C	77	ILE
3	C	90	ASP
3	C	110	THR
3	C	133	ILE
3	C	141	GLY
3	C	149	LYS
3	C	161	LYS
3	C	173	ALA
3	C	174	ALA
3	C	175	ALA
3	C	215	GLU
3	C	216	GLY
3	C	237	SER
3	C	269	LYS
4	D	3	VAL
4	D	12	ARG
4	D	19	GLU
4	D	52	LEU
4	D	169	SER
5	E	43	LYS
5	E	45	LYS
5	E	73	PRO
5	E	106	GLN
5	E	115	ASN
5	E	129	PRO
5	E	130	ALA
5	E	174	GLN
5	E	192	ARG
5	E	206	GLY
6	F	71	GLU
6	F	72	LYS
6	F	81	THR
6	F	139	PRO
7	G	2	PHE
7	G	120	THR
7	G	139	ILE
7	G	154	VAL
8	H	42	ILE
8	H	78	SER
8	H	84	ALA
8	H	87	ARG
8	H	92	ASP

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Mol	Chain	Res	Type
8	H	128	ASN
8	H	131	ASN
8	H	140	ALA
9	I	8	ARG
9	I	11	ASN
9	I	79	HIS
9	I	95	THR
9	I	106	CYS
10	J	2	ILE
10	J	64	ASN
11	K	14	GLU
11	K	79	GLU
12	L	40	LEU
12	L	42	ARG
12	L	50	ASP
12	L	55	ILE
12	L	59	ALA
12	L	60	ARG
1	A	57	ARG
1	A	70	CYS
1	A	74	MET
1	A	93	VAL
1	A	96	ILE
1	A	131	SER
1	A	148	CYS
1	A	281	HIS
1	A	283	GLY
1	A	313	GLN
1	A	332	LYS
1	A	399	HIS
1	A	419	LYS
1	A	556	TRP
1	A	591	PHE
1	A	600	PRO
1	A	619	LYS
1	A	706	HIS
1	A	719	VAL
1	A	752	LYS
1	A	780	VAL
1	A	789	LYS
1	A	871	ASP
1	A	922	ASP

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Mol	Chain	Res	Type
1	A	969	GLN
1	A	972	HIS
1	A	1050	GLU
1	A	1064	VAL
1	A	1140	HIS
1	A	1206	ASP
1	A	1221	LYS
1	A	1279	ILE
1	A	1302	PRO
1	A	1316	VAL
1	A	1393	ASN
1	A	1437	GLY
2	B	21	GLU
2	B	45	SER
2	B	48	LEU
2	B	56	ASP
2	B	65	GLU
2	B	134	LYS
2	B	135	ARG
2	B	257	LYS
2	B	259	TYR
2	B	277	LYS
2	B	278	GLN
2	B	312	GLU
2	B	327	ARG
2	B	341	LEU
2	B	364	ILE
2	B	450	ALA
2	B	470	LYS
2	B	483	LEU
2	B	506	GLY
2	B	512	ARG
2	B	577	ALA
2	B	709	ASP
2	B	727	LYS
2	B	752	ALA
2	B	754	SER
2	B	894	ASP
2	B	943	SER
2	B	951	GLN
2	B	956	THR
2	B	1075	GLY

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Mol	Chain	Res	Type
2	B	1099	VAL
2	B	1100	ASP
2	B	1131	GLY
2	B	1167	GLY
2	B	1184	GLY
2	B	1223	ASP
3	C	61	GLU
3	C	78	GLU
3	C	128	ASN
3	C	240	VAL
4	D	20	GLU
4	D	47	LEU
4	D	119	ARG
4	D	131	GLU
4	D	192	LYS
4	D	218	GLU
4	D	220	LEU
5	E	3	GLN
5	E	76	GLY
5	E	97	VAL
5	E	121	MET
6	F	150	GLU
7	G	63	PRO
7	G	64	THR
7	G	114	LEU
8	H	18	GLY
8	H	63	LEU
8	H	81	PRO
8	H	82	PRO
8	H	90	ALA
8	H	119	GLY
8	H	137	GLN
9	I	2	THR
9	I	3	THR
9	I	32	CYS
9	I	56	ALA
10	J	17	LYS
10	J	24	LEU
10	J	32	GLU
11	K	15	GLY
12	L	28	LYS
12	L	37	LYS

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Mol	Chain	Res	Type
12	L	53	HIS
12	L	56	LEU
1	A	5	GLN
1	A	38	PRO
1	A	42	ASP
1	A	77	CYS
1	A	86	LEU
1	A	128	ILE
1	A	222	LEU
1	A	232	GLU
1	A	287	HIS
1	A	423	ASP
1	A	424	ILE
1	A	568	PRO
1	A	601	LYS
1	A	604	GLY
1	A	661	GLY
1	A	847	ASP
1	A	885	THR
1	A	979	SER
1	A	1067	LEU
1	A	1105	LEU
1	A	1124	HIS
1	A	1127	ASP
1	A	1165	GLU
1	A	1229	SER
1	A	1331	SER
1	A	1405	THR
1	A	1450	LEU
2	B	37	PHE
2	B	100	PRO
2	B	184	ALA
2	B	265	SER
2	B	295	GLY
2	B	304	ASP
2	B	333	PHE
2	B	343	ILE
2	B	368	GLU
2	B	409	ALA
2	B	559	SER
2	B	591	ARG
2	B	711	GLU

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Mol	Chain	Res	Type
2	B	746	SER
2	B	815	ARG
2	B	848	ARG
2	B	878	GLN
2	B	892	LYS
2	B	909	ASP
2	B	1003	ALA
2	B	1035	ALA
2	B	1082	MET
2	B	1126	GLY
2	B	1155	SER
2	B	1157	ALA
2	B	1176	ASN
3	C	132	PRO
3	C	142	VAL
3	C	213	PRO
4	D	21	GLU
4	D	25	ALA
4	D	32	GLU
4	D	59	ILE
4	D	139	LYS
4	D	168	LYS
4	D	198	LEU
4	D	199	ASN
5	E	48	ASP
5	E	74	ASP
5	E	93	MET
5	E	104	ASN
5	E	173	SER
7	G	141	SER
8	H	2	SER
8	H	107	VAL
8	H	108	SER
8	H	109	LYS
8	H	110	ASP
9	I	47	GLU
10	J	6	ARG
10	J	18	TRP
1	A	55	ASP
1	A	59	GLY
1	A	63	ARG
1	A	126	LEU

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Mol	Chain	Res	Type
1	A	164	ARG
1	A	190	ALA
1	A	196	GLU
1	A	257	ARG
1	A	286	HIS
1	A	300	VAL
1	A	322	VAL
1	A	330	LYS
1	A	409	SER
1	A	525	GLN
1	A	535	THR
1	A	557	ASP
1	A	592	ASP
1	A	738	LYS
1	A	765	VAL
1	A	854	ASN
1	A	1005	GLU
1	A	1068	ALA
1	A	1240	CYS
1	A	1242	VAL
1	A	1366	ARG
1	A	1377	THR
1	A	1399	ARG
1	A	1402	PHE
2	B	41	LYS
2	B	115	GLN
2	B	131	ASP
2	B	267	ARG
2	B	531	GLN
2	B	642	ASP
2	B	688	GLY
2	B	699	GLU
2	B	868	MET
2	B	881	ASN
2	B	891	ASP
2	B	1017	ILE
3	C	108	GLU
3	C	191	TYR
3	C	214	ASN
4	D	4	SER
4	D	13	ARG
4	D	118	THR

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Mol	Chain	Res	Type
5	E	122	LYS
5	E	179	GLN
7	G	118	ASP
8	H	17	PRO
8	H	41	ASP
8	H	52	GLN
8	H	83	GLN
9	I	93	LYS
9	I	107	SER
10	J	9	SER
10	J	14	VAL
10	J	33	GLY
12	L	35	SER
1	A	35	ILE
1	A	52	GLY
1	A	113	LEU
1	A	234	MET
1	A	294	SER
1	A	917	SER
1	A	958	VAL
1	A	986	ILE
1	A	1006	ILE
1	A	1133	LEU
1	A	1211	GLN
2	B	24	PRO
2	B	49	ASP
2	B	171	PRO
2	B	283	VAL
2	B	311	LEU
2	B	456	GLY
2	B	480	SER
2	B	510	LYS
2	B	579	ARG
2	B	594	ALA
2	B	643	ASP
2	B	655	LYS
2	B	793	ALA
2	B	1042	GLY
3	C	11	ARG
4	D	191	ALA
5	E	56	LYS
5	E	148	GLU

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Mol	Chain	Res	Type
7	G	20	PRO
8	H	21	ASN
8	H	132	LEU
10	J	13	VAL
10	J	42	LYS
12	L	36	SER
12	L	46	VAL
1	A	24	PRO
1	A	170	THR
1	A	314	ALA
1	A	517	ASN
1	A	652	VAL
1	A	704	ALA
1	A	818	MET
1	A	845	LEU
1	A	1454	MET
2	B	67	SER
2	B	219	ALA
2	B	903	VAL
2	B	1080	LYS
2	B	1214	PRO
3	C	3	GLU
3	C	36	VAL
3	C	89	GLU
3	C	218	PRO
10	J	55	ASP
12	L	25	ALA
1	A	231	PRO
1	A	244	PRO
1	A	910	PRO
2	B	436	VAL
2	B	478	GLY
2	B	503	GLY
3	C	25	VAL
8	H	120	GLY
1	A	258	GLY
2	B	315	LYS
2	B	780	VAL
9	I	62	ILE
1	A	250	ILE
2	B	305	VAL
2	B	636	PRO

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Mol	Chain	Res	Type
2	B	744	HIS
5	E	86	PRO
7	G	92	VAL
9	I	57	GLY
10	J	57	ILE
1	A	51	GLY
1	A	197	PRO
1	A	718	VAL
1	A	1162	VAL
2	B	114	PRO
2	B	464	GLY
2	B	658	ILE
5	E	53	PRO
8	H	12	VAL
1	A	78	PRO
2	B	334	ILE
3	C	10	ILE
8	H	44	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1249/1520 (82%)	1125 (90%)	124 (10%)	7	28
2	B	974/1061 (92%)	880 (90%)	94 (10%)	8	28
3	C	238/280 (85%)	217 (91%)	21 (9%)	9	32
4	D	164/200 (82%)	143 (87%)	21 (13%)	4	20
5	E	196/197 (100%)	178 (91%)	18 (9%)	8	30
6	F	78/137 (57%)	68 (87%)	10 (13%)	4	20
7	G	152/152 (100%)	142 (93%)	10 (7%)	15	41
8	H	121/128 (94%)	112 (93%)	9 (7%)	13	38
9	I	111/116 (96%)	103 (93%)	8 (7%)	13	39
10	J	60/65 (92%)	55 (92%)	5 (8%)	10	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	99/102 (97%)	89 (90%)	10 (10%)	7	27
12	L	41/57 (72%)	33 (80%)	8 (20%)	1	9
All	All	3483/4015 (87%)	3145 (90%)	338 (10%)	8	28

All (338) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	34	LYS
1	A	37	PHE
1	A	38	PRO
1	A	41	MET
1	A	54	ASN
1	A	69	THR
1	A	70	CYS
1	A	85	ASP
1	A	93	VAL
1	A	157	ASP
1	A	200	ARG
1	A	231	PRO
1	A	236	LEU
1	A	245	PRO
1	A	262	LEU
1	A	265	LYS
1	A	275	SER
1	A	295	LEU
1	A	307	ASP
1	A	312	PRO
1	A	320	ARG
1	A	322	VAL
1	A	326	ARG
1	A	335	ARG
1	A	345	VAL
1	A	352	VAL
1	A	375	THR
1	A	379	VAL
1	A	385	ILE
1	A	406	ILE
1	A	407	ARG
1	A	408	ASP
1	A	419	LYS

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Mol	Chain	Res	Type
1	A	438	ASP
1	A	442	VAL
1	A	443	LEU
1	A	445	ASN
1	A	449	SER
1	A	450	LEU
1	A	451	HIS
1	A	456	MET
1	A	462	VAL
1	A	466	SER
1	A	481	ASP
1	A	489	LEU
1	A	493	GLN
1	A	503	GLN
1	A	511	ILE
1	A	518	LYS
1	A	540	PHE
1	A	542	GLU
1	A	552	TRP
1	A	557	ASP
1	A	590	ARG
1	A	618	GLU
1	A	629	LEU
1	A	634	THR
1	A	635	ARG
1	A	666	ILE
1	A	720	ARG
1	A	758	ILE
1	A	779	PHE
1	A	821	ARG
1	A	825	ILE
1	A	830	LYS
1	A	833	GLU
1	A	842	VAL
1	A	854	ASN
1	A	858	ASN
1	A	918	GLU
1	A	920	LEU
1	A	929	LEU
1	A	942	PHE
1	A	947	PHE
1	A	948	VAL

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Mol	Chain	Res	Type
1	A	949	ASP
1	A	965	GLN
1	A	976	THR
1	A	995	GLU
1	A	1001	ARG
1	A	1017	LEU
1	A	1019	CYS
1	A	1029	ARG
1	A	1037	LEU
1	A	1067	LEU
1	A	1077	THR
1	A	1111	MET
1	A	1120	LEU
1	A	1122	PRO
1	A	1124	HIS
1	A	1163	ILE
1	A	1166	ASP
1	A	1170	ILE
1	A	1178	ASP
1	A	1206	ASP
1	A	1233	ASP
1	A	1240	CYS
1	A	1245	PRO
1	A	1255	GLU
1	A	1257	ASP
1	A	1259	MET
1	A	1260	LEU
1	A	1264	GLU
1	A	1271	ILE
1	A	1280	GLU
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1300	LYS
1	A	1308	THR
1	A	1314	SER
1	A	1325	THR
1	A	1332	PHE
1	A	1333	ILE
1	A	1336	MET
1	A	1359	ASP
1	A	1389	PHE

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Mol	Chain	Res	Type
1	A	1393	ASN
1	A	1394	THR
1	A	1400	CYS
1	A	1443	VAL
1	A	1445	ILE
1	A	1454	MET
2	B	20	ASP
2	B	57	TYR
2	B	70	ILE
2	B	100	PRO
2	B	164	LYS
2	B	167	ILE
2	B	169	ARG
2	B	174	LEU
2	B	175	ARG
2	B	180	TYR
2	B	194	GLU
2	B	217	ARG
2	B	244	LEU
2	B	268	THR
2	B	272	THR
2	B	294	ASP
2	B	324	ILE
2	B	332	ASP
2	B	364	ILE
2	B	365	THR
2	B	371	GLU
2	B	378	LEU
2	B	393	LYS
2	B	396	ASP
2	B	428	ILE
2	B	429	PHE
2	B	465	ASN
2	B	473	MET
2	B	485	ARG
2	B	502	ILE
2	B	510	LYS
2	B	516	ASN
2	B	547	VAL
2	B	555	ILE
2	B	563	MET
2	B	570	VAL

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Mol	Chain	Res	Type
2	B	572	HIS
2	B	582	VAL
2	B	591	ARG
2	B	597	MET
2	B	603	LEU
2	B	609	ILE
2	B	615	MET
2	B	616	ILE
2	B	628	THR
2	B	636	PRO
2	B	680	THR
2	B	685	LEU
2	B	694	ASP
2	B	737	THR
2	B	742	GLU
2	B	743	ILE
2	B	748	ILE
2	B	766	ARG
2	B	776	GLN
2	B	785	TYR
2	B	790	ASP
2	B	811	TYR
2	B	830	TYR
2	B	839	MET
2	B	854	LEU
2	B	860	MET
2	B	878	GLN
2	B	879	ARG
2	B	895	ASP
2	B	901	PRO
2	B	909	ASP
2	B	918	ILE
2	B	944	THR
2	B	955	THR
2	B	999	MET
2	B	1046	PRO
2	B	1047	PHE
2	B	1050	ILE
2	B	1069	PHE
2	B	1077	THR
2	B	1084	GLN
2	B	1095	LEU

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Mol	Chain	Res	Type
2	B	1098	MET
2	B	1103	ILE
2	B	1113	VAL
2	B	1150	ARG
2	B	1151	LEU
2	B	1159	ARG
2	B	1170	THR
2	B	1181	GLU
2	B	1182	CYS
2	B	1189	ILE
2	B	1196	ILE
2	B	1202	LEU
2	B	1207	LEU
2	B	1218	THR
2	B	1221	SER
2	B	1223	ASP
3	C	1	MET
3	C	29	MET
3	C	35	ARG
3	C	38	ILE
3	C	54	ASN
3	C	56	THR
3	C	58	LEU
3	C	77	ILE
3	C	99	LEU
3	C	106	GLU
3	C	138	GLU
3	C	147	LEU
3	C	166	GLU
3	C	193	TYR
3	C	209	TYR
3	C	226	ASP
3	C	233	GLU
3	C	235	VAL
3	C	240	VAL
3	C	250	THR
3	C	269	LYS
4	D	13	ARG
4	D	15	LEU
4	D	22	GLU
4	D	32	GLU
4	D	37	GLN

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Mol	Chain	Res	Type
4	D	40	HIS
4	D	47	LEU
4	D	63	LEU
4	D	70	PHE
4	D	118	THR
4	D	127	ASP
4	D	137	ASN
4	D	148	LEU
4	D	149	THR
4	D	189	ASP
4	D	192	LYS
4	D	211	LEU
4	D	214	LEU
4	D	215	SER
4	D	219	THR
4	D	221	TYR
5	E	17	ARG
5	E	22	MET
5	E	31	THR
5	E	52	ARG
5	E	60	PHE
5	E	74	ASP
5	E	86	PRO
5	E	104	ASN
5	E	114	ASN
5	E	131	THR
5	E	132	ILE
5	E	149	LEU
5	E	169	ARG
5	E	172	GLU
5	E	173	SER
5	E	175	LEU
5	E	178	ILE
5	E	190	LEU
6	F	71	GLU
6	F	72	LYS
6	F	79	ARG
6	F	99	LEU
6	F	111	LEU
6	F	118	LEU
6	F	122	MET
6	F	148	VAL

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Mol	Chain	Res	Type
6	F	151	LEU
6	F	152	ILE
7	G	1	MET
7	G	13	LEU
7	G	17	PHE
7	G	21	ARG
7	G	49	LEU
7	G	52	ASP
7	G	73	LYS
7	G	74	TYR
7	G	79	PHE
7	G	171	ILE
8	H	17	PRO
8	H	42	ILE
8	H	63	LEU
8	H	64	ASN
8	H	86	ASP
8	H	88	SER
8	H	89	LEU
8	H	102	TYR
8	H	110	ASP
9	I	4	PHE
9	I	6	PHE
9	I	8	ARG
9	I	85	PHE
9	I	86	PHE
9	I	94	ASP
9	I	100	PHE
9	I	101	PHE
10	J	22	LEU
10	J	23	ASN
10	J	43	ARG
10	J	44	TYR
10	J	46	CYS
11	K	5	ASP
11	K	6	ARG
11	K	10	PHE
11	K	25	THR
11	K	41	THR
11	K	47	ARG
11	K	50	LEU
11	K	61	TYR

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Mol	Chain	Res	Type
11	K	111	LEU
11	K	114	LEU
12	L	27	LEU
12	L	33	GLU
12	L	34	CYS
12	L	54	ARG
12	L	55	ILE
12	L	64	LEU
12	L	65	VAL
12	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (132) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	83	HIS
1	A	92	HIS
1	A	109	HIS
1	A	169	ASN
1	A	225	ASN
1	A	253	ASN
1	A	256	GLN
1	A	299	HIS
1	A	306	ASN
1	A	339	ASN
1	A	358	ASN
1	A	399	HIS
1	A	445	ASN
1	A	447	GLN
1	A	631	HIS
1	A	659	HIS
1	A	700	ASN
1	A	723	ASN
1	A	736	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	767	GLN
1	A	768	GLN
1	A	786	HIS
1	A	851	HIS
1	A	858	ASN

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Mol	Chain	Res	Type
1	A	903	ASN
1	A	926	GLN
1	A	959	ASN
1	A	969	GLN
1	A	1004	ASN
1	A	1009	ASN
1	A	1070	GLN
1	A	1106	ASN
1	A	1130	GLN
1	A	1140	HIS
1	A	1188	GLN
1	A	1203	ASN
1	A	1278	ASN
1	A	1364	ASN
1	A	1393	ASN
1	A	1427	ASN
1	A	1432	GLN
2	B	46	GLN
2	B	52	ASN
2	B	60	GLN
2	B	178	ASN
2	B	224	GLN
2	B	236	HIS
2	B	366	GLN
2	B	383	ASN
2	B	415	GLN
2	B	465	ASN
2	B	484	ASN
2	B	499	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	587	HIS
2	B	686	ASN
2	B	706	GLN
2	B	744	HIS
2	B	763	GLN
2	B	786	ASN
2	B	794	ASN
2	B	821	GLN
2	B	842	ASN

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Mol	Chain	Res	Type
2	B	862	GLN
2	B	878	GLN
2	B	951	GLN
2	B	975	GLN
2	B	1015	HIS
2	B	1040	ASN
2	B	1065	GLN
2	B	1076	HIS
2	B	1084	GLN
2	B	1117	GLN
2	B	1141	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	102	GLN
3	C	112	ASN
3	C	140	ASN
3	C	167	HIS
3	C	231	ASN
4	D	2	ASN
4	D	9	GLN
4	D	31	GLN
4	D	39	ASN
4	D	40	HIS
4	D	74	GLN
4	D	132	GLN
4	D	137	ASN
4	D	143	ASN
4	D	179	GLN
4	D	216	ASN
5	E	101	GLN
5	E	104	ASN
5	E	114	ASN
5	E	147	HIS
6	F	100	GLN
7	G	53	ASN
7	G	97	HIS
7	G	122	ASN
7	G	126	ASN

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Mol	Chain	Res	Type
7	G	158	HIS
8	H	33	GLN
8	H	35	GLN
8	H	131	ASN
8	H	134	ASN
8	H	137	GLN
9	I	12	ASN
9	I	79	HIS
9	I	89	GLN
9	I	90	GLN
9	I	108	HIS
9	I	114	GLN
10	J	64	ASN
11	K	44	ASN
11	K	52	ASN
11	K	65	HIS
11	K	76	GLN
11	K	104	ASN
11	K	110	ASN
12	L	53	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/16 (56%)	2 (22%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	10	A
15	P	11	U

There are no RNA pucker outliers to report.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	8OG	T	19	15,13	22,25,26	1.08	1 (4%)	26,37,40	1.59	3 (11%)
13	BRU	T	23	15,13	18,21,22	3.95	1 (5%)	25,30,33	0.99	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	8OG	T	19	15,13	-	2/7/21/22	0/3/3/3
13	BRU	T	23	15,13	-	1/7/21/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	23	BRU	BR-C5	-16.71	1.49	1.88
13	T	19	8OG	C8-N7	-4.16	1.30	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	19	8OG	N7-C8-N9	5.90	113.18	106.61
13	T	19	8OG	C5-N7-C8	-3.83	104.19	109.47
13	T	19	8OG	C4-C5-N7	2.60	110.81	106.06
13	T	23	BRU	C6-C5-C4	-2.58	118.05	120.67
13	T	23	BRU	O3'-C3'-C2'	-2.22	103.15	110.88

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	T	19	8OG	O4'-C4'-C5'-O5'
13	T	19	8OG	C3'-C4'-C5'-O5'
13	T	23	BRU	C2'-C1'-N1-C2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T	19	8OG	3	0
13	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1429/1733 (82%)	0.13	24 (1%) 69 48	73, 132, 187, 200	0
2	B	1125/1224 (91%)	0.36	60 (5%) 32 25	79, 146, 196, 200	0
3	C	270/324 (83%)	0.11	1 (0%) 88 74	92, 133, 183, 200	0
4	D	182/221 (82%)	0.37	12 (6%) 24 21	122, 160, 195, 200	0
5	E	214/215 (99%)	0.16	1 (0%) 87 72	111, 170, 198, 200	0
6	F	88/155 (56%)	0.04	1 (1%) 78 57	77, 110, 145, 175	0
7	G	171/171 (100%)	0.19	2 (1%) 76 55	113, 140, 176, 182	0
8	H	137/146 (93%)	0.70	15 (10%) 10 13	147, 178, 198, 200	0
9	I	117/122 (95%)	0.40	6 (5%) 33 26	126, 178, 197, 200	0
10	J	65/70 (92%)	0.17	0 100 100	112, 129, 171, 180	0
11	K	116/120 (96%)	-0.00	1 (0%) 81 62	96, 135, 160, 199	0
12	L	47/70 (67%)	0.55	1 (2%) 63 44	128, 169, 190, 200	0
13	T	18/26 (69%)	1.22	2 (11%) 10 13	182, 200, 200, 200	0
14	N	11/12 (91%)	1.53	3 (27%) 1 3	196, 200, 200, 200	0
15	P	10/16 (62%)	1.10	2 (20%) 3 5	199, 200, 200, 200	0
All	All	4000/4625 (86%)	0.25	131 (3%) 49 34	73, 142, 196, 200	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	1	MET	5.5
2	B	510	LYS	5.1
9	I	1	MET	4.8
2	B	310	MET	4.5
2	B	70	ILE	4.5
2	B	471	LYS	4.4
1	A	2	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	715	ALA	4.2
2	B	504	ARG	3.9
11	K	116	ALA	3.9
2	B	734	HIS	3.8
8	H	140	ALA	3.7
12	L	27	LEU	3.7
4	D	13	ARG	3.6
8	H	119	GLY	3.6
2	B	164	LYS	3.5
1	A	252	PHE	3.5
8	H	142	LEU	3.5
2	B	964	VAL	3.4
9	I	93	LYS	3.4
1	A	1081	LEU	3.4
2	B	468	GLU	3.4
1	A	1080	THR	3.3
1	A	480	ALA	3.3
2	B	436	VAL	3.3
8	H	1	MET	3.3
2	B	266	ALA	3.2
1	A	51	GLY	3.2
2	B	392	ARG	3.2
2	B	709	ASP	3.2
8	H	29	ALA	3.1
15	P	2	U	3.1
1	A	250	ILE	3.1
2	B	134	LYS	3.1
1	A	4	GLN	3.0
2	B	723	VAL	3.0
2	B	138	GLU	3.0
15	P	11	U	3.0
2	B	646	LEU	2.9
8	H	84	ALA	2.9
2	B	503	GLY	2.8
2	B	736	THR	2.8
2	B	470	LYS	2.8
2	B	933	SER	2.8
14	N	11	DC	2.8
2	B	446	LEU	2.8
1	A	1217	LYS	2.8
2	B	860	MET	2.7
3	C	222	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
9	I	4	PHE	2.7
2	B	888	GLY	2.7
2	B	726	ALA	2.7
1	A	1246	LYS	2.7
4	D	3	VAL	2.7
2	B	341	LEU	2.7
13	T	26	DT	2.7
1	A	975	HIS	2.6
2	B	508	LEU	2.6
1	A	1254	ALA	2.6
8	H	57	VAL	2.6
2	B	507	LYS	2.6
1	A	309	ALA	2.6
7	G	51	TYR	2.6
8	H	116	TYR	2.6
8	H	19	ARG	2.6
2	B	887	HIS	2.6
1	A	1187	GLN	2.6
2	B	1224	PHE	2.6
1	A	251	SER	2.5
4	D	137	ASN	2.5
6	F	72	LYS	2.5
2	B	648	HIS	2.5
2	B	245	GLU	2.5
2	B	735	ALA	2.5
8	H	132	LEU	2.5
2	B	250	PHE	2.5
2	B	881	ASN	2.5
2	B	509	ALA	2.5
4	D	26	THR	2.4
2	B	502	ILE	2.4
1	A	310	GLY	2.4
2	B	486	TYR	2.4
4	D	168	LYS	2.4
2	B	1222	ARG	2.4
8	H	144	ILE	2.4
1	A	270	LEU	2.4
1	A	1177	LEU	2.4
13	T	7	DC	2.4
1	A	792	TYR	2.4
2	B	713	ALA	2.4
4	D	180	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
9	I	13	MET	2.3
2	B	561	TRP	2.3
2	B	1173	ALA	2.3
2	B	216	GLU	2.3
7	G	113	HIS	2.3
1	A	830	LYS	2.3
9	I	117	LYS	2.3
4	D	4	SER	2.3
1	A	176	LYS	2.3
2	B	474	SER	2.2
8	H	76	THR	2.2
1	A	68	GLN	2.2
4	D	76	LYS	2.2
2	B	241	ARG	2.2
2	B	312	GLU	2.2
2	B	732	SER	2.2
2	B	505	ASP	2.2
2	B	712	PRO	2.2
1	A	893	PHE	2.2
2	B	92	PHE	2.2
4	D	18	VAL	2.2
14	N	8	DG	2.2
5	E	152	LYS	2.2
9	I	97	MET	2.2
2	B	246	LYS	2.1
2	B	472	ALA	2.1
2	B	311	LEU	2.1
4	D	2	ASN	2.1
2	B	90	ILE	2.1
2	B	301	ILE	2.1
4	D	17	LYS	2.1
2	B	473	MET	2.1
14	N	9	DA	2.1
8	H	143	LEU	2.1
2	B	469	GLN	2.1
1	A	69	THR	2.0
2	B	573	GLN	2.0
8	H	136	LYS	2.0
2	B	466	TRP	2.0
8	H	78	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
13	BRU	T	23	20/21	0.70	0.16	198,199,200,200	0
13	8OG	T	19	23/24	0.91	0.10	186,193,198,199	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
16	MG	A	2458	1/1	0.92	0.09	200,200,200,200	0
17	ZN	I	1122	1/1	0.98	0.04	198,198,198,198	0
17	ZN	A	2456	1/1	0.99	0.03	150,150,150,150	0
17	ZN	J	1066	1/1	0.99	0.05	135,135,135,135	0
17	ZN	L	1071	1/1	0.99	0.02	158,158,158,158	0
17	ZN	I	1121	1/1	1.00	0.03	140,140,140,140	0
17	ZN	A	2457	1/1	1.00	0.04	107,107,107,107	0
17	ZN	B	2225	1/1	1.00	0.05	106,106,106,106	0
17	ZN	C	1269	1/1	1.00	0.05	101,101,101,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.