



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:01 AM UTC

PDB ID : 2R92 / pdb_00002r92
Title : Elongation complex of RNA polymerase II with artificial RdRP scaffold
Authors : Lehmann, E.; Brueckner, F.; Cramer, P.
Deposited on : 2007-09-12
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

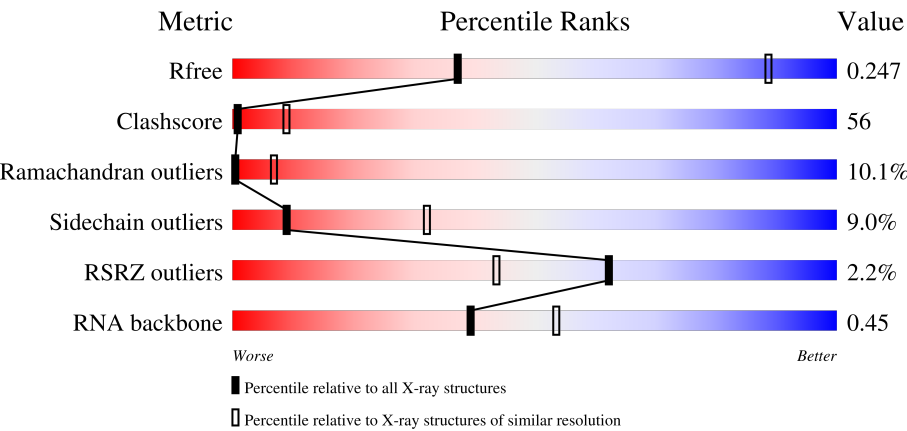
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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.



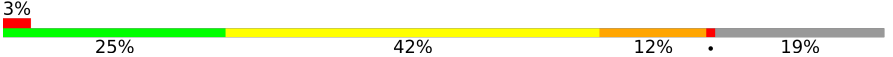
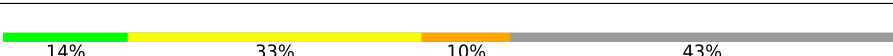
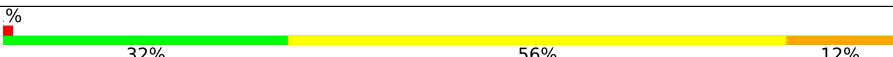
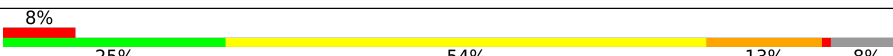
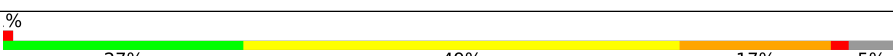
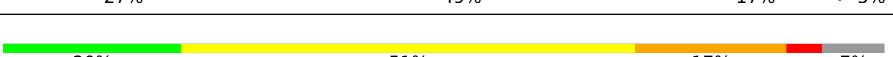
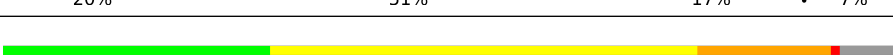
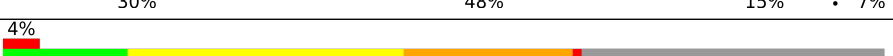
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)
RNA backbone	3983	1007 (4.50-3.10)

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	P	16	25% 12% 38% 6% 44%
2	T	17	47% 6% 29% 18% 6% 41%
3	A	1733	% 25% 44% 12% • 18%
4	B	1224	2% 24% 53% 13% • 9%

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Mol	Chain	Length	Quality of chain
5	C	318	
6	D	221	
7	E	215	
8	F	155	
9	G	171	
10	H	146	
11	I	122	
12	J	70	
13	K	120	
14	L	70	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 31611 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 RNA chain called RNA (5'-R(*UP*GP*CP*AP*UP*AP*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	9	Total	C	N	O	P	0	0	0
			192	87	39	58	8			

- Molecule 2 is a RNA chain called RNA (5'-R(*CP*UP*UP*GP*AP*CP*GP*CP*CP*UP*GP*GP*UP*CP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	10	Total	C	N	O	P	0	0	0
			208	94	36	69	9			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1422	Total	C	N	O	S	0	0	0
			11194	7054	1959	2119	62			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	1112	Total	C	N	O	S	0	0	0
			8841	5596	1550	1640	55			

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB4.

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

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	88	Total	C	N	O	S	0	0	0
			712	455	120	134	3			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	135	Total	C	N	O	S	0	0	0
			1084	683	183	214	4			

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	116	Total	C	N	O	S	0	0	0
			944	581	172	181	10			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	112	Total	C	N	O	S	0	0	0
			904	580	154	168	2			

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

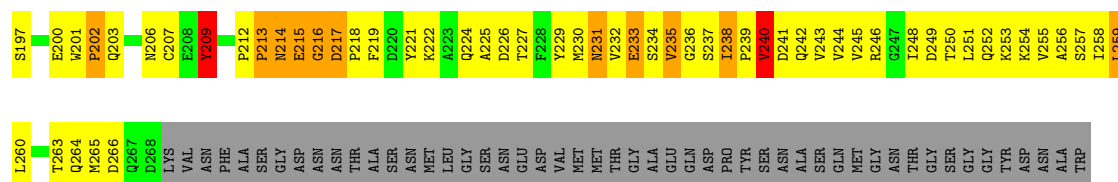
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	2	Total	Zn	0	0
			2	2		
15	B	1	Total	Zn	0	0
			1	1		
15	C	1	Total	Zn	0	0
			1	1		
15	I	2	Total	Zn	0	0
			2	2		
15	J	1	Total	Zn	0	0
			1	1		
15	L	1	Total	Zn	0	0
			1	1		

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

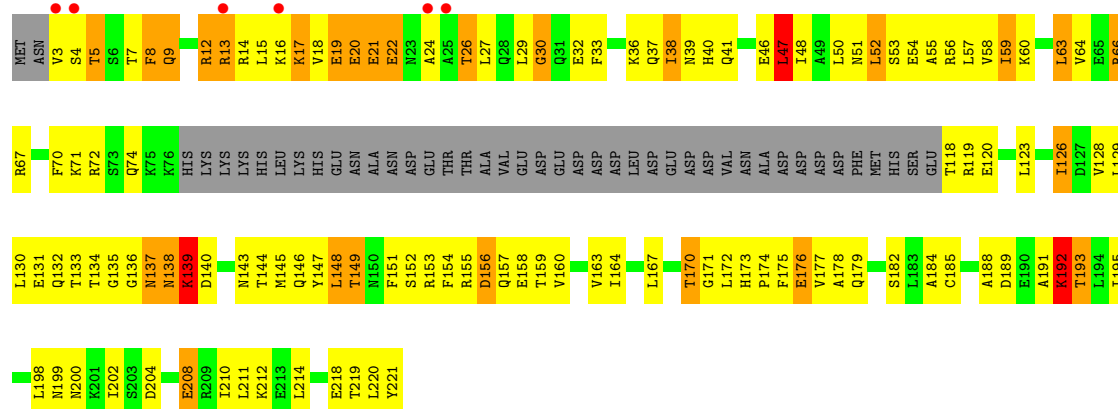
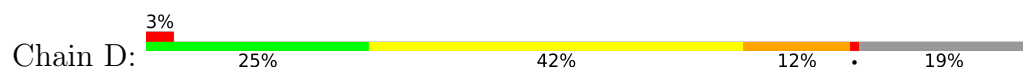
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		



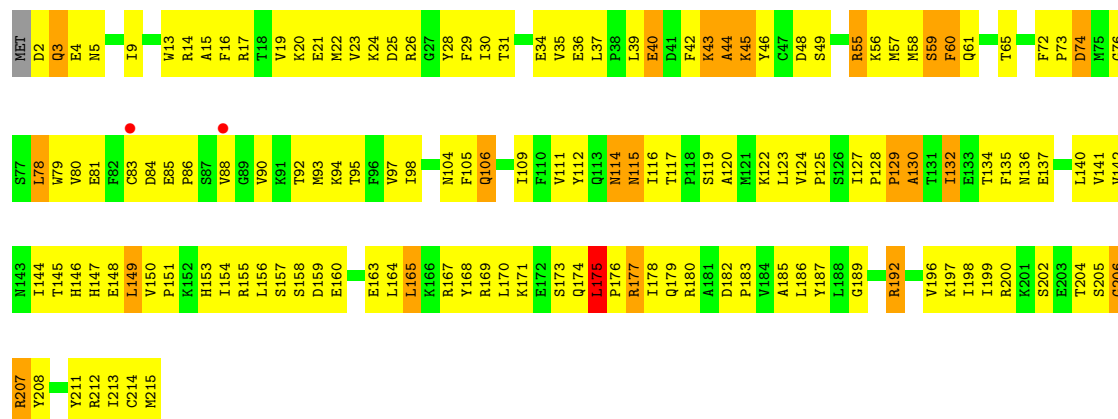




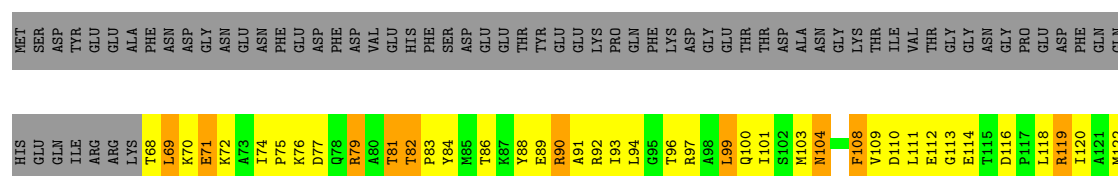
• Molecule 6: DNA-directed RNA polymerase II subunit RPB4

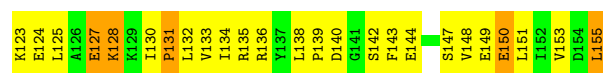


• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

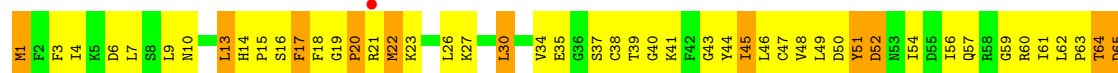


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

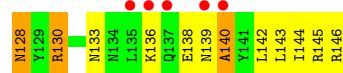
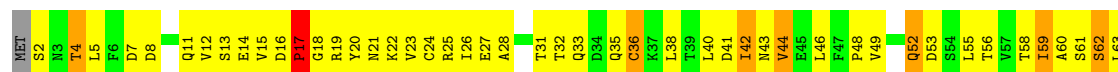




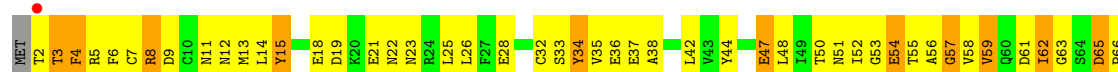
• Molecule 9: DNA-directed RNA polymerase II subunit RPB7



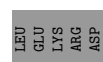
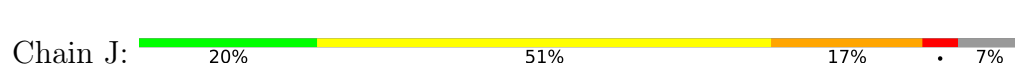
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 11: DNA-directed RNA polymerase II subunit RPB9

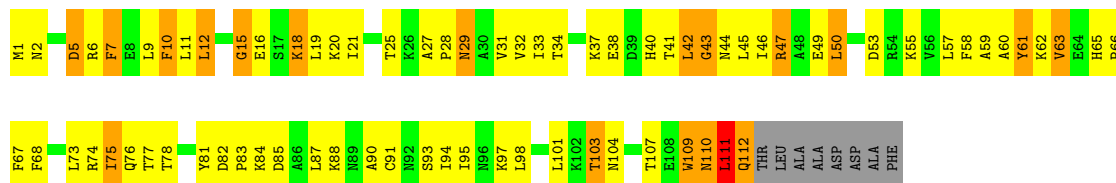


• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC5



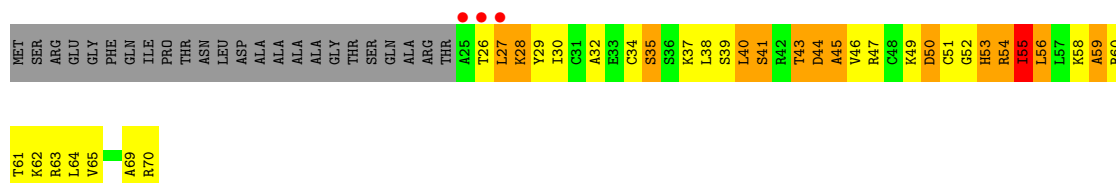
- Molecule 13: DNA-directed RNA polymerase II subunit RPB11

Chain K: 



- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.68Å 393.85Å 283.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 50.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.80) 99.9 (50.00-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.44 (at 3.77Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.212 , 0.246 0.217 , 0.247	Depositor DCC
R_{free} test set	2431 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	114.7	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 77.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.038 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.037 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31611	wwPDB-VP
Average B, all atoms (Å ²)	128.0	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: MG, ZN

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	P	0.46	0/215	0.69	0/334
2	T	0.53	0/231	1.12	2/358 (0.6%)
3	A	0.52	3/11394 (0.0%)	1.10	89/15407 (0.6%)
4	B	0.48	0/9012	1.03	53/12149 (0.4%)
5	C	0.52	0/2138	1.11	19/2896 (0.7%)
6	D	0.47	0/1444	1.05	11/1935 (0.6%)
7	E	0.46	0/1788	1.00	9/2406 (0.4%)
8	F	0.55	0/724	1.19	7/977 (0.7%)
9	G	0.49	0/1368	1.08	12/1844 (0.7%)
10	H	0.44	0/1102	0.93	2/1492 (0.1%)
11	I	0.44	0/962	1.00	4/1295 (0.3%)
12	J	0.53	0/541	1.01	2/727 (0.3%)
13	K	0.51	0/922	1.03	5/1244 (0.4%)
14	L	0.54	0/366	0.91	0/485
All	All	0.50	3/32207 (0.0%)	1.06	215/43549 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1177	LEU	CG-CD2	-5.21	1.35	1.52
3	A	1080	THR	CA-CB	5.14	1.59	1.53
3	A	1176	LEU	CA-CB	5.12	1.62	1.53

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	452	LYS	N-CA-C	-13.99	94.48	111.69
3	A	56	PRO	N-CA-C	-11.54	102.68	114.68
3	A	1175	SER	N-CA-C	-10.96	100.15	113.19
4	B	1185	CYS	N-CA-C	-10.87	100.02	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	26	THR	N-CA-C	-10.18	99.74	112.88
4	B	427	ASP	N-CA-C	-9.45	102.32	114.04
8	F	71	GLU	N-CA-C	-9.19	102.20	113.97
3	A	60	SER	N-CA-C	8.96	119.74	108.19
3	A	266	LEU	N-CA-C	-8.89	101.54	111.14
4	B	1201	LYS	N-CA-C	-8.67	101.80	111.07
3	A	1176	LEU	CA-CB-CG	8.55	146.23	116.30
3	A	1261	LYS	N-CA-C	-8.40	103.89	114.56
3	A	998	LEU	N-CA-C	8.33	122.00	109.25
4	B	473	MET	N-CA-C	-8.21	103.29	112.57
3	A	242	PRO	CA-C-N	8.06	128.68	120.38
3	A	242	PRO	C-N-CA	8.06	128.68	120.38
9	G	52	ASP	N-CA-C	7.89	119.51	111.07
4	B	296	GLU	N-CA-C	-7.87	102.31	112.23
2	T	12	G	N9-C1'-C2'	7.84	125.76	114.00
3	A	1176	LEU	CA-C-O	7.81	131.68	120.51
3	A	1096	SER	N-CA-C	7.64	119.31	108.00
4	B	1009	ASP	N-CA-C	-7.62	104.51	113.88
9	G	129	SER	N-CA-C	7.55	118.57	108.38
3	A	472	LEU	N-CA-C	7.48	119.33	111.03
5	C	173	ALA	N-CA-C	7.37	119.00	110.97
4	B	208	SER	N-CA-C	7.36	120.88	110.50
4	B	555	ILE	N-CA-C	-7.34	103.52	110.42
3	A	301	ALA	N-CA-C	-7.24	103.06	112.68
3	A	288	ALA	N-CA-C	-7.23	102.47	113.89
3	A	982	THR	N-CA-C	-7.22	100.80	110.55
3	A	236	LEU	N-CA-C	7.19	119.50	109.15
4	B	111	ALA	N-CA-C	-7.14	96.91	108.41
9	G	62	LEU	CA-C-N	-7.09	110.97	119.84
9	G	62	LEU	C-N-CA	-7.09	110.97	119.84
3	A	950	GLY	N-CA-C	-7.07	104.74	114.64
3	A	682	THR	N-CA-C	-7.07	104.13	112.89
6	D	38	ILE	N-CA-C	7.05	118.04	108.17
3	A	567	LYS	CA-C-N	-7.04	111.05	119.84
3	A	567	LYS	C-N-CA	-7.04	111.05	119.84
4	B	112	LEU	N-CA-C	7.00	121.26	110.20
4	B	291	ILE	CA-C-N	6.96	124.62	120.24
4	B	291	ILE	C-N-CA	6.96	124.62	120.24
3	A	344	ARG	N-CA-C	-6.95	100.24	110.52
3	A	1177	LEU	CD1-CG-CD2	-6.89	95.65	110.80
6	D	157	GLN	N-CA-C	-6.86	104.63	112.87
3	A	1176	LEU	CB-CA-C	-6.84	96.81	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	710	LEU	N-CA-C	-6.70	103.97	111.28
3	A	1177	LEU	N-CA-C	-6.69	92.26	111.00
5	C	38	ILE	N-CA-C	6.69	116.85	110.42
4	B	66	ASP	N-CA-C	-6.66	103.75	112.41
5	C	96	SER	N-CA-C	6.65	119.17	109.07
4	B	1099	VAL	N-CA-C	6.61	117.10	110.23
8	F	127	GLU	N-CA-C	-6.60	103.83	112.41
5	C	200	GLU	N-CA-C	6.59	119.29	111.71
4	B	468	GLU	CB-CA-C	-6.58	108.97	116.54
6	D	171	GLY	N-CA-C	-6.58	106.61	115.36
4	B	1045	SER	CA-C-N	6.57	128.05	119.84
4	B	1045	SER	C-N-CA	6.57	128.05	119.84
9	G	19	GLY	CA-C-N	6.56	128.04	119.84
9	G	19	GLY	C-N-CA	6.56	128.04	119.84
3	A	436	ILE	N-CA-C	-6.51	101.19	109.58
4	B	1033	LYS	N-CA-C	-6.50	105.32	113.18
3	A	539	THR	N-CA-C	6.49	119.18	109.25
5	C	165	LYS	N-CA-C	-6.44	102.76	112.04
3	A	598	LEU	N-CA-C	-6.41	102.68	112.99
6	D	176	GLU	N-CA-C	-6.36	103.64	111.40
3	A	636	GLU	N-CA-C	6.35	117.89	110.97
3	A	466	SER	N-CA-C	6.35	120.95	111.81
3	A	311	GLN	N-CA-C	6.31	123.76	109.81
7	E	171	LYS	N-CA-C	-6.30	100.30	110.32
3	A	1422	ARG	N-CA-C	-6.28	106.20	114.31
3	A	215	SER	N-CA-C	6.28	118.41	110.24
9	G	65	ASP	N-CA-C	-6.28	100.91	110.14
3	A	3	GLY	N-CA-C	-6.25	106.80	114.92
3	A	1403	GLU	N-CA-C	6.24	124.09	110.80
3	A	983	ILE	N-CA-C	-6.24	103.30	111.09
6	D	72	ARG	N-CA-C	-6.23	104.59	111.82
4	B	732	SER	N-CA-C	6.18	116.44	108.34
7	E	65	THR	N-CA-C	-6.18	102.38	110.53
3	A	143	LYS	N-CA-C	-6.16	105.73	113.18
4	B	472	ALA	N-CA-C	6.13	117.60	107.73
9	G	45	ILE	N-CA-C	-6.12	99.76	108.58
4	B	1008	PRO	N-CA-C	6.11	119.78	111.22
3	A	1262	LYS	N-CA-C	-6.11	104.53	112.23
6	D	188	ALA	N-CA-C	-6.11	105.09	112.54
3	A	453	MET	N-CA-C	6.09	119.81	112.38
4	B	127	GLY	N-CA-C	6.09	121.20	111.64
3	A	1102	LYS	N-CA-C	-6.08	104.65	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	111	VAL	N-CA-C	6.08	115.49	106.85
8	F	108	PHE	N-CA-C	6.08	120.32	113.02
3	A	281	HIS	N-CA-C	-6.06	103.59	111.71
4	B	395	GLN	N-CA-C	-6.05	102.68	110.19
11	I	18	GLU	N-CA-C	6.05	119.33	109.59
3	A	1313	LEU	N-CA-C	6.04	117.56	110.97
8	F	119	ARG	N-CA-C	-6.02	104.08	112.45
4	B	851	PHE	N-CA-C	6.01	119.83	111.90
12	J	44	TYR	N-CA-C	6.01	119.44	111.75
5	C	27	LEU	N-CA-C	-5.97	103.95	111.11
4	B	934	LYS	N-CA-C	5.96	119.46	107.41
8	F	82	THR	CA-C-N	5.96	125.83	119.28
8	F	82	THR	C-N-CA	5.96	125.83	119.28
3	A	1005	GLU	N-CA-C	5.95	117.57	111.14
6	D	66	ARG	N-CA-C	-5.94	104.78	112.68
5	C	39	ALA	N-CA-C	5.92	122.49	113.61
3	A	834	THR	N-CA-C	-5.91	104.84	111.28
5	C	225	ALA	N-CA-C	5.85	118.43	108.02
3	A	360	GLU	N-CA-C	-5.84	102.78	110.43
11	I	65	ASP	CA-C-N	5.83	125.70	119.28
11	I	65	ASP	C-N-CA	5.83	125.70	119.28
5	C	235	VAL	N-CA-C	-5.81	106.81	111.81
7	E	177	ARG	N-CA-C	5.77	119.37	110.42
11	I	115	LYS	N-CA-C	-5.77	104.78	113.89
2	T	12	G	O4'-C1'-C2'	5.77	111.57	105.80
9	G	30	LEU	N-CA-C	-5.76	103.99	111.02
7	E	55	ARG	N-CA-C	5.75	117.22	111.07
3	A	227	VAL	CB-CA-C	-5.74	104.95	111.55
4	B	840	ILE	CB-CA-C	-5.74	102.89	110.98
3	A	320	ARG	CA-C-N	5.71	126.98	119.84
3	A	320	ARG	C-N-CA	5.71	126.98	119.84
3	A	861	GLY	N-CA-C	-5.68	106.94	114.95
3	A	1360	GLY	N-CA-C	-5.67	107.44	115.43
3	A	584	ASN	N-CA-C	5.67	118.20	110.55
3	A	1311	VAL	N-CA-C	5.67	116.99	107.18
3	A	1445	ILE	CB-CA-C	-5.66	105.12	111.23
9	G	76	ALA	N-CA-C	5.66	116.01	108.38
3	A	293	GLU	N-CA-C	-5.65	105.11	112.23
5	C	135	GLN	N-CA-C	-5.64	105.81	114.16
4	B	628	THR	N-CA-C	-5.61	105.03	113.89
9	G	145	VAL	N-CA-C	5.60	117.88	109.20
4	B	366	GLN	N-CA-C	-5.59	105.80	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	173	THR	N-CA-C	-5.59	103.11	110.43
4	B	292	ILE	CB-CA-C	-5.58	108.44	114.35
7	E	173	SER	N-CA-C	5.57	119.69	113.01
4	B	835	GLN	N-CA-C	5.55	117.71	110.43
3	A	289	ILE	N-CA-C	-5.54	105.71	111.58
13	K	20	LYS	N-CA-C	-5.54	98.61	108.13
5	C	131	HIS	CA-C-N	5.50	126.72	119.84
5	C	131	HIS	C-N-CA	5.50	126.72	119.84
4	B	99	LYS	CA-C-N	5.50	126.72	119.84
4	B	99	LYS	C-N-CA	5.50	126.72	119.84
3	A	1376	THR	N-CA-C	5.50	119.97	111.56
13	K	75	ILE	N-CA-C	5.49	115.79	108.11
4	B	573	GLN	N-CA-C	-5.49	105.32	112.23
3	A	833	GLU	N-CA-C	-5.47	105.73	112.90
12	J	24	LEU	N-CA-C	-5.46	106.69	113.19
4	B	840	ILE	N-CA-C	-5.46	100.57	108.71
3	A	227	VAL	N-CA-C	5.45	116.50	111.81
4	B	1112	GLN	CA-C-N	-5.45	117.37	122.66
4	B	1112	GLN	C-N-CA	-5.45	117.37	122.66
4	B	292	ILE	N-CA-C	5.45	120.51	112.61
3	A	683	ILE	N-CA-C	-5.44	105.79	110.74
3	A	1096	SER	CB-CA-C	-5.44	108.72	116.34
6	D	146	GLN	N-CA-C	-5.43	105.27	111.14
3	A	562	THR	CA-C-N	5.43	125.74	119.93
3	A	562	THR	C-N-CA	5.43	125.74	119.93
5	C	155	LEU	CB-CA-C	-5.43	108.55	116.53
9	G	22	MET	N-CA-C	-5.42	105.47	112.68
4	B	1071	VAL	N-CA-C	-5.40	101.94	109.45
4	B	681	TRP	N-CA-C	-5.40	104.81	111.40
8	F	112	GLU	N-CA-C	-5.39	105.86	113.20
4	B	41	LYS	N-CA-C	5.39	118.19	111.24
3	A	81	PHE	N-CA-C	5.38	117.88	110.35
7	E	175	LEU	CA-C-N	5.38	125.64	119.83
7	E	175	LEU	C-N-CA	5.38	125.64	119.83
3	A	425	GLN	N-CA-C	-5.34	100.47	109.07
4	B	1129	ARG	N-CA-C	5.34	117.78	108.76
3	A	1291	VAL	CA-C-N	5.34	126.17	119.98
3	A	1291	VAL	C-N-CA	5.34	126.17	119.98
10	H	4	THR	N-CA-C	-5.33	102.57	110.46
3	A	467	THR	N-CA-C	5.33	117.48	109.23
3	A	1345	ARG	N-CA-C	-5.32	104.89	111.33
4	B	516	ASN	N-CA-C	-5.32	105.39	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	729	ALA	N-CA-C	-5.32	105.56	111.36
4	B	648	HIS	CA-C-O	5.32	121.02	117.94
3	A	158	PRO	N-CA-C	-5.31	107.72	114.35
3	A	507	VAL	CB-CA-C	-5.30	108.73	114.35
3	A	82	GLY	N-CA-C	-5.29	103.27	112.06
3	A	552	TRP	N-CA-C	5.29	117.79	111.71
4	B	361	LEU	CA-C-N	5.28	126.44	119.84
4	B	361	LEU	C-N-CA	5.28	126.44	119.84
10	H	16	ASP	N-CA-C	5.28	117.85	109.40
3	A	776	ALA	N-CA-C	5.27	118.12	110.17
4	B	774	GLY	N-CA-C	-5.23	106.39	113.24
5	C	75	MET	N-CA-C	-5.22	106.98	113.55
5	C	162	GLY	N-CA-C	5.21	118.55	111.72
3	A	291	GLU	N-CA-C	-5.21	106.61	113.17
13	K	18	LYS	N-CA-C	-5.20	104.87	111.11
7	E	4	GLU	N-CA-C	5.19	116.93	111.28
3	A	987	VAL	N-CA-C	5.16	118.29	111.17
5	C	40	GLU	N-CA-C	5.16	120.21	112.94
3	A	30	ILE	CB-CA-C	-5.15	105.29	111.88
13	K	12	LEU	N-CA-C	-5.15	103.74	110.53
4	B	949	VAL	N-CA-C	-5.15	101.65	109.78
4	B	288	ALA	N-CA-C	-5.14	106.10	112.38
4	B	580	VAL	N-CA-C	5.13	115.97	108.53
13	K	63	VAL	N-CA-C	-5.13	100.38	108.23
6	D	36	LYS	N-CA-C	5.13	116.97	107.73
4	B	606	LYS	N-CA-C	-5.12	107.09	113.55
4	B	964	VAL	N-CA-C	5.12	115.11	108.35
3	A	977	LYS	CA-C-N	5.12	125.33	120.31
3	A	977	LYS	C-N-CA	5.12	125.33	120.31
3	A	398	GLU	N-CA-C	-5.11	103.30	110.50
3	A	928	LEU	N-CA-C	-5.09	105.62	111.07
5	C	193	TYR	N-CA-C	5.09	115.01	108.34
4	B	648	HIS	CB-CA-C	-5.08	109.76	117.07
6	D	138	ASN	N-CA-C	-5.07	104.60	111.55
3	A	886	ILE	N-CA-C	5.07	115.35	110.74
5	C	40	GLU	CA-C-N	-5.07	118.94	122.59
5	C	40	GLU	C-N-CA	-5.07	118.94	122.59
3	A	543	LEU	N-CA-C	5.05	121.56	110.80
3	A	30	ILE	N-CA-C	5.04	115.65	110.36
3	A	864	ILE	N-CA-C	-5.04	107.92	112.96
4	B	1078	GLY	N-CA-C	-5.02	107.77	115.00
3	A	513	SER	CA-C-N	5.00	124.61	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	513	SER	C-N-CA	5.00	124.61	119.56

There are no chirality outliers.

There are no planarity outliers.

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	P	192	0	101	6	0
2	T	208	0	110	16	0
3	A	11194	0	11278	1330	0
4	B	8841	0	8874	1076	0
5	C	2101	0	2055	289	0
6	D	1434	0	1460	157	0
7	E	1752	0	1776	173	0
8	F	712	0	738	96	0
9	G	1340	0	1357	194	0
10	H	1084	0	1057	147	0
11	I	944	0	903	123	0
12	J	532	0	542	95	0
13	K	904	0	911	98	0
14	L	364	0	388	55	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	A	1	0	0	0	0
All	All	31611	0	31550	3515	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 56.

All (3515) 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)
3:A:58:LEU:HD12	3:A:59:GLY:H	0.99	1.11
4:B:343:ILE:HG23	4:B:347:LYS:HB2	1.25	1.09
4:B:510:LYS:HG2	4:B:511:PRO:HD3	1.22	1.08
3:A:53:LEU:HD23	3:A:54:ASN:N	1.68	1.08
5:C:43:THR:HG22	5:C:44:LEU:H	0.98	1.07
6:D:40:HIS:HB3	9:G:73:LYS:HZ3	1.12	1.06
3:A:868:TYR:CE1	3:A:1064:VAL:HG11	1.90	1.05
12:J:5:VAL:HG12	12:J:6:ARG:HG3	1.39	1.05
4:B:589:VAL:HG12	4:B:590:HIS:H	1.20	1.04
4:B:882:THR:HG22	4:B:884:ARG:H	1.18	1.04
4:B:521:LEU:HD22	4:B:633:VAL:HG12	1.38	1.03
7:E:94:LYS:HE2	7:E:98:ILE:HD11	1.35	1.03
4:B:37:PHE:HE1	4:B:41:LYS:HG3	1.25	1.02
4:B:273:LEU:HB2	4:B:276:ILE:HD12	1.37	1.02
3:A:901:LEU:H	3:A:926:GLN:NE2	1.55	1.02
3:A:254:GLU:HB2	4:B:935:ARG:HH12	1.25	1.02
10:H:100:THR:HG23	10:H:138:GLU:HA	1.40	1.02
3:A:53:LEU:HD23	3:A:54:ASN:H	0.89	1.00
3:A:744:LYS:HG2	3:A:748:MET:HE2	1.42	1.00
3:A:115:LEU:HB2	3:A:122:MET:HE2	1.43	1.00
11:I:115:LYS:HD3	11:I:117:LYS:HE3	1.40	0.99
3:A:1161:THR:HG22	3:A:1163:ILE:H	1.25	0.98
3:A:1329:THR:HG22	3:A:1331:SER:H	1.27	0.98
4:B:583:ASN:HD21	4:B:628:THR:HG22	1.26	0.98
9:G:15:PRO:HA	9:G:18:PHE:CD1	1.99	0.97
3:A:34:LYS:HE2	3:A:57:ARG:HH22	1.28	0.97
4:B:37:PHE:CE1	4:B:41:LYS:HG3	1.98	0.97
3:A:567:LYS:CG	3:A:568:PRO:HD2	1.96	0.96
3:A:225:ASN:HD22	3:A:228:PHE:H	1.08	0.96
10:H:4:THR:HA	10:H:60:ALA:HB2	1.42	0.96
3:A:754:SER:H	3:A:757:ASN:HD22	1.00	0.95
4:B:287:ARG:HG2	4:B:292:ILE:HA	1.46	0.95
3:A:446:ARG:HD3	3:A:480:ALA:HB2	1.48	0.95
9:G:138:THR:HG22	9:G:139:ILE:H	1.32	0.95
4:B:364:ILE:HG12	4:B:585:VAL:HG13	1.44	0.95
12:J:64:ASN:HB3	12:J:65:PRO:CD	1.97	0.95
3:A:1063:MET:SD	3:A:1436:ILE:HG12	2.07	0.95
3:A:541:ILE:HD13	3:A:549:MET:HE1	1.47	0.94
4:B:1072:MET:CE	4:B:1085:ILE:HB	1.97	0.94
11:I:34:TYR:HD2	11:I:35:VAL:N	1.63	0.94
3:A:58:LEU:HD12	3:A:59:GLY:N	1.82	0.94
3:A:63:ARG:HA	3:A:74:MET:HE1	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:779:PHE:HE1	3:A:785:PRO:HD3	1.29	0.94
13:K:49:GLU:HG3	13:K:94:ILE:HG12	1.49	0.94
3:A:855:THR:HG21	3:A:857:ARG:HE	1.32	0.93
2:T:13:U:O2'	2:T:14:C:O5'	1.84	0.93
5:C:43:THR:CG2	5:C:44:LEU:H	1.82	0.93
6:D:40:HIS:HB3	9:G:73:LYS:NZ	1.84	0.93
4:B:1002:THR:HG23	4:B:1006:ILE:HG13	1.50	0.93
3:A:767:GLN:NE2	3:A:774:ARG:HB3	1.84	0.93
6:D:56:ARG:HB2	6:D:148:LEU:HD22	1.50	0.93
14:L:32:ALA:HB3	14:L:55:ILE:HD12	1.51	0.93
3:A:535:THR:HG21	3:A:616:VAL:HA	1.49	0.92
5:C:47:ASP:HA	14:L:69:ALA:HB3	1.52	0.92
4:B:999:MET:HG3	4:B:1000:PRO:HD2	1.52	0.92
5:C:57:VAL:HG11	12:J:60:PHE:HB3	1.49	0.92
3:A:58:LEU:CD1	3:A:59:GLY:H	1.83	0.92
5:C:39:ALA:HA	5:C:164:ALA:HB3	1.48	0.92
4:B:313:MET:HE3	4:B:386:LEU:HD22	1.52	0.92
10:H:130:ARG:H	10:H:130:ARG:HD2	1.35	0.92
4:B:746:SER:HB2	4:B:1046:PRO:HG2	1.51	0.91
5:C:43:THR:HG22	5:C:44:LEU:N	1.80	0.91
4:B:806:THR:HG22	4:B:808:ALA:H	1.33	0.91
6:D:17:LYS:HA	6:D:17:LYS:HE3	1.52	0.91
3:A:1127:ASP:HB3	3:A:1130:GLN:HB3	1.52	0.91
4:B:336:ARG:HG2	4:B:348:ARG:HD3	1.50	0.91
7:E:19:VAL:O	7:E:23:VAL:HG23	1.71	0.91
4:B:637:LEU:HD12	4:B:693:ILE:HD12	1.53	0.90
3:A:903:ASN:HD22	3:A:904:THR:N	1.69	0.90
3:A:1438:THR:HB	4:B:1144:ALA:HB3	1.50	0.90
4:B:172:ILE:HD13	4:B:178:ASN:HB3	1.51	0.90
12:J:1:MET:H1	12:J:57:ILE:H	0.93	0.90
3:A:563:PRO:HG3	3:A:572:TRP:CZ2	2.07	0.90
3:A:1445:ILE:H	3:A:1445:ILE:HD12	1.37	0.90
4:B:247:GLY:H	4:B:418:LYS:NZ	1.70	0.90
3:A:53:LEU:CD2	3:A:54:ASN:H	1.82	0.89
4:B:510:LYS:HG2	4:B:511:PRO:CD	2.02	0.89
4:B:1177:HIS:HB2	4:B:1179:GLN:HE21	1.35	0.89
5:C:32:SER:O	5:C:36:VAL:HG23	1.72	0.89
4:B:1159:ARG:HD3	4:B:1193:GLN:HG3	1.54	0.89
3:A:1004:ASN:ND2	7:E:167:ARG:HD2	1.86	0.89
12:J:16:ASP:OD1	12:J:17:LYS:HD2	1.72	0.89
3:A:399:HIS:HB3	3:A:400:PRO:HD3	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:879:ARG:NH1	4:B:883:LEU:HD22	1.85	0.89
4:B:800:GLN:HB3	12:J:52:THR:HG21	1.54	0.89
12:J:3:VAL:HG21	12:J:18:TRP:HB2	1.51	0.89
3:A:605:MET:HE1	3:A:612:ILE:HG23	1.55	0.88
9:G:39:THR:HG22	9:G:40:GLY:H	1.37	0.88
3:A:658:LEU:HD13	4:B:831:SER:H	1.37	0.88
3:A:19:PHE:O	3:A:1416:ALA:HA	1.73	0.88
5:C:22:LEU:HD13	5:C:230:MET:HE1	1.55	0.88
4:B:549:THR:HG22	4:B:550:ASP:H	1.37	0.88
3:A:567:LYS:HB3	10:H:96:VAL:H	1.38	0.88
4:B:577:ALA:HB1	4:B:589:VAL:HG11	1.56	0.88
3:A:901:LEU:H	3:A:926:GLN:HE21	0.90	0.88
4:B:999:MET:HA	4:B:999:MET:HE3	1.53	0.88
12:J:64:ASN:HB3	12:J:65:PRO:HD3	1.56	0.88
3:A:567:LYS:CD	3:A:568:PRO:HD2	2.04	0.87
4:B:515:HIS:H	4:B:518:HIS:HD2	1.22	0.87
3:A:1444:MET:HE1	8:F:135:ARG:HB2	1.56	0.87
9:G:111:THR:HG22	9:G:113:HIS:H	1.37	0.87
3:A:763:ALA:O	3:A:803:SER:HB3	1.74	0.87
11:I:26:LEU:HD23	11:I:37:GLU:HA	1.53	0.87
7:E:180:ARG:HH21	7:E:192:ARG:HB2	1.38	0.87
3:A:93:VAL:HG13	3:A:301:ALA:HB1	1.57	0.86
5:C:101:LEU:HD13	5:C:118:LEU:HD23	1.58	0.86
6:D:144:THR:O	6:D:148:LEU:HB2	1.73	0.86
3:A:356:ASP:HB2	3:A:469:ARG:NH1	1.89	0.86
4:B:467:GLY:H	4:B:475:SER:HB3	1.37	0.86
3:A:590:ARG:NH2	3:A:620:LYS:HB3	1.91	0.86
13:K:47:ARG:HB3	13:K:47:ARG:HH11	1.41	0.86
9:G:26:LEU:HD12	9:G:56:ILE:HD13	1.58	0.85
3:A:963:ILE:HD11	3:A:1048:ASN:HB3	1.58	0.85
5:C:164:ALA:HA	5:C:167:HIS:O	1.75	0.85
3:A:868:TYR:HE1	3:A:1064:VAL:HG11	1.38	0.85
5:C:166:GLU:HG3	13:K:10:PHE:HZ	1.42	0.85
3:A:1345:ARG:HG3	3:A:1376:THR:HG21	1.58	0.85
1:P:9:G:H2'	1:P:10:A:C8	2.12	0.85
13:K:65:HIS:HD2	13:K:67:PHE:H	1.24	0.85
11:I:34:TYR:CD2	11:I:35:VAL:N	2.45	0.85
11:I:85:PHE:H	11:I:85:PHE:HD2	1.25	0.85
3:A:63:ARG:HD3	3:A:74:MET:HE1	1.59	0.84
4:B:112:LEU:HD12	4:B:113:TYR:H	1.40	0.84
5:C:6:PRO:HB3	5:C:25:VAL:HG12	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:560:ILE:HG13	10:H:78:SER:HB2	1.59	0.84
9:G:7:LEU:HB2	9:G:74:TYR:CE2	2.11	0.84
3:A:33:ALA:HB1	3:A:56:PRO:HB2	1.58	0.84
3:A:40:THR:HG22	3:A:41:MET:HG3	1.56	0.84
3:A:164:ARG:HG3	3:A:165:GLY:H	1.42	0.84
4:B:879:ARG:HH11	4:B:883:LEU:HD22	1.39	0.84
5:C:44:LEU:HB2	5:C:77:ILE:HD11	1.57	0.84
5:C:99:LEU:HD12	5:C:118:LEU:HB3	1.60	0.84
7:E:198:ILE:HD11	7:E:212:ARG:HG3	1.60	0.84
3:A:308:ILE:HG22	3:A:309:ALA:H	1.42	0.84
3:A:714:PHE:HB2	11:I:97:MET:HE1	1.59	0.84
3:A:1017:LEU:HB2	7:E:206:GLY:H	1.41	0.84
4:B:343:ILE:CG2	4:B:347:LYS:HB2	2.07	0.84
3:A:265:LYS:HD2	3:A:265:LYS:H	1.42	0.83
3:A:901:LEU:N	3:A:926:GLN:HE21	1.75	0.83
4:B:1201:LYS:HE2	4:B:1205:GLN:OE1	1.78	0.83
12:J:1:MET:H1	12:J:57:ILE:N	1.74	0.83
9:G:143:ILE:HG22	9:G:144:ARG:N	1.93	0.83
5:C:98:VAL:O	5:C:99:LEU:HD22	1.78	0.83
8:F:69:LEU:C	8:F:71:GLU:H	1.83	0.83
3:A:858:ASN:C	3:A:858:ASN:HD22	1.84	0.83
4:B:212:LEU:HD23	4:B:480:SER:HB2	1.59	0.83
4:B:789:MET:HE2	4:B:953:LEU:HD22	1.61	0.83
3:A:34:LYS:HE2	3:A:57:ARG:NH2	1.93	0.83
3:A:899:VAL:HB	3:A:929:LEU:HD11	1.61	0.83
3:A:699:ALA:HB1	11:I:114:GLN:HB2	1.58	0.83
3:A:1420:ASP:HB3	3:A:1422:ARG:HG3	1.59	0.83
4:B:1072:MET:HE3	4:B:1085:ILE:HB	1.59	0.83
5:C:77:ILE:HG23	5:C:161:LYS:HE3	1.61	0.82
9:G:1:MET:SD	9:G:79:PHE:HD1	2.03	0.82
9:G:138:THR:HG22	9:G:139:ILE:N	1.92	0.82
8:F:99:LEU:O	8:F:103:MET:HG2	1.80	0.82
6:D:40:HIS:CB	9:G:73:LYS:NZ	2.41	0.82
4:B:613:VAL:HG13	4:B:627:PHE:O	1.79	0.82
4:B:770:GLN:OE1	4:B:983:ARG:HA	1.78	0.82
13:K:21:ILE:HG12	13:K:33:ILE:HG12	1.59	0.82
3:A:265:LYS:HD2	3:A:265:LYS:N	1.94	0.82
6:D:47:LEU:HD13	6:D:48:ILE:N	1.95	0.81
8:F:93:ILE:HD11	8:F:134:ILE:HD11	1.59	0.81
3:A:1424:VAL:HG11	4:B:1139:ILE:HD13	1.61	0.81
11:I:8:ARG:HG3	11:I:34:TYR:HE1	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:75:CYS:HG	11:I:78:CYS:HG	1.23	0.81
3:A:866:PHE:C	3:A:867:ILE:HD12	2.06	0.81
3:A:913:LEU:HD12	3:A:914:GLU:H	1.46	0.81
5:C:239:PRO:HB2	5:C:241:ASP:OD1	1.81	0.81
3:A:779:PHE:CE1	3:A:785:PRO:HD3	2.15	0.81
3:A:1325:THR:O	7:E:148:GLU:HB2	1.79	0.81
4:B:121:ASN:HA	4:B:207:GLY:HA2	1.61	0.81
3:A:34:LYS:CE	3:A:57:ARG:HH12	1.92	0.81
3:A:58:LEU:HD11	3:A:243:PRO:HB3	1.61	0.81
3:A:666:ILE:HD12	3:A:667:GLY:H	1.46	0.81
4:B:115:GLN:HG2	4:B:193:LYS:HB2	1.63	0.81
6:D:134:THR:HG22	6:D:135:GLY:N	1.95	0.81
3:A:679:ILE:HG12	3:A:732:LEU:HD12	1.62	0.81
3:A:1028:THR:O	3:A:1032:LEU:HD12	1.79	0.81
4:B:654:ARG:H	4:B:657:HIS:HD2	1.28	0.81
3:A:442:VAL:HB	3:A:489:LEU:HD11	1.61	0.81
3:A:225:ASN:ND2	3:A:228:PHE:H	1.79	0.81
3:A:451:HIS:CD2	3:A:1074:GLU:HG3	2.16	0.81
3:A:1312:ASN:O	3:A:1316:VAL:HG23	1.81	0.81
3:A:518:LYS:HE2	3:A:624:SER:O	1.80	0.80
4:B:35:SER:O	4:B:39:ARG:HG3	1.82	0.80
4:B:778:MET:CE	4:B:1094:ARG:HD3	2.10	0.80
4:B:1007:VAL:HG22	4:B:1008:PRO:HD2	1.63	0.80
7:E:16:PHE:CZ	7:E:20:LYS:HE2	2.15	0.80
9:G:1:MET:SD	9:G:79:PHE:CD1	2.75	0.80
3:A:598:LEU:HA	10:H:122:LEU:HD13	1.64	0.80
7:E:22:MET:HE3	7:E:26:ARG:HE	1.46	0.80
3:A:629:LEU:O	3:A:633:VAL:HG23	1.82	0.80
4:B:1169:MET:HE1	4:B:1201:LYS:HA	1.64	0.80
3:A:1189:SER:O	3:A:1241:ARG:HD3	1.82	0.80
5:C:238:ILE:HG23	5:C:242:GLN:HB2	1.63	0.80
10:H:93:TYR:HB3	10:H:144:ILE:O	1.82	0.80
11:I:8:ARG:HG3	11:I:34:TYR:CE1	2.17	0.80
3:A:1120:LEU:HD12	3:A:1120:LEU:N	1.98	0.79
4:B:902:GLY:O	14:L:65:VAL:HG11	1.82	0.79
3:A:567:LYS:HD2	3:A:568:PRO:HD2	1.63	0.79
4:B:22:SER:HA	4:B:654:ARG:CB	2.11	0.79
5:C:66:ARG:NH1	12:J:2:ILE:HG21	1.97	0.79
3:A:70:CYS:O	3:A:72:GLU:HG2	1.82	0.79
13:K:40:HIS:HD1	13:K:61:TYR:HH	1.27	0.79
4:B:370:PHE:HE2	4:B:373:ARG:HH11	1.31	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:86:THR:OG1	8:F:89:GLU:HG3	1.83	0.79
9:G:49:LEU:HD21	9:G:77:VAL:HG23	1.65	0.79
4:B:882:THR:HG22	4:B:884:ARG:N	1.98	0.79
9:G:127:PRO:HG2	9:G:138:THR:HG21	1.63	0.79
3:A:868:TYR:HD2	3:A:1058:VAL:HG21	1.45	0.79
3:A:577:ILE:O	3:A:580:VAL:HG23	1.82	0.79
6:D:159:THR:O	6:D:163:VAL:HG23	1.82	0.79
3:A:58:LEU:HD11	3:A:243:PRO:CB	2.12	0.78
3:A:541:ILE:HG21	3:A:549:MET:HE1	1.63	0.78
3:A:567:LYS:HD3	10:H:95:TYR:CD2	2.18	0.78
3:A:855:THR:HG21	3:A:857:ARG:NE	1.98	0.78
3:A:244:PRO:HG2	3:A:245:PRO:HD3	1.64	0.78
3:A:1336:MET:HE3	3:A:1381:LEU:HG	1.63	0.78
4:B:467:GLY:N	4:B:475:SER:HB3	1.97	0.78
4:B:23:ALA:HB1	4:B:24:PRO:HD2	1.66	0.78
4:B:899:ILE:HD11	4:B:911:ILE:HA	1.64	0.78
9:G:13:LEU:HD21	9:G:17:PHE:HB2	1.64	0.78
13:K:49:GLU:HG3	13:K:94:ILE:CG1	2.13	0.78
4:B:65:GLU:HG3	4:B:66:ASP:H	1.48	0.78
4:B:622:LYS:HE2	11:I:59:VAL:HG22	1.65	0.78
4:B:1183:LYS:N	4:B:1183:LYS:HE3	1.99	0.78
4:B:1072:MET:HE1	4:B:1085:ILE:HB	1.65	0.78
4:B:955:THR:HG22	4:B:956:THR:N	1.97	0.77
9:G:122:ASN:ND2	9:G:125:SER:HB3	1.99	0.77
9:G:34:VAL:HG12	9:G:45:ILE:HG21	1.64	0.77
3:A:665:GLY:O	3:A:667:GLY:N	2.18	0.77
3:A:709:THR:HG22	3:A:711:ARG:H	1.49	0.77
4:B:906:SER:O	4:B:941:LEU:HD23	1.85	0.77
4:B:1095:LEU:H	4:B:1095:LEU:HD12	1.49	0.77
6:D:153:ARG:NH2	6:D:184:ALA:HA	2.00	0.77
12:J:36:LEU:HD22	12:J:41:LEU:HD12	1.66	0.77
4:B:579:ARG:HB2	4:B:586:TRP:NE1	1.99	0.77
4:B:860:MET:HB2	4:B:965:LYS:HG2	1.67	0.77
3:A:23:SER:HA	3:A:233:TRP:NE1	2.00	0.77
3:A:381:THR:HG23	3:A:383:TYR:H	1.50	0.77
5:C:18:VAL:HG12	5:C:18:VAL:O	1.84	0.77
4:B:232:SER:HB3	4:B:261:ARG:HH21	1.50	0.77
4:B:580:VAL:HG22	4:B:624:LEU:HB3	1.66	0.77
4:B:801:LYS:O	12:J:52:THR:HG23	1.84	0.77
10:H:89:LEU:C	10:H:91:ASP:H	1.92	0.77
4:B:516:ASN:HD22	4:B:516:ASN:N	1.80	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:124:VAL:HG13	7:E:132:ILE:HD12	1.67	0.76
3:A:69:THR:C	3:A:71:GLN:H	1.93	0.76
3:A:1032:LEU:O	3:A:1036:ARG:HD3	1.85	0.76
3:A:1341:ILE:HD12	3:A:1379:GLY:O	1.85	0.76
3:A:61:ILE:HG22	3:A:62:ASP:H	1.49	0.76
3:A:332:LYS:HG3	3:A:333:GLU:HG2	1.67	0.76
4:B:502:ILE:H	4:B:502:ILE:HD12	1.48	0.76
6:D:39:ASN:HD21	6:D:41:GLN:NE2	1.82	0.76
3:A:384:ASN:OD1	3:A:388:LEU:HD12	1.85	0.76
7:E:192:ARG:HH11	7:E:192:ARG:HG3	1.50	0.76
12:J:43:ARG:HG3	12:J:45:CYS:SG	2.26	0.76
3:A:902:LEU:HG	3:A:926:GLN:HG3	1.67	0.76
3:A:353:ILE:HD13	3:A:487:MET:HE2	1.67	0.76
4:B:22:SER:HA	4:B:654:ARG:HB3	1.66	0.76
4:B:515:HIS:HD2	4:B:517:THR:H	1.31	0.76
13:K:65:HIS:CD2	13:K:67:PHE:H	2.04	0.76
4:B:216:GLU:OE1	4:B:537:LYS:HE2	1.85	0.76
4:B:589:VAL:HG12	4:B:590:HIS:N	2.00	0.76
5:C:241:ASP:O	5:C:245:VAL:HG23	1.86	0.76
9:G:88:ASP:HB3	9:G:144:ARG:HA	1.68	0.76
3:A:738:LYS:HB2	3:A:740:LEU:HG	1.67	0.76
3:A:768:GLN:HG2	3:A:816:HIS:HA	1.66	0.76
3:A:1002:GLY:HA3	3:A:1007:ILE:HG21	1.67	0.76
4:B:882:THR:CG2	4:B:884:ARG:HB2	2.16	0.76
4:B:1202:LEU:O	4:B:1206:GLU:HG3	1.85	0.75
6:D:173:HIS:O	6:D:177:VAL:HG23	1.86	0.75
4:B:806:THR:HG22	4:B:808:ALA:N	2.00	0.75
4:B:1065:GLN:HE21	4:B:1067:ARG:H	1.34	0.75
4:B:1065:GLN:HE21	4:B:1067:ARG:N	1.84	0.75
3:A:93:VAL:HG22	3:A:301:ALA:HA	1.68	0.75
3:A:821:ARG:HB2	3:A:821:ARG:HH11	1.51	0.75
3:A:87:ALA:CB	3:A:276:LEU:HD23	2.17	0.75
4:B:642:ASP:HB3	4:B:649:LYS:HD2	1.69	0.75
3:A:164:ARG:HG3	3:A:165:GLY:N	2.01	0.75
4:B:114:PRO:HG2	4:B:115:GLN:H	1.51	0.75
4:B:798:TYR:HE2	5:C:62:PHE:CE2	2.04	0.75
7:E:202:SER:HB3	7:E:205:SER:O	1.86	0.75
3:A:321:PRO:O	3:A:322:VAL:HB	1.87	0.75
3:A:382:PRO:HB3	3:A:428:TYR:HE2	1.50	0.75
3:A:567:LYS:HG3	3:A:568:PRO:HD2	1.67	0.75
3:A:1329:THR:HG22	3:A:1331:SER:N	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1332:PHE:H	3:A:1332:PHE:HD2	1.34	0.75
2:T:12:G:O2'	2:T:13:U:O5'	2.02	0.75
4:B:611:PRO:HB3	4:B:685:LEU:HD11	1.68	0.75
4:B:1163:CYS:SG	4:B:1165:ILE:HB	2.25	0.75
6:D:12:ARG:HG2	6:D:14:ARG:HG3	1.69	0.75
3:A:699:ALA:HB3	3:A:701:LEU:HG	1.68	0.74
4:B:800:GLN:HB3	12:J:52:THR:CG2	2.17	0.74
3:A:249:SER:O	3:A:250:ILE:HG13	1.87	0.74
4:B:1162:ILE:HD11	4:B:1194:ILE:HD13	1.67	0.74
3:A:34:LYS:CE	3:A:57:ARG:HH22	2.00	0.74
3:A:69:THR:O	3:A:71:GLN:N	2.20	0.74
4:B:758:PHE:CE1	4:B:1027:ILE:HG22	2.22	0.74
11:I:34:TYR:HE2	11:I:36:GLU:HB3	1.52	0.74
3:A:351:THR:HB	4:B:1103:ILE:HD12	1.70	0.74
4:B:642:ASP:HA	4:B:649:LYS:HA	1.67	0.74
10:H:59:ILE:HG22	10:H:60:ALA:N	2.01	0.74
10:H:102:TYR:OH	10:H:122:LEU:HD22	1.88	0.74
3:A:337:ARG:HD3	4:B:1132:GLU:OE1	1.88	0.74
3:A:853:ASP:O	3:A:854:ASN:HB2	1.86	0.74
4:B:53:GLN:HG2	4:B:547:VAL:HG22	1.69	0.74
5:C:8:VAL:HG12	5:C:9:LYS:H	1.53	0.74
9:G:14:HIS:ND1	9:G:15:PRO:HD2	2.03	0.74
3:A:67:CYS:O	3:A:70:CYS:HB3	1.87	0.74
3:A:239:LEU:HD12	3:A:240:PRO:HD2	1.69	0.74
3:A:605:MET:HE2	3:A:607:ILE:CG1	2.17	0.74
4:B:60:GLN:O	4:B:63:ILE:HG22	1.88	0.74
3:A:62:ASP:HB3	3:A:64:ASN:ND2	2.02	0.74
10:H:40:LEU:HD13	10:H:123:MET:HB2	1.70	0.74
3:A:534:LEU:O	3:A:574:GLY:HA3	1.85	0.74
3:A:783:THR:HG21	3:A:815:PHE:CZ	2.22	0.74
3:A:50:ILE:C	3:A:52:GLY:H	1.96	0.74
3:A:774:ARG:NH2	3:A:797:LYS:HG3	2.03	0.74
3:A:836:TYR:CE2	3:A:840:ARG:HD2	2.23	0.73
4:B:483:LEU:HD11	4:B:491:THR:HG23	1.70	0.73
5:C:212:PRO:HB3	5:C:213:PRO:HD2	1.69	0.73
10:H:38:LEU:HD12	10:H:124:ARG:O	1.87	0.73
13:K:45:LEU:HG	13:K:94:ILE:HD13	1.68	0.73
4:B:336:ARG:HH22	4:B:345:LYS:HE2	1.54	0.73
3:A:605:MET:HE2	3:A:607:ILE:HG13	1.69	0.73
3:A:1100:ARG:HH21	3:A:1351:GLU:HG2	1.53	0.73
4:B:745:PRO:O	4:B:748:ILE:HG12	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:153:ARG:HB3	6:D:154:PHE:CE1	2.22	0.73
9:G:119:LEU:HD12	9:G:131:GLN:O	1.88	0.73
10:H:4:THR:HA	10:H:60:ALA:CB	2.18	0.73
3:A:114:LEU:HD13	3:A:171:GLN:HE22	1.53	0.73
3:A:1030:ARG:HG3	3:A:1034:GLU:CD	2.13	0.73
3:A:1244:ARG:HB3	3:A:1245:PRO:HD2	1.69	0.73
4:B:615:MET:C	4:B:616:ILE:HD12	2.14	0.73
13:K:21:ILE:HG23	13:K:31:VAL:HG11	1.71	0.73
13:K:90:ALA:O	13:K:94:ILE:HG13	1.88	0.73
7:E:22:MET:HE3	7:E:26:ARG:NE	2.02	0.73
10:H:89:LEU:O	10:H:91:ASP:N	2.22	0.73
3:A:55:ASP:N	3:A:56:PRO:HD3	2.04	0.73
3:A:152:VAL:CG1	3:A:153:PRO:HD2	2.17	0.73
3:A:868:TYR:CD2	3:A:1058:VAL:HG21	2.23	0.73
3:A:1118:VAL:HG12	3:A:1327:ILE:HG13	1.69	0.73
1:P:11:C:H2'	1:P:12:C:H6	1.54	0.73
3:A:754:SER:N	3:A:757:ASN:HD22	1.83	0.73
3:A:896:ARG:HD3	3:A:897:TYR:HE1	1.54	0.73
3:A:1116:LEU:N	3:A:1308:THR:HG22	2.04	0.73
3:A:1198:ASP:HB3	3:A:1201:ALA:HB3	1.68	0.73
4:B:244:LEU:HD11	4:B:366:GLN:HE22	1.54	0.73
4:B:579:ARG:HB2	4:B:586:TRP:HE1	1.54	0.73
6:D:47:LEU:HD13	6:D:48:ILE:H	1.53	0.73
6:D:189:ASP:O	6:D:193:THR:HB	1.88	0.73
3:A:34:LYS:HE2	3:A:57:ARG:HH12	1.52	0.72
3:A:1174:PHE:HA	3:A:1176:LEU:HD23	1.70	0.72
4:B:1187:ASN:O	4:B:1188:LYS:HB2	1.89	0.72
6:D:134:THR:HG22	6:D:135:GLY:H	1.52	0.72
3:A:345:VAL:HG21	4:B:1150:ARG:NH1	2.04	0.72
4:B:167:ILE:HG22	4:B:453:ILE:HD12	1.70	0.72
4:B:359:GLU:O	4:B:362:PRO:HD3	1.89	0.72
4:B:642:ASP:HB3	4:B:649:LYS:CD	2.19	0.72
4:B:1172:ILE:HG22	4:B:1172:ILE:O	1.89	0.72
14:L:30:ILE:O	14:L:56:LEU:HA	1.88	0.72
4:B:863:GLU:OE2	4:B:873:THR:HA	1.89	0.72
7:E:157:SER:OG	7:E:160:GLU:HG3	1.88	0.72
3:A:244:PRO:HG2	3:A:245:PRO:CD	2.19	0.72
3:A:285:PRO:HG2	3:A:288:ALA:HB3	1.71	0.72
3:A:63:ARG:HA	3:A:74:MET:CE	2.18	0.72
3:A:230:ARG:H	3:A:233:TRP:HE3	1.32	0.72
4:B:336:ARG:NH2	4:B:345:LYS:HE2	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:340:ALA:CB	4:B:343:ILE:HD12	2.18	0.72
5:C:189:THR:HG22	5:C:190:ASP:N	2.03	0.72
3:A:1242:VAL:HG12	3:A:1243:VAL:H	1.55	0.72
4:B:365:THR:HG23	4:B:367:LEU:H	1.54	0.72
4:B:880:THR:O	4:B:881:ASN:HB2	1.88	0.72
10:H:100:THR:OG1	10:H:138:GLU:HG3	1.88	0.72
12:J:57:ILE:HA	12:J:60:PHE:HD2	1.54	0.72
4:B:1115:THR:HG22	4:B:1117:GLN:HG3	1.70	0.72
5:C:238:ILE:HD11	5:C:246:ARG:NH1	2.04	0.72
10:H:41:ASP:O	10:H:42:ILE:HG13	1.89	0.72
3:A:896:ARG:NH2	3:A:1030:ARG:HH21	1.88	0.72
3:A:1017:LEU:HB2	7:E:206:GLY:N	2.02	0.72
4:B:1159:ARG:HE	4:B:1193:GLN:HE21	1.35	0.72
8:F:103:MET:CE	9:G:66:GLY:H	2.03	0.72
9:G:143:ILE:HG22	9:G:144:ARG:H	1.52	0.72
3:A:885:THR:O	3:A:940:ARG:HD2	1.90	0.72
4:B:582:VAL:HG23	4:B:626:ILE:HB	1.70	0.72
12:J:3:VAL:HG21	12:J:18:TRP:CB	2.19	0.72
2:T:10:U:H2'	2:T:11:G:O4'	1.89	0.71
4:B:247:GLY:H	4:B:418:LYS:HZ1	1.35	0.71
4:B:847:ASP:HB3	5:C:167:HIS:NE2	2.05	0.71
3:A:32:VAL:HG21	3:A:68:GLN:NE2	2.05	0.71
3:A:855:THR:HG23	3:A:857:ARG:HG3	1.71	0.71
3:A:1116:LEU:HB2	3:A:1329:THR:OG1	1.90	0.71
3:A:1120:LEU:CD1	3:A:1120:LEU:H	2.03	0.71
3:A:1124:HIS:HB3	3:A:1130:GLN:HG2	1.71	0.71
8:F:69:LEU:O	8:F:71:GLU:N	2.23	0.71
3:A:986:ILE:HG22	3:A:987:VAL:N	2.05	0.71
4:B:193:LYS:NZ	14:L:32:ALA:HB1	2.05	0.71
4:B:975:GLN:HG2	4:B:976:ILE:H	1.56	0.71
12:J:7:CYS:SG	12:J:49:MET:HE3	2.30	0.71
4:B:859:TYR:OH	4:B:941:LEU:HD12	1.91	0.71
6:D:170:THR:HB	6:D:172:LEU:HG	1.70	0.71
14:L:32:ALA:HB3	14:L:55:ILE:CD1	2.20	0.71
3:A:913:LEU:HD12	3:A:914:GLU:N	2.05	0.71
4:B:842:ASN:ND2	4:B:845:SER:H	1.88	0.71
5:C:36:VAL:HG21	5:C:251:LEU:HD22	1.72	0.71
3:A:821:ARG:HB2	3:A:821:ARG:NH1	2.05	0.71
4:B:112:LEU:HD12	4:B:113:TYR:N	2.06	0.71
4:B:815:ARG:HD3	4:B:1041:GLU:OE2	1.91	0.71
5:C:35:ARG:NH1	13:K:41:THR:N	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2:VAL:HG21	4:B:1157:ALA:HB1	1.73	0.71
3:A:477:PRO:HG2	3:A:521:MET:HG2	1.72	0.71
3:A:960:ILE:O	3:A:963:ILE:HG22	1.91	0.71
3:A:1030:ARG:HG3	3:A:1034:GLU:OE2	1.91	0.71
3:A:438:ASP:O	3:A:439:ASN:HB2	1.88	0.70
3:A:646:PHE:O	3:A:650:GLN:HG3	1.91	0.70
3:A:1115:SER:O	3:A:1116:LEU:HB3	1.89	0.70
4:B:708:GLU:O	4:B:710:LEU:N	2.24	0.70
4:B:862:GLN:HG2	4:B:963:PHE:HD1	1.54	0.70
7:E:157:SER:C	7:E:159:ASP:H	1.99	0.70
3:A:139:TRP:O	3:A:143:LYS:HB3	1.90	0.70
5:C:46:ILE:HD12	5:C:67:LEU:HB3	1.72	0.70
5:C:213:PRO:O	5:C:214:ASN:HB2	1.91	0.70
9:G:81:PRO:HG3	9:G:106:MET:SD	2.31	0.70
14:L:58:LYS:O	14:L:58:LYS:HG2	1.90	0.70
3:A:58:LEU:HD13	3:A:80:HIS:O	1.91	0.70
3:A:445:ASN:HB2	3:A:455:MET:HG2	1.73	0.70
3:A:1121:GLU:HG2	3:A:1122:PRO:HD2	1.72	0.70
3:A:1343:ALA:HB2	7:E:150:VAL:HG22	1.73	0.70
4:B:39:ARG:NH2	4:B:665:GLU:HG2	2.05	0.70
3:A:35:ILE:HG22	3:A:35:ILE:O	1.90	0.70
5:C:209:TYR:HD1	5:C:209:TYR:H	1.40	0.70
11:I:82:GLU:OE2	11:I:104:LEU:HD12	1.90	0.70
3:A:745:GLN:HA	3:A:748:MET:HE3	1.72	0.70
3:A:1202:MET:HE1	3:A:1212:VAL:HG21	1.72	0.70
4:B:343:ILE:CG2	4:B:348:ARG:HG3	2.22	0.70
6:D:40:HIS:CE1	6:D:41:GLN:HG3	2.27	0.70
8:F:103:MET:O	8:F:104:ASN:HB2	1.90	0.70
8:F:119:ARG:HH11	8:F:119:ARG:HG3	1.56	0.70
12:J:12:LYS:O	12:J:14:VAL:HG23	1.92	0.70
3:A:761:MET:HA	3:A:804:TYR:HB2	1.72	0.70
3:A:899:VAL:HB	3:A:929:LEU:CD1	2.21	0.70
3:A:1208:THR:O	3:A:1212:VAL:HG23	1.92	0.70
4:B:205:ILE:N	4:B:205:ILE:HD12	2.07	0.70
6:D:130:LEU:C	6:D:132:GLN:H	2.00	0.70
3:A:34:LYS:NZ	3:A:57:ARG:HH12	1.90	0.70
3:A:794:PRO:HG2	3:A:795:GLU:OE2	1.91	0.70
3:A:993:LEU:HD22	3:A:1046:LEU:HD22	1.73	0.70
3:A:412:ARG:NH2	4:B:1108:ARG:NH1	2.39	0.70
3:A:1161:THR:HG22	3:A:1163:ILE:N	2.05	0.70
4:B:498:THR:HG22	4:B:537:LYS:H	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:971:THR:OG1	5:C:61:GLU:HG3	1.92	0.70
10:H:126:GLU:C	10:H:130:ARG:HH22	2.00	0.70
3:A:451:HIS:NE2	3:A:1074:GLU:HG3	2.07	0.69
3:A:1261:LYS:O	3:A:1264:GLU:HB3	1.92	0.69
9:G:143:ILE:CG2	9:G:144:ARG:H	2.05	0.69
4:B:98:THR:O	4:B:126:SER:HB2	1.91	0.69
4:B:847:ASP:C	4:B:849:GLY:H	1.98	0.69
13:K:46:ILE:O	13:K:50:LEU:HB2	1.92	0.69
6:D:175:PHE:HZ	9:G:85:GLU:HG3	1.57	0.69
12:J:36:LEU:HD12	12:J:47:ARG:NH1	2.07	0.69
5:C:232:VAL:HG21	5:C:244:VAL:HG22	1.73	0.69
3:A:79:GLY:HA3	3:A:243:PRO:HG3	1.74	0.69
3:A:541:ILE:HG21	3:A:549:MET:CE	2.21	0.69
3:A:901:LEU:N	3:A:926:GLN:NE2	2.37	0.69
4:B:168:GLY:H	4:B:450:ALA:HB1	1.57	0.69
5:C:66:ARG:NH2	12:J:3:VAL:O	2.24	0.69
7:E:48:ASP:CG	7:E:49:SER:H	2.00	0.69
11:I:50:THR:HG22	11:I:52:ILE:H	1.58	0.69
10:H:61:SER:O	10:H:62:SER:HB3	1.91	0.69
10:H:127:GLY:O	10:H:128:ASN:HB2	1.93	0.69
3:A:254:GLU:HB2	4:B:935:ARG:NH1	2.03	0.69
3:A:472:LEU:HD11	4:B:835:GLN:NE2	2.08	0.69
3:A:709:THR:HG23	11:I:94:ASP:HA	1.73	0.69
4:B:975:GLN:O	4:B:990:ILE:HD12	1.93	0.69
3:A:84:ILE:HD11	3:A:270:LEU:HD13	1.74	0.69
3:A:1015:VAL:HG12	3:A:1019:CYS:SG	2.33	0.69
4:B:811:TYR:N	4:B:811:TYR:CD1	2.60	0.69
4:B:830:TYR:CE2	4:B:1000:PRO:HD3	2.28	0.69
5:C:184:ASN:ND2	5:C:187:LYS:HA	2.08	0.69
7:E:117:THR:HG22	7:E:119:SER:H	1.58	0.69
3:A:443:LEU:HD21	3:A:455:MET:HB3	1.75	0.69
3:A:446:ARG:CD	3:A:480:ALA:HB2	2.22	0.69
3:A:567:LYS:HB3	10:H:96:VAL:N	2.07	0.69
4:B:515:HIS:CD2	4:B:516:ASN:H	2.10	0.69
4:B:597:MET:HA	4:B:597:MET:HE3	1.74	0.69
4:B:25:ILE:HD11	4:B:653:VAL:O	1.92	0.69
4:B:710:LEU:HA	4:B:733:HIS:HB3	1.75	0.69
3:A:344:ARG:HD2	4:B:1118:PRO:O	1.92	0.68
3:A:477:PRO:CG	3:A:521:MET:HG2	2.23	0.68
3:A:1171:GLN:HA	3:A:1174:PHE:CD1	2.29	0.68
9:G:143:ILE:CG2	9:G:144:ARG:N	2.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:68:GLN:C	3:A:70:CYS:H	2.00	0.68
4:B:1006:ILE:HD13	12:J:44:TYR:HE2	1.58	0.68
3:A:567:LYS:HD3	10:H:95:TYR:CG	2.28	0.68
3:A:903:ASN:ND2	3:A:904:THR:N	2.42	0.68
4:B:65:GLU:HG3	4:B:66:ASP:N	2.08	0.68
4:B:295:GLY:H	4:B:298:LEU:HD23	1.57	0.68
4:B:378:LEU:HD12	4:B:378:LEU:O	1.93	0.68
4:B:526:GLU:HG2	4:B:538:ASN:HD22	1.58	0.68
4:B:1087:PHE:HD2	4:B:1088:GLY:N	1.91	0.68
11:I:111:THR:HG22	11:I:112:SER:N	2.08	0.68
3:A:903:ASN:HD22	3:A:904:THR:H	1.41	0.68
10:H:36:CYS:HA	10:H:126:GLU:O	1.92	0.68
3:A:311:GLN:O	3:A:312:PRO:C	2.36	0.68
3:A:528:LEU:O	3:A:531:ILE:HG22	1.93	0.68
3:A:590:ARG:HD3	3:A:604:GLY:HA2	1.74	0.68
3:A:886:ILE:HD11	3:A:943:LEU:HB3	1.74	0.68
4:B:1006:ILE:HD13	12:J:44:TYR:CE2	2.29	0.68
5:C:191:TYR:HD2	5:C:201:TRP:CD1	2.11	0.68
9:G:128:PRO:O	9:G:138:THR:HG23	1.93	0.68
3:A:694:THR:O	3:A:698:GLN:HG3	1.93	0.68
4:B:351:TYR:O	4:B:355:ILE:HG13	1.94	0.68
6:D:17:LYS:HE3	6:D:17:LYS:CA	2.23	0.68
8:F:90:ARG:HD3	8:F:155:LEU:CD1	2.23	0.68
8:F:109:VAL:HG11	8:F:123:LYS:HD3	1.74	0.68
3:A:443:LEU:HD12	4:B:1146:PHE:CE2	2.28	0.68
3:A:836:TYR:CD2	3:A:840:ARG:HD2	2.27	0.68
4:B:661:LEU:HD11	4:B:684:LEU:HD21	1.74	0.68
10:H:84:ALA:HA	10:H:87:ARG:HB2	1.76	0.68
3:A:535:THR:CG2	3:A:616:VAL:HA	2.24	0.68
6:D:50:LEU:HD13	6:D:55:ALA:HA	1.76	0.68
10:H:58:THR:HG22	10:H:59:ILE:H	1.59	0.68
4:B:288:ALA:HA	4:B:331:LEU:HD12	1.73	0.68
4:B:653:VAL:HG22	4:B:689:LEU:HB3	1.76	0.68
5:C:40:GLU:HA	5:C:163:ILE:HG21	1.74	0.68
5:C:73:GLN:HB3	5:C:131:HIS:H	1.58	0.68
10:H:59:ILE:HG22	10:H:60:ALA:H	1.58	0.68
13:K:58:PHE:HB3	13:K:76:GLN:HB3	1.76	0.68
3:A:1402:PHE:CE1	3:A:1403:GLU:HG3	2.28	0.67
7:E:55:ARG:C	7:E:57:MET:H	2.00	0.67
3:A:18:GLN:HB2	4:B:1215:ARG:HB2	1.77	0.67
4:B:113:TYR:HB3	4:B:114:PRO:HD2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:123:THR:OG1	4:B:458:LYS:HE2	1.94	0.67
5:C:189:THR:HG22	5:C:190:ASP:H	1.59	0.67
10:H:25:ARG:HA	10:H:41:ASP:HA	1.76	0.67
3:A:567:LYS:HB3	10:H:95:TYR:HA	1.76	0.67
4:B:1085:ILE:N	4:B:1085:ILE:HD12	2.09	0.67
5:C:40:GLU:HA	5:C:163:ILE:CG2	2.24	0.67
5:C:244:VAL:O	5:C:248:ILE:HG13	1.94	0.67
3:A:182:VAL:HG22	3:A:201:VAL:HA	1.75	0.67
3:A:224:PHE:CZ	3:A:234:MET:HE2	2.30	0.67
3:A:1094:VAL:HG12	3:A:1095:THR:H	1.60	0.67
4:B:859:TYR:CZ	4:B:941:LEU:HD12	2.30	0.67
6:D:56:ARG:HA	6:D:148:LEU:HD13	1.76	0.67
12:J:1:MET:N	12:J:57:ILE:H	1.81	0.67
3:A:963:ILE:HD11	3:A:1048:ASN:CB	2.25	0.67
4:B:467:GLY:H	4:B:475:SER:CB	2.07	0.67
4:B:654:ARG:H	4:B:657:HIS:CD2	2.12	0.67
4:B:1096:ARG:O	4:B:1097:HIS:HB2	1.93	0.67
5:C:35:ARG:HH12	13:K:41:THR:H	1.41	0.67
8:F:69:LEU:C	8:F:71:GLU:N	2.52	0.67
8:F:118:LEU:O	8:F:122:MET:HG3	1.95	0.67
3:A:666:ILE:H	4:B:1026:LEU:HD13	1.59	0.67
6:D:47:LEU:HD11	9:G:3:PHE:CD2	2.30	0.67
3:A:388:LEU:O	3:A:392:VAL:HG23	1.95	0.67
3:A:714:PHE:CB	11:I:97:MET:HE1	2.24	0.67
4:B:606:LYS:HD2	4:B:608:ASP:OD2	1.94	0.67
4:B:778:MET:HE1	4:B:1094:ARG:HD3	1.77	0.67
5:C:183:TRP:CZ2	5:C:207:CYS:HB3	2.30	0.67
7:E:207:ARG:HB2	7:E:207:ARG:HH11	1.60	0.67
10:H:64:ASN:O	10:H:65:LEU:HB2	1.94	0.67
3:A:253:ASN:HB3	4:B:935:ARG:CZ	2.24	0.67
3:A:1120:LEU:HD12	3:A:1120:LEU:H	1.59	0.67
4:B:408:LEU:HD22	4:B:545:ILE:HD12	1.77	0.67
4:B:603:LEU:HD13	4:B:608:ASP:HB2	1.77	0.67
5:C:34:ARG:O	5:C:38:ILE:HG13	1.95	0.67
6:D:134:THR:HG22	6:D:136:GLY:H	1.59	0.67
11:I:111:THR:HG22	11:I:112:SER:H	1.59	0.67
12:J:57:ILE:HA	12:J:60:PHE:CD2	2.30	0.67
2:T:8:C:H4'	3:A:447:GLN:NE2	2.09	0.67
3:A:92:HIS:O	3:A:94:GLY:N	2.28	0.67
3:A:335:ARG:HA	3:A:339:ASN:HB2	1.77	0.67
4:B:532:ALA:HA	4:B:535:LEU:HD12	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:133:ILE:CD1	5:C:237:SER:HA	2.25	0.67
6:D:13:ARG:HA	6:D:17:LYS:HZ3	1.59	0.67
3:A:152:VAL:HG12	3:A:153:PRO:HD2	1.77	0.67
3:A:1420:ASP:O	3:A:1421:CYS:HB2	1.95	0.67
4:B:604:ARG:NH1	4:B:691:GLU:OE2	2.28	0.67
3:A:34:LYS:HE2	3:A:57:ARG:NH1	2.10	0.66
5:C:251:LEU:O	5:C:255:VAL:HG23	1.96	0.66
8:F:130:ILE:HB	8:F:148:VAL:HG21	1.76	0.66
10:H:81:PRO:CB	10:H:82:PRO:HD2	2.25	0.66
11:I:52:ILE:HG13	11:I:52:ILE:O	1.95	0.66
11:I:55:THR:HG22	11:I:58:VAL:CG2	2.26	0.66
11:I:85:PHE:CD1	11:I:99:LEU:HD13	2.30	0.66
3:A:356:ASP:HB2	3:A:469:ARG:HH12	1.58	0.66
3:A:458:HIS:CE1	3:A:507:VAL:HG21	2.31	0.66
3:A:1100:ARG:O	3:A:1103:GLU:HB3	1.96	0.66
5:C:8:VAL:HG12	5:C:9:LYS:N	2.10	0.66
6:D:8:PHE:CE2	9:G:6:ASP:HB2	2.30	0.66
3:A:341:MET:HE2	3:A:843:LYS:HZ1	1.61	0.66
3:A:396:PRO:HG3	3:A:416:ARG:HB3	1.78	0.66
4:B:737:THR:HG21	11:I:66:PRO:HA	1.76	0.66
7:E:135:PHE:HB3	7:E:140:LEU:HD11	1.76	0.66
12:J:14:VAL:HG12	12:J:50:ILE:HD11	1.77	0.66
3:A:335:ARG:NH1	4:B:1202:LEU:HD13	2.10	0.66
3:A:466:SER:O	4:B:1103:ILE:HD11	1.94	0.66
3:A:1027:ALA:O	3:A:1031:VAL:HG23	1.95	0.66
3:A:746:MET:HE3	4:B:1018:PRO:HG2	1.76	0.66
3:A:798:GLY:HA2	3:A:815:PHE:CD1	2.30	0.66
3:A:1127:ASP:HB3	3:A:1130:GLN:CB	2.25	0.66
4:B:60:GLN:HE22	4:B:94:LYS:HA	1.61	0.66
5:C:35:ARG:NH1	13:K:41:THR:H	1.92	0.66
2:T:12:G:O2'	2:T:13:U:H3'	1.94	0.66
3:A:1100:ARG:HH21	3:A:1351:GLU:CG	2.07	0.66
4:B:955:THR:CG2	4:B:956:THR:N	2.59	0.66
4:B:999:MET:HB3	4:B:1007:VAL:HG21	1.76	0.66
3:A:698:GLN:HA	11:I:97:MET:O	1.96	0.66
3:A:1436:ILE:O	3:A:1437:GLY:C	2.39	0.66
4:B:361:LEU:HD21	4:B:377:PHE:CD2	2.31	0.66
4:B:792:MET:HA	4:B:856:PHE:O	1.96	0.66
6:D:40:HIS:CB	9:G:73:LYS:HZ3	1.93	0.66
8:F:116:ASP:HB3	8:F:119:ARG:HB2	1.78	0.66
3:A:254:GLU:O	3:A:256:GLN:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:856:THR:HB	3:A:865:GLN:HB2	1.77	0.66
4:B:642:ASP:O	4:B:644:GLU:N	2.28	0.66
4:B:857:ARG:HD2	4:B:945:GLU:OE1	1.94	0.66
3:A:541:ILE:HG22	3:A:546:VAL:HG23	1.76	0.66
4:B:121:ASN:HA	4:B:207:GLY:CA	2.26	0.66
4:B:999:MET:HA	4:B:999:MET:CE	2.26	0.66
9:G:96:GLN:HG3	9:G:97:HIS:HD2	1.60	0.66
3:A:63:ARG:HD3	3:A:74:MET:CE	2.26	0.66
3:A:1372:VAL:O	3:A:1376:THR:HG22	1.95	0.66
4:B:35:SER:HA	4:B:811:TYR:HE2	1.61	0.66
4:B:114:PRO:HG3	4:B:181:LEU:HD11	1.77	0.66
4:B:525:ALA:O	4:B:768:THR:HA	1.96	0.66
4:B:1023:VAL:O	4:B:1026:LEU:HB2	1.95	0.66
6:D:58:VAL:HG11	9:G:4:ILE:HD11	1.78	0.66
13:K:65:HIS:CD2	13:K:67:PHE:HB2	2.31	0.66
3:A:1094:VAL:HG13	3:A:1113:THR:HG21	1.77	0.65
3:A:1373:ASP:HA	3:A:1376:THR:CG2	2.26	0.65
4:B:830:TYR:O	4:B:832:GLY:N	2.29	0.65
5:C:11:ARG:HD3	5:C:209:TYR:CE2	2.31	0.65
5:C:161:LYS:O	5:C:170:TRP:NE1	2.28	0.65
3:A:87:ALA:HB3	3:A:276:LEU:HD23	1.77	0.65
3:A:590:ARG:NH2	3:A:620:LYS:CB	2.59	0.65
3:A:842:VAL:HG11	4:B:1136:ASP:OD2	1.95	0.65
6:D:47:LEU:HD11	9:G:3:PHE:CE2	2.31	0.65
11:I:76:PRO:CG	11:I:110:PHE:HB3	2.27	0.65
4:B:39:ARG:HG2	4:B:39:ARG:HH11	1.61	0.65
4:B:364:ILE:HG12	4:B:585:VAL:CG1	2.25	0.65
5:C:146:LYS:HB2	12:J:61:LEU:HD11	1.78	0.65
6:D:130:LEU:O	6:D:132:GLN:N	2.29	0.65
10:H:42:ILE:HG23	10:H:95:TYR:HE1	1.61	0.65
10:H:81:PRO:HB2	10:H:82:PRO:HD2	1.78	0.65
3:A:35:ILE:HA	3:A:52:GLY:O	1.97	0.65
3:A:254:GLU:HG3	4:B:935:ARG:HH22	1.60	0.65
3:A:1130:GLN:HE21	3:A:1134:ILE:HD11	1.61	0.65
3:A:1164:PRO:HG2	3:A:1165:GLU:H	1.59	0.65
4:B:799:PRO:HB3	4:B:818:PRO:HG2	1.77	0.65
4:B:1162:ILE:HD11	4:B:1194:ILE:CD1	2.27	0.65
11:I:58:VAL:HG13	11:I:62:ILE:HD13	1.78	0.65
4:B:351:TYR:CE1	4:B:355:ILE:HD11	2.32	0.65
4:B:763:GLN:HG2	4:B:765:PRO:HD2	1.79	0.65
7:E:176:PRO:O	7:E:212:ARG:HA	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:1:MET:HG3	9:G:85:GLU:OE2	1.96	0.65
3:A:356:ASP:OD2	13:K:65:HIS:HE1	1.78	0.65
3:A:416:ARG:C	3:A:417:TYR:HD2	2.05	0.65
3:A:450:LEU:HB3	3:A:838:GLN:HE21	1.61	0.65
4:B:601:ARG:O	4:B:605:ARG:HG3	1.97	0.65
8:F:111:LEU:HD12	8:F:111:LEU:H	1.60	0.65
13:K:31:VAL:HG12	13:K:32:VAL:N	2.12	0.65
14:L:70:ARG:HG2	14:L:70:ARG:HH11	1.62	0.65
3:A:211:PHE:HA	3:A:214:ILE:HG13	1.78	0.65
3:A:896:ARG:HD3	3:A:897:TYR:CE1	2.31	0.65
3:A:1038:THR:H	3:A:1041:ALA:HB3	1.62	0.65
4:B:807:ARG:HG2	4:B:1045:SER:OG	1.97	0.65
10:H:62:SER:HB2	10:H:64:ASN:HD22	1.61	0.65
3:A:809:THR:H	3:A:812:GLU:HB2	1.62	0.65
4:B:294:ASP:O	4:B:296:GLU:N	2.29	0.65
4:B:549:THR:HB	4:B:628:THR:OG1	1.97	0.65
9:G:122:ASN:HD22	9:G:125:SER:HB3	1.61	0.65
3:A:698:GLN:NE2	11:I:99:LEU:HD21	2.12	0.65
3:A:743:VAL:O	3:A:747:VAL:HG23	1.97	0.65
4:B:515:HIS:CD2	4:B:517:THR:H	2.15	0.65
4:B:953:LEU:HD21	4:B:965:LYS:HB2	1.78	0.65
7:E:93:MET:HE3	7:E:120:ALA:O	1.96	0.65
2:T:13:U:O2'	2:T:14:C:H6	1.80	0.65
3:A:475:THR:HG23	3:A:476:SER:N	2.10	0.65
3:A:596:THR:C	3:A:598:LEU:H	2.05	0.65
4:B:38:PHE:HD1	4:B:811:TYR:CD2	2.15	0.65
4:B:782:LEU:HD12	4:B:788:ARG:HH11	1.62	0.65
4:B:842:ASN:O	4:B:846:ILE:HG13	1.97	0.65
4:B:1180:PHE:HB3	4:B:1191:ILE:HD12	1.77	0.65
6:D:29:LEU:HB3	9:G:82:PHE:HE2	1.60	0.65
9:G:18:PHE:HA	9:G:22:MET:CE	2.27	0.65
3:A:366:VAL:HG21	3:A:460:VAL:HG22	1.78	0.64
3:A:1118:VAL:O	3:A:1305:VAL:HG13	1.97	0.64
4:B:1069:PHE:H	4:B:1069:PHE:HD1	1.44	0.64
5:C:39:ALA:CA	5:C:164:ALA:HB3	2.26	0.64
4:B:185:THR:H	4:B:188:ASP:HB2	1.62	0.64
6:D:67:ARG:HB2	6:D:133:THR:HG21	1.78	0.64
9:G:51:TYR:C	9:G:51:TYR:CD2	2.75	0.64
3:A:547:LEU:HD22	13:K:58:PHE:CE1	2.32	0.64
3:A:628:GLY:O	3:A:632:VAL:HG23	1.97	0.64
4:B:1159:ARG:NE	4:B:1193:GLN:HE21	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:174:ALA:HB2	5:C:235:VAL:HG22	1.80	0.64
3:A:738:LYS:HD2	3:A:740:LEU:HD21	1.80	0.64
3:A:853:ASP:OD1	3:A:855:THR:HB	1.98	0.64
4:B:705:MET:H	4:B:710:LEU:CD1	2.11	0.64
6:D:29:LEU:HD22	9:G:82:PHE:CE2	2.32	0.64
8:F:68:THR:HB	8:F:71:GLU:HB2	1.80	0.64
3:A:88:LYS:HE3	3:A:280:GLU:OE2	1.98	0.64
3:A:215:SER:HB3	3:A:218:ASP:HB2	1.79	0.64
5:C:18:VAL:HG23	5:C:240:VAL:HB	1.80	0.64
9:G:45:ILE:HD13	9:G:78:VAL:HG13	1.78	0.64
11:I:55:THR:HG23	11:I:86:PHE:HZ	1.62	0.64
3:A:1317:MET:O	3:A:1322:ILE:HD11	1.96	0.64
4:B:46:GLN:HG3	4:B:47:GLN:H	1.62	0.64
4:B:705:MET:HA	4:B:705:MET:HE3	1.79	0.64
4:B:865:LYS:NZ	4:B:869:SER:HA	2.12	0.64
4:B:955:THR:HG22	4:B:956:THR:H	1.61	0.64
5:C:67:LEU:HD11	5:C:155:LEU:CD1	2.27	0.64
7:E:198:ILE:HD11	7:E:212:ARG:CG	2.28	0.64
8:F:90:ARG:HD3	8:F:155:LEU:HD11	1.79	0.64
3:A:144:THR:O	3:A:146:MET:HE2	1.97	0.64
3:A:325:ILE:HG22	4:B:1210:MET:HE2	1.80	0.64
3:A:537:ARG:HD2	10:H:20:TYR:CE1	2.33	0.64
3:A:886:ILE:HG13	3:A:943:LEU:HD12	1.78	0.64
4:B:798:TYR:HE2	5:C:62:PHE:CZ	2.16	0.64
9:G:1:MET:HE1	9:G:80:LYS:N	2.13	0.64
3:A:42:ASP:HB3	3:A:45:GLN:H	1.63	0.64
3:A:844:ALA:O	3:A:845:LEU:HD23	1.97	0.64
4:B:603:LEU:HD12	4:B:609:ILE:HG13	1.80	0.64
4:B:955:THR:CG2	4:B:956:THR:H	2.11	0.64
4:B:1002:THR:CG2	4:B:1006:ILE:HG13	2.27	0.64
7:E:114:ASN:O	7:E:115:ASN:HB3	1.97	0.64
8:F:99:LEU:O	8:F:99:LEU:HD12	1.96	0.64
9:G:119:LEU:HD13	9:G:132:SER:HB2	1.80	0.64
3:A:372:LYS:HA	3:A:435:HIS:ND1	2.13	0.64
5:C:6:PRO:CB	5:C:25:VAL:HG12	2.28	0.64
9:G:1:MET:HE1	9:G:80:LYS:H	1.61	0.64
3:A:55:ASP:C	3:A:57:ARG:H	2.05	0.63
3:A:79:GLY:HA3	3:A:243:PRO:CG	2.29	0.63
3:A:154:SER:HB3	3:A:162:VAL:HG21	1.79	0.63
3:A:441:PRO:HD2	3:A:498:ARG:NH2	2.13	0.63
3:A:590:ARG:HH21	3:A:620:LYS:HB3	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:616:VAL:HG12	3:A:617:VAL:H	1.64	0.63
4:B:434:ARG:O	4:B:437:GLU:HB2	1.98	0.63
3:A:215:SER:HB3	3:A:218:ASP:OD2	1.99	0.63
3:A:728:LYS:O	3:A:732:LEU:HG	1.97	0.63
3:A:1313:LEU:HD23	3:A:1338:VAL:HG21	1.80	0.63
3:A:1329:THR:CG2	3:A:1331:SER:H	2.06	0.63
3:A:1438:THR:HB	4:B:1144:ALA:CB	2.28	0.63
4:B:847:ASP:HB3	5:C:167:HIS:CD2	2.34	0.63
8:F:103:MET:HE3	9:G:66:GLY:H	1.61	0.63
3:A:105:CYS:O	3:A:114:LEU:HG	1.98	0.63
3:A:914:GLU:HB2	3:A:979:SER:O	1.98	0.63
4:B:824:ILE:CG2	4:B:1087:PHE:HE2	2.12	0.63
4:B:1138:MET:HE2	4:B:1146:PHE:CD2	2.34	0.63
5:C:253:LYS:O	5:C:256:ALA:HB3	1.98	0.63
3:A:168:GLY:O	3:A:169:ASN:C	2.42	0.63
3:A:310:GLY:O	3:A:312:PRO:HD2	1.99	0.63
4:B:273:LEU:HD12	4:B:280:ILE:HD12	1.80	0.63
4:B:411:PRO:O	4:B:414:ALA:HB3	1.97	0.63
5:C:67:LEU:HA	5:C:70:ILE:HD12	1.79	0.63
6:D:71:LYS:HA	6:D:74:GLN:HB2	1.79	0.63
7:E:192:ARG:HG3	7:E:192:ARG:NH1	2.13	0.63
8:F:130:ILE:O	8:F:148:VAL:HG21	1.98	0.63
3:A:567:LYS:HB2	3:A:568:PRO:CD	2.29	0.63
4:B:305:VAL:O	4:B:305:VAL:HG12	1.99	0.63
4:B:952:VAL:HG12	4:B:953:LEU:N	2.13	0.63
11:I:34:TYR:CE2	11:I:36:GLU:HB3	2.33	0.63
12:J:3:VAL:HG21	12:J:18:TRP:CG	2.34	0.63
3:A:34:LYS:O	3:A:35:ILE:HB	1.99	0.63
4:B:227:LYS:HB2	4:B:395:GLN:OE1	1.98	0.63
5:C:179:GLU:HG2	5:C:180:TYR:N	2.13	0.63
3:A:144:THR:O	3:A:146:MET:HG3	1.98	0.63
3:A:984:LYS:O	3:A:988:LEU:HB2	1.98	0.63
4:B:1001:PHE:CZ	4:B:1073:TYR:HB2	2.33	0.63
5:C:101:LEU:HD13	5:C:118:LEU:CD2	2.27	0.63
6:D:134:THR:CG2	6:D:135:GLY:H	2.10	0.63
6:D:134:THR:CG2	6:D:135:GLY:N	2.61	0.63
7:E:5:ASN:O	7:E:9:ILE:HG13	1.98	0.63
9:G:1:MET:HE2	9:G:3:PHE:HE1	1.64	0.63
3:A:871:ASP:OD2	3:A:873:MET:HB2	1.98	0.63
5:C:45:ALA:HA	5:C:72:LEU:CD1	2.28	0.63
12:J:2:ILE:H	12:J:57:ILE:CG2	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:13:U:HO2'	2:T:14:C:C5'	2.08	0.62
3:A:1006:ILE:HD12	7:E:163:GLU:HG3	1.80	0.62
4:B:557:PHE:C	4:B:557:PHE:CD2	2.76	0.62
4:B:792:MET:HG3	4:B:855:PHE:CE1	2.34	0.62
5:C:73:GLN:CB	5:C:131:HIS:H	2.11	0.62
3:A:858:ASN:ND2	3:A:860:LEU:H	1.97	0.62
4:B:219:ALA:HB2	4:B:405:ARG:NH1	2.14	0.62
4:B:363:HIS:O	4:B:364:ILE:HB	1.99	0.62
6:D:22:GLU:H	6:D:22:GLU:CD	2.07	0.62
3:A:427:GLN:HB2	3:A:430:TRP:CE2	2.34	0.62
3:A:442:VAL:HG21	3:A:460:VAL:HG23	1.80	0.62
3:A:685:GLU:HG3	3:A:686:ALA:N	2.15	0.62
3:A:1385:THR:HG22	3:A:1386:ARG:N	2.13	0.62
5:C:17:ASN:O	5:C:18:VAL:HG23	1.99	0.62
10:H:62:SER:C	10:H:64:ASN:H	2.06	0.62
3:A:7:SER:HB3	4:B:1175:LEU:HD22	1.81	0.62
3:A:69:THR:C	3:A:71:GLN:N	2.56	0.62
4:B:429:PHE:HA	4:B:432:MET:HE3	1.80	0.62
4:B:658:ILE:HG22	4:B:662:MET:HE2	1.81	0.62
4:B:792:MET:HG3	4:B:855:PHE:HE1	1.64	0.62
4:B:997:GLU:CD	4:B:997:GLU:H	2.06	0.62
3:A:55:ASP:CG	3:A:55:ASP:O	2.41	0.62
4:B:842:ASN:HD22	4:B:845:SER:CB	2.13	0.62
4:B:1099:VAL:CG1	4:B:1100:ASP:N	2.62	0.62
9:G:165:GLU:HB2	9:G:168:LEU:HD12	1.80	0.62
10:H:139:ASN:O	10:H:140:ALA:HB2	1.99	0.62
12:J:44:TYR:HD2	12:J:44:TYR:N	1.98	0.62
4:B:516:ASN:N	4:B:516:ASN:ND2	2.46	0.62
9:G:51:TYR:O	9:G:54:ILE:HG13	1.99	0.62
3:A:202:LEU:HB3	3:A:207:ILE:HD11	1.81	0.62
3:A:252:PHE:O	3:A:253:ASN:HB2	1.99	0.62
3:A:714:PHE:O	3:A:718:VAL:HG23	2.00	0.62
4:B:218:SER:HB3	4:B:241:ARG:NH1	2.15	0.62
4:B:1180:PHE:O	4:B:1181:GLU:O	2.18	0.62
6:D:12:ARG:NE	6:D:14:ARG:HD2	2.15	0.62
7:E:22:MET:CE	7:E:26:ARG:HH21	2.12	0.62
7:E:124:VAL:HG13	7:E:132:ILE:HB	1.81	0.62
12:J:44:TYR:HA	12:J:47:ARG:CB	2.30	0.62
13:K:42:LEU:CD2	13:K:46:ILE:HD11	2.30	0.62
3:A:215:SER:HB3	3:A:218:ASP:CG	2.24	0.62
3:A:1036:ARG:HG2	3:A:1036:ARG:HH11	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1375:MET:HE3	3:A:1384:VAL:HG23	1.82	0.62
7:E:213:ILE:HG12	7:E:214:CYS:N	2.13	0.62
13:K:60:ALA:O	13:K:73:LEU:HD12	1.99	0.62
4:B:224:GLN:HA	4:B:396:ASP:OD2	2.00	0.62
4:B:616:ILE:HD12	4:B:616:ILE:N	2.14	0.62
5:C:69:LEU:N	5:C:69:LEU:HD12	2.15	0.62
7:E:124:VAL:HA	7:E:132:ILE:HD12	1.82	0.62
8:F:89:GLU:OE2	8:F:134:ILE:HG21	1.99	0.62
14:L:27:LEU:O	14:L:28:LYS:HG2	2.00	0.62
3:A:767:GLN:HE22	3:A:774:ARG:HB3	1.62	0.61
3:A:993:LEU:HD22	3:A:1046:LEU:CD2	2.30	0.61
4:B:751:VAL:HG13	4:B:812:LEU:HD22	1.81	0.61
4:B:1106:ARG:NH2	4:B:1111:MET:HE2	2.15	0.61
4:B:373:ARG:HG3	4:B:566:LEU:HD23	1.80	0.61
4:B:744:HIS:HD2	4:B:746:SER:OG	1.82	0.61
6:D:4:SER:O	6:D:5:THR:HB	1.99	0.61
3:A:42:ASP:C	3:A:44:THR:H	2.06	0.61
3:A:399:HIS:HB3	3:A:400:PRO:CD	2.29	0.61
3:A:785:PRO:HG2	3:A:786:HIS:HD2	1.65	0.61
3:A:786:HIS:N	3:A:786:HIS:CD2	2.67	0.61
3:A:870:GLU:HG2	7:E:208:TYR:CG	2.36	0.61
3:A:1095:THR:O	3:A:1095:THR:HG22	2.00	0.61
3:A:1227:ILE:HG22	3:A:1228:TRP:N	2.14	0.61
3:A:1348:LEU:O	3:A:1352:VAL:HG23	2.00	0.61
4:B:1183:LYS:N	4:B:1183:LYS:CE	2.62	0.61
4:B:1181:GLU:HG3	4:B:1188:LYS:HE3	1.80	0.61
5:C:20:PHE:HE1	5:C:22:LEU:HD12	1.65	0.61
9:G:131:GLN:HG2	9:G:136:VAL:HG22	1.83	0.61
3:A:107:CYS:N	3:A:114:LEU:HD21	2.15	0.61
3:A:115:LEU:CB	3:A:122:MET:HE2	2.25	0.61
3:A:1114:PRO:O	3:A:1115:SER:O	2.18	0.61
3:A:1174:PHE:C	3:A:1176:LEU:N	2.53	0.61
4:B:58:THR:O	4:B:62:ILE:HG13	2.00	0.61
4:B:745:PRO:C	4:B:747:MET:H	2.08	0.61
4:B:1002:THR:O	4:B:1004:GLU:N	2.32	0.61
7:E:144:ILE:HG13	7:E:145:THR:N	2.14	0.61
3:A:818:MET:HA	4:B:514:LEU:HB3	1.82	0.61
3:A:984:LYS:HG2	3:A:988:LEU:HD12	1.81	0.61
4:B:217:ARG:HE	4:B:405:ARG:HB2	1.66	0.61
4:B:515:HIS:CD2	4:B:516:ASN:N	2.69	0.61
4:B:1138:MET:HE2	4:B:1146:PHE:HD2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:22:MET:HE3	7:E:26:ARG:NH2	2.16	0.61
9:G:48:VAL:HG13	9:G:74:TYR:HD1	1.65	0.61
10:H:84:ALA:CB	10:H:87:ARG:HB2	2.29	0.61
3:A:349:ALA:C	4:B:1128:LEU:HD11	2.25	0.61
3:A:418:SER:C	3:A:420:ARG:H	2.08	0.61
3:A:567:LYS:CB	10:H:95:TYR:HA	2.30	0.61
3:A:1121:GLU:CG	3:A:1122:PRO:HD2	2.30	0.61
3:A:1224:LEU:HD11	3:A:1240:CYS:HB2	1.83	0.61
4:B:118:ARG:HH22	4:B:194:GLU:CD	2.08	0.61
4:B:1177:HIS:HB2	4:B:1179:GLN:NE2	2.12	0.61
5:C:45:ALA:HA	5:C:72:LEU:HD13	1.83	0.61
5:C:107:SER:C	5:C:109:SER:H	2.09	0.61
7:E:22:MET:HE3	7:E:26:ARG:HH21	1.65	0.61
3:A:1279:ILE:HD11	3:A:1316:VAL:HG21	1.83	0.61
3:A:87:ALA:HB1	3:A:276:LEU:HD23	1.82	0.61
3:A:1226:VAL:HG22	3:A:1240:CYS:HB3	1.83	0.61
3:A:1313:LEU:O	3:A:1315:GLU:N	2.34	0.61
4:B:278:GLN:HG2	4:B:279:ASP:H	1.65	0.61
4:B:393:LYS:HA	4:B:393:LYS:HE3	1.82	0.61
4:B:557:PHE:C	4:B:557:PHE:HD2	2.08	0.61
4:B:842:ASN:HB3	4:B:845:SER:OG	2.00	0.61
7:E:84:ASP:O	7:E:86:PRO:HD3	2.00	0.61
9:G:39:THR:HG22	9:G:40:GLY:N	2.12	0.61
3:A:268:ASP:HB3	3:A:299:HIS:ND1	2.16	0.61
3:A:1206:ASP:HB3	3:A:1274:ARG:HH12	1.65	0.61
4:B:39:ARG:HH21	4:B:665:GLU:HG2	1.64	0.61
4:B:428:ILE:HG22	4:B:432:MET:HE2	1.82	0.61
4:B:900:ALA:O	4:B:903:VAL:HG23	2.01	0.61
5:C:112:ASN:HB2	5:C:114:TYR:CE1	2.36	0.61
2:T:12:G:HO2'	2:T:13:U:C5'	2.11	0.60
3:A:1451:VAL:O	3:A:1454:MET:HG2	2.00	0.60
4:B:291:ILE:HD13	4:B:300:HIS:NE2	2.16	0.60
4:B:583:ASN:ND2	4:B:628:THR:HG22	2.09	0.60
5:C:66:ARG:CZ	12:J:2:ILE:HG21	2.30	0.60
5:C:98:VAL:HG23	5:C:122:SER:HB3	1.82	0.60
5:C:105:GLY:HA3	5:C:149:LYS:O	2.00	0.60
7:E:207:ARG:HH11	7:E:207:ARG:CB	2.14	0.60
11:I:61:ASP:C	11:I:63:GLY:H	2.09	0.60
3:A:549:MET:SD	3:A:577:ILE:HD11	2.41	0.60
3:A:552:TRP:HE3	3:A:651:LYS:HB3	1.66	0.60
3:A:1305:VAL:HG12	3:A:1306:LEU:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1348:LEU:HG	3:A:1372:VAL:HG23	1.82	0.60
4:B:97:VAL:HG12	4:B:178:ASN:HD21	1.65	0.60
4:B:166:PHE:C	4:B:167:ILE:HG13	2.25	0.60
4:B:234:ILE:HG12	4:B:257:LYS:HD3	1.83	0.60
4:B:770:GLN:CD	4:B:983:ARG:HA	2.26	0.60
4:B:803:LEU:HD13	4:B:1032:SER:HB3	1.82	0.60
4:B:1180:PHE:HB3	4:B:1191:ILE:CD1	2.31	0.60
6:D:24:ALA:C	6:D:26:THR:H	2.09	0.60
6:D:173:HIS:ND1	6:D:174:PRO:HD2	2.16	0.60
9:G:39:THR:HG22	9:G:41:LYS:H	1.64	0.60
1:P:11:C:H2'	1:P:12:C:C6	2.35	0.60
3:A:381:THR:CG2	3:A:383:TYR:H	2.14	0.60
3:A:578:LEU:HD23	3:A:612:ILE:CD1	2.31	0.60
3:A:672:ASP:HB2	3:A:736:ASN:OD1	2.01	0.60
3:A:1174:PHE:C	3:A:1176:LEU:H	2.07	0.60
3:A:1293:SER:OG	3:A:1294:PRO:HD2	2.01	0.60
4:B:796:LEU:HD12	4:B:852:ARG:O	2.01	0.60
4:B:839:MET:HE1	4:B:980:PHE:HB2	1.82	0.60
5:C:98:VAL:C	5:C:99:LEU:HD22	2.25	0.60
5:C:175:ALA:HB2	12:J:10:CYS:HB2	1.82	0.60
5:C:187:LYS:C	5:C:189:THR:H	2.10	0.60
5:C:238:ILE:CG2	5:C:242:GLN:HB2	2.31	0.60
10:H:11:GLN:HA	10:H:53:ASP:O	2.01	0.60
11:I:55:THR:HG23	11:I:86:PHE:CZ	2.37	0.60
2:T:13:U:C2'	2:T:14:C:O5'	2.49	0.60
3:A:11:LEU:O	3:A:11:LEU:HD23	2.01	0.60
3:A:401:GLY:C	3:A:435:HIS:HD2	2.09	0.60
3:A:471:ASN:OD1	3:A:472:LEU:N	2.34	0.60
4:B:364:ILE:CG1	4:B:585:VAL:HG13	2.25	0.60
4:B:378:LEU:O	4:B:382:ILE:HG13	2.01	0.60
4:B:866:TYR:HB2	4:B:870:ILE:HB	1.83	0.60
6:D:192:LYS:HE3	6:D:204:ASP:OD1	2.02	0.60
3:A:41:MET:HB3	3:A:49:LYS:HA	1.83	0.60
3:A:423:ASP:O	3:A:424:ILE:HB	2.02	0.60
3:A:1073:GLY:O	3:A:1076:ALA:HB3	2.02	0.60
4:B:547:VAL:HG12	4:B:612:GLU:OE2	2.01	0.60
4:B:1001:PHE:CD2	5:C:34:ARG:NH2	2.69	0.60
4:B:1034:VAL:HG12	4:B:1035:ALA:N	2.16	0.60
12:J:44:TYR:N	12:J:44:TYR:CD2	2.68	0.60
3:A:600:PRO:HG2	3:A:601:LYS:H	1.65	0.60
3:A:829:VAL:C	3:A:831:THR:H	2.10	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:852:TYR:CD2	3:A:1060:PRO:HB2	2.37	0.60
4:B:976:ILE:O	4:B:990:ILE:HB	2.01	0.60
4:B:1031:LEU:HD11	4:B:1042:GLY:HA3	1.84	0.60
4:B:1115:THR:O	4:B:1116:ARG:HB2	2.02	0.60
11:I:106:CYS:O	11:I:107:SER:HB2	2.02	0.60
12:J:27:GLU:C	12:J:29:GLU:H	2.10	0.60
13:K:53:ASP:OD1	13:K:55:LYS:HB2	2.02	0.60
3:A:565:ILE:O	3:A:570:PRO:HA	2.02	0.60
4:B:269:ILE:HD11	4:B:386:LEU:HD21	1.83	0.60
4:B:873:THR:O	4:B:914:LYS:HA	2.02	0.60
7:E:55:ARG:C	7:E:57:MET:N	2.60	0.60
11:I:25:LEU:HB3	11:I:38:ALA:HB2	1.82	0.60
13:K:47:ARG:C	13:K:47:ARG:HD2	2.27	0.60
3:A:34:LYS:HG2	3:A:57:ARG:HH22	1.66	0.60
3:A:709:THR:HB	3:A:712:GLU:HG3	1.83	0.60
3:A:1004:ASN:O	3:A:1008:GLN:HB2	2.01	0.60
4:B:232:SER:HB3	4:B:261:ARG:NH2	2.17	0.60
4:B:821:GLN:HE22	4:B:851:PHE:HA	1.67	0.60
4:B:847:ASP:C	4:B:849:GLY:N	2.59	0.60
7:E:39:LEU:O	7:E:42:PHE:HB3	2.01	0.60
3:A:709:THR:HG22	3:A:710:LEU:N	2.17	0.60
5:C:144:ILE:O	5:C:145:CYS:HB3	2.01	0.60
5:C:168:ALA:C	5:C:170:TRP:H	2.10	0.60
5:C:263:THR:C	5:C:265:MET:H	2.09	0.60
9:G:27:LYS:HE2	9:G:54:ILE:HB	1.84	0.60
10:H:48:PRO:O	10:H:49:VAL:HG23	2.02	0.60
11:I:101:PHE:N	11:I:101:PHE:CD1	2.70	0.60
13:K:101:LEU:O	13:K:101:LEU:HD23	2.01	0.60
3:A:14:VAL:N	3:A:1432:GLN:HE22	2.00	0.60
3:A:56:PRO:O	3:A:57:ARG:NE	2.35	0.60
3:A:284:ALA:O	3:A:286:HIS:N	2.34	0.60
3:A:567:LYS:CB	3:A:568:PRO:CD	2.80	0.60
3:A:683:ILE:HD13	3:A:801:GLU:HG3	1.84	0.60
4:B:100:PRO:HD3	4:B:172:ILE:HD12	1.84	0.60
10:H:84:ALA:CA	10:H:87:ARG:HB2	2.32	0.60
3:A:12:ARG:HE	4:B:1192:TYR:HE2	1.50	0.59
3:A:49:LYS:HZ1	3:A:61:ILE:HG13	1.65	0.59
3:A:53:LEU:HD22	3:A:54:ASN:HD22	1.66	0.59
3:A:427:GLN:HG3	3:A:430:TRP:CZ2	2.36	0.59
4:B:483:LEU:HD11	4:B:491:THR:CG2	2.31	0.59
7:E:13:TRP:O	7:E:16:PHE:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:35:GLU:OE2	9:G:48:VAL:HG23	2.01	0.59
3:A:683:ILE:HG21	3:A:801:GLU:HG3	1.84	0.59
3:A:768:GLN:CG	3:A:816:HIS:HA	2.31	0.59
3:A:1076:ALA:HA	3:A:1079:MET:CE	2.31	0.59
3:A:1289:ARG:HD2	3:A:1303:GLU:OE2	2.02	0.59
3:A:1341:ILE:HG23	3:A:1342:GLU:N	2.18	0.59
4:B:431:TYR:CE2	4:B:447:ALA:HB2	2.37	0.59
4:B:696:GLU:O	4:B:699:GLU:HB2	2.02	0.59
6:D:119:ARG:HD3	6:D:221:TYR:CE2	2.37	0.59
7:E:78:LEU:HD21	7:E:80:VAL:HG23	1.83	0.59
9:G:1:MET:HE3	9:G:80:LYS:O	2.02	0.59
9:G:117:GLN:C	9:G:119:LEU:H	2.09	0.59
3:A:369:SER:HB2	13:K:2:ASN:OD1	2.02	0.59
3:A:407:ARG:HG2	3:A:430:TRP:CZ2	2.37	0.59
4:B:487:THR:O	4:B:490:SER:HB3	2.02	0.59
8:F:90:ARG:HG3	8:F:91:ALA:N	2.17	0.59
9:G:144:ARG:HG2	9:G:168:LEU:HD23	1.84	0.59
10:H:81:PRO:CB	10:H:82:PRO:CD	2.81	0.59
10:H:95:TYR:HB3	10:H:144:ILE:HB	1.84	0.59
3:A:14:VAL:H	3:A:1432:GLN:HE22	1.50	0.59
3:A:90:VAL:CG1	3:A:297:GLN:HA	2.32	0.59
3:A:414:ASP:OD1	3:A:416:ARG:HG2	2.02	0.59
4:B:265:SER:O	4:B:266:ALA:HB3	2.03	0.59
4:B:446:LEU:O	4:B:447:ALA:HB3	2.02	0.59
4:B:871:THR:HG22	4:B:872:GLU:O	2.01	0.59
5:C:238:ILE:HG22	5:C:243:VAL:HG23	1.84	0.59
6:D:7:THR:HG21	6:D:32:GLU:OE2	2.01	0.59
9:G:1:MET:O	9:G:3:PHE:CD1	2.56	0.59
3:A:34:LYS:HB3	3:A:36:ARG:HE	1.67	0.59
3:A:49:LYS:NZ	3:A:61:ILE:HG13	2.18	0.59
3:A:53:LEU:CD2	3:A:54:ASN:HD22	2.15	0.59
3:A:224:PHE:CE2	3:A:231:PRO:HG3	2.37	0.59
3:A:630:ILE:HD13	3:A:646:PHE:CZ	2.38	0.59
3:A:682:THR:HA	3:A:685:GLU:HG2	1.85	0.59
4:B:705:MET:N	4:B:710:LEU:HD12	2.18	0.59
4:B:803:LEU:CD1	4:B:1032:SER:HB3	2.32	0.59
4:B:1077:THR:HG22	13:K:44:ASN:ND2	2.17	0.59
5:C:165:LYS:O	13:K:6:ARG:NH1	2.35	0.59
3:A:496:GLU:O	3:A:499:ALA:HB3	2.02	0.59
3:A:547:LEU:HD22	13:K:58:PHE:CD1	2.38	0.59
3:A:710:LEU:HD13	11:I:94:ASP:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:745:PRO:O	4:B:747:MET:N	2.35	0.59
7:E:60:PHE:CE2	7:E:80:VAL:HB	2.37	0.59
7:E:157:SER:C	7:E:159:ASP:N	2.60	0.59
7:E:212:ARG:HG3	7:E:212:ARG:HH11	1.68	0.59
10:H:58:THR:HB	10:H:143:LEU:HD13	1.84	0.59
12:J:48:ARG:HE	12:J:49:MET:CE	2.14	0.59
3:A:34:LYS:HE2	3:A:57:ARG:CZ	2.33	0.59
3:A:53:LEU:CD2	3:A:54:ASN:N	2.55	0.59
3:A:60:SER:C	3:A:61:ILE:HG13	2.26	0.59
3:A:90:VAL:HG13	3:A:297:GLN:HA	1.84	0.59
3:A:981:LEU:CD2	3:A:1039:LYS:HA	2.33	0.59
3:A:1198:ASP:O	3:A:1202:MET:HG2	2.02	0.59
3:A:1242:VAL:HG12	3:A:1243:VAL:N	2.18	0.59
3:A:1447:GLU:OE2	9:G:23:LYS:HB2	2.02	0.59
4:B:824:ILE:HG23	4:B:1087:PHE:HE2	1.68	0.59
3:A:1171:GLN:HA	3:A:1174:PHE:HD1	1.68	0.59
4:B:39:ARG:HH21	4:B:665:GLU:CD	2.11	0.59
4:B:309:GLN:HG3	11:I:52:ILE:CD1	2.33	0.59
4:B:653:VAL:CG2	4:B:689:LEU:HB3	2.32	0.59
4:B:1187:ASN:O	4:B:1188:LYS:CB	2.51	0.59
3:A:427:GLN:HB2	3:A:430:TRP:NE1	2.18	0.59
4:B:641:GLU:HB3	4:B:643:ASP:OD2	2.03	0.59
6:D:29:LEU:HD13	9:G:82:PHE:CZ	2.37	0.59
9:G:49:LEU:HG	9:G:76:ALA:HA	1.83	0.59
11:I:50:THR:HG22	11:I:51:ASN:N	2.16	0.59
14:L:38:LEU:O	14:L:39:SER:HB3	2.01	0.59
3:A:34:LYS:NZ	3:A:57:ARG:NH1	2.50	0.59
3:A:783:THR:HG21	3:A:815:PHE:CE2	2.38	0.59
3:A:855:THR:CG2	3:A:857:ARG:HE	2.13	0.59
3:A:1370:LEU:O	3:A:1374:VAL:HG23	2.03	0.59
4:B:247:GLY:H	4:B:418:LYS:HZ3	1.49	0.59
5:C:203:GLN:HG2	5:C:207:CYS:SG	2.41	0.59
9:G:88:ASP:OD2	9:G:88:ASP:N	2.35	0.59
12:J:14:VAL:HG12	12:J:14:VAL:O	2.03	0.59
3:A:23:SER:HB3	3:A:233:TRP:CZ2	2.38	0.58
3:A:332:LYS:H	3:A:337:ARG:HB3	1.68	0.58
3:A:722:LEU:HD22	3:A:799:PHE:CD1	2.37	0.58
3:A:1030:ARG:NH1	3:A:1035:TYR:OH	2.35	0.58
4:B:221:ASN:N	4:B:241:ARG:O	2.30	0.58
4:B:546:SER:OG	4:B:631:GLY:N	2.32	0.58
3:A:897:TYR:HD2	3:A:936:LEU:HD13	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:911:ILE:HD11	4:B:941:LEU:HD13	1.86	0.58
5:C:145:CYS:HA	12:J:2:ILE:HD11	1.85	0.58
6:D:53:SER:H	6:D:148:LEU:CD2	2.15	0.58
9:G:1:MET:SD	9:G:1:MET:C	2.86	0.58
3:A:782:ARG:NH2	4:B:699:GLU:O	2.36	0.58
3:A:901:LEU:HD22	3:A:919:ILE:CG2	2.33	0.58
3:A:1373:ASP:HA	3:A:1376:THR:HG22	1.85	0.58
4:B:217:ARG:HD2	4:B:217:ARG:C	2.28	0.58
4:B:337:ARG:C	4:B:338:GLY:N	2.61	0.58
4:B:702:LEU:HD12	4:B:703:ILE:H	1.67	0.58
10:H:23:VAL:HG22	10:H:43:ASN:HA	1.85	0.58
13:K:21:ILE:HG23	13:K:31:VAL:CG1	2.33	0.58
3:A:444:PHE:HB2	3:A:458:HIS:HD2	1.67	0.58
3:A:596:THR:O	3:A:598:LEU:N	2.35	0.58
8:F:109:VAL:HG12	8:F:110:ASP:N	2.18	0.58
10:H:102:TYR:N	10:H:102:TYR:CD2	2.72	0.58
11:I:115:LYS:HB3	11:I:117:LYS:HG3	1.85	0.58
12:J:44:TYR:HA	12:J:47:ARG:HB2	1.85	0.58
3:A:1100:ARG:NH2	3:A:1351:GLU:HG2	2.19	0.58
4:B:995:ARG:HH12	5:C:165:LYS:HG2	1.69	0.58
5:C:254:LYS:O	5:C:258:ILE:HD13	2.02	0.58
8:F:130:ILE:O	8:F:148:VAL:CG2	2.51	0.58
3:A:1004:ASN:CG	7:E:167:ARG:HD2	2.28	0.58
3:A:1450:LEU:O	3:A:1450:LEU:HG	2.03	0.58
4:B:418:LYS:HG2	4:B:422:LYS:HE3	1.86	0.58
4:B:792:MET:HE2	4:B:857:ARG:NH2	2.17	0.58
4:B:856:PHE:HD2	4:B:967:ARG:HD2	1.68	0.58
4:B:1065:GLN:HG3	4:B:1067:ARG:H	1.68	0.58
5:C:17:ASN:N	5:C:240:VAL:HG11	2.18	0.58
9:G:80:LYS:O	9:G:80:LYS:HG2	2.02	0.58
11:I:76:PRO:HG2	11:I:110:PHE:HB3	1.84	0.58
12:J:2:ILE:H	12:J:57:ILE:HG22	1.67	0.58
3:A:399:HIS:CB	3:A:400:PRO:HD3	2.30	0.58
3:A:524:VAL:HG12	3:A:525:GLN:H	1.69	0.58
3:A:828:ALA:CB	4:B:530:GLY:HA2	2.34	0.58
3:A:845:LEU:HD22	3:A:1374:VAL:HG21	1.84	0.58
3:A:1445:ILE:HD12	3:A:1445:ILE:N	2.13	0.58
4:B:1152:MET:CE	4:B:1157:ALA:HA	2.34	0.58
5:C:131:HIS:O	5:C:133:ILE:N	2.36	0.58
6:D:64:VAL:C	6:D:66:ARG:H	2.10	0.58
11:I:85:PHE:CE1	11:I:99:LEU:HD13	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:1:MET:N	12:J:57:ILE:HG22	2.19	0.58
3:A:470:LEU:HD22	3:A:487:MET:HE3	1.86	0.58
3:A:774:ARG:O	3:A:775:ILE:C	2.45	0.58
3:A:871:ASP:OD1	3:A:1366:ARG:NH2	2.37	0.58
3:A:901:LEU:HD22	3:A:919:ILE:HG22	1.85	0.58
3:A:1147:THR:HB	11:I:48:LEU:HD12	1.84	0.58
4:B:580:VAL:HG22	4:B:624:LEU:CB	2.33	0.58
4:B:1147:LEU:C	4:B:1147:LEU:HD23	2.28	0.58
5:C:209:TYR:N	5:C:209:TYR:CD1	2.72	0.58
7:E:60:PHE:HE2	7:E:80:VAL:HB	1.68	0.58
10:H:12:VAL:HG13	10:H:26:ILE:HG23	1.86	0.58
10:H:17:PRO:HB3	10:H:24:CYS:SG	2.43	0.58
10:H:40:LEU:HD22	10:H:123:MET:CE	2.33	0.58
11:I:50:THR:CG2	11:I:52:ILE:HG12	2.34	0.58
3:A:23:SER:HA	3:A:233:TRP:CD1	2.38	0.58
3:A:940:ARG:HG2	3:A:940:ARG:HH11	1.69	0.58
3:A:1141:THR:OG1	3:A:1205:LYS:HD3	2.04	0.58
4:B:542:MET:SD	4:B:747:MET:HE2	2.44	0.58
9:G:138:THR:CG2	9:G:139:ILE:H	2.02	0.58
3:A:264:PHE:O	3:A:267:ALA:HB3	2.04	0.58
3:A:547:LEU:HD13	13:K:58:PHE:CD1	2.38	0.58
3:A:935:GLN:HE21	3:A:1023:ARG:NH1	2.01	0.58
3:A:1445:ILE:H	3:A:1445:ILE:CD1	2.04	0.58
4:B:193:LYS:HZ2	14:L:32:ALA:HB1	1.68	0.58
4:B:309:GLN:HG3	11:I:52:ILE:HD11	1.85	0.58
4:B:583:ASN:HD21	4:B:628:THR:CG2	2.08	0.58
9:G:59:GLY:HA3	9:G:70:PHE:CD2	2.38	0.58
3:A:64:ASN:O	3:A:65:LEU:C	2.46	0.57
3:A:172:PRO:HD3	3:A:185:TRP:NE1	2.18	0.57
3:A:1343:ALA:O	3:A:1346:ALA:HB3	2.03	0.57
4:B:357:GLN:O	4:B:366:GLN:HA	2.03	0.57
4:B:365:THR:HG23	4:B:367:LEU:N	2.18	0.57
4:B:969:ARG:NH1	5:C:61:GLU:OE1	2.37	0.57
5:C:124:LEU:O	5:C:127:ARG:HG2	2.04	0.57
7:E:24:LYS:HB3	7:E:30:ILE:HD12	1.85	0.57
9:G:14:HIS:CD2	9:G:16:SER:HB2	2.40	0.57
2:T:13:U:HO2'	2:T:14:C:P	2.24	0.57
3:A:117:GLU:H	3:A:117:GLU:CD	2.12	0.57
3:A:1227:ILE:HG22	3:A:1228:TRP:H	1.67	0.57
3:A:1445:ILE:HD11	9:G:68:ALA:HB1	1.87	0.57
4:B:185:THR:O	4:B:188:ASP:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:218:SER:HB3	4:B:241:ARG:HH11	1.70	0.57
4:B:846:ILE:HG23	4:B:974:PRO:HG2	1.85	0.57
5:C:212:PRO:CB	5:C:213:PRO:HD2	2.34	0.57
14:L:28:LYS:HB2	14:L:39:SER:HB2	1.86	0.57
3:A:382:PRO:CB	3:A:428:TYR:HE2	2.18	0.57
3:A:598:LEU:HD22	10:H:25:ARG:NH1	2.19	0.57
3:A:1002:GLY:HA3	3:A:1007:ILE:CG2	2.33	0.57
4:B:214:ALA:HB3	4:B:498:THR:HA	1.86	0.57
4:B:1103:ILE:O	4:B:1122:ARG:NH1	2.37	0.57
5:C:31:ASN:OD1	5:C:34:ARG:HD3	2.04	0.57
5:C:172:PRO:O	5:C:235:VAL:HG23	2.05	0.57
12:J:1:MET:N	12:J:56:LEU:N	2.53	0.57
3:A:24:PRO:HD2	3:A:233:TRP:CD1	2.38	0.57
3:A:325:ILE:CG2	4:B:1210:MET:HE2	2.34	0.57
3:A:1097:GLY:O	3:A:1100:ARG:HB3	2.05	0.57
3:A:1342:GLU:OE2	7:E:212:ARG:NH1	2.38	0.57
7:E:153:HIS:HB3	7:E:196:VAL:HG11	1.86	0.57
10:H:100:THR:HG22	10:H:101:ALA:N	2.19	0.57
12:J:64:ASN:CB	12:J:65:PRO:CD	2.79	0.57
14:L:40:LEU:HD22	14:L:44:ASP:CB	2.34	0.57
3:A:427:GLN:HB2	3:A:430:TRP:CD1	2.40	0.57
3:A:535:THR:HG21	3:A:616:VAL:CA	2.30	0.57
3:A:675:THR:OG1	3:A:736:ASN:ND2	2.37	0.57
3:A:875:ALA:HA	3:A:878:ILE:CD1	2.34	0.57
4:B:340:ALA:HB2	4:B:343:ILE:HD12	1.86	0.57
4:B:641:GLU:C	4:B:643:ASP:H	2.12	0.57
4:B:865:LYS:HZ3	4:B:869:SER:HA	1.69	0.57
4:B:1222:ARG:O	4:B:1222:ARG:HG2	2.05	0.57
6:D:4:SER:O	6:D:5:THR:CB	2.51	0.57
7:E:154:ILE:H	7:E:196:VAL:HG13	1.70	0.57
7:E:207:ARG:HB2	7:E:207:ARG:NH1	2.18	0.57
3:A:567:LYS:HD2	3:A:568:PRO:CD	2.33	0.57
3:A:754:SER:H	3:A:757:ASN:ND2	1.86	0.57
3:A:886:ILE:HG13	3:A:943:LEU:CD1	2.34	0.57
3:A:979:SER:OG	3:A:980:ASP:N	2.35	0.57
3:A:1193:LEU:HD12	3:A:1194:ARG:N	2.20	0.57
4:B:27:ALA:O	4:B:29:ASP:N	2.37	0.57
4:B:189:LEU:O	4:B:192:LEU:N	2.34	0.57
4:B:466:TRP:O	4:B:468:GLU:N	2.37	0.57
4:B:549:THR:HG22	4:B:550:ASP:N	2.15	0.57
4:B:872:GLU:HG2	4:B:916:THR:OG1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:36:VAL:HG21	5:C:251:LEU:HB2	1.85	0.57
6:D:119:ARG:HG2	6:D:120:GLU:N	2.19	0.57
10:H:40:LEU:HD22	10:H:123:MET:HE3	1.87	0.57
10:H:41:ASP:OD2	10:H:122:LEU:N	2.37	0.57
2:T:8:C:H4'	3:A:447:GLN:HE22	1.70	0.57
3:A:222:LEU:O	3:A:224:PHE:N	2.37	0.57
3:A:738:LYS:C	3:A:740:LEU:H	2.13	0.57
3:A:841:LEU:O	3:A:845:LEU:HG	2.05	0.57
3:A:886:ILE:HG22	3:A:887:GLY:N	2.18	0.57
3:A:1377:THR:O	3:A:1379:GLY:N	2.38	0.57
4:B:128:LEU:HD11	4:B:170:LEU:HB2	1.87	0.57
4:B:237:VAL:HG22	4:B:257:LYS:HA	1.87	0.57
8:F:68:THR:HG21	8:F:71:GLU:OE2	2.03	0.57
8:F:119:ARG:HG3	8:F:119:ARG:NH1	2.20	0.57
9:G:1:MET:O	9:G:3:PHE:CE1	2.58	0.57
9:G:145:VAL:HG12	9:G:146:LYS:N	2.19	0.57
3:A:119:ASN:O	3:A:122:MET:HB3	2.05	0.57
3:A:996:ASN:C	3:A:998:LEU:HD12	2.29	0.57
4:B:751:VAL:HG13	4:B:812:LEU:CD2	2.35	0.57
4:B:843:GLN:O	4:B:844:SER:C	2.48	0.57
4:B:957:ASN:O	4:B:959:ASP:N	2.38	0.57
4:B:1096:ARG:O	4:B:1097:HIS:CB	2.53	0.57
13:K:59:ALA:HA	13:K:74:ARG:O	2.05	0.57
3:A:341:MET:CE	3:A:843:LYS:NZ	2.68	0.57
3:A:351:THR:HB	4:B:1103:ILE:CD1	2.35	0.57
3:A:821:ARG:HD2	3:A:825:ILE:HD11	1.87	0.57
3:A:1244:ARG:HB3	3:A:1245:PRO:CD	2.35	0.57
4:B:118:ARG:HH11	4:B:204:ILE:HD11	1.69	0.57
4:B:203:PHE:N	4:B:203:PHE:CD1	2.73	0.57
5:C:99:LEU:HB2	5:C:157:CYS:HB2	1.87	0.57
9:G:17:PHE:N	9:G:17:PHE:CD2	2.71	0.57
3:A:61:ILE:O	3:A:63:ARG:N	2.38	0.57
3:A:901:LEU:HB2	3:A:926:GLN:HG2	1.86	0.57
3:A:1222:ASN:O	3:A:1223:ASP:HB3	2.05	0.57
3:A:1299:VAL:HG12	3:A:1300:LYS:N	2.20	0.57
4:B:758:PHE:CE2	4:B:1044:ALA:HA	2.40	0.57
4:B:1099:VAL:HG13	4:B:1100:ASP:N	2.19	0.57
6:D:55:ALA:HB3	6:D:148:LEU:HD21	1.86	0.57
8:F:97:ARG:O	8:F:101:ILE:HG13	2.05	0.57
10:H:143:LEU:HD12	10:H:143:LEU:N	2.20	0.57
11:I:55:THR:HG22	11:I:58:VAL:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:268:ASP:HB3	3:A:299:HIS:CE1	2.39	0.56
3:A:666:ILE:HG23	4:B:1026:LEU:HB3	1.87	0.56
4:B:217:ARG:NE	4:B:405:ARG:HB2	2.20	0.56
4:B:242:SER:HB2	4:B:362:PRO:HG2	1.86	0.56
4:B:899:ILE:CD1	4:B:911:ILE:HA	2.34	0.56
4:B:1073:TYR:CE2	4:B:1080:LYS:HG2	2.39	0.56
5:C:2:SER:N	5:C:3:GLU:N	2.53	0.56
7:E:135:PHE:HD2	7:E:140:LEU:HD21	1.70	0.56
9:G:20:PRO:HG2	9:G:21:ARG:H	1.69	0.56
13:K:12:LEU:H	13:K:12:LEU:HD12	1.69	0.56
3:A:84:ILE:HG22	3:A:239:LEU:HB3	1.87	0.56
3:A:779:PHE:O	3:A:780:VAL:C	2.48	0.56
6:D:18:VAL:HG13	6:D:18:VAL:O	2.05	0.56
6:D:160:VAL:O	6:D:164:ILE:HG13	2.05	0.56
9:G:1:MET:SD	9:G:1:MET:O	2.63	0.56
1:P:9:G:H2'	1:P:10:A:H8	1.67	0.56
3:A:114:LEU:HD13	3:A:171:GLN:NE2	2.19	0.56
3:A:244:PRO:CG	3:A:245:PRO:HD3	2.35	0.56
3:A:298:PHE:CZ	3:A:314:ALA:HB2	2.41	0.56
3:A:450:LEU:HB3	3:A:838:GLN:NE2	2.21	0.56
3:A:590:ARG:O	3:A:591:PHE:HB2	2.04	0.56
3:A:798:GLY:HA2	3:A:815:PHE:HD1	1.70	0.56
3:A:1035:TYR:O	3:A:1037:LEU:N	2.38	0.56
3:A:1213:GLY:O	3:A:1216:ILE:N	2.39	0.56
3:A:1289:ARG:NH1	3:A:1326:ARG:NH1	2.54	0.56
4:B:126:SER:OG	4:B:172:ILE:HD11	2.04	0.56
4:B:562:GLY:C	4:B:590:HIS:HD1	2.13	0.56
4:B:865:LYS:HE2	4:B:871:THR:OG1	2.05	0.56
5:C:133:ILE:HD12	5:C:237:SER:HA	1.87	0.56
5:C:147:LEU:HB2	5:C:151:GLN:HB2	1.86	0.56
7:E:22:MET:HE3	7:E:26:ARG:CZ	2.35	0.56
7:E:46:TYR:CD2	7:E:58:MET:HG2	2.41	0.56
7:E:153:HIS:HB3	7:E:196:VAL:CG1	2.35	0.56
8:F:79:ARG:HG3	8:F:144:GLU:OE1	2.05	0.56
8:F:111:LEU:C	8:F:113:GLY:H	2.13	0.56
9:G:3:PHE:CD1	9:G:80:LYS:NZ	2.72	0.56
10:H:99:GLY:HA3	10:H:118:PHE:HA	1.86	0.56
3:A:563:PRO:HG3	3:A:572:TRP:CE2	2.40	0.56
3:A:601:LYS:HB2	3:A:603:ASN:HD21	1.70	0.56
3:A:785:PRO:HG2	3:A:786:HIS:CD2	2.41	0.56
3:A:1369:ALA:O	3:A:1372:VAL:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:811:TYR:H	4:B:811:TYR:HD1	1.53	0.56
4:B:819:ALA:O	4:B:1093:GLN:HG2	2.05	0.56
4:B:1001:PHE:CE1	4:B:1073:TYR:HB2	2.39	0.56
10:H:89:LEU:C	10:H:91:ASP:N	2.59	0.56
3:A:288:ALA:HA	3:A:291:GLU:OE2	2.05	0.56
3:A:345:VAL:HG21	4:B:1150:ARG:HH11	1.70	0.56
3:A:1454:MET:O	3:A:1454:MET:HG3	2.04	0.56
4:B:900:ALA:HB3	14:L:61:THR:OG1	2.06	0.56
5:C:66:ARG:NH2	12:J:5:VAL:HG23	2.20	0.56
6:D:8:PHE:O	6:D:8:PHE:CD1	2.58	0.56
6:D:52:LEU:HD21	6:D:147:TYR:HE2	1.69	0.56
9:G:47:CYS:O	9:G:76:ALA:HB1	2.05	0.56
3:A:18:GLN:O	4:B:1215:ARG:HG2	2.06	0.56
3:A:41:MET:HB3	3:A:48:ALA:O	2.06	0.56
3:A:215:SER:HB3	3:A:218:ASP:CB	2.36	0.56
3:A:1445:ILE:HD12	9:G:59:GLY:O	2.05	0.56
4:B:39:ARG:HG2	4:B:39:ARG:NH1	2.19	0.56
4:B:844:SER:O	4:B:847:ASP:HB2	2.05	0.56
5:C:31:ASN:O	5:C:34:ARG:HB3	2.05	0.56
3:A:34:LYS:CE	3:A:57:ARG:NH1	2.66	0.56
3:A:154:SER:CB	3:A:162:VAL:HG21	2.36	0.56
3:A:504:LEU:HD12	3:A:504:LEU:N	2.21	0.56
4:B:1106:ARG:NH1	4:B:1110:PRO:HG2	2.21	0.56
3:A:106:VAL:HG13	3:A:112:LYS:O	2.06	0.56
3:A:794:PRO:C	3:A:796:SER:H	2.13	0.56
3:A:1412:ALA:HA	3:A:1417:GLU:OE2	2.06	0.56
4:B:424:LEU:O	4:B:428:ILE:HG13	2.05	0.56
4:B:872:GLU:CD	4:B:914:LYS:HE2	2.31	0.56
7:E:198:ILE:CD1	7:E:212:ARG:HG3	2.35	0.56
9:G:138:THR:HG22	9:G:139:ILE:HG13	1.88	0.56
13:K:109:TRP:O	13:K:111:LEU:N	2.39	0.56
3:A:869:GLY:O	7:E:204:THR:HG21	2.05	0.56
4:B:295:GLY:N	4:B:298:LEU:HD23	2.20	0.56
4:B:785:TYR:CD1	4:B:785:TYR:C	2.83	0.56
4:B:810:GLU:HG3	4:B:815:ARG:HH22	1.69	0.56
10:H:113:ALA:HB1	10:H:125:LEU:O	2.06	0.56
2:T:12:G:O2'	2:T:13:U:C3'	2.54	0.56
3:A:963:ILE:HD13	3:A:1049:ILE:CG1	2.36	0.56
4:B:125:SER:HA	4:B:171:PRO:HA	1.88	0.56
4:B:280:ILE:HG21	4:B:285:ILE:HG13	1.87	0.56
4:B:431:TYR:CZ	4:B:447:ALA:HB2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:582:VAL:HG12	4:B:587:HIS:CD2	2.41	0.56
8:F:75:PRO:O	8:F:77:ASP:O	2.23	0.56
13:K:15:GLY:O	13:K:16:GLU:HG3	2.06	0.56
3:A:265:LYS:O	3:A:269:ILE:HG13	2.06	0.55
3:A:470:LEU:HD22	3:A:487:MET:CE	2.36	0.55
3:A:696:GLU:O	3:A:696:GLU:HG2	2.06	0.55
3:A:1166:ASP:OD2	3:A:1239:ARG:HD2	2.05	0.55
4:B:282:ILE:HD12	4:B:382:ILE:HD13	1.89	0.55
4:B:589:VAL:CG1	4:B:590:HIS:H	2.03	0.55
5:C:18:VAL:O	5:C:20:PHE:HD2	1.89	0.55
6:D:29:LEU:HB3	9:G:82:PHE:CE2	2.41	0.55
7:E:79:TRP:HE1	7:E:81:GLU:HB2	1.71	0.55
7:E:124:VAL:HG13	7:E:132:ILE:CD1	2.36	0.55
4:B:308:TRP:HA	4:B:311:LEU:HD12	1.88	0.55
4:B:638:PHE:HD2	4:B:690:VAL:HG22	1.71	0.55
9:G:27:LYS:O	9:G:30:LEU:HB3	2.06	0.55
3:A:84:ILE:O	3:A:84:ILE:HG23	2.06	0.55
3:A:543:LEU:H	3:A:572:TRP:HZ3	1.54	0.55
3:A:683:ILE:HD13	3:A:801:GLU:CG	2.36	0.55
3:A:863:VAL:HG11	3:A:866:PHE:CD2	2.41	0.55
3:A:907:THR:CG2	3:A:908:LEU:N	2.68	0.55
4:B:247:GLY:N	4:B:418:LYS:HZ1	2.04	0.55
4:B:336:ARG:NE	4:B:348:ARG:HH11	2.03	0.55
4:B:757:PRO:HG3	4:B:1028:GLU:OE2	2.06	0.55
4:B:955:THR:HG23	14:L:54:ARG:O	2.07	0.55
4:B:978:ASP:OD2	4:B:1098:MET:HG2	2.06	0.55
9:G:9:LEU:HD12	9:G:10:ASN:H	1.71	0.55
13:K:65:HIS:HD2	13:K:67:PHE:HB2	1.71	0.55
3:A:58:LEU:HD21	3:A:243:PRO:HA	1.88	0.55
3:A:250:ILE:O	3:A:258:GLY:HA3	2.05	0.55
3:A:450:LEU:HD12	3:A:450:LEU:N	2.22	0.55
4:B:850:LEU:HD12	4:B:851:PHE:H	1.72	0.55
4:B:997:GLU:OE2	4:B:997:GLU:N	2.29	0.55
7:E:169:ARG:HH12	8:F:74:ILE:HD11	1.72	0.55
11:I:26:LEU:CD2	11:I:37:GLU:HA	2.30	0.55
11:I:105:SER:O	11:I:106:CYS:HB3	2.06	0.55
3:A:500:GLU:OE2	4:B:1145:SER:HB2	2.06	0.55
3:A:507:VAL:HG13	3:A:521:MET:HE1	1.87	0.55
3:A:590:ARG:HH22	3:A:620:LYS:HB3	1.72	0.55
3:A:663:SER:OG	3:A:664:THR:N	2.40	0.55
3:A:857:ARG:NH1	8:F:139:PRO:HB2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1332:PHE:CD2	3:A:1332:PHE:N	2.73	0.55
4:B:95:ILE:HG13	4:B:130:VAL:HG22	1.86	0.55
4:B:95:ILE:CG1	4:B:130:VAL:HG22	2.37	0.55
4:B:190:TYR:CE2	12:J:62:ARG:HB3	2.41	0.55
4:B:243:ALA:HA	4:B:250:PHE:O	2.07	0.55
3:A:648:ASN:O	3:A:649:ILE:C	2.48	0.55
3:A:825:ILE:HG22	3:A:826:ASP:N	2.21	0.55
3:A:973:ILE:HD11	3:A:1041:ALA:HB2	1.87	0.55
4:B:909:ASP:OD1	4:B:909:ASP:N	2.40	0.55
4:B:999:MET:HB3	4:B:1007:VAL:CG2	2.36	0.55
5:C:31:ASN:O	5:C:32:SER:C	2.50	0.55
5:C:257:SER:HA	5:C:260:LEU:HB3	1.88	0.55
7:E:85:GLU:HB2	7:E:88:VAL:HG22	1.87	0.55
11:I:115:LYS:HD3	11:I:117:LYS:CE	2.26	0.55
3:A:44:THR:O	3:A:45:GLN:HB2	2.06	0.55
3:A:53:LEU:HD22	3:A:54:ASN:ND2	2.21	0.55
3:A:469:ARG:HB3	3:A:469:ARG:HH11	1.71	0.55
3:A:1008:GLN:O	3:A:1011:GLN:HB3	2.07	0.55
4:B:129:PHE:HA	4:B:165:VAL:O	2.06	0.55
4:B:1223:ASP:O	4:B:1224:PHE:HB2	2.07	0.55
6:D:153:ARG:C	6:D:154:PHE:CD1	2.85	0.55
7:E:197:LYS:HE2	7:E:199:ILE:HD11	1.89	0.55
14:L:34:CYS:O	14:L:34:CYS:SG	2.64	0.55
3:A:407:ARG:HG2	3:A:430:TRP:CH2	2.41	0.55
3:A:567:LYS:CB	3:A:568:PRO:HD2	2.36	0.55
3:A:567:LYS:NZ	10:H:46:LEU:HB2	2.21	0.55
3:A:849:MET:CE	3:A:1061:GLY:HA2	2.37	0.55
3:A:1198:ASP:HB3	3:A:1201:ALA:CB	2.36	0.55
3:A:1323:ASP:C	3:A:1325:THR:H	2.15	0.55
4:B:336:ARG:CZ	4:B:348:ARG:HH11	2.20	0.55
4:B:899:ILE:CG2	4:B:949:VAL:HG21	2.37	0.55
4:B:1174:LYS:O	4:B:1176:ASN:N	2.39	0.55
5:C:145:CYS:HA	12:J:2:ILE:CD1	2.37	0.55
5:C:263:THR:C	5:C:265:MET:N	2.64	0.55
6:D:145:MET:O	6:D:149:THR:HB	2.07	0.55
7:E:23:VAL:O	7:E:28:TYR:HB2	2.06	0.55
13:K:19:LEU:HD22	13:K:33:ILE:CG2	2.37	0.55
3:A:266:LEU:HD21	3:A:303:TYR:CE1	2.41	0.55
3:A:590:ARG:HG3	3:A:590:ARG:NH1	2.21	0.55
3:A:1064:VAL:O	3:A:1064:VAL:HG12	2.05	0.55
4:B:287:ARG:NH1	4:B:324:ILE:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:640:VAL:O	4:B:641:GLU:C	2.49	0.55
4:B:687:GLU:O	4:B:689:LEU:HG	2.06	0.55
4:B:1177:HIS:CB	4:B:1179:GLN:HE21	2.14	0.55
12:J:1:MET:H3	12:J:56:LEU:N	2.05	0.55
3:A:537:ARG:HD2	10:H:20:TYR:HE1	1.72	0.55
3:A:537:ARG:HH12	10:H:122:LEU:HG	1.71	0.55
3:A:1076:ALA:HA	3:A:1079:MET:HE2	1.88	0.55
3:A:1116:LEU:HD11	3:A:1118:VAL:HG13	1.88	0.55
3:A:1364:ASN:O	3:A:1365:TYR:C	2.50	0.55
3:A:1409:LEU:O	3:A:1412:ALA:HB3	2.06	0.55
6:D:167:LEU:O	6:D:170:THR:OG1	2.25	0.55
7:E:44:ALA:O	7:E:45:LYS:HB2	2.06	0.55
10:H:38:LEU:HD13	10:H:125:LEU:HD13	1.87	0.55
14:L:29:TYR:CD2	14:L:29:TYR:N	2.73	0.55
3:A:719:VAL:C	3:A:721:PHE:H	2.14	0.54
3:A:767:GLN:HA	3:A:799:PHE:HA	1.88	0.54
3:A:903:ASN:HD22	3:A:903:ASN:C	2.10	0.54
4:B:63:ILE:HD12	4:B:421:PHE:CE2	2.41	0.54
4:B:557:PHE:HE1	4:B:603:LEU:HD11	1.72	0.54
4:B:789:MET:HE3	4:B:965:LYS:HB3	1.89	0.54
4:B:1176:ASN:C	4:B:1178:ASN:H	2.15	0.54
8:F:111:LEU:HD12	8:F:111:LEU:N	2.22	0.54
9:G:13:LEU:CD2	9:G:17:PHE:HB2	2.36	0.54
3:A:222:LEU:O	3:A:224:PHE:HD1	1.90	0.54
3:A:472:LEU:O	3:A:475:THR:HB	2.06	0.54
3:A:559:VAL:O	3:A:559:VAL:HG12	2.06	0.54
4:B:847:ASP:O	4:B:849:GLY:N	2.40	0.54
5:C:186:LEU:HD21	5:C:224:GLN:O	2.08	0.54
5:C:234:SER:CB	5:C:240:VAL:HG13	2.38	0.54
8:F:76:LYS:O	8:F:79:ARG:HD3	2.07	0.54
10:H:15:VAL:HG22	10:H:26:ILE:HG12	1.90	0.54
10:H:83:GLN:C	10:H:85:GLY:H	2.15	0.54
3:A:356:ASP:HB2	3:A:469:ARG:HH11	1.72	0.54
3:A:845:LEU:O	3:A:846:GLU:C	2.50	0.54
3:A:1349:TYR:HB2	3:A:1372:VAL:HG21	1.90	0.54
4:B:575:PRO:HG2	4:B:576:ASP:H	1.72	0.54
4:B:654:ARG:C	4:B:656:GLY:H	2.15	0.54
4:B:792:MET:HE2	4:B:857:ARG:HH22	1.72	0.54
4:B:1182:CYS:C	4:B:1183:LYS:HE3	2.32	0.54
5:C:166:GLU:HG3	13:K:10:PHE:CZ	2.33	0.54
3:A:346:ASP:HB3	4:B:1108:ARG:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:478:TYR:O	3:A:479:ASN:HB3	2.06	0.54
3:A:720:ARG:HB3	3:A:720:ARG:NH1	2.21	0.54
3:A:1340:GLY:HA2	7:E:183:PRO:HD2	1.89	0.54
4:B:209:GLU:OE2	4:B:483:LEU:HD23	2.07	0.54
4:B:1182:CYS:O	4:B:1182:CYS:SG	2.65	0.54
6:D:208:GLU:O	6:D:212:LYS:HG3	2.06	0.54
8:F:82:THR:HG22	8:F:84:TYR:H	1.70	0.54
11:I:50:THR:HG22	11:I:51:ASN:H	1.72	0.54
12:J:31:ASP:O	12:J:32:GLU:C	2.50	0.54
14:L:70:ARG:HG2	14:L:70:ARG:NH1	2.21	0.54
3:A:7:SER:C	3:A:9:ALA:H	2.15	0.54
3:A:1025:ARG:O	3:A:1026:LEU:HD23	2.07	0.54
3:A:1176:LEU:HD12	3:A:1177:LEU:O	2.07	0.54
4:B:102:VAL:HG23	4:B:112:LEU:HB2	1.88	0.54
4:B:615:MET:HB3	4:B:626:ILE:HG12	1.89	0.54
4:B:1007:VAL:CG2	4:B:1008:PRO:HD2	2.37	0.54
3:A:58:LEU:CD1	3:A:243:PRO:HB3	2.32	0.54
3:A:673:GLY:O	3:A:676:MET:HB2	2.07	0.54
3:A:746:MET:CE	4:B:1018:PRO:HG2	2.38	0.54
4:B:44:VAL:HG11	4:B:199:MET:HG2	1.89	0.54
4:B:192:LEU:O	4:B:193:LYS:HB2	2.07	0.54
6:D:40:HIS:CB	9:G:73:LYS:HZ2	2.18	0.54
7:E:93:MET:SD	7:E:97:VAL:HG23	2.47	0.54
10:H:123:MET:HE1	10:H:142:LEU:HD11	1.90	0.54
11:I:58:VAL:HG13	11:I:62:ILE:CD1	2.37	0.54
11:I:90:GLN:NE2	11:I:92:ARG:HD3	2.23	0.54
3:A:37:PHE:N	3:A:37:PHE:CD1	2.76	0.54
3:A:666:ILE:HD11	4:B:1067:ARG:O	2.06	0.54
3:A:1062:GLU:OE2	8:F:88:TYR:OH	2.24	0.54
4:B:228:LYS:CB	4:B:261:ARG:HH22	2.21	0.54
4:B:731:VAL:HG12	4:B:732:SER:N	2.23	0.54
3:A:89:PRO:HB2	3:A:204:THR:HG22	1.88	0.54
3:A:345:VAL:HG23	3:A:346:ASP:O	2.07	0.54
3:A:404:TYR:HB2	3:A:433:GLU:HB2	1.89	0.54
3:A:1211:GLN:O	3:A:1212:VAL:C	2.51	0.54
4:B:57:TYR:N	4:B:57:TYR:HD1	2.05	0.54
4:B:798:TYR:CE2	5:C:62:PHE:CE2	2.92	0.54
4:B:806:THR:O	4:B:809:MET:HG3	2.08	0.54
4:B:952:VAL:HG12	4:B:953:LEU:H	1.71	0.54
4:B:1065:GLN:NE2	4:B:1066:SER:N	2.56	0.54
6:D:220:LEU:O	6:D:221:TYR:HD1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:125:LEU:HB2	8:F:130:ILE:HD11	1.88	0.54
4:B:39:ARG:HH21	4:B:665:GLU:CG	2.20	0.54
4:B:96:TYR:HB2	4:B:129:PHE:HB2	1.89	0.54
4:B:247:GLY:N	4:B:418:LYS:NZ	2.50	0.54
4:B:616:ILE:HG13	4:B:697:GLU:HG3	1.90	0.54
4:B:1216:LEU:C	4:B:1217:TYR:HD1	2.16	0.54
6:D:71:LYS:HA	6:D:74:GLN:CB	2.37	0.54
9:G:51:TYR:C	9:G:51:TYR:HD2	2.16	0.54
11:I:7:CYS:N	11:I:14:LEU:HD21	2.22	0.54
11:I:8:ARG:CG	11:I:34:TYR:HE1	2.17	0.54
13:K:42:LEU:HD21	13:K:46:ILE:HD11	1.90	0.54
14:L:53:HIS:HB3	14:L:55:ILE:CD1	2.38	0.54
3:A:19:PHE:HB3	3:A:1413:GLY:HA2	1.88	0.54
3:A:207:ILE:O	3:A:211:PHE:HD1	1.91	0.54
3:A:224:PHE:HZ	3:A:234:MET:HE2	1.70	0.54
3:A:903:ASN:ND2	3:A:903:ASN:C	2.64	0.54
3:A:1102:LYS:O	3:A:1106:ASN:ND2	2.40	0.54
3:A:1130:GLN:O	3:A:1134:ILE:HG13	2.08	0.54
3:A:1272:THR:C	3:A:1273:LEU:HD12	2.33	0.54
4:B:126:SER:O	4:B:169:ARG:HA	2.07	0.54
4:B:459:TYR:CE1	4:B:469:GLN:HG2	2.43	0.54
4:B:769:TYR:C	4:B:771:SER:N	2.65	0.54
5:C:7:GLN:HG2	13:K:104:ASN:HD22	1.72	0.54
6:D:191:ALA:O	6:D:193:THR:N	2.41	0.54
8:F:89:GLU:HB3	8:F:134:ILE:CD1	2.37	0.54
10:H:40:LEU:CD1	10:H:123:MET:HB2	2.36	0.54
11:I:2:THR:O	11:I:3:THR:C	2.51	0.54
13:K:6:ARG:O	13:K:9:LEU:HG	2.08	0.54
14:L:49:LYS:O	14:L:50:ASP:CB	2.55	0.54
3:A:350:ARG:HH11	3:A:350:ARG:HG3	1.74	0.53
3:A:1435:PRO:HA	3:A:1439:GLY:O	2.08	0.53
4:B:311:LEU:O	4:B:312:GLU:C	2.49	0.53
4:B:570:VAL:CG2	4:B:573:GLN:HB3	2.38	0.53
4:B:590:HIS:HD2	4:B:593:PRO:HB3	1.73	0.53
4:B:866:TYR:O	4:B:867:GLY:C	2.52	0.53
5:C:168:ALA:C	5:C:170:TRP:N	2.65	0.53
10:H:15:VAL:HG22	10:H:26:ILE:CD1	2.38	0.53
13:K:63:VAL:HG23	13:K:63:VAL:O	2.08	0.53
3:A:49:LYS:HZ1	3:A:61:ILE:CG1	2.21	0.53
3:A:1239:ARG:HH22	3:A:1241:ARG:HH22	1.55	0.53
4:B:315:LYS:N	4:B:316:PRO:HD2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:459:TYR:CZ	4:B:469:GLN:HG2	2.42	0.53
4:B:591:ARG:O	4:B:593:PRO:HD3	2.08	0.53
4:B:654:ARG:O	4:B:656:GLY:N	2.42	0.53
4:B:704:ALA:HB2	4:B:738:PHE:CD2	2.44	0.53
4:B:1196:ILE:HB	4:B:1197:PRO:HD2	1.89	0.53
5:C:23:SER:O	5:C:24:ASN:HB3	2.07	0.53
6:D:153:ARG:HB3	6:D:154:PHE:CD1	2.43	0.53
11:I:34:TYR:HD2	11:I:34:TYR:C	2.16	0.53
13:K:10:PHE:N	13:K:10:PHE:CD2	2.76	0.53
3:A:399:HIS:O	3:A:401:GLY:N	2.41	0.53
3:A:442:VAL:CG2	3:A:460:VAL:HG23	2.38	0.53
3:A:596:THR:C	3:A:598:LEU:N	2.65	0.53
3:A:699:ALA:CB	3:A:701:LEU:HG	2.36	0.53
4:B:476:ARG:NH2	4:B:501:PRO:HG3	2.23	0.53
4:B:705:MET:H	4:B:710:LEU:HD12	1.73	0.53
4:B:758:PHE:CE1	4:B:1027:ILE:CG2	2.92	0.53
5:C:46:ILE:HG23	5:C:157:CYS:HB3	1.89	0.53
8:F:109:VAL:HG13	8:F:127:GLU:OE1	2.08	0.53
9:G:114:LEU:HG	9:G:162:SER:HB3	1.91	0.53
11:I:34:TYR:CD2	11:I:34:TYR:C	2.86	0.53
13:K:61:TYR:C	13:K:61:TYR:CD2	2.85	0.53
3:A:4:GLN:O	3:A:5:GLN:HB2	2.08	0.53
3:A:166:GLY:O	3:A:167:CYS:SG	2.67	0.53
3:A:816:HIS:HE2	4:B:764:SER:H	1.55	0.53
3:A:1430:LEU:O	4:B:1196:ILE:HG22	2.09	0.53
4:B:57:TYR:N	4:B:57:TYR:CD1	2.74	0.53
4:B:326:ASP:OD2	4:B:328:GLU:HB2	2.07	0.53
4:B:758:PHE:CZ	4:B:1044:ALA:HA	2.43	0.53
4:B:825:VAL:CG1	4:B:826:ALA:N	2.71	0.53
4:B:1034:VAL:O	4:B:1037:LEU:N	2.41	0.53
5:C:17:ASN:O	5:C:18:VAL:CG2	2.57	0.53
3:A:236:LEU:HD11	3:A:304:MET:HE1	1.90	0.53
3:A:339:ASN:O	3:A:343:LYS:HG2	2.09	0.53
3:A:1291:VAL:HG22	3:A:1292:PRO:HD2	1.90	0.53
3:A:1325:THR:OG1	7:E:146:HIS:O	2.27	0.53
4:B:189:LEU:O	4:B:192:LEU:HB2	2.08	0.53
4:B:240:ILE:CG2	4:B:254:LEU:HB3	2.38	0.53
4:B:594:ALA:HA	4:B:617:ARG:NH1	2.24	0.53
4:B:785:TYR:CD1	4:B:786:ASN:N	2.76	0.53
5:C:181:ASP:CG	5:C:186:LEU:HD13	2.32	0.53
7:E:154:ILE:O	7:E:196:VAL:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:69:PRO:HG2	11:I:85:PHE:CE2	2.44	0.53
3:A:49:LYS:HZ2	3:A:60:SER:HA	1.72	0.53
3:A:666:ILE:HD12	3:A:667:GLY:N	2.20	0.53
3:A:698:GLN:HE21	11:I:99:LEU:HD21	1.73	0.53
3:A:1280:GLU:O	3:A:1281:ARG:C	2.52	0.53
4:B:129:PHE:HD2	4:B:166:PHE:HA	1.72	0.53
4:B:746:SER:CB	4:B:1046:PRO:HG2	2.32	0.53
4:B:893:LEU:HD22	4:B:897:GLY:C	2.34	0.53
4:B:983:ARG:HD2	4:B:1091:TYR:HB3	1.89	0.53
4:B:1102:LYS:O	4:B:1103:ILE:C	2.52	0.53
10:H:58:THR:HG22	10:H:59:ILE:N	2.24	0.53
3:A:30:ILE:HG23	4:B:1170:THR:HG23	1.91	0.53
3:A:73:GLY:O	3:A:75:ASN:N	2.42	0.53
3:A:711:ARG:NH2	11:I:87:GLN:OE1	2.41	0.53
3:A:862:ASN:HA	7:E:174:GLN:HB3	1.91	0.53
3:A:1134:ILE:O	3:A:1138:ILE:HG13	2.08	0.53
3:A:1394:THR:HG21	3:A:1398:MET:SD	2.48	0.53
3:A:1397:LEU:O	3:A:1400:CYS:HB3	2.09	0.53
4:B:233:PRO:HG2	4:B:234:ILE:CD1	2.39	0.53
4:B:343:ILE:HG21	4:B:348:ARG:HG3	1.90	0.53
4:B:479:VAL:O	4:B:480:SER:HB3	2.08	0.53
5:C:3:GLU:O	5:C:4:GLU:HB2	2.06	0.53
3:A:347:PHE:CE2	3:A:375:THR:HG23	2.43	0.53
3:A:618:GLU:O	3:A:620:LYS:N	2.42	0.53
3:A:710:LEU:H	3:A:710:LEU:HD12	1.74	0.53
4:B:642:ASP:HB3	4:B:649:LYS:CG	2.38	0.53
7:E:78:LEU:HD23	7:E:78:LEU:C	2.33	0.53
10:H:64:ASN:O	10:H:65:LEU:CB	2.57	0.53
10:H:91:ASP:C	10:H:93:TYR:H	2.15	0.53
3:A:340:LEU:HD21	4:B:1200:ALA:N	2.24	0.53
3:A:472:LEU:CD1	4:B:835:GLN:NE2	2.71	0.53
3:A:828:ALA:HB2	4:B:530:GLY:HA2	1.91	0.53
3:A:997:LEU:HD13	3:A:1018:PHE:CE2	2.44	0.53
3:A:1308:THR:HG23	3:A:1309:ASP:N	2.23	0.53
3:A:1444:MET:HG3	9:G:60:ARG:HA	1.90	0.53
4:B:102:VAL:CG2	4:B:112:LEU:HD22	2.38	0.53
4:B:233:PRO:HG2	4:B:234:ILE:HD12	1.90	0.53
4:B:502:ILE:HD12	4:B:502:ILE:N	2.20	0.53
4:B:550:ASP:OD1	4:B:552:MET:HE3	2.09	0.53
4:B:986:GLN:OE1	4:B:986:GLN:HA	2.09	0.53
4:B:1071:VAL:O	4:B:1072:MET:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1106:ARG:HH21	4:B:1111:MET:HE2	1.74	0.53
5:C:214:ASN:HB3	5:C:217:ASP:OD2	2.09	0.53
6:D:135:GLY:C	6:D:137:ASN:H	2.16	0.53
7:E:28:TYR:CE1	7:E:78:LEU:HD13	2.44	0.53
12:J:9:SER:HB2	12:J:45:CYS:HB2	1.90	0.53
13:K:47:ARG:HH11	13:K:47:ARG:CB	2.17	0.53
3:A:50:ILE:O	3:A:52:GLY:N	2.42	0.53
3:A:61:ILE:HG22	3:A:62:ASP:N	2.23	0.53
3:A:475:THR:CG2	3:A:476:SER:N	2.72	0.53
3:A:901:LEU:HA	3:A:907:THR:OG1	2.09	0.53
4:B:582:VAL:HA	4:B:626:ILE:O	2.09	0.53
4:B:1065:GLN:NE2	4:B:1066:SER:H	2.07	0.53
6:D:191:ALA:C	6:D:193:THR:H	2.17	0.53
8:F:109:VAL:HG21	8:F:124:GLU:HA	1.90	0.53
9:G:18:PHE:HA	9:G:22:MET:HE3	1.90	0.53
3:A:219:PHE:CE2	3:A:231:PRO:HD2	2.43	0.52
3:A:382:PRO:HB3	3:A:428:TYR:CE2	2.38	0.52
3:A:446:ARG:HB2	3:A:487:MET:SD	2.49	0.52
3:A:474:VAL:C	3:A:477:PRO:HD2	2.34	0.52
3:A:1348:LEU:HG	3:A:1372:VAL:CG2	2.39	0.52
4:B:169:ARG:HB2	4:B:454:THR:HG23	1.91	0.52
4:B:487:THR:CG2	4:B:488:TYR:N	2.73	0.52
4:B:519:TRP:C	4:B:519:TRP:CD1	2.87	0.52
4:B:693:ILE:HD11	4:B:740:HIS:CD2	2.44	0.52
4:B:693:ILE:HD13	4:B:701:ILE:HD13	1.90	0.52
4:B:766:ARG:NH2	4:B:1020:ARG:HH11	2.06	0.52
4:B:822:ASN:O	12:J:48:ARG:NH1	2.41	0.52
4:B:1001:PHE:CE2	5:C:34:ARG:NE	2.77	0.52
8:F:103:MET:HE1	9:G:65:ASP:HB2	1.90	0.52
11:I:32:CYS:SG	11:I:33:SER:N	2.81	0.52
3:A:113:LEU:HG	3:A:218:ASP:OD1	2.09	0.52
3:A:300:VAL:O	3:A:300:VAL:HG12	2.08	0.52
3:A:326:ARG:NH2	3:A:1407:GLU:HG3	2.24	0.52
3:A:767:GLN:HE21	3:A:774:ARG:HB3	1.71	0.52
3:A:858:ASN:C	3:A:858:ASN:ND2	2.56	0.52
4:B:216:GLU:HA	4:B:406:LEU:CD2	2.40	0.52
4:B:378:LEU:HD12	4:B:378:LEU:C	2.34	0.52
4:B:797:TYR:HE1	4:B:854:LEU:CD2	2.23	0.52
4:B:797:TYR:HE1	4:B:854:LEU:HD23	1.72	0.52
5:C:177:GLU:HB2	5:C:231:ASN:HB3	1.89	0.52
8:F:100:GLN:O	8:F:103:MET:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:15:PRO:HA	9:G:18:PHE:CE1	2.43	0.52
10:H:123:MET:HE1	10:H:142:LEU:CD1	2.40	0.52
13:K:31:VAL:CG1	13:K:32:VAL:N	2.71	0.52
3:A:34:LYS:HB3	3:A:36:ARG:NE	2.24	0.52
3:A:98:LYS:O	3:A:99:ILE:C	2.52	0.52
3:A:1215:ARG:HA	3:A:1218:GLN:HG2	1.90	0.52
4:B:294:ASP:C	4:B:296:GLU:H	2.16	0.52
4:B:464:GLY:HA2	4:B:479:VAL:O	2.09	0.52
4:B:515:HIS:H	4:B:518:HIS:CD2	2.14	0.52
4:B:604:ARG:NH2	4:B:615:MET:HE2	2.25	0.52
6:D:8:PHE:HE1	6:D:38:ILE:H	1.57	0.52
6:D:56:ARG:NH2	6:D:57:LEU:HD21	2.23	0.52
7:E:202:SER:OG	7:E:204:THR:HG22	2.09	0.52
9:G:94:CYS:HA	9:G:99:PHE:HA	1.90	0.52
12:J:20:SER:O	12:J:24:LEU:HG	2.09	0.52
13:K:93:SER:O	13:K:97:LYS:HG3	2.09	0.52
3:A:120:GLU:C	3:A:122:MET:N	2.66	0.52
3:A:208:LEU:HD21	3:A:212:LYS:HE3	1.90	0.52
3:A:471:ASN:O	3:A:474:VAL:HG12	2.10	0.52
3:A:504:LEU:HD11	8:F:91:ALA:HB1	1.92	0.52
4:B:745:PRO:C	4:B:747:MET:N	2.66	0.52
4:B:1039:GLY:HA2	12:J:51:LEU:HD21	1.91	0.52
4:B:1072:MET:HE3	4:B:1085:ILE:HD13	1.92	0.52
5:C:15:LYS:O	5:C:240:VAL:HG22	2.09	0.52
5:C:146:LYS:C	5:C:147:LEU:HD23	2.33	0.52
9:G:106:MET:HG2	9:G:107:LYS:N	2.22	0.52
10:H:130:ARG:HB3	10:H:133:ASN:HB2	1.91	0.52
11:I:7:CYS:HB3	11:I:14:LEU:HD21	1.90	0.52
13:K:42:LEU:O	13:K:46:ILE:HG13	2.08	0.52
3:A:12:ARG:O	4:B:1194:ILE:HG22	2.09	0.52
3:A:335:ARG:O	3:A:339:ASN:HB2	2.08	0.52
3:A:341:MET:CE	3:A:843:LYS:HZ1	2.21	0.52
3:A:960:ILE:HA	3:A:963:ILE:HG22	1.90	0.52
3:A:971:PHE:CE2	3:A:1040:GLN:HG2	2.45	0.52
3:A:1017:LEU:CB	7:E:206:GLY:H	2.20	0.52
3:A:1048:ASN:O	3:A:1049:ILE:C	2.52	0.52
3:A:1324:PRO:HB2	7:E:142:VAL:HG11	1.91	0.52
3:A:1333:ILE:O	3:A:1337:GLU:HG3	2.09	0.52
3:A:1376:THR:O	3:A:1377:THR:C	2.53	0.52
3:A:1445:ILE:HG12	9:G:18:PHE:CE2	2.44	0.52
4:B:1081:LEU:HD12	4:B:1085:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:109:VAL:CG1	8:F:123:LYS:HD3	2.39	0.52
10:H:24:CYS:HB2	10:H:44:VAL:HG21	1.92	0.52
11:I:101:PHE:HB2	11:I:110:PHE:CE2	2.45	0.52
12:J:27:GLU:O	12:J:29:GLU:N	2.41	0.52
3:A:90:VAL:HG13	3:A:297:GLN:CD	2.35	0.52
3:A:514:PRO:C	3:A:516:SER:H	2.16	0.52
3:A:546:VAL:HG21	3:A:572:TRP:CE3	2.44	0.52
3:A:898:ARG:HB2	3:A:933:TYR:HE1	1.75	0.52
4:B:44:VAL:O	4:B:45:SER:C	2.52	0.52
4:B:47:GLN:O	4:B:173:MET:HE1	2.09	0.52
4:B:225:VAL:HA	4:B:237:VAL:O	2.10	0.52
4:B:563:MET:CE	4:B:580:VAL:HB	2.40	0.52
5:C:215:GLU:O	5:C:216:GLY:C	2.51	0.52
10:H:4:THR:CA	10:H:60:ALA:HB2	2.28	0.52
3:A:68:GLN:O	3:A:70:CYS:N	2.37	0.52
3:A:298:PHE:HZ	3:A:314:ALA:HB2	1.74	0.52
3:A:567:LYS:HE3	10:H:46:LEU:HB2	1.90	0.52
3:A:626:ASN:O	3:A:631:HIS:CD2	2.63	0.52
3:A:1147:THR:HB	11:I:48:LEU:CD1	2.39	0.52
3:A:1397:LEU:HB2	3:A:1426:GLU:OE1	2.10	0.52
4:B:171:PRO:HD2	4:B:457:LEU:HD13	1.90	0.52
4:B:281:PRO:HG2	4:B:284:ILE:HG13	1.92	0.52
4:B:604:ARG:C	4:B:606:LYS:H	2.17	0.52
5:C:182:PRO:HG3	5:C:206:ASN:O	2.09	0.52
5:C:189:THR:CG2	5:C:190:ASP:H	2.21	0.52
6:D:198:LEU:O	6:D:200:ASN:N	2.43	0.52
9:G:96:GLN:HB3	9:G:121:PHE:CE2	2.45	0.52
9:G:119:LEU:CD1	9:G:132:SER:HB2	2.39	0.52
3:A:265:LYS:HE2	3:A:322:VAL:HG11	1.91	0.52
4:B:824:ILE:HG12	12:J:48:ARG:HH12	1.75	0.52
4:B:834:ASN:HA	4:B:838:SER:O	2.09	0.52
4:B:1124:ARG:O	4:B:1125:ASP:HB3	2.08	0.52
5:C:69:LEU:O	12:J:6:ARG:HD2	2.09	0.52
5:C:251:LEU:O	5:C:251:LEU:HD12	2.09	0.52
11:I:62:ILE:O	11:I:62:ILE:HG12	2.10	0.52
13:K:18:LYS:NZ	13:K:37:LYS:O	2.43	0.52
3:A:253:ASN:HB3	4:B:935:ARG:NH2	2.24	0.52
3:A:512:VAL:HA	3:A:519:PRO:HA	1.92	0.52
3:A:1313:LEU:C	3:A:1315:GLU:H	2.18	0.52
4:B:228:LYS:HB2	4:B:261:ARG:HH22	1.75	0.52
4:B:247:GLY:C	4:B:249:ARG:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:769:TYR:C	4:B:771:SER:H	2.17	0.52
4:B:878:GLN:O	4:B:879:ARG:C	2.52	0.52
4:B:995:ARG:NH1	5:C:165:LYS:HG2	2.24	0.52
4:B:1097:HIS:H	4:B:1098:MET:HE2	1.75	0.52
5:C:34:ARG:NH1	5:C:35:ARG:HG2	2.25	0.52
6:D:5:THR:O	6:D:5:THR:HG23	2.10	0.52
9:G:1:MET:HE2	9:G:1:MET:O	2.10	0.52
9:G:73:LYS:HE2	9:G:74:TYR:O	2.10	0.52
11:I:71:SER:OG	11:I:83:ASN:HB2	2.08	0.52
13:K:55:LYS:HB3	13:K:81:TYR:CD1	2.45	0.52
4:B:244:LEU:HD11	4:B:366:GLN:NE2	2.25	0.52
4:B:363:HIS:CD2	4:B:585:VAL:HG22	2.45	0.52
4:B:370:PHE:HE2	4:B:373:ARG:NH1	2.05	0.52
4:B:466:TRP:HA	4:B:466:TRP:CE3	2.43	0.52
4:B:616:ILE:CG1	4:B:697:GLU:HA	2.40	0.52
4:B:871:THR:HG22	4:B:872:GLU:N	2.24	0.52
4:B:948:ILE:HG22	4:B:949:VAL:O	2.09	0.52
4:B:1166:CYS:HB2	4:B:1215:ARG:NH1	2.24	0.52
9:G:79:PHE:HZ	9:G:106:MET:HE2	1.75	0.52
10:H:18:GLY:O	10:H:19:ARG:HB2	2.10	0.52
12:J:2:ILE:HG12	12:J:57:ILE:HD12	1.92	0.52
14:L:52:GLY:O	14:L:53:HIS:C	2.53	0.52
3:A:42:ASP:HA	3:A:46:THR:O	2.10	0.51
3:A:54:ASN:N	3:A:54:ASN:HD22	2.08	0.51
3:A:666:ILE:N	4:B:1026:LEU:HD13	2.25	0.51
3:A:722:LEU:O	3:A:725:ALA:HB3	2.11	0.51
3:A:1236:LEU:C	3:A:1237:ILE:HG13	2.35	0.51
4:B:681:TRP:HA	4:B:684:LEU:CD1	2.40	0.51
4:B:1065:GLN:HB2	5:C:201:TRP:CZ3	2.44	0.51
6:D:29:LEU:HD22	9:G:82:PHE:CD2	2.45	0.51
13:K:110:ASN:O	13:K:111:LEU:CB	2.57	0.51
3:A:1400:CYS:O	3:A:1405:THR:HG23	2.10	0.51
4:B:809:MET:HE2	4:B:814:PHE:CD2	2.45	0.51
4:B:824:ILE:HG12	12:J:48:ARG:NH1	2.25	0.51
4:B:1063:GLY:O	5:C:202:PRO:HG2	2.11	0.51
9:G:56:ILE:O	9:G:57:GLN:HB2	2.09	0.51
3:A:846:GLU:OE1	3:A:1425:SER:OG	2.29	0.51
3:A:1018:PHE:O	3:A:1021:LEU:HB3	2.11	0.51
3:A:1120:LEU:O	3:A:1323:ASP:HB2	2.10	0.51
3:A:1305:VAL:CG1	3:A:1306:LEU:N	2.73	0.51
4:B:542:MET:HG2	4:B:747:MET:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:882:THR:HG22	4:B:884:ARG:HB2	1.93	0.51
4:B:1087:PHE:HD2	4:B:1088:GLY:H	1.58	0.51
4:B:1197:PRO:HG2	4:B:1200:ALA:CB	2.41	0.51
5:C:3:GLU:O	5:C:4:GLU:CB	2.59	0.51
7:E:127:ILE:O	7:E:127:ILE:HG13	2.08	0.51
9:G:99:PHE:CD1	9:G:99:PHE:C	2.87	0.51
10:H:113:ALA:HB2	10:H:126:GLU:HG3	1.92	0.51
13:K:57:LEU:HD12	13:K:77:THR:O	2.10	0.51
3:A:172:PRO:HD3	3:A:185:TRP:HE1	1.76	0.51
3:A:475:THR:HG23	3:A:476:SER:H	1.76	0.51
3:A:666:ILE:HD11	4:B:1086:PHE:HE1	1.75	0.51
3:A:806:ARG:HH12	4:B:729:ILE:CD1	2.23	0.51
4:B:1074:ASN:HB2	4:B:1081:LEU:HD21	1.92	0.51
4:B:1106:ARG:HH21	4:B:1111:MET:CE	2.24	0.51
5:C:52:GLU:HA	14:L:64:LEU:HD22	1.91	0.51
5:C:235:VAL:HG13	12:J:13:VAL:HG23	1.92	0.51
6:D:130:LEU:C	6:D:132:GLN:N	2.68	0.51
7:E:16:PHE:HZ	7:E:20:LYS:HE2	1.70	0.51
7:E:35:VAL:C	7:E:37:LEU:H	2.19	0.51
8:F:77:ASP:C	8:F:79:ARG:H	2.16	0.51
9:G:99:PHE:HZ	9:G:163:ILE:HD13	1.76	0.51
10:H:130:ARG:HD2	10:H:130:ARG:N	2.16	0.51
11:I:53:GLY:C	11:I:55:THR:H	2.19	0.51
3:A:29:ALA:HB1	4:B:1184:GLY:HA2	1.93	0.51
3:A:42:ASP:C	3:A:44:THR:N	2.67	0.51
3:A:152:VAL:HG12	3:A:153:PRO:CD	2.40	0.51
3:A:525:GLN:HG3	4:B:835:GLN:HG2	1.93	0.51
3:A:897:TYR:CD2	3:A:936:LEU:HD13	2.45	0.51
3:A:907:THR:HG23	3:A:908:LEU:N	2.26	0.51
4:B:340:ALA:HB1	4:B:343:ILE:HD12	1.92	0.51
4:B:833:TYR:N	4:B:833:TYR:CD1	2.77	0.51
4:B:862:GLN:CG	4:B:963:PHE:HD1	2.21	0.51
4:B:1050:ILE:HG22	4:B:1051:THR:N	2.26	0.51
5:C:183:TRP:O	5:C:185:LYS:N	2.43	0.51
6:D:63:LEU:HD23	9:G:47:CYS:SG	2.51	0.51
6:D:173:HIS:CD2	6:D:175:PHE:H	2.29	0.51
9:G:149:GLY:O	9:G:159:ALA:HB1	2.11	0.51
10:H:127:GLY:N	10:H:130:ARG:HH22	2.07	0.51
14:L:43:THR:HG22	14:L:43:THR:O	2.10	0.51
3:A:49:LYS:HZ1	3:A:61:ILE:N	2.09	0.51
3:A:62:ASP:HB3	3:A:64:ASN:HD21	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:332:LYS:HB2	3:A:337:ARG:CZ	2.41	0.51
3:A:382:PRO:HD3	3:A:428:TYR:CD2	2.45	0.51
3:A:719:VAL:C	3:A:721:PHE:N	2.67	0.51
3:A:898:ARG:HB2	3:A:933:TYR:CE1	2.46	0.51
3:A:1283:VAL:HG12	3:A:1284:MET:N	2.25	0.51
3:A:1436:ILE:CD1	4:B:1139:ILE:HG23	2.41	0.51
4:B:29:ASP:OD1	4:B:658:ILE:HD13	2.10	0.51
4:B:212:LEU:CD2	4:B:480:SER:HB2	2.36	0.51
4:B:336:ARG:CZ	4:B:348:ARG:NH1	2.73	0.51
4:B:343:ILE:HG22	4:B:348:ARG:HG3	1.91	0.51
5:C:20:PHE:CE1	5:C:22:LEU:HD12	2.45	0.51
6:D:8:PHE:CD2	9:G:6:ASP:O	2.63	0.51
9:G:99:PHE:CE2	9:G:115:MET:HE2	2.45	0.51
3:A:116:ASP:O	3:A:118:HIS:N	2.43	0.51
3:A:148:CYS:O	3:A:168:GLY:HA2	2.09	0.51
3:A:412:ARG:NH2	4:B:1108:ARG:HH12	2.08	0.51
3:A:1377:THR:O	3:A:1378:GLN:C	2.53	0.51
4:B:168:GLY:HA2	4:B:454:THR:OG1	2.11	0.51
4:B:1098:MET:HE3	4:B:1098:MET:H	1.74	0.51
7:E:22:MET:CE	7:E:26:ARG:NH2	2.74	0.51
7:E:48:ASP:CG	7:E:49:SER:N	2.68	0.51
7:E:165:LEU:N	7:E:165:LEU:HD23	2.25	0.51
11:I:69:PRO:HG2	11:I:85:PHE:CD2	2.46	0.51
11:I:85:PHE:HD2	11:I:85:PHE:N	2.02	0.51
3:A:351:THR:HG22	4:B:1103:ILE:HA	1.91	0.51
3:A:1066:VAL:O	3:A:1070:GLN:HG3	2.10	0.51
4:B:361:LEU:N	4:B:362:PRO:CD	2.73	0.51
4:B:460:ALA:HB1	4:B:466:TRP:CZ3	2.46	0.51
4:B:984:HIS:NE2	4:B:1025:HIS:HA	2.26	0.51
4:B:1001:PHE:CE2	5:C:34:ARG:CZ	2.94	0.51
5:C:259:LEU:HD13	13:K:91:CYS:CB	2.40	0.51
6:D:123:LEU:HD23	6:D:149:THR:HG21	1.93	0.51
8:F:131:PRO:C	8:F:132:LEU:HD23	2.36	0.51
9:G:79:PHE:CZ	9:G:106:MET:HE2	2.45	0.51
3:A:106:VAL:HG13	3:A:112:LYS:C	2.35	0.51
3:A:896:ARG:NH2	3:A:1030:ARG:NH2	2.59	0.51
3:A:1371:LEU:O	3:A:1375:MET:HG3	2.10	0.51
4:B:216:GLU:HA	4:B:406:LEU:HD23	1.93	0.51
4:B:840:ILE:HG21	4:B:994:TYR:HD1	1.75	0.51
4:B:944:THR:HG21	4:B:1122:ARG:NH2	2.26	0.51
4:B:957:ASN:O	4:B:958:GLN:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:213:PRO:O	5:C:214:ASN:CB	2.58	0.51
7:E:24:LYS:HG3	7:E:25:ASP:N	2.26	0.51
7:E:55:ARG:O	7:E:57:MET:N	2.44	0.51
8:F:96:THR:O	8:F:100:GLN:HG3	2.11	0.51
3:A:58:LEU:HD11	3:A:244:PRO:HD2	1.91	0.51
3:A:89:PRO:HB3	3:A:208:LEU:HD12	1.93	0.51
3:A:116:ASP:C	3:A:118:HIS:N	2.66	0.51
3:A:1220:PHE:O	3:A:1221:LYS:HB2	2.11	0.51
4:B:176:SER:O	4:B:182:SER:HB3	2.11	0.51
4:B:288:ALA:O	4:B:331:LEU:HD11	2.11	0.51
4:B:329:THR:O	4:B:332:ASP:HB3	2.10	0.51
4:B:773:MET:HE2	4:B:985:GLY:HA2	1.92	0.51
4:B:885:MET:HA	4:B:936:ASP:HB2	1.92	0.51
5:C:97:VAL:HB	5:C:159:ALA:HB3	1.93	0.51
10:H:128:ASN:OD1	10:H:128:ASN:O	2.29	0.51
11:I:7:CYS:SG	11:I:8:ARG:O	2.69	0.51
3:A:50:ILE:C	3:A:52:GLY:N	2.62	0.50
3:A:75:ASN:O	3:A:76:GLU:CB	2.59	0.50
3:A:152:VAL:HG13	3:A:153:PRO:HD2	1.90	0.50
3:A:347:PHE:H	4:B:1107:ALA:HA	1.76	0.50
3:A:527:THR:CG2	3:A:650:GLN:HA	2.41	0.50
3:A:591:PHE:HA	3:A:595:THR:HG21	1.92	0.50
3:A:982:THR:O	3:A:985:ASP:HB2	2.11	0.50
3:A:1149:ALA:HB2	11:I:47:GLU:HA	1.92	0.50
4:B:23:ALA:H	4:B:654:ARG:HB3	1.77	0.50
4:B:637:LEU:O	4:B:690:VAL:HG13	2.11	0.50
4:B:1040:ASN:O	4:B:1042:GLY:N	2.43	0.50
5:C:62:PHE:O	5:C:66:ARG:HG3	2.10	0.50
5:C:112:ASN:HB2	5:C:114:TYR:HE1	1.74	0.50
5:C:184:ASN:HD21	5:C:187:LYS:HA	1.76	0.50
9:G:22:MET:O	9:G:23:LYS:C	2.54	0.50
9:G:127:PRO:HG2	9:G:138:THR:CG2	2.37	0.50
3:A:1121:GLU:O	3:A:1122:PRO:C	2.53	0.50
3:A:1197:LEU:HD11	3:A:1238:ILE:HD11	1.93	0.50
3:A:1410:PHE:HD2	4:B:1212:ILE:HD12	1.76	0.50
3:A:1446:ASP:HB2	8:F:133:VAL:HG23	1.93	0.50
4:B:185:THR:O	4:B:186:GLU:C	2.54	0.50
4:B:215:GLN:OE1	4:B:479:VAL:HG22	2.11	0.50
4:B:309:GLN:OE1	11:I:52:ILE:HD11	2.11	0.50
4:B:731:VAL:HG12	4:B:732:SER:H	1.76	0.50
4:B:882:THR:HB	4:B:934:LYS:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:133:ILE:HD13	5:C:236:GLY:C	2.37	0.50
5:C:242:GLN:C	5:C:244:VAL:N	2.69	0.50
7:E:205:SER:O	7:E:206:GLY:C	2.54	0.50
9:G:1:MET:HE2	9:G:3:PHE:CE1	2.46	0.50
11:I:6:PHE:HA	11:I:14:LEU:HG	1.92	0.50
12:J:56:LEU:O	12:J:57:ILE:C	2.55	0.50
3:A:317:LYS:O	3:A:318:SER:CB	2.58	0.50
3:A:357:PRO:HD2	4:B:833:TYR:CE1	2.46	0.50
3:A:718:VAL:O	3:A:721:PHE:HB2	2.10	0.50
3:A:805:LEU:CD1	4:B:1052:VAL:HG21	2.42	0.50
3:A:1149:ALA:CB	11:I:47:GLU:HA	2.41	0.50
3:A:1425:SER:O	3:A:1429:ILE:HG13	2.11	0.50
4:B:822:ASN:ND2	12:J:52:THR:HG21	2.26	0.50
5:C:138:GLU:OE1	5:C:138:GLU:N	2.42	0.50
5:C:241:ASP:OD1	5:C:242:GLN:N	2.42	0.50
6:D:4:SER:OG	6:D:5:THR:N	2.45	0.50
6:D:8:PHE:O	6:D:9:GLN:HB2	2.11	0.50
7:E:112:TYR:CE1	7:E:136:ASN:HB2	2.46	0.50
10:H:91:ASP:O	10:H:93:TYR:N	2.41	0.50
12:J:14:VAL:CG1	12:J:50:ILE:HD11	2.39	0.50
3:A:31:SER:HA	3:A:81:PHE:O	2.12	0.50
3:A:103:CYS:SG	3:A:108:MET:HE1	2.51	0.50
3:A:207:ILE:HG22	3:A:211:PHE:CE1	2.47	0.50
3:A:325:ILE:HG21	4:B:1210:MET:HG3	1.94	0.50
3:A:720:ARG:HB3	3:A:720:ARG:CZ	2.42	0.50
6:D:13:ARG:CA	6:D:17:LYS:HZ3	2.25	0.50
6:D:63:LEU:HD13	6:D:133:THR:OG1	2.10	0.50
9:G:35:GLU:CG	9:G:48:VAL:HG23	2.41	0.50
3:A:295:LEU:O	3:A:298:PHE:HB3	2.11	0.50
3:A:571:LEU:HD22	10:H:46:LEU:HD11	1.94	0.50
3:A:837:ILE:HA	3:A:840:ARG:HD3	1.92	0.50
3:A:852:TYR:CD1	8:F:136:ARG:HB3	2.46	0.50
4:B:295:GLY:O	4:B:299:GLU:HG2	2.12	0.50
4:B:683:SER:O	4:B:687:GLU:HB2	2.12	0.50
4:B:798:TYR:HE2	5:C:62:PHE:HE2	1.56	0.50
5:C:70:ILE:HD11	5:C:144:ILE:HG12	1.93	0.50
6:D:56:ARG:HD3	6:D:149:THR:HA	1.91	0.50
9:G:44:TYR:CD2	9:G:105:PRO:HB2	2.47	0.50
10:H:26:ILE:CG2	10:H:27:GLU:N	2.75	0.50
3:A:16:GLU:HB3	3:A:1418:LEU:HD11	1.94	0.50
3:A:675:THR:O	3:A:679:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1120:LEU:O	3:A:1323:ASP:N	2.44	0.50
4:B:526:GLU:OE2	4:B:752:ALA:HB2	2.12	0.50
4:B:558:LEU:C	4:B:560:GLU:H	2.19	0.50
4:B:638:PHE:HB3	4:B:651:LEU:HD22	1.94	0.50
4:B:824:ILE:CG2	4:B:1087:PHE:CE2	2.93	0.50
5:C:89:GLU:O	5:C:90:ASP:HB3	2.11	0.50
9:G:34:VAL:CG1	9:G:45:ILE:HG21	2.37	0.50
3:A:224:PHE:HD2	3:A:229:SER:O	1.95	0.50
3:A:455:MET:HE3	4:B:1134:GLU:HG3	1.93	0.50
3:A:683:ILE:HG21	3:A:801:GLU:CD	2.36	0.50
3:A:1101:LEU:HB2	3:A:1355:VAL:HG11	1.93	0.50
4:B:25:ILE:HD11	4:B:653:VAL:C	2.36	0.50
4:B:100:PRO:HB2	4:B:180:TYR:HE1	1.75	0.50
4:B:169:ARG:HD2	4:B:454:THR:HG21	1.93	0.50
6:D:39:ASN:HD21	6:D:41:GLN:HE21	1.54	0.50
6:D:195:ILE:HG22	6:D:198:LEU:HG	1.93	0.50
7:E:145:THR:HG21	7:E:187:TYR:CD2	2.46	0.50
8:F:68:THR:O	8:F:69:LEU:HB3	2.12	0.50
9:G:80:LYS:N	9:G:80:LYS:HD3	2.26	0.50
9:G:137:ILE:HG21	9:G:143:ILE:HD11	1.94	0.50
12:J:7:CYS:O	12:J:11:GLY:HA2	2.12	0.50
12:J:55:ASP:OD2	12:J:58:GLU:HG2	2.12	0.50
3:A:180:LYS:NZ	3:A:294:SER:HB3	2.26	0.50
3:A:606:LEU:HG	3:A:613:ILE:HD12	1.93	0.50
3:A:853:ASP:OD1	3:A:855:THR:CB	2.60	0.50
3:A:920:LEU:HD23	3:A:921:GLY:N	2.27	0.50
3:A:1120:LEU:CD1	3:A:1304:TRP:O	2.60	0.50
3:A:1144:LYS:HB2	3:A:1268:LEU:O	2.11	0.50
4:B:289:LEU:HD13	4:B:375:ALA:HB2	1.93	0.50
4:B:291:ILE:HD13	4:B:300:HIS:CD2	2.47	0.50
4:B:639:ILE:HG22	4:B:641:GLU:HG2	1.94	0.50
4:B:1162:ILE:HG22	4:B:1163:CYS:H	1.77	0.50
9:G:115:MET:CB	9:G:116:PRO:HD2	2.42	0.50
14:L:40:LEU:HD13	14:L:44:ASP:HB3	1.94	0.50
3:A:43:GLU:O	3:A:44:THR:HB	2.12	0.50
3:A:346:ASP:HB3	4:B:1108:ARG:N	2.25	0.50
3:A:852:TYR:CE2	3:A:1060:PRO:HB2	2.47	0.50
3:A:1410:PHE:C	3:A:1412:ALA:H	2.20	0.50
3:A:1446:ASP:HB2	8:F:133:VAL:CG2	2.41	0.50
4:B:171:PRO:HD2	4:B:457:LEU:CD1	2.42	0.50
4:B:281:PRO:O	4:B:283:VAL:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:840:ILE:HD13	4:B:994:TYR:HE1	1.77	0.50
4:B:976:ILE:O	4:B:978:ASP:N	2.45	0.50
4:B:1045:SER:O	4:B:1046:PRO:O	2.30	0.50
4:B:1152:MET:HE3	4:B:1157:ALA:HA	1.94	0.50
5:C:11:ARG:HD3	5:C:209:TYR:CZ	2.46	0.50
5:C:16:ASP:O	5:C:17:ASN:CG	2.55	0.50
8:F:114:GLU:OE2	8:F:119:ARG:HG2	2.12	0.50
9:G:115:MET:HB3	9:G:116:PRO:HD2	1.93	0.50
10:H:55:LEU:HD22	10:H:144:ILE:CG2	2.42	0.50
3:A:7:SER:CB	4:B:1175:LEU:HD22	2.42	0.49
3:A:399:HIS:O	3:A:400:PRO:C	2.53	0.49
3:A:427:GLN:O	3:A:428:TYR:C	2.52	0.49
3:A:695:LYS:C	3:A:697:ALA:H	2.20	0.49
3:A:827:THR:O	3:A:831:THR:HB	2.11	0.49
3:A:844:ALA:C	3:A:845:LEU:HD23	2.36	0.49
3:A:963:ILE:HD13	3:A:1049:ILE:HG13	1.93	0.49
3:A:1017:LEU:HB3	7:E:205:SER:HA	1.93	0.49
3:A:1401:SER:O	3:A:1402:PHE:HB2	2.11	0.49
4:B:33:VAL:O	4:B:36:ALA:HB3	2.11	0.49
5:C:18:VAL:CG2	5:C:240:VAL:HB	2.42	0.49
6:D:126:ILE:HD13	6:D:145:MET:HE2	1.93	0.49
7:E:124:VAL:HG13	7:E:132:ILE:CG1	2.42	0.49
8:F:109:VAL:HG23	8:F:124:GLU:HG2	1.94	0.49
9:G:80:LYS:O	9:G:82:PHE:CE1	2.65	0.49
9:G:96:GLN:HG3	9:G:97:HIS:CD2	2.45	0.49
11:I:14:LEU:HD22	11:I:28:GLU:O	2.12	0.49
3:A:93:VAL:CG2	3:A:301:ALA:HA	2.41	0.49
3:A:224:PHE:CD2	3:A:231:PRO:HG3	2.47	0.49
3:A:616:VAL:HG12	3:A:617:VAL:N	2.27	0.49
3:A:621:THR:O	3:A:629:LEU:HB2	2.12	0.49
3:A:720:ARG:O	3:A:724:GLU:HB2	2.11	0.49
3:A:981:LEU:HD21	3:A:1039:LYS:HA	1.94	0.49
3:A:1313:LEU:HD23	3:A:1338:VAL:CG2	2.41	0.49
3:A:1389:PHE:CD1	3:A:1389:PHE:C	2.90	0.49
3:A:1450:LEU:O	3:A:1450:LEU:CG	2.59	0.49
4:B:521:LEU:HB3	4:B:633:VAL:HG11	1.94	0.49
4:B:640:VAL:O	4:B:640:VAL:HG12	2.11	0.49
4:B:1077:THR:HG22	13:K:44:ASN:HD21	1.77	0.49
5:C:74:SER:HB2	5:C:77:ILE:HG12	1.95	0.49
5:C:76:ASP:OD2	5:C:128:ASN:N	2.44	0.49
9:G:145:VAL:CG1	9:G:146:LYS:N	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:128:ASN:O	10:H:128:ASN:CG	2.55	0.49
3:A:322:VAL:O	3:A:322:VAL:HG12	2.11	0.49
3:A:997:LEU:HD13	3:A:1018:PHE:HE2	1.76	0.49
3:A:1007:ILE:HD13	7:E:168:TYR:HE2	1.77	0.49
4:B:281:PRO:HB3	4:B:320:ASP:OD2	2.12	0.49
6:D:64:VAL:C	6:D:66:ARG:N	2.70	0.49
9:G:14:HIS:CD2	9:G:16:SER:CB	2.95	0.49
9:G:50:ASP:O	9:G:51:TYR:C	2.54	0.49
11:I:15:TYR:N	11:I:15:TYR:CD1	2.80	0.49
3:A:783:THR:HG22	3:A:784:LEU:HG	1.93	0.49
3:A:808:LEU:HD23	3:A:813:PHE:HA	1.93	0.49
3:A:857:ARG:CZ	8:F:139:PRO:HG3	2.43	0.49
3:A:1006:ILE:HB	7:E:167:ARG:HG3	1.95	0.49
7:E:156:LEU:HA	7:E:160:GLU:OE1	2.12	0.49
7:E:157:SER:O	7:E:159:ASP:N	2.45	0.49
10:H:13:SER:O	10:H:14:GLU:HB2	2.13	0.49
10:H:101:ALA:HB2	10:H:116:TYR:CE1	2.48	0.49
3:A:106:VAL:HG12	3:A:107:CYS:N	2.28	0.49
3:A:438:ASP:OD1	3:A:461:LYS:HA	2.12	0.49
3:A:440:ASP:O	3:A:442:VAL:HG22	2.12	0.49
3:A:541:ILE:CD1	3:A:549:MET:HE1	2.31	0.49
3:A:939:ASP:OD1	3:A:1023:ARG:NH1	2.46	0.49
3:A:1283:VAL:HG12	3:A:1284:MET:H	1.78	0.49
4:B:37:PHE:CD1	4:B:41:LYS:HG3	2.45	0.49
4:B:409:ALA:O	4:B:413:LEU:HG	2.12	0.49
4:B:680:THR:O	4:B:684:LEU:HD12	2.12	0.49
4:B:777:ALA:HA	4:B:1095:LEU:HA	1.94	0.49
4:B:1174:LYS:O	4:B:1176:ASN:HB2	2.11	0.49
10:H:87:ARG:O	10:H:89:LEU:HG	2.12	0.49
14:L:39:SER:O	14:L:40:LEU:HG	2.11	0.49
3:A:51:GLY:HA2	3:A:56:PRO:HA	1.94	0.49
4:B:204:ILE:O	4:B:204:ILE:HG22	2.12	0.49
4:B:843:GLN:O	4:B:846:ILE:N	2.45	0.49
4:B:1182:CYS:O	4:B:1183:LYS:C	2.55	0.49
5:C:22:LEU:HB2	5:C:230:MET:HE3	1.94	0.49
7:E:23:VAL:HB	7:E:30:ILE:HD11	1.95	0.49
11:I:51:ASN:O	11:I:54:GLU:HG3	2.12	0.49
11:I:85:PHE:HD1	11:I:99:LEU:HD13	1.75	0.49
3:A:35:ILE:HD13	3:A:241:VAL:HG11	1.94	0.49
3:A:40:THR:CG2	3:A:41:MET:HE2	2.42	0.49
3:A:364:VAL:O	3:A:364:VAL:HG13	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:416:ARG:C	3:A:417:TYR:CD2	2.89	0.49
3:A:578:LEU:O	3:A:578:LEU:HG	2.13	0.49
3:A:806:ARG:NH1	4:B:729:ILE:HG13	2.28	0.49
3:A:1004:ASN:HD21	7:E:167:ARG:HD2	1.73	0.49
3:A:1385:THR:C	3:A:1387:HIS:N	2.69	0.49
4:B:189:LEU:CD1	4:B:196:PRO:HA	2.42	0.49
4:B:784:ASN:O	4:B:788:ARG:HG3	2.13	0.49
4:B:882:THR:HG21	4:B:884:ARG:HB2	1.93	0.49
9:G:88:ASP:HB3	9:G:144:ARG:CA	2.42	0.49
9:G:117:GLN:C	9:G:119:LEU:N	2.70	0.49
12:J:56:LEU:O	12:J:59:LYS:N	2.44	0.49
3:A:269:ILE:HG23	3:A:300:VAL:CG2	2.43	0.49
3:A:310:GLY:C	3:A:312:PRO:HD2	2.38	0.49
3:A:590:ARG:HH21	3:A:620:LYS:CB	2.22	0.49
3:A:1256:GLU:O	3:A:1260:LEU:HB3	2.12	0.49
4:B:280:ILE:CG2	4:B:285:ILE:HG13	2.42	0.49
4:B:642:ASP:CA	4:B:649:LYS:HA	2.40	0.49
4:B:729:ILE:O	4:B:729:ILE:HG22	2.11	0.49
4:B:1220:ARG:HB3	4:B:1220:ARG:CZ	2.43	0.49
5:C:146:LYS:HB2	12:J:57:ILE:HD11	1.93	0.49
5:C:254:LYS:C	5:C:256:ALA:N	2.70	0.49
6:D:39:ASN:HD22	6:D:41:GLN:HB2	1.78	0.49
6:D:210:ILE:O	6:D:214:LEU:HG	2.13	0.49
7:E:13:TRP:CE3	7:E:39:LEU:HD13	2.47	0.49
7:E:135:PHE:CD2	7:E:140:LEU:HD21	2.48	0.49
9:G:7:LEU:CD1	9:G:45:ILE:HD11	2.43	0.49
9:G:106:MET:CG	9:G:107:LYS:N	2.75	0.49
9:G:129:SER:HB3	9:G:138:THR:OG1	2.12	0.49
13:K:110:ASN:O	13:K:111:LEU:HB3	2.12	0.49
3:A:70:CYS:O	3:A:70:CYS:SG	2.71	0.49
3:A:735:VAL:O	3:A:735:VAL:HG12	2.12	0.49
3:A:853:ASP:OD1	3:A:853:ASP:C	2.56	0.49
3:A:984:LYS:HG2	3:A:988:LEU:CD1	2.43	0.49
4:B:658:ILE:CG2	4:B:662:MET:HE2	2.42	0.49
5:C:112:ASN:CB	5:C:114:TYR:CE1	2.95	0.49
5:C:234:SER:HB3	5:C:240:VAL:HG13	1.95	0.49
8:F:128:LYS:HD3	8:F:149:GLU:O	2.12	0.49
9:G:7:LEU:O	9:G:73:LYS:HD2	2.13	0.49
9:G:74:TYR:H	9:G:74:TYR:HD2	1.61	0.49
10:H:12:VAL:HB	10:H:52:GLN:H	1.77	0.49
13:K:47:ARG:HD2	13:K:47:ARG:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1213:GLY:O	3:A:1214:GLU:C	2.56	0.49
4:B:770:GLN:HG2	4:B:983:ARG:O	2.13	0.49
4:B:850:LEU:HD12	4:B:851:PHE:N	2.28	0.49
4:B:1001:PHE:CD1	4:B:1001:PHE:C	2.91	0.49
5:C:46:ILE:CD1	5:C:67:LEU:HB3	2.40	0.49
5:C:147:LEU:HD23	5:C:147:LEU:N	2.28	0.49
6:D:19:GLU:O	6:D:21:GLU:N	2.46	0.49
7:E:28:TYR:HE1	7:E:78:LEU:HD13	1.78	0.49
14:L:32:ALA:CB	14:L:55:ILE:HD12	2.33	0.49
3:A:29:ALA:HB1	4:B:1184:GLY:CA	2.43	0.48
3:A:335:ARG:HA	3:A:339:ASN:HD22	1.78	0.48
3:A:527:THR:O	3:A:653:VAL:HG11	2.13	0.48
3:A:546:VAL:O	3:A:550:LEU:HG	2.13	0.48
3:A:981:LEU:HD21	3:A:1038:THR:O	2.13	0.48
3:A:1116:LEU:C	3:A:1116:LEU:HD12	2.38	0.48
4:B:234:ILE:HD12	4:B:234:ILE:N	2.28	0.48
4:B:550:ASP:OD1	4:B:551:PRO:HD2	2.13	0.48
4:B:992:ILE:HD11	13:K:66:PRO:HB2	1.95	0.48
4:B:1084:GLN:OE1	5:C:189:THR:CG2	2.61	0.48
5:C:226:ASP:O	5:C:227:THR:HB	2.12	0.48
5:C:243:VAL:O	5:C:243:VAL:HG12	2.13	0.48
6:D:53:SER:H	6:D:148:LEU:HD23	1.78	0.48
7:E:124:VAL:HB	7:E:125:PRO:HD3	1.95	0.48
3:A:18:GLN:HB3	4:B:1215:ARG:HG3	1.94	0.48
3:A:166:GLY:O	3:A:167:CYS:CB	2.61	0.48
3:A:227:VAL:HG12	6:D:15:LEU:HD23	1.94	0.48
3:A:573:SER:OG	3:A:576:GLN:HB2	2.12	0.48
4:B:129:PHE:CD2	4:B:166:PHE:HA	2.48	0.48
4:B:615:MET:HA	4:B:625:LYS:O	2.13	0.48
4:B:896:ASP:CG	14:L:58:LYS:HZ2	2.21	0.48
6:D:51:ASN:O	6:D:52:LEU:C	2.56	0.48
7:E:15:ALA:O	7:E:19:VAL:HG23	2.13	0.48
11:I:21:GLU:O	11:I:21:GLU:HG2	2.14	0.48
13:K:65:HIS:HD2	13:K:67:PHE:N	2.03	0.48
3:A:618:GLU:O	3:A:621:THR:N	2.41	0.48
3:A:1219:THR:HG21	3:A:1271:ILE:HD11	1.94	0.48
3:A:1385:THR:CG2	3:A:1386:ARG:N	2.76	0.48
4:B:542:MET:HE2	4:B:743:ILE:HG13	1.95	0.48
4:B:737:THR:CG2	11:I:66:PRO:HA	2.43	0.48
4:B:806:THR:HA	4:B:1045:SER:OG	2.13	0.48
4:B:810:GLU:HB3	4:B:811:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:879:ARG:O	4:B:880:THR:HB	2.13	0.48
4:B:1022:THR:HG23	4:B:1022:THR:O	2.12	0.48
4:B:1068:GLY:O	4:B:1069:PHE:O	2.32	0.48
4:B:1166:CYS:SG	4:B:1166:CYS:O	2.70	0.48
5:C:26:ASP:O	5:C:27:LEU:C	2.56	0.48
5:C:70:ILE:HG12	5:C:142:VAL:HG11	1.95	0.48
5:C:75:MET:HE2	5:C:239:PRO:HD3	1.95	0.48
11:I:56:ALA:O	11:I:57:GLY:O	2.31	0.48
3:A:18:GLN:H	4:B:1215:ARG:HB2	1.79	0.48
3:A:507:VAL:N	3:A:508:PRO:CD	2.77	0.48
3:A:849:MET:HE1	3:A:1061:GLY:HA2	1.95	0.48
4:B:54:PHE:HA	4:B:58:THR:HB	1.93	0.48
4:B:581:PHE:HA	4:B:585:VAL:O	2.13	0.48
7:E:129:PRO:O	7:E:130:ALA:C	2.57	0.48
8:F:90:ARG:HD3	8:F:155:LEU:HD12	1.93	0.48
10:H:142:LEU:C	10:H:143:LEU:HD12	2.37	0.48
10:H:145:ARG:O	10:H:146:ARG:HB2	2.13	0.48
13:K:7:PHE:CD1	13:K:7:PHE:C	2.91	0.48
3:A:608:ILE:C	3:A:610:GLY:H	2.21	0.48
3:A:966:ASN:O	3:A:967:ALA:C	2.56	0.48
3:A:1094:VAL:HG12	3:A:1095:THR:N	2.26	0.48
3:A:1265:ASN:C	3:A:1267:MET:N	2.68	0.48
3:A:1319:VAL:HG13	3:A:1320:PRO:HD2	1.96	0.48
4:B:363:HIS:HD2	4:B:585:VAL:HG22	1.78	0.48
4:B:365:THR:HG23	4:B:367:LEU:HG	1.96	0.48
4:B:498:THR:O	4:B:536:VAL:HA	2.13	0.48
5:C:221:TYR:CE1	5:C:222:LYS:HG3	2.49	0.48
7:E:13:TRP:CZ3	7:E:39:LEU:HB2	2.48	0.48
11:I:111:THR:CG2	11:I:112:SER:N	2.77	0.48
12:J:44:TYR:HA	12:J:47:ARG:HB3	1.95	0.48
3:A:98:LYS:O	3:A:102:VAL:HG23	2.14	0.48
3:A:187:LYS:NZ	3:A:198:GLU:OE2	2.39	0.48
3:A:218:ASP:O	3:A:219:PHE:C	2.57	0.48
3:A:423:ASP:O	3:A:424:ILE:CB	2.62	0.48
3:A:475:THR:CG2	3:A:476:SER:H	2.26	0.48
3:A:981:LEU:HD23	3:A:1039:LYS:HA	1.96	0.48
3:A:1029:ARG:HH11	3:A:1029:ARG:HG3	1.79	0.48
3:A:1444:MET:CG	9:G:60:ARG:HA	2.43	0.48
4:B:324:ILE:HD13	4:B:330:ALA:HA	1.96	0.48
4:B:711:GLU:H	4:B:712:PRO:HD2	1.78	0.48
4:B:913:GLY:HA2	4:B:938:SER:OG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1167:GLY:N	4:B:1217:TYR:HE1	2.11	0.48
5:C:249:ASP:O	5:C:252:GLN:HB3	2.13	0.48
7:E:2:ASP:HB3	7:E:3:GLN:H	1.46	0.48
10:H:82:PRO:C	10:H:84:ALA:H	2.21	0.48
11:I:3:THR:O	11:I:3:THR:HG22	2.13	0.48
14:L:34:CYS:O	14:L:35:SER:C	2.57	0.48
3:A:167:CYS:SG	3:A:167:CYS:O	2.72	0.48
3:A:185:TRP:CZ3	3:A:200:ARG:HG2	2.48	0.48
3:A:1005:GLU:O	3:A:1009:ASN:HB2	2.13	0.48
3:A:1409:LEU:HD13	4:B:1207:LEU:HD21	1.95	0.48
4:B:98:THR:OG1	4:B:101:MET:HE2	2.13	0.48
4:B:954:VAL:O	14:L:55:ILE:O	2.31	0.48
4:B:1072:MET:CE	4:B:1087:PHE:HD1	2.26	0.48
5:C:11:ARG:HH21	5:C:229:TYR:HB3	1.79	0.48
5:C:82:TYR:O	5:C:83:SER:C	2.56	0.48
5:C:242:GLN:C	5:C:244:VAL:H	2.20	0.48
7:E:55:ARG:HD2	7:E:83:CYS:O	2.14	0.48
3:A:207:ILE:CG2	3:A:211:PHE:CE1	2.97	0.48
3:A:407:ARG:HD2	3:A:413:ILE:HD11	1.96	0.48
3:A:442:VAL:CB	3:A:489:LEU:HD11	2.40	0.48
3:A:456:MET:HE3	3:A:478:TYR:CZ	2.49	0.48
3:A:613:ILE:O	3:A:614:PHE:HB3	2.13	0.48
3:A:666:ILE:CD1	3:A:667:GLY:H	2.20	0.48
3:A:1237:ILE:HG22	3:A:1238:ILE:N	2.28	0.48
4:B:121:ASN:OD1	4:B:963:PHE:HZ	1.96	0.48
4:B:314:LEU:O	4:B:317:CYS:HB3	2.14	0.48
4:B:383:ASN:O	4:B:384:ARG:C	2.57	0.48
4:B:744:HIS:CG	4:B:745:PRO:HD2	2.49	0.48
4:B:1072:MET:SD	4:B:1087:PHE:HD1	2.37	0.48
4:B:1106:ARG:NH2	4:B:1111:MET:CE	2.76	0.48
5:C:147:LEU:HD12	5:C:151:GLN:O	2.13	0.48
5:C:174:ALA:O	5:C:175:ALA:HB2	2.14	0.48
7:E:213:ILE:HG12	7:E:214:CYS:H	1.78	0.48
10:H:116:TYR:HE2	10:H:140:ALA:CB	2.27	0.48
12:J:1:MET:H2	12:J:57:ILE:HG22	1.78	0.48
14:L:47:ARG:HH21	14:L:54:ARG:NH2	2.12	0.48
3:A:399:HIS:CB	3:A:400:PRO:CD	2.90	0.48
3:A:1315:GLU:C	3:A:1317:MET:N	2.70	0.48
3:A:1398:MET:HB2	3:A:1426:GLU:OE2	2.13	0.48
4:B:345:LYS:O	4:B:348:ARG:N	2.47	0.48
4:B:790:ASP:OD2	4:B:790:ASP:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1138:MET:HE3	4:B:1143:ALA:HB3	1.96	0.48
6:D:51:ASN:O	6:D:52:LEU:O	2.32	0.48
10:H:99:GLY:CA	10:H:118:PHE:HA	2.44	0.48
3:A:79:GLY:H	4:B:1205:GLN:HE22	1.61	0.48
3:A:401:GLY:C	3:A:435:HIS:CD2	2.89	0.48
3:A:568:PRO:HB2	5:C:221:TYR:CZ	2.49	0.48
3:A:577:ILE:C	3:A:579:SER:N	2.71	0.48
3:A:608:ILE:HD12	3:A:613:ILE:CD1	2.44	0.48
3:A:1120:LEU:HD13	3:A:1304:TRP:O	2.14	0.48
4:B:557:PHE:HD2	4:B:557:PHE:O	1.96	0.48
4:B:954:VAL:HA	4:B:964:VAL:HG22	1.95	0.48
4:B:1034:VAL:C	4:B:1036:ALA:N	2.71	0.48
6:D:4:SER:C	6:D:5:THR:HG22	2.39	0.48
9:G:153:GLN:CG	9:G:154:VAL:HG23	2.44	0.48
10:H:20:TYR:O	10:H:22:LYS:N	2.46	0.48
14:L:61:THR:HG22	14:L:62:LYS:N	2.28	0.48
3:A:208:LEU:HD23	3:A:208:LEU:C	2.39	0.47
3:A:444:PHE:CB	3:A:458:HIS:HD2	2.26	0.47
3:A:456:MET:HE3	3:A:478:TYR:CE1	2.49	0.47
3:A:1438:THR:CG2	8:F:92:ARG:HD2	2.44	0.47
3:A:1438:THR:HG22	8:F:92:ARG:HD2	1.96	0.47
4:B:955:THR:HG22	4:B:956:THR:O	2.14	0.47
5:C:186:LEU:N	5:C:186:LEU:HD12	2.29	0.47
7:E:42:PHE:O	7:E:43:LYS:C	2.57	0.47
8:F:138:LEU:HB3	8:F:139:PRO:HD2	1.95	0.47
9:G:43:GLY:HA3	9:G:80:LYS:HB3	1.96	0.47
3:A:146:MET:HA	3:A:171:GLN:HB2	1.97	0.47
3:A:903:ASN:ND2	3:A:905:ASP:H	2.12	0.47
3:A:1349:TYR:CA	3:A:1372:VAL:HG21	2.44	0.47
3:A:1349:TYR:O	3:A:1350:LYS:C	2.56	0.47
4:B:43:LEU:HD11	4:B:811:TYR:O	2.15	0.47
4:B:193:LYS:HZ1	14:L:32:ALA:HB1	1.74	0.47
4:B:200:GLY:HA2	4:B:202:TYR:CE2	2.49	0.47
4:B:801:LYS:O	12:J:52:THR:CG2	2.58	0.47
4:B:1023:VAL:O	4:B:1026:LEU:N	2.47	0.47
5:C:35:ARG:HH11	13:K:41:THR:CA	2.27	0.47
5:C:107:SER:C	5:C:109:SER:N	2.72	0.47
6:D:52:LEU:CD2	6:D:147:TYR:HE2	2.27	0.47
8:F:68:THR:O	8:F:69:LEU:CB	2.62	0.47
3:A:282:ASN:O	3:A:284:ALA:N	2.47	0.47
3:A:352:VAL:O	3:A:467:THR:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:353:ILE:HG21	3:A:487:MET:HE3	1.96	0.47
4:B:38:PHE:CD1	4:B:811:TYR:CD2	3.00	0.47
4:B:314:LEU:O	4:B:318:VAL:HG23	2.15	0.47
4:B:557:PHE:CD2	4:B:557:PHE:O	2.67	0.47
4:B:628:THR:HG23	4:B:628:THR:O	2.14	0.47
4:B:842:ASN:ND2	4:B:845:SER:OG	2.38	0.47
5:C:263:THR:O	5:C:265:MET:N	2.47	0.47
10:H:62:SER:C	10:H:64:ASN:N	2.73	0.47
11:I:99:LEU:C	11:I:100:PHE:HD1	2.21	0.47
3:A:353:ILE:CD1	3:A:487:MET:HE2	2.39	0.47
3:A:939:ASP:O	3:A:940:ARG:C	2.58	0.47
3:A:961:ARG:HH11	3:A:961:ARG:HG3	1.80	0.47
4:B:300:HIS:O	4:B:303:TYR:HE2	1.98	0.47
4:B:310:MET:O	4:B:313:MET:HB2	2.13	0.47
4:B:838:SER:HB2	4:B:989:THR:O	2.15	0.47
4:B:897:GLY:O	4:B:898:LEU:HD23	2.13	0.47
4:B:1198:TYR:CD2	4:B:1198:TYR:O	2.67	0.47
5:C:18:VAL:O	5:C:18:VAL:CG1	2.56	0.47
5:C:43:THR:CG2	5:C:44:LEU:N	2.52	0.47
6:D:185:CYS:O	6:D:211:LEU:HD22	2.14	0.47
7:E:164:LEU:HD11	7:E:211:TYR:CE1	2.50	0.47
8:F:74:ILE:HG23	8:F:75:PRO:HD2	1.96	0.47
10:H:123:MET:HG2	10:H:124:ARG:N	2.28	0.47
3:A:65:LEU:O	3:A:66:LYS:C	2.57	0.47
3:A:262:LEU:O	3:A:264:PHE:N	2.47	0.47
3:A:332:LYS:C	3:A:334:GLY:H	2.20	0.47
4:B:118:ARG:CG	4:B:204:ILE:HD13	2.45	0.47
4:B:298:LEU:N	4:B:298:LEU:CD2	2.78	0.47
4:B:360:PHE:C	4:B:360:PHE:CD2	2.92	0.47
4:B:360:PHE:O	4:B:361:LEU:C	2.58	0.47
4:B:1069:PHE:HA	4:B:1085:ILE:O	2.14	0.47
5:C:22:LEU:O	5:C:227:THR:HA	2.15	0.47
5:C:67:LEU:HD11	5:C:155:LEU:HD12	1.97	0.47
6:D:151:PHE:CD1	6:D:151:PHE:N	2.81	0.47
3:A:55:ASP:C	3:A:57:ARG:N	2.71	0.47
3:A:614:PHE:CD1	3:A:614:PHE:C	2.92	0.47
3:A:1161:THR:C	3:A:1163:ILE:H	2.22	0.47
4:B:51:PHE:CD2	4:B:173:MET:HB3	2.49	0.47
4:B:258:LEU:HG	4:B:258:LEU:O	2.13	0.47
4:B:293:PRO:HG2	4:B:296:GLU:CB	2.44	0.47
4:B:376:PHE:O	4:B:586:TRP:HZ3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:867:GLY:C	4:B:869:SER:H	2.22	0.47
5:C:84:ARG:NE	13:K:11:LEU:HD11	2.29	0.47
7:E:145:THR:HG21	7:E:187:TYR:CE2	2.50	0.47
3:A:120:GLU:C	3:A:122:MET:H	2.23	0.47
3:A:289:ILE:C	3:A:291:GLU:H	2.23	0.47
3:A:567:LYS:CG	3:A:568:PRO:CD	2.80	0.47
3:A:598:LEU:O	3:A:599:SER:C	2.57	0.47
3:A:626:ASN:C	3:A:628:GLY:H	2.22	0.47
3:A:816:HIS:CD2	4:B:764:SER:HB2	2.50	0.47
3:A:1015:VAL:O	3:A:1016:THR:C	2.57	0.47
4:B:114:PRO:O	4:B:116:GLU:N	2.48	0.47
4:B:220:GLY:O	4:B:222:ILE:HG13	2.14	0.47
4:B:273:LEU:CB	4:B:276:ILE:HD12	2.27	0.47
4:B:455:SER:O	4:B:456:GLY:C	2.58	0.47
4:B:460:ALA:HB1	4:B:466:TRP:CE3	2.50	0.47
4:B:604:ARG:O	4:B:606:LYS:N	2.47	0.47
5:C:69:LEU:HB3	12:J:6:ARG:HD3	1.97	0.47
5:C:100:THR:OG1	5:C:121:VAL:HG21	2.14	0.47
5:C:116:LYS:HD3	5:C:140:ASN:HA	1.96	0.47
5:C:189:THR:CG2	5:C:190:ASP:N	2.69	0.47
6:D:48:ILE:HG21	9:G:4:ILE:HB	1.96	0.47
6:D:54:GLU:O	6:D:58:VAL:HG23	2.14	0.47
7:E:117:THR:C	7:E:119:SER:H	2.22	0.47
11:I:22:ASN:O	11:I:23:ASN:HB2	2.15	0.47
3:A:47:ARG:O	3:A:48:ALA:HB2	2.15	0.47
3:A:55:ASP:N	3:A:56:PRO:CD	2.77	0.47
3:A:902:LEU:CG	3:A:926:GLN:HG3	2.43	0.47
3:A:1036:ARG:HH11	3:A:1036:ARG:CG	2.28	0.47
4:B:54:PHE:O	4:B:58:THR:HB	2.15	0.47
4:B:485:ARG:HG3	4:B:781:PHE:CD1	2.49	0.47
4:B:578:THR:C	4:B:589:VAL:HG13	2.40	0.47
4:B:735:ALA:O	4:B:738:PHE:HE1	1.98	0.47
4:B:882:THR:HG21	4:B:934:LYS:O	2.15	0.47
5:C:98:VAL:HG12	5:C:99:LEU:N	2.29	0.47
5:C:259:LEU:HD13	13:K:91:CYS:HB2	1.96	0.47
6:D:24:ALA:C	6:D:26:THR:N	2.73	0.47
6:D:156:ASP:C	6:D:158:GLU:N	2.70	0.47
7:E:93:MET:SD	7:E:97:VAL:CG2	3.03	0.47
7:E:144:ILE:HG13	7:E:145:THR:H	1.79	0.47
11:I:53:GLY:C	11:I:55:THR:N	2.70	0.47
3:A:40:THR:C	3:A:41:MET:HG3	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:211:PHE:HA	3:A:214:ILE:CD1	2.45	0.47
3:A:590:ARG:HG3	3:A:590:ARG:HH11	1.79	0.47
3:A:829:VAL:C	3:A:831:THR:N	2.70	0.47
3:A:1114:PRO:HB2	3:A:1311:VAL:HG23	1.95	0.47
3:A:1453:TYR:O	3:A:1454:MET:HB3	2.14	0.47
4:B:205:ILE:O	4:B:206:ASN:C	2.58	0.47
4:B:569:TYR:CE1	4:B:589:VAL:HG21	2.49	0.47
4:B:826:ALA:HB2	4:B:1008:PRO:HB3	1.96	0.47
4:B:882:THR:CB	4:B:934:LYS:O	2.62	0.47
4:B:903:VAL:HG12	4:B:904:ARG:N	2.30	0.47
5:C:18:VAL:O	5:C:19:ASP:C	2.58	0.47
5:C:100:THR:HG22	5:C:101:LEU:N	2.30	0.47
5:C:121:VAL:O	5:C:121:VAL:HG12	2.15	0.47
5:C:254:LYS:C	5:C:256:ALA:H	2.23	0.47
6:D:185:CYS:HB2	6:D:211:LEU:HD21	1.97	0.47
10:H:7:ASP:O	10:H:8:ASP:HB2	2.15	0.47
10:H:99:GLY:HA3	10:H:117:SER:O	2.14	0.47
11:I:5:ARG:HD3	11:I:36:GLU:OE2	2.15	0.47
14:L:38:LEU:CD1	14:L:49:LYS:HE2	2.44	0.47
3:A:246:VAL:O	3:A:328:ARG:NH1	2.41	0.47
3:A:453:MET:O	3:A:456:MET:HE2	2.14	0.47
3:A:506:ALA:HB1	3:A:508:PRO:HD2	1.96	0.47
3:A:601:LYS:HB2	3:A:603:ASN:ND2	2.29	0.47
3:A:652:VAL:O	3:A:653:VAL:C	2.58	0.47
3:A:793:SER:HB2	3:A:794:PRO:HD2	1.96	0.47
4:B:44:VAL:HG21	4:B:199:MET:O	2.15	0.47
4:B:373:ARG:CG	4:B:566:LEU:HD23	2.45	0.47
4:B:616:ILE:HG12	4:B:697:GLU:HA	1.97	0.47
4:B:642:ASP:H	4:B:649:LYS:HE3	1.79	0.47
4:B:1161:HIS:NE2	4:B:1175:LEU:HD21	2.30	0.47
4:B:1167:GLY:H	4:B:1215:ARG:HD2	1.80	0.47
5:C:22:LEU:HD13	5:C:230:MET:CE	2.36	0.47
5:C:179:GLU:HG2	5:C:180:TYR:H	1.78	0.47
7:E:78:LEU:HD11	7:E:109:ILE:HD12	1.97	0.47
9:G:126:ASN:HD22	9:G:127:PRO:HA	1.80	0.47
3:A:254:GLU:CG	4:B:935:ARG:HH22	2.27	0.46
3:A:453:MET:C	3:A:455:MET:H	2.23	0.46
3:A:705:LYS:HB2	3:A:708:MET:HE3	1.97	0.46
3:A:794:PRO:C	3:A:796:SER:N	2.73	0.46
3:A:1336:MET:HE3	3:A:1381:LEU:CG	2.41	0.46
4:B:195:CYS:SG	4:B:197:PHE:HB2	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:449:ASN:C	4:B:451:LYS:H	2.23	0.46
4:B:525:ALA:O	4:B:768:THR:HG23	2.15	0.46
4:B:860:MET:CB	4:B:965:LYS:HG2	2.43	0.46
4:B:1070:GLU:O	4:B:1084:GLN:HB3	2.16	0.46
5:C:112:ASN:HD22	5:C:112:ASN:N	2.13	0.46
5:C:234:SER:OG	5:C:235:VAL:N	2.46	0.46
9:G:87:VAL:HB	9:G:103:VAL:HG11	1.97	0.46
9:G:91:VAL:HA	9:G:101:VAL:HA	1.97	0.46
10:H:11:GLN:C	10:H:28:ALA:HB1	2.41	0.46
10:H:26:ILE:HG22	10:H:27:GLU:N	2.31	0.46
3:A:347:PHE:HE2	3:A:375:THR:HG23	1.79	0.46
3:A:418:SER:C	3:A:420:ARG:N	2.69	0.46
3:A:961:ARG:O	3:A:965:GLN:HG3	2.15	0.46
3:A:1015:VAL:CG1	3:A:1019:CYS:SG	3.03	0.46
4:B:115:GLN:HG2	4:B:193:LYS:CB	2.40	0.46
4:B:307:ASP:O	4:B:308:TRP:C	2.57	0.46
4:B:383:ASN:C	4:B:387:LEU:HD13	2.40	0.46
4:B:773:MET:CE	4:B:985:GLY:HA2	2.45	0.46
4:B:1183:LYS:HE3	4:B:1183:LYS:O	2.15	0.46
7:E:151:PRO:HB3	7:E:200:ARG:HB3	1.96	0.46
9:G:115:MET:CB	9:G:116:PRO:CD	2.93	0.46
14:L:40:LEU:HD22	14:L:44:ASP:CG	2.40	0.46
3:A:90:VAL:HG13	3:A:297:GLN:OE1	2.14	0.46
3:A:247:ARG:HH11	3:A:247:ARG:HG3	1.81	0.46
3:A:350:ARG:HG3	3:A:350:ARG:NH1	2.31	0.46
3:A:567:LYS:CE	10:H:46:LEU:HB2	2.44	0.46
3:A:967:ALA:HA	3:A:1044:TRP:CZ3	2.51	0.46
4:B:654:ARG:C	4:B:656:GLY:N	2.72	0.46
5:C:47:ASP:HA	14:L:69:ALA:CB	2.33	0.46
6:D:33:PHE:CE1	9:G:80:LYS:HE3	2.50	0.46
7:E:61:GLN:NE2	7:E:105:PHE:CZ	2.82	0.46
7:E:124:VAL:CA	7:E:132:ILE:HD12	2.46	0.46
10:H:11:GLN:O	10:H:28:ALA:HB1	2.15	0.46
10:H:38:LEU:HD13	10:H:125:LEU:CD1	2.46	0.46
10:H:139:ASN:O	10:H:140:ALA:CB	2.63	0.46
3:A:371:ALA:HB2	3:A:462:VAL:HG12	1.97	0.46
3:A:537:ARG:NH1	10:H:120:GLY:O	2.47	0.46
3:A:709:THR:HG21	11:I:93:LYS:O	2.15	0.46
3:A:957:PRO:O	3:A:958:VAL:HB	2.16	0.46
3:A:963:ILE:HD13	3:A:1049:ILE:HG12	1.96	0.46
4:B:372:SER:O	4:B:376:PHE:HD1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:840:ILE:HD13	4:B:994:TYR:CE1	2.51	0.46
5:C:27:LEU:O	5:C:28:ALA:C	2.58	0.46
5:C:124:LEU:CD2	5:C:129:ILE:HG22	2.46	0.46
6:D:156:ASP:C	6:D:158:GLU:H	2.23	0.46
9:G:61:ILE:HG23	9:G:66:GLY:O	2.16	0.46
11:I:106:CYS:SG	11:I:107:SER:N	2.89	0.46
13:K:7:PHE:HA	13:K:10:PHE:CE2	2.50	0.46
14:L:46:VAL:CG1	14:L:56:LEU:HD12	2.46	0.46
2:T:6:C:H2'	2:T:7:G:O4'	2.16	0.46
3:A:211:PHE:HA	3:A:214:ILE:CG1	2.46	0.46
3:A:262:LEU:C	3:A:264:PHE:N	2.71	0.46
3:A:577:ILE:O	3:A:578:LEU:C	2.59	0.46
3:A:701:LEU:HD23	11:I:115:LYS:HG3	1.96	0.46
3:A:787:PHE:CE1	3:A:796:SER:HA	2.51	0.46
3:A:986:ILE:CG2	3:A:987:VAL:N	2.76	0.46
4:B:1064:TYR:O	4:B:1065:GLN:C	2.59	0.46
5:C:74:SER:CB	5:C:77:ILE:HG12	2.46	0.46
5:C:175:ALA:HB3	12:J:43:ARG:HH22	1.79	0.46
6:D:154:PHE:CE2	6:D:163:VAL:HG21	2.50	0.46
6:D:219:THR:HG22	6:D:220:LEU:N	2.30	0.46
10:H:27:GLU:HA	10:H:38:LEU:O	2.15	0.46
3:A:377:PRO:HD3	3:A:493:GLN:OE1	2.15	0.46
3:A:562:THR:HA	3:A:563:PRO:HD3	1.82	0.46
3:A:676:MET:O	3:A:679:ILE:HB	2.16	0.46
3:A:683:ILE:HG21	3:A:801:GLU:CG	2.45	0.46
3:A:1205:LYS:O	3:A:1206:ASP:C	2.58	0.46
4:B:240:ILE:HG23	4:B:240:ILE:O	2.14	0.46
4:B:344:LYS:O	4:B:346:GLU:N	2.48	0.46
4:B:616:ILE:HG23	4:B:700:SER:OG	2.15	0.46
4:B:973:ILE:HG23	4:B:974:PRO:HD2	1.98	0.46
5:C:234:SER:HB2	5:C:240:VAL:HG13	1.98	0.46
9:G:48:VAL:HG13	9:G:74:TYR:CD1	2.49	0.46
13:K:67:PHE:C	13:K:68:PHE:HD2	2.24	0.46
3:A:230:ARG:HB2	3:A:233:TRP:CE3	2.51	0.46
3:A:701:LEU:CD2	11:I:115:LYS:HG3	2.45	0.46
3:A:768:GLN:HG2	3:A:816:HIS:CA	2.42	0.46
3:A:899:VAL:CB	3:A:929:LEU:HD11	2.39	0.46
3:A:1279:ILE:CD1	3:A:1316:VAL:HG21	2.46	0.46
3:A:1345:ARG:HG3	3:A:1376:THR:CG2	2.39	0.46
4:B:189:LEU:HD12	4:B:196:PRO:HA	1.97	0.46
4:B:212:LEU:HD21	4:B:461:LEU:HG	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:280:ILE:HD13	4:B:334:ILE:HG12	1.98	0.46
5:C:73:GLN:CD	5:C:74:SER:H	2.24	0.46
6:D:40:HIS:CG	6:D:41:GLN:N	2.83	0.46
6:D:144:THR:HG21	9:G:46:LEU:HD13	1.98	0.46
7:E:92:THR:O	7:E:95:THR:HB	2.15	0.46
9:G:18:PHE:HZ	9:G:68:ALA:HB2	1.81	0.46
12:J:45:CYS:O	12:J:48:ARG:HG3	2.15	0.46
13:K:18:LYS:HZ2	13:K:38:GLU:HG2	1.80	0.46
14:L:30:ILE:HD11	14:L:59:ALA:HB2	1.98	0.46
4:B:343:ILE:HG21	4:B:348:ARG:N	2.30	0.46
4:B:839:MET:CE	4:B:980:PHE:HB2	2.44	0.46
7:E:42:PHE:CE1	7:E:58:MET:HE3	2.51	0.46
7:E:90:VAL:O	7:E:93:MET:HB3	2.16	0.46
9:G:106:MET:HE2	9:G:106:MET:HB3	1.63	0.46
10:H:59:ILE:O	10:H:60:ALA:HB3	2.16	0.46
10:H:91:ASP:O	10:H:91:ASP:CG	2.57	0.46
10:H:95:TYR:CE2	10:H:97:MET:HG3	2.51	0.46
14:L:61:THR:HG21	14:L:63:ARG:CG	2.46	0.46
3:A:65:LEU:O	3:A:66:LYS:O	2.34	0.46
3:A:241:VAL:HG13	3:A:266:LEU:HD13	1.97	0.46
3:A:269:ILE:CG2	3:A:300:VAL:HG22	2.46	0.46
3:A:302:THR:HA	3:A:305:ASP:O	2.16	0.46
3:A:608:ILE:C	3:A:610:GLY:N	2.72	0.46
3:A:1116:LEU:CD1	3:A:1118:VAL:HG13	2.45	0.46
4:B:96:TYR:N	4:B:129:PHE:O	2.39	0.46
4:B:376:PHE:CE2	4:B:569:TYR:HD2	2.34	0.46
4:B:834:ASN:O	4:B:838:SER:O	2.34	0.46
4:B:1034:VAL:C	4:B:1036:ALA:H	2.22	0.46
6:D:185:CYS:HB2	6:D:211:LEU:CD2	2.46	0.46
7:E:17:ARG:O	7:E:20:LYS:HB2	2.16	0.46
7:E:90:VAL:HG23	7:E:120:ALA:HA	1.97	0.46
7:E:179:GLN:HB2	7:E:182:ASP:HB2	1.97	0.46
9:G:44:TYR:O	9:G:78:VAL:HG12	2.16	0.46
14:L:46:VAL:O	14:L:46:VAL:HG12	2.14	0.46
3:A:84:ILE:O	3:A:84:ILE:CG2	2.64	0.46
3:A:219:PHE:O	3:A:222:LEU:O	2.34	0.46
3:A:308:ILE:HG22	3:A:309:ALA:N	2.20	0.46
3:A:710:LEU:N	3:A:710:LEU:HD12	2.29	0.46
3:A:873:MET:HE3	3:A:957:PRO:HG3	1.98	0.46
3:A:900:ASP:HA	3:A:926:GLN:NE2	2.31	0.46
4:B:758:PHE:HZ	4:B:1031:LEU:HD22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:800:GLN:O	4:B:801:LYS:C	2.58	0.46
4:B:824:ILE:HG22	4:B:824:ILE:O	2.15	0.46
4:B:1151:LEU:N	4:B:1151:LEU:CD1	2.78	0.46
5:C:2:SER:N	5:C:3:GLU:O	2.49	0.46
5:C:160:LYS:O	5:C:161:LYS:O	2.34	0.46
5:C:256:ALA:O	5:C:259:LEU:N	2.47	0.46
6:D:56:ARG:CA	6:D:148:LEU:HD13	2.45	0.46
10:H:44:VAL:O	10:H:44:VAL:HG12	2.16	0.46
11:I:19:ASP:OD1	11:I:22:ASN:HB2	2.16	0.46
12:J:2:ILE:HG22	12:J:3:VAL:O	2.16	0.46
12:J:6:ARG:HG2	12:J:13:VAL:HA	1.98	0.46
14:L:27:LEU:HD23	14:L:27:LEU:N	2.30	0.46
3:A:335:ARG:NH1	4:B:1202:LEU:HD22	2.31	0.45
3:A:425:GLN:OE1	3:A:425:GLN:N	2.49	0.45
3:A:728:LYS:HA	3:A:731:ARG:HB2	1.98	0.45
3:A:852:TYR:HA	3:A:1060:PRO:HB3	1.97	0.45
3:A:883:LEU:CD2	3:A:1021:LEU:HB2	2.46	0.45
4:B:570:VAL:HG23	4:B:573:GLN:HB3	1.98	0.45
4:B:798:TYR:CE2	5:C:62:PHE:HE2	2.30	0.45
4:B:860:MET:HG2	4:B:861:ASP:N	2.31	0.45
5:C:67:LEU:HD11	5:C:155:LEU:HD13	1.98	0.45
5:C:75:MET:HE3	5:C:75:MET:HB2	1.68	0.45
5:C:104:PHE:HD2	5:C:105:GLY:N	2.14	0.45
5:C:254:LYS:O	5:C:256:ALA:N	2.49	0.45
6:D:137:ASN:C	6:D:137:ASN:HD22	2.23	0.45
6:D:195:ILE:HB	6:D:198:LEU:CD1	2.46	0.45
11:I:6:PHE:C	11:I:14:LEU:HD11	2.41	0.45
11:I:70:ARG:HA	11:I:83:ASN:O	2.15	0.45
3:A:7:SER:OG	4:B:1193:GLN:NE2	2.50	0.45
3:A:384:ASN:O	3:A:385:ILE:C	2.59	0.45
3:A:954:TRP:HB3	3:A:955:PRO:HD2	1.98	0.45
3:A:964:ILE:O	3:A:967:ALA:HB3	2.16	0.45
4:B:283:VAL:O	4:B:286:PHE:N	2.45	0.45
4:B:827:ILE:HD12	4:B:1086:PHE:HD2	1.81	0.45
4:B:827:ILE:HD12	4:B:1086:PHE:CD2	2.51	0.45
4:B:880:THR:O	4:B:880:THR:HG22	2.17	0.45
5:C:11:ARG:NH2	5:C:229:TYR:HB3	2.31	0.45
5:C:40:GLU:HA	5:C:163:ILE:HG22	1.98	0.45
6:D:175:PHE:O	6:D:179:GLN:HG2	2.16	0.45
7:E:178:ILE:CD1	7:E:185:ALA:HB2	2.47	0.45
14:L:43:THR:C	14:L:45:ALA:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:416:ARG:O	3:A:417:TYR:HD2	2.00	0.45
3:A:546:VAL:HA	3:A:549:MET:HE3	1.97	0.45
3:A:901:LEU:O	3:A:921:GLY:N	2.35	0.45
3:A:1362:TYR:CD1	3:A:1363:VAL:N	2.84	0.45
4:B:232:SER:CB	4:B:261:ARG:HH21	2.24	0.45
4:B:293:PRO:C	4:B:294:ASP:O	2.58	0.45
4:B:579:ARG:HG2	4:B:579:ARG:HH11	1.81	0.45
4:B:1159:ARG:CD	4:B:1193:GLN:HE21	2.30	0.45
9:G:37:SER:OG	9:G:45:ILE:HB	2.16	0.45
11:I:68:LEU:HB3	11:I:84:VAL:HG23	1.98	0.45
11:I:111:THR:CG2	11:I:112:SER:H	2.27	0.45
13:K:110:ASN:O	13:K:111:LEU:HD23	2.17	0.45
3:A:33:ALA:CB	3:A:56:PRO:HB2	2.38	0.45
3:A:59:GLY:HA2	3:A:67:CYS:SG	2.56	0.45
3:A:248:PRO:O	3:A:260:ASP:HB2	2.15	0.45
3:A:878:ILE:HG22	3:A:956:LEU:N	2.30	0.45
3:A:919:ILE:HD13	3:A:983:ILE:HD12	1.97	0.45
4:B:401:PHE:HB2	4:B:517:THR:OG1	2.16	0.45
4:B:469:GLN:HB2	4:B:470:LYS:H	1.50	0.45
4:B:603:LEU:HB3	4:B:609:ILE:CD1	2.47	0.45
4:B:792:MET:HE2	4:B:857:ARG:CZ	2.47	0.45
4:B:980:PHE:HE2	4:B:1094:ARG:HB2	1.81	0.45
6:D:8:PHE:O	6:D:8:PHE:HD1	1.99	0.45
6:D:176:GLU:C	6:D:178:ALA:N	2.73	0.45
9:G:13:LEU:O	9:G:67:SER:HA	2.17	0.45
11:I:101:PHE:HE1	11:I:112:SER:HB2	1.80	0.45
12:J:64:ASN:HB3	12:J:65:PRO:HD2	1.90	0.45
14:L:58:LYS:O	14:L:59:ALA:O	2.34	0.45
3:A:21:LEU:HD11	3:A:1414:ALA:HA	1.98	0.45
3:A:89:PRO:C	3:A:204:THR:HG21	2.42	0.45
3:A:150:THR:HG22	3:A:150:THR:O	2.16	0.45
3:A:445:ASN:HB2	3:A:454:SER:O	2.17	0.45
3:A:469:ARG:NH1	3:A:469:ARG:HB3	2.31	0.45
3:A:961:ARG:HG2	3:A:965:GLN:HE21	1.81	0.45
3:A:967:ALA:O	3:A:968:GLN:O	2.35	0.45
4:B:63:ILE:O	4:B:67:SER:HB3	2.16	0.45
4:B:95:ILE:CB	4:B:130:VAL:HG22	2.47	0.45
4:B:118:ARG:HG2	4:B:204:ILE:HD13	1.98	0.45
4:B:265:SER:O	4:B:266:ALA:CB	2.65	0.45
4:B:520:GLY:H	4:B:748:ILE:HG22	1.81	0.45
4:B:591:ARG:O	4:B:592:ASN:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:744:HIS:ND1	4:B:745:PRO:HD2	2.31	0.45
4:B:780:VAL:HG12	4:B:782:LEU:O	2.17	0.45
4:B:792:MET:HE2	4:B:857:ARG:NH1	2.31	0.45
4:B:979:LYS:HG2	4:B:1095:LEU:HD13	1.97	0.45
4:B:1197:PRO:HG2	4:B:1200:ALA:HB2	1.99	0.45
8:F:147:SER:OG	8:F:150:GLU:HG3	2.16	0.45
9:G:18:PHE:HA	9:G:22:MET:HE2	1.98	0.45
14:L:61:THR:CG2	14:L:63:ARG:HG2	2.47	0.45
3:A:185:TRP:HZ3	3:A:200:ARG:HG2	1.81	0.45
3:A:317:LYS:O	3:A:318:SER:HB3	2.17	0.45
3:A:374:LEU:HD13	3:A:491:VAL:CG2	2.47	0.45
3:A:590:ARG:HH11	3:A:590:ARG:CG	2.29	0.45
3:A:774:ARG:NH2	3:A:797:LYS:CG	2.78	0.45
4:B:542:MET:CE	4:B:743:ILE:HG13	2.47	0.45
4:B:563:MET:HE3	4:B:580:VAL:HB	1.97	0.45
4:B:1034:VAL:O	4:B:1036:ALA:N	2.50	0.45
5:C:45:ALA:HA	5:C:72:LEU:HD12	1.97	0.45
6:D:128:VAL:C	6:D:130:LEU:N	2.74	0.45
7:E:19:VAL:HG11	7:E:80:VAL:HG11	1.98	0.45
9:G:101:VAL:HG12	9:G:102:GLN:N	2.31	0.45
10:H:43:ASN:OD1	10:H:46:LEU:HG	2.17	0.45
10:H:106:GLU:O	10:H:108:SER:N	2.50	0.45
13:K:50:LEU:HD11	13:K:75:ILE:CD1	2.47	0.45
13:K:67:PHE:C	13:K:68:PHE:CD2	2.94	0.45
3:A:24:PRO:HB3	3:A:237:THR:HB	1.99	0.45
3:A:95:PHE:O	3:A:96:ILE:C	2.58	0.45
3:A:107:CYS:SG	3:A:171:GLN:HG2	2.57	0.45
3:A:547:LEU:HD22	13:K:58:PHE:HE1	1.80	0.45
3:A:586:ILE:HD11	3:A:633:VAL:HA	1.99	0.45
3:A:1074:GLU:C	3:A:1076:ALA:H	2.25	0.45
3:A:1265:ASN:O	3:A:1268:LEU:N	2.48	0.45
3:A:1438:THR:HG23	8:F:92:ARG:HB2	1.99	0.45
4:B:55:VAL:CG1	4:B:97:VAL:HG21	2.47	0.45
4:B:226:PHE:CD1	4:B:398:ARG:NH2	2.84	0.45
4:B:758:PHE:HB2	4:B:1024:ALA:HB1	1.98	0.45
4:B:806:THR:CG2	4:B:808:ALA:HB3	2.47	0.45
4:B:980:PHE:CE2	4:B:1094:ARG:HG3	2.51	0.45
4:B:1130:PHE:HZ	4:B:1138:MET:HG2	1.82	0.45
5:C:56:THR:HG22	5:C:57:VAL:H	1.81	0.45
6:D:155:ARG:HG2	6:D:155:ARG:O	2.15	0.45
6:D:191:ALA:C	6:D:193:THR:N	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:14:ARG:HH21	7:E:141:VAL:HG12	1.82	0.45
7:E:31:THR:O	7:E:35:VAL:HG23	2.16	0.45
8:F:111:LEU:C	8:F:113:GLY:N	2.73	0.45
9:G:1:MET:O	9:G:1:MET:CE	2.64	0.45
9:G:138:THR:CG2	9:G:139:ILE:N	2.62	0.45
3:A:53:LEU:O	3:A:54:ASN:C	2.60	0.45
3:A:353:ILE:HG21	3:A:487:MET:HG3	1.98	0.45
3:A:578:LEU:HD23	3:A:612:ILE:HD11	1.99	0.45
4:B:30:SER:HB3	4:B:743:ILE:O	2.17	0.45
4:B:114:PRO:O	4:B:115:GLN:C	2.60	0.45
4:B:799:PRO:CB	4:B:818:PRO:HG2	2.43	0.45
4:B:860:MET:HG2	4:B:861:ASP:H	1.81	0.45
4:B:1045:SER:HB3	4:B:1046:PRO:HD2	1.99	0.45
5:C:187:LYS:C	5:C:189:THR:N	2.75	0.45
7:E:124:VAL:HG13	7:E:132:ILE:CB	2.45	0.45
8:F:97:ARG:HD2	8:F:97:ARG:HA	1.82	0.45
9:G:38:CYS:HB3	9:G:155:SER:HA	1.97	0.45
3:A:57:ARG:O	3:A:68:GLN:HG3	2.16	0.45
3:A:78:PRO:HA	4:B:1201:LYS:NZ	2.32	0.45
3:A:347:PHE:N	3:A:347:PHE:CD1	2.85	0.45
3:A:560:ILE:HG13	10:H:78:SER:CB	2.40	0.45
3:A:657:LEU:O	3:A:657:LEU:HD12	2.16	0.45
3:A:1341:ILE:CG2	3:A:1342:GLU:N	2.79	0.45
4:B:879:ARG:HH11	4:B:883:LEU:CD2	2.20	0.45
4:B:1081:LEU:O	4:B:1082:MET:C	2.59	0.45
6:D:67:ARG:CB	6:D:133:THR:HG21	2.45	0.45
6:D:176:GLU:C	6:D:178:ALA:H	2.25	0.45
7:E:112:TYR:CZ	7:E:136:ASN:HB2	2.52	0.45
8:F:125:LEU:HB2	8:F:130:ILE:CD1	2.47	0.45
13:K:61:TYR:CD2	13:K:61:TYR:O	2.69	0.45
2:T:12:G:H4'	2:T:13:U:OP1	2.17	0.45
3:A:417:TYR:CD2	3:A:417:TYR:N	2.85	0.45
3:A:709:THR:CG2	3:A:710:LEU:N	2.80	0.45
3:A:795:GLU:CD	3:A:795:GLU:H	2.25	0.45
3:A:875:ALA:HA	3:A:878:ILE:HD11	1.98	0.45
3:A:1021:LEU:O	3:A:1024:SER:HB3	2.17	0.45
3:A:1115:SER:OG	3:A:1116:LEU:N	2.50	0.45
3:A:1299:VAL:CG1	3:A:1300:LYS:N	2.79	0.45
3:A:1369:ALA:O	3:A:1370:LEU:C	2.58	0.45
4:B:27:ALA:C	4:B:29:ASP:N	2.74	0.45
4:B:99:LYS:HB3	4:B:100:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:644:GLU:C	4:B:646:LEU:H	2.25	0.45
4:B:1017:ILE:HB	4:B:1018:PRO:HD3	1.98	0.45
4:B:1099:VAL:C	4:B:1101:ASP:H	2.25	0.45
5:C:76:ASP:O	5:C:77:ILE:C	2.58	0.45
7:E:31:THR:OG1	7:E:34:GLU:N	2.47	0.45
10:H:127:GLY:O	10:H:128:ASN:CB	2.59	0.45
11:I:55:THR:HG22	11:I:55:THR:O	2.16	0.45
11:I:77:LYS:C	11:I:79:HIS:H	2.25	0.45
14:L:53:HIS:O	14:L:55:ILE:HG12	2.16	0.45
3:A:58:LEU:CD1	3:A:59:GLY:N	2.62	0.44
3:A:603:ASN:O	3:A:604:GLY:C	2.60	0.44
3:A:817:ALA:O	3:A:818:MET:C	2.59	0.44
4:B:29:ASP:O	4:B:30:SER:C	2.61	0.44
4:B:294:ASP:C	4:B:296:GLU:N	2.75	0.44
4:B:953:LEU:HD23	4:B:953:LEU:O	2.17	0.44
4:B:1162:ILE:HG22	4:B:1163:CYS:N	2.31	0.44
7:E:151:PRO:CB	7:E:200:ARG:HB3	2.47	0.44
8:F:99:LEU:HD12	8:F:99:LEU:C	2.42	0.44
9:G:15:PRO:O	9:G:16:SER:C	2.59	0.44
9:G:125:SER:OG	9:G:128:PRO:HA	2.16	0.44
3:A:93:VAL:HG21	3:A:301:ALA:O	2.17	0.44
3:A:590:ARG:HD3	3:A:604:GLY:CA	2.45	0.44
3:A:1115:SER:C	3:A:1308:THR:HG22	2.42	0.44
3:A:1202:MET:HE1	3:A:1212:VAL:CG2	2.44	0.44
3:A:1239:ARG:C	3:A:1240:CYS:SG	3.01	0.44
3:A:1291:VAL:HG22	3:A:1292:PRO:CD	2.47	0.44
4:B:471:LYS:O	4:B:472:ALA:HB2	2.17	0.44
4:B:566:LEU:O	4:B:567:GLU:C	2.60	0.44
4:B:641:GLU:C	4:B:643:ASP:N	2.76	0.44
4:B:874:PHE:HA	4:B:913:GLY:O	2.16	0.44
4:B:1079:LYS:CA	5:C:27:LEU:HD21	2.47	0.44
8:F:86:THR:HG23	8:F:89:GLU:OE1	2.18	0.44
9:G:20:PRO:HG2	9:G:21:ARG:N	2.32	0.44
3:A:207:ILE:HG23	3:A:211:PHE:HE1	1.82	0.44
3:A:266:LEU:O	3:A:267:ALA:C	2.61	0.44
3:A:341:MET:CE	4:B:1135:ARG:NH1	2.80	0.44
3:A:418:SER:O	3:A:420:ARG:N	2.50	0.44
3:A:717:ASN:HA	3:A:720:ARG:HH12	1.81	0.44
3:A:786:HIS:CD2	3:A:786:HIS:H	2.35	0.44
3:A:1219:THR:HG21	3:A:1271:ILE:CD1	2.47	0.44
3:A:1293:SER:OG	3:A:1295:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:128:LEU:HD11	4:B:170:LEU:CB	2.48	0.44
4:B:339:THR:O	4:B:339:THR:HG22	2.16	0.44
4:B:611:PRO:O	4:B:692:TYR:HB2	2.17	0.44
5:C:66:ARG:NH1	5:C:144:ILE:O	2.50	0.44
5:C:87:PHE:H	5:C:87:PHE:HD1	1.65	0.44
5:C:87:PHE:N	5:C:87:PHE:CD1	2.86	0.44
6:D:119:ARG:HD3	6:D:221:TYR:CD2	2.53	0.44
7:E:180:ARG:HH21	7:E:192:ARG:CB	2.20	0.44
9:G:10:ASN:OD1	9:G:71:ASN:HA	2.18	0.44
9:G:48:VAL:HA	9:G:76:ALA:HB2	1.98	0.44
9:G:153:GLN:HG2	9:G:154:VAL:HG23	1.97	0.44
13:K:12:LEU:HD12	13:K:12:LEU:N	2.32	0.44
3:A:34:LYS:HG2	3:A:57:ARG:NH2	2.32	0.44
3:A:343:LYS:NZ	4:B:1151:LEU:O	2.41	0.44
3:A:406:ILE:HG13	3:A:431:LYS:HB2	2.00	0.44
3:A:543:LEU:N	3:A:572:TRP:HZ3	2.15	0.44
3:A:693:VAL:HA	3:A:696:GLU:HB3	2.00	0.44
3:A:705:LYS:O	3:A:706:HIS:C	2.60	0.44
3:A:806:ARG:HD3	4:B:728:ARG:HA	1.99	0.44
3:A:1072:ILE:O	3:A:1075:PRO:HG2	2.17	0.44
3:A:1445:ILE:HG12	9:G:18:PHE:HE2	1.83	0.44
4:B:168:GLY:HA2	4:B:454:THR:HG1	1.82	0.44
4:B:833:TYR:N	4:B:833:TYR:HD1	2.15	0.44
4:B:1095:LEU:HD12	4:B:1095:LEU:N	2.25	0.44
4:B:1165:ILE:HG22	4:B:1166:CYS:N	2.32	0.44
6:D:46:GLU:C	6:D:47:LEU:O	2.61	0.44
9:G:110:VAL:HG22	9:G:161:GLY:O	2.16	0.44
9:G:126:ASN:HD22	9:G:126:ASN:HA	1.60	0.44
10:H:40:LEU:HB2	10:H:123:MET:HG3	1.98	0.44
1:P:13:A:O2'	1:P:14:G:H5'	2.18	0.44
3:A:415:LEU:HD23	3:A:415:LEU:HA	1.80	0.44
3:A:600:PRO:C	3:A:602:ASP:H	2.25	0.44
3:A:608:ILE:HG13	3:A:613:ILE:HD12	1.99	0.44
3:A:1313:LEU:C	3:A:1315:GLU:N	2.76	0.44
4:B:94:LYS:HG2	4:B:95:ILE:N	2.32	0.44
4:B:205:ILE:N	4:B:205:ILE:CD1	2.74	0.44
4:B:356:LEU:O	4:B:374:LYS:NZ	2.48	0.44
4:B:834:ASN:HB3	4:B:840:ILE:HG13	1.98	0.44
5:C:35:ARG:HH11	13:K:41:THR:N	2.13	0.44
5:C:69:LEU:N	5:C:69:LEU:CD1	2.81	0.44
5:C:90:ASP:O	5:C:91:HIS:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:186:LEU:O	7:E:189:GLY:N	2.50	0.44
10:H:143:LEU:C	10:H:144:ILE:HG13	2.43	0.44
11:I:98:VAL:HG12	11:I:99:LEU:N	2.33	0.44
3:A:23:SER:O	3:A:24:PRO:C	2.60	0.44
3:A:31:SER:OG	3:A:82:GLY:HA2	2.18	0.44
3:A:108:MET:O	3:A:109:HIS:HB2	2.18	0.44
3:A:1409:LEU:HD13	4:B:1207:LEU:CD2	2.48	0.44
4:B:234:ILE:HG21	4:B:237:VAL:CG2	2.48	0.44
4:B:562:GLY:HA3	4:B:590:HIS:CE1	2.52	0.44
4:B:957:ASN:HD22	4:B:961:LEU:HD12	1.83	0.44
4:B:1116:ARG:HD2	4:B:1198:TYR:CD1	2.53	0.44
5:C:8:VAL:O	5:C:9:LYS:HG3	2.17	0.44
5:C:44:LEU:HD21	5:C:159:ALA:HB1	1.99	0.44
5:C:193:TYR:HD2	5:C:197:SER:HB3	1.83	0.44
6:D:47:LEU:HD11	9:G:3:PHE:HD2	1.81	0.44
7:E:124:VAL:CG1	7:E:132:ILE:HD12	2.43	0.44
7:E:182:ASP:OD1	7:E:183:PRO:HD2	2.17	0.44
9:G:154:VAL:HG12	9:G:155:SER:N	2.32	0.44
11:I:12:ASN:HB3	11:I:13:MET:H	1.55	0.44
14:L:28:LYS:HB2	14:L:39:SER:CB	2.48	0.44
3:A:77:CYS:C	3:A:78:PRO:O	2.58	0.44
3:A:889:SER:HB3	3:A:1297:GLU:HG2	1.99	0.44
3:A:1226:VAL:HG13	3:A:1239:ARG:O	2.17	0.44
3:A:1436:ILE:HD11	4:B:1139:ILE:HG23	2.00	0.44
3:A:1445:ILE:HG21	9:G:18:PHE:CD2	2.53	0.44
4:B:387:LEU:O	4:B:392:ARG:HB2	2.17	0.44
4:B:401:PHE:HA	4:B:404:LYS:HG3	1.99	0.44
4:B:882:THR:O	4:B:883:LEU:HB2	2.17	0.44
6:D:29:LEU:O	6:D:30:GLY:C	2.61	0.44
7:E:14:ARG:O	7:E:15:ALA:C	2.60	0.44
9:G:20:PRO:CG	9:G:21:ARG:H	2.31	0.44
10:H:89:LEU:HB3	10:H:91:ASP:OD1	2.18	0.44
10:H:99:GLY:N	10:H:118:PHE:CD2	2.86	0.44
11:I:78:CYS:SG	11:I:106:CYS:HB3	2.58	0.44
3:A:7:SER:C	3:A:9:ALA:N	2.75	0.44
3:A:600:PRO:HA	10:H:25:ARG:NH2	2.32	0.44
3:A:719:VAL:O	3:A:721:PHE:N	2.50	0.44
3:A:738:LYS:CD	3:A:740:LEU:HD21	2.46	0.44
3:A:818:MET:N	4:B:514:LEU:HD23	2.33	0.44
3:A:821:ARG:HD2	3:A:825:ILE:CD1	2.47	0.44
3:A:1115:SER:C	3:A:1308:THR:CG2	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1209:MET:SD	3:A:1236:LEU:HD22	2.57	0.44
3:A:1345:ARG:HD2	3:A:1373:ASP:OD1	2.17	0.44
4:B:263:GLY:O	4:B:264:SER:C	2.61	0.44
4:B:558:LEU:C	4:B:560:GLU:N	2.75	0.44
4:B:766:ARG:HD3	4:B:766:ARG:HA	1.69	0.44
4:B:999:MET:HE3	4:B:999:MET:CA	2.38	0.44
4:B:1207:LEU:HB3	4:B:1212:ILE:HG22	2.00	0.44
6:D:8:PHE:CE2	9:G:6:ASP:O	2.71	0.44
10:H:4:THR:HG22	10:H:5:LEU:H	1.83	0.44
13:K:55:LYS:HB3	13:K:81:TYR:CE1	2.52	0.44
13:K:82:ASP:O	13:K:85:ASP:HB2	2.18	0.44
3:A:14:VAL:HG21	4:B:1216:LEU:CD1	2.48	0.44
3:A:382:PRO:HD3	3:A:428:TYR:HD2	1.83	0.44
3:A:442:VAL:O	3:A:457:ALA:HA	2.18	0.44
3:A:896:ARG:HB3	3:A:897:TYR:CD1	2.53	0.44
3:A:986:ILE:HD12	3:A:1032:LEU:HD11	1.99	0.44
3:A:1011:GLN:HE21	3:A:1015:VAL:HG21	1.83	0.44
3:A:1191:TRP:HB3	3:A:1260:LEU:HD23	2.00	0.44
3:A:1259:MET:C	3:A:1261:LYS:H	2.25	0.44
3:A:1410:PHE:HA	4:B:1212:ILE:HD11	2.00	0.44
3:A:1444:MET:HE1	8:F:135:ARG:CB	2.37	0.44
4:B:199:MET:SD	4:B:199:MET:N	2.88	0.44
4:B:274:PRO:O	4:B:275:TYR:HB2	2.18	0.44
4:B:298:LEU:N	4:B:298:LEU:HD22	2.33	0.44
4:B:408:LEU:HD12	4:B:408:LEU:HA	1.75	0.44
7:E:169:ARG:HB3	8:F:140:ASP:OD2	2.17	0.44
10:H:12:VAL:HB	10:H:52:GLN:N	2.33	0.44
12:J:41:LEU:HD23	12:J:41:LEU:N	2.33	0.44
13:K:68:PHE:CD2	13:K:68:PHE:N	2.83	0.44
3:A:42:ASP:HB3	3:A:45:GLN:N	2.33	0.43
3:A:113:LEU:C	3:A:114:LEU:HD23	2.42	0.43
3:A:164:ARG:CG	3:A:165:GLY:H	2.12	0.43
3:A:285:PRO:CG	3:A:288:ALA:HB3	2.44	0.43
3:A:621:THR:O	3:A:621:THR:HG22	2.18	0.43
3:A:805:LEU:HD11	4:B:1052:VAL:HG21	1.98	0.43
3:A:814:PHE:O	3:A:817:ALA:HB3	2.17	0.43
3:A:897:TYR:CD1	3:A:897:TYR:N	2.86	0.43
3:A:1225:PHE:CE2	3:A:1227:ILE:HD11	2.52	0.43
4:B:210:LYS:HE2	4:B:462:ALA:HA	2.00	0.43
4:B:281:PRO:O	4:B:282:ILE:C	2.60	0.43
4:B:515:HIS:HD2	4:B:516:ASN:N	2.14	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1166:CYS:SG	4:B:1168:LEU:HD12	2.57	0.43
5:C:98:VAL:CG2	5:C:122:SER:HB3	2.48	0.43
5:C:113:VAL:O	5:C:144:ILE:N	2.50	0.43
5:C:250:THR:O	5:C:251:LEU:C	2.61	0.43
6:D:138:ASN:C	6:D:140:ASP:N	2.76	0.43
7:E:168:TYR:HB2	7:E:170:LEU:HG	2.00	0.43
7:E:178:ILE:HG22	7:E:213:ILE:O	2.18	0.43
8:F:72:LYS:O	8:F:142:SER:HA	2.18	0.43
12:J:1:MET:HG3	12:J:1:MET:O	2.17	0.43
13:K:10:PHE:HA	13:K:37:LYS:HB3	2.00	0.43
13:K:43:GLY:HA3	13:K:61:TYR:CE1	2.53	0.43
14:L:40:LEU:HD22	14:L:44:ASP:HB3	1.99	0.43
3:A:279:LEU:O	3:A:284:ALA:HB2	2.17	0.43
3:A:514:PRO:CB	3:A:875:ALA:HB3	2.47	0.43
3:A:523:ILE:CD1	3:A:649:ILE:HG21	2.48	0.43
3:A:1076:ALA:HA	3:A:1079:MET:HE3	2.00	0.43
3:A:1147:THR:O	11:I:48:LEU:HD12	2.18	0.43
3:A:1151:GLU:HA	11:I:44:TYR:O	2.17	0.43
4:B:497:ARG:NH2	4:B:775:LYS:NZ	2.66	0.43
4:B:593:PRO:HG2	4:B:617:ARG:NH2	2.33	0.43
4:B:769:TYR:O	4:B:771:SER:N	2.51	0.43
4:B:1115:THR:CG2	4:B:1117:GLN:HG3	2.43	0.43
4:B:1197:PRO:O	4:B:1200:ALA:N	2.48	0.43
5:C:101:LEU:HD12	5:C:101:LEU:HA	1.79	0.43
5:C:113:VAL:HG23	5:C:147:LEU:HD21	1.99	0.43
5:C:131:HIS:HA	5:C:132:PRO:HD3	1.89	0.43
6:D:8:PHE:CE1	6:D:37:GLN:HB2	2.53	0.43
9:G:34:VAL:HG11	9:G:74:TYR:CE1	2.54	0.43
12:J:27:GLU:C	12:J:29:GLU:N	2.75	0.43
3:A:18:GLN:HB2	4:B:1215:ARG:CB	2.47	0.43
3:A:278:THR:O	3:A:282:ASN:HB2	2.18	0.43
3:A:472:LEU:HD11	4:B:835:GLN:CD	2.43	0.43
3:A:858:ASN:ND2	3:A:861:GLY:H	2.15	0.43
3:A:965:GLN:HA	3:A:968:GLN:HG3	2.00	0.43
3:A:1153:TYR:CE1	11:I:42:LEU:HD13	2.54	0.43
4:B:95:ILE:HB	4:B:130:VAL:HG22	2.00	0.43
4:B:278:GLN:HG2	4:B:279:ASP:N	2.33	0.43
4:B:309:GLN:CG	11:I:52:ILE:HD11	2.48	0.43
4:B:756:ILE:O	4:B:759:PRO:HD3	2.19	0.43
4:B:773:MET:HB3	4:B:1095:LEU:HD23	2.01	0.43
4:B:839:MET:HE1	4:B:980:PHE:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:996:ARG:HG2	4:B:1007:VAL:HG11	1.99	0.43
4:B:1156:ASP:HB3	4:B:1198:TYR:H	1.84	0.43
6:D:40:HIS:HB2	9:G:73:LYS:HZ2	1.83	0.43
7:E:147:HIS:CD2	7:E:149:LEU:H	2.36	0.43
8:F:81:THR:HB	8:F:136:ARG:HH11	1.83	0.43
11:I:7:CYS:HB2	11:I:34:TYR:CD1	2.53	0.43
12:J:41:LEU:HD11	12:J:50:ILE:HG13	2.00	0.43
3:A:58:LEU:O	3:A:59:GLY:O	2.37	0.43
3:A:86:LEU:HD12	3:A:236:LEU:O	2.18	0.43
3:A:244:PRO:CG	3:A:245:PRO:CD	2.92	0.43
3:A:351:THR:CB	4:B:1103:ILE:HD12	2.46	0.43
3:A:560:ILE:CG1	10:H:78:SER:HB2	2.39	0.43
3:A:753:GLY:HA2	3:A:757:ASN:ND2	2.33	0.43
3:A:1095:THR:OG1	3:A:1113:THR:HB	2.19	0.43
3:A:1409:LEU:HD23	3:A:1409:LEU:HA	1.87	0.43
3:A:1410:PHE:HA	4:B:1212:ILE:CD1	2.48	0.43
4:B:750:GLY:O	4:B:751:VAL:C	2.60	0.43
4:B:885:MET:HA	4:B:936:ASP:CB	2.47	0.43
4:B:1001:PHE:HD2	5:C:34:ARG:NH2	2.14	0.43
7:E:149:LEU:N	7:E:149:LEU:HD23	2.33	0.43
8:F:147:SER:HG	8:F:150:GLU:HG3	1.83	0.43
12:J:3:VAL:CG2	12:J:18:TRP:CG	3.02	0.43
12:J:53:HIS:CD2	12:J:54:VAL:N	2.86	0.43
3:A:738:LYS:C	3:A:740:LEU:N	2.76	0.43
3:A:806:ARG:HH12	4:B:729:ILE:HD12	1.83	0.43
3:A:1011:GLN:O	3:A:1015:VAL:HG23	2.19	0.43
3:A:1162:VAL:O	3:A:1162:VAL:HG12	2.17	0.43
4:B:46:GLN:OE1	4:B:47:GLN:HG2	2.19	0.43
4:B:53:GLN:HG2	4:B:547:VAL:CG2	2.45	0.43
4:B:102:VAL:O	4:B:109:THR:HA	2.18	0.43
4:B:114:PRO:HG2	4:B:115:GLN:N	2.28	0.43
4:B:221:ASN:OD1	4:B:242:SER:HA	2.18	0.43
4:B:303:TYR:CD2	4:B:303:TYR:N	2.86	0.43
4:B:351:TYR:CD1	4:B:355:ILE:HD11	2.54	0.43
4:B:977:GLY:HA3	4:B:1099:VAL:HB	2.01	0.43
5:C:12:GLU:O	5:C:13:ALA:HB2	2.18	0.43
7:E:94:LYS:CE	7:E:98:ILE:HD11	2.26	0.43
10:H:48:PRO:O	10:H:49:VAL:CG2	2.66	0.43
13:K:10:PHE:CD1	13:K:11:LEU:CD2	3.01	0.43
3:A:17:VAL:HA	4:B:1215:ARG:O	2.18	0.43
3:A:247:ARG:HG3	3:A:247:ARG:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:402:ALA:CB	3:A:434:ARG:HA	2.49	0.43
3:A:667:GLY:HA3	5:C:192:TRP:CH2	2.54	0.43
3:A:746:MET:HE3	4:B:1018:PRO:CG	2.47	0.43
3:A:1171:GLN:HA	3:A:1174:PHE:CE1	2.54	0.43
3:A:1285:MET:O	3:A:1304:TRP:HA	2.18	0.43
3:A:1311:VAL:HG11	3:A:1329:THR:HG21	1.99	0.43
4:B:29:ASP:HB3	4:B:658:ILE:CD1	2.49	0.43
4:B:97:VAL:HG12	4:B:178:ASN:ND2	2.32	0.43
4:B:225:VAL:HG11	4:B:385:LEU:HA	2.01	0.43
4:B:383:ASN:O	4:B:387:LEU:HD13	2.18	0.43
4:B:519:TRP:HE1	4:B:635:ARG:NH2	2.16	0.43
5:C:8:VAL:CG1	5:C:9:LYS:N	2.80	0.43
7:E:178:ILE:HD11	7:E:185:ALA:HB2	2.01	0.43
11:I:4:PHE:CD1	11:I:4:PHE:C	2.96	0.43
3:A:316:GLN:O	3:A:317:LYS:C	2.61	0.43
3:A:369:SER:CB	13:K:2:ASN:OD1	2.67	0.43
3:A:453:MET:C	3:A:455:MET:N	2.75	0.43
3:A:477:PRO:HG3	3:A:521:MET:HG2	1.98	0.43
3:A:500:GLU:OE1	4:B:1143:ALA:C	2.62	0.43
3:A:604:GLY:O	3:A:605:MET:HB2	2.19	0.43
3:A:647:GLY:O	3:A:651:LYS:HG3	2.19	0.43
3:A:818:MET:HG2	4:B:514:LEU:HG	2.01	0.43
3:A:1118:VAL:HG12	3:A:1327:ILE:CG1	2.43	0.43
3:A:1135:ARG:C	3:A:1137:ALA:H	2.27	0.43
4:B:37:PHE:CD1	4:B:37:PHE:C	2.96	0.43
4:B:282:ILE:CD1	4:B:382:ILE:HD13	2.48	0.43
4:B:700:SER:O	4:B:701:ILE:HG22	2.19	0.43
4:B:1074:ASN:HB2	4:B:1081:LEU:CD2	2.49	0.43
4:B:1159:ARG:HB3	4:B:1159:ARG:NH1	2.34	0.43
6:D:119:ARG:HG2	6:D:120:GLU:H	1.81	0.43
7:E:72:PHE:CE2	7:E:155:ARG:NH2	2.87	0.43
7:E:128:PRO:HA	7:E:129:PRO:C	2.44	0.43
7:E:175:LEU:HD23	7:E:176:PRO:HD2	2.00	0.43
10:H:2:SER:HA	10:H:62:SER:OG	2.19	0.43
11:I:101:PHE:HD1	11:I:101:PHE:H	1.66	0.43
13:K:49:GLU:OE2	13:K:97:LYS:HE3	2.19	0.43
14:L:61:THR:CG2	14:L:63:ARG:CG	2.97	0.43
3:A:50:ILE:HG22	3:A:52:GLY:N	2.33	0.43
3:A:89:PRO:HB2	3:A:204:THR:CG2	2.49	0.43
3:A:346:ASP:CG	4:B:1108:ARG:HA	2.44	0.43
3:A:497:THR:O	3:A:498:ARG:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:567:LYS:HB3	10:H:95:TYR:CA	2.46	0.43
3:A:658:LEU:HD12	4:B:830:TYR:CD1	2.53	0.43
3:A:665:GLY:C	3:A:666:ILE:HD12	2.44	0.43
3:A:717:ASN:HA	3:A:720:ARG:NH1	2.34	0.43
3:A:971:PHE:HE2	3:A:1040:GLN:HG2	1.83	0.43
3:A:1156:PRO:HA	3:A:1190:PRO:CB	2.49	0.43
3:A:1193:LEU:HB2	3:A:1260:LEU:HD11	2.01	0.43
3:A:1451:VAL:C	3:A:1453:TYR:N	2.76	0.43
4:B:168:GLY:N	4:B:450:ALA:HB1	2.29	0.43
4:B:701:ILE:HD11	4:B:703:ILE:HD11	2.01	0.43
4:B:839:MET:HG3	4:B:1010:LEU:HD11	2.01	0.43
4:B:1031:LEU:HD11	4:B:1042:GLY:CA	2.48	0.43
8:F:103:MET:HE2	9:G:66:GLY:H	1.79	0.43
14:L:28:LYS:C	14:L:29:TYR:HD2	2.27	0.43
3:A:37:PHE:HD1	3:A:37:PHE:H	1.66	0.43
3:A:184:SER:HB3	3:A:199:LEU:CD2	2.48	0.43
3:A:335:ARG:HH11	4:B:1202:LEU:HD13	1.82	0.43
3:A:535:THR:CG2	3:A:575:LYS:HE2	2.48	0.43
3:A:551:TYR:CE2	13:K:62:LYS:HG2	2.53	0.43
3:A:722:LEU:HD22	3:A:799:PHE:CG	2.54	0.43
3:A:765:VAL:HG23	3:A:802:ASN:O	2.18	0.43
3:A:1066:VAL:HG11	4:B:1136:ASP:O	2.19	0.43
3:A:1161:THR:C	3:A:1163:ILE:N	2.76	0.43
3:A:1215:ARG:HG2	3:A:1215:ARG:HH11	1.83	0.43
4:B:38:PHE:HD1	4:B:811:TYR:HD2	1.64	0.43
4:B:609:ILE:O	4:B:610:ASN:C	2.61	0.43
4:B:681:TRP:C	4:B:683:SER:N	2.76	0.43
4:B:687:GLU:O	4:B:688:GLY:C	2.62	0.43
4:B:758:PHE:N	4:B:759:PRO:CD	2.82	0.43
4:B:980:PHE:CE2	4:B:1094:ARG:HB2	2.54	0.43
4:B:1060:ARG:HA	4:B:1060:ARG:HD2	1.57	0.43
4:B:1079:LYS:HA	5:C:27:LEU:HD21	2.01	0.43
5:C:47:ASP:CA	14:L:69:ALA:HB3	2.36	0.43
5:C:116:LYS:C	5:C:118:LEU:H	2.27	0.43
5:C:120:ILE:CD1	5:C:124:LEU:HD11	2.48	0.43
6:D:66:ARG:HD2	6:D:133:THR:HB	2.00	0.43
7:E:177:ARG:HD3	7:E:215:MET:HG3	2.01	0.43
3:A:302:THR:HG22	3:A:303:TYR:N	2.34	0.43
3:A:515:GLN:O	3:A:516:SER:HB3	2.18	0.43
3:A:527:THR:HG23	3:A:650:GLN:HA	2.00	0.43
3:A:789:LYS:NZ	4:B:620:ARG:HH11	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:866:PHE:O	3:A:867:ILE:HD12	2.19	0.43
4:B:412:LEU:HB3	4:B:466:TRP:CZ2	2.54	0.43
4:B:764:SER:HB3	4:B:765:PRO:CD	2.49	0.43
5:C:8:VAL:CG1	5:C:9:LYS:H	2.27	0.43
5:C:236:GLY:C	5:C:238:ILE:N	2.76	0.43
5:C:252:GLN:HB2	13:K:98:LEU:HD13	2.01	0.43
8:F:93:ILE:HD13	8:F:148:VAL:HG12	2.01	0.43
8:F:111:LEU:H	8:F:111:LEU:CD1	2.29	0.43
11:I:53:GLY:O	11:I:55:THR:N	2.52	0.43
3:A:116:ASP:C	3:A:118:HIS:H	2.27	0.42
3:A:478:TYR:O	3:A:479:ASN:CB	2.65	0.42
3:A:1004:ASN:HD21	3:A:1007:ILE:HG12	1.84	0.42
3:A:1424:VAL:HG11	4:B:1139:ILE:CD1	2.40	0.42
3:A:1434:ALA:HA	3:A:1435:PRO:HD3	1.90	0.42
4:B:205:ILE:O	4:B:207:GLY:N	2.52	0.42
4:B:642:ASP:CA	4:B:649:LYS:HG3	2.48	0.42
4:B:769:TYR:O	4:B:772:ALA:N	2.52	0.42
4:B:1065:GLN:NE2	4:B:1067:ARG:H	2.11	0.42
5:C:214:ASN:O	5:C:215:GLU:C	2.62	0.42
5:C:238:ILE:HD11	5:C:246:ARG:CZ	2.47	0.42
6:D:59:ILE:O	6:D:60:LYS:C	2.60	0.42
7:E:105:PHE:O	7:E:106:GLN:HB2	2.19	0.42
7:E:204:THR:HG23	7:E:205:SER:N	2.34	0.42
9:G:14:HIS:ND1	9:G:15:PRO:CD	2.77	0.42
11:I:100:PHE:N	11:I:100:PHE:CD1	2.87	0.42
14:L:40:LEU:HD13	14:L:44:ASP:CB	2.49	0.42
3:A:37:PHE:HB2	3:A:52:GLY:HA3	2.01	0.42
3:A:336:ILE:HG22	3:A:337:ARG:N	2.33	0.42
3:A:367:PRO:HB3	3:A:465:TYR:O	2.19	0.42
3:A:629:LEU:HD22	3:A:633:VAL:CG2	2.50	0.42
3:A:767:GLN:OE1	3:A:799:PHE:HB2	2.19	0.42
3:A:943:LEU:C	3:A:945:GLU:H	2.26	0.42
3:A:976:THR:HG23	10:H:136:LYS:HZ3	1.83	0.42
3:A:1163:ILE:HG22	3:A:1164:PRO:HD2	2.01	0.42
3:A:1191:TRP:CD1	3:A:1256:GLU:HB2	2.54	0.42
3:A:1280:GLU:O	3:A:1281:ARG:O	2.37	0.42
4:B:51:PHE:HE2	4:B:172:ILE:HG23	1.84	0.42
4:B:100:PRO:HB2	4:B:180:TYR:CE1	2.53	0.42
4:B:820:GLY:C	4:B:1091:TYR:CE1	2.98	0.42
4:B:952:VAL:CG1	4:B:953:LEU:N	2.81	0.42
1:P:14:G:O2'	1:P:15:G:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:40:THR:HG21	3:A:41:MET:HE2	2.02	0.42
3:A:172:PRO:HB3	3:A:185:TRP:CE2	2.54	0.42
3:A:560:ILE:H	3:A:560:ILE:HG12	1.55	0.42
3:A:645:LEU:CD1	3:A:649:ILE:HG13	2.50	0.42
3:A:742:ASN:O	3:A:745:GLN:HB2	2.19	0.42
3:A:1215:ARG:HA	3:A:1218:GLN:HE21	1.84	0.42
3:A:1239:ARG:HH22	3:A:1241:ARG:NH2	2.15	0.42
3:A:1280:GLU:O	3:A:1282:VAL:HG23	2.19	0.42
3:A:1444:MET:HE3	3:A:1444:MET:HB2	1.78	0.42
4:B:502:ILE:N	4:B:502:ILE:CD1	2.82	0.42
4:B:515:HIS:CD2	4:B:517:THR:HG23	2.54	0.42
4:B:515:HIS:N	4:B:518:HIS:HD2	2.03	0.42
5:C:133:ILE:HD13	5:C:236:GLY:O	2.18	0.42
6:D:56:ARG:CB	6:D:148:LEU:HD22	2.36	0.42
7:E:157:SER:HG	7:E:160:GLU:HG3	1.82	0.42
9:G:79:PHE:HZ	9:G:106:MET:CE	2.31	0.42
13:K:87:LEU:O	13:K:88:LYS:C	2.62	0.42
3:A:41:MET:HB2	3:A:42:ASP:H	1.39	0.42
3:A:224:PHE:CD2	3:A:231:PRO:HD3	2.54	0.42
3:A:386:ASP:O	3:A:387:ARG:C	2.63	0.42
3:A:481:ASP:OD1	3:A:483:ASP:OD2	2.37	0.42
3:A:553:VAL:HG22	3:A:652:VAL:CG2	2.49	0.42
3:A:577:ILE:HG13	3:A:578:LEU:N	2.33	0.42
3:A:894:GLU:HG3	3:A:933:TYR:OH	2.18	0.42
3:A:896:ARG:HB3	3:A:897:TYR:HD1	1.84	0.42
3:A:1394:THR:CG2	3:A:1398:MET:SD	3.06	0.42
3:A:1424:VAL:HG13	3:A:1436:ILE:HD12	2.02	0.42
4:B:259:TYR:HB2	4:B:268:THR:HG23	2.01	0.42
4:B:467:GLY:CA	4:B:475:SER:HB3	2.48	0.42
4:B:519:TRP:C	4:B:521:LEU:H	2.28	0.42
4:B:707:PRO:HG2	4:B:708:GLU:H	1.82	0.42
4:B:1040:ASN:O	4:B:1041:GLU:C	2.62	0.42
5:C:69:LEU:HB3	12:J:6:ARG:CD	2.49	0.42
5:C:147:LEU:HA	12:J:61:LEU:HD21	2.01	0.42
6:D:29:LEU:HD23	6:D:29:LEU:N	2.33	0.42
7:E:42:PHE:CZ	7:E:58:MET:HE3	2.54	0.42
7:E:149:LEU:O	7:E:151:PRO:HD3	2.19	0.42
10:H:84:ALA:HB1	10:H:87:ARG:HB2	1.98	0.42
10:H:91:ASP:C	10:H:93:TYR:N	2.77	0.42
3:A:332:LYS:HG3	3:A:333:GLU:CG	2.43	0.42
3:A:362:ASP:OD2	3:A:459:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:514:PRO:HB2	3:A:875:ALA:HB3	2.01	0.42
3:A:977:LYS:HB3	3:A:978:PRO:HD2	2.00	0.42
3:A:1074:GLU:C	3:A:1076:ALA:N	2.78	0.42
3:A:1164:PRO:HG2	3:A:1165:GLU:HG3	2.02	0.42
3:A:1332:PHE:HA	3:A:1335:ILE:HB	2.00	0.42
4:B:352:ALA:O	4:B:353:LYS:C	2.62	0.42
4:B:429:PHE:HA	4:B:432:MET:CE	2.46	0.42
4:B:1010:LEU:HD12	4:B:1010:LEU:HA	1.74	0.42
4:B:1167:GLY:O	4:B:1215:ARG:HA	2.20	0.42
5:C:73:GLN:HB2	5:C:131:HIS:HB2	2.00	0.42
7:E:16:PHE:O	7:E:17:ARG:C	2.62	0.42
9:G:35:GLU:CD	9:G:48:VAL:HG23	2.44	0.42
9:G:83:LYS:HE2	9:G:150:CYS:H	1.84	0.42
9:G:117:GLN:O	9:G:119:LEU:N	2.53	0.42
10:H:4:THR:O	10:H:5:LEU:HD23	2.19	0.42
10:H:95:TYR:HE2	10:H:97:MET:CG	2.31	0.42
10:H:110:ASP:O	10:H:128:ASN:ND2	2.53	0.42
13:K:103:THR:HG22	13:K:104:ASN:N	2.34	0.42
3:A:244:PRO:CB	3:A:245:PRO:HD3	2.49	0.42
3:A:346:ASP:OD1	4:B:1108:ARG:HA	2.19	0.42
3:A:622:VAL:O	3:A:622:VAL:HG13	2.19	0.42
3:A:780:VAL:O	3:A:780:VAL:HG12	2.19	0.42
4:B:45:SER:O	4:B:46:GLN:C	2.61	0.42
4:B:96:TYR:HE1	4:B:131:ASP:OD2	2.02	0.42
4:B:377:PHE:HE1	4:B:581:PHE:HE2	1.66	0.42
4:B:1097:HIS:N	4:B:1098:MET:HE2	2.34	0.42
4:B:1159:ARG:HD3	4:B:1193:GLN:CG	2.39	0.42
5:C:114:TYR:CD2	5:C:140:ASN:HB2	2.55	0.42
6:D:67:ARG:CA	6:D:133:THR:HG21	2.49	0.42
7:E:85:GLU:O	7:E:88:VAL:HG23	2.19	0.42
7:E:179:GLN:O	7:E:182:ASP:HB2	2.20	0.42
8:F:77:ASP:C	8:F:79:ARG:N	2.75	0.42
11:I:90:GLN:HE21	11:I:92:ARG:HB2	1.85	0.42
11:I:101:PHE:CE1	11:I:112:SER:HB2	2.55	0.42
13:K:111:LEU:O	13:K:112:GLN:CB	2.67	0.42
14:L:53:HIS:HB3	14:L:55:ILE:HD11	2.01	0.42
3:A:20:GLY:O	3:A:21:LEU:HD23	2.20	0.42
3:A:74:MET:HE3	3:A:74:MET:HB2	1.93	0.42
3:A:154:SER:OG	3:A:162:VAL:HG21	2.20	0.42
3:A:388:LEU:HD22	3:A:432:VAL:HB	2.01	0.42
3:A:541:ILE:HD13	3:A:549:MET:CE	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:890:ASP:H	3:A:1296:GLY:HA3	1.84	0.42
3:A:919:ILE:HD13	3:A:983:ILE:CD1	2.50	0.42
3:A:960:ILE:HA	3:A:963:ILE:CG2	2.50	0.42
3:A:1107:VAL:HG12	3:A:1107:VAL:O	2.19	0.42
3:A:1265:ASN:O	3:A:1267:MET:N	2.53	0.42
3:A:1385:THR:O	3:A:1387:HIS:N	2.52	0.42
4:B:332:ASP:OD1	4:B:336:ARG:NE	2.53	0.42
4:B:1039:GLY:HA2	12:J:51:LEU:CD2	2.48	0.42
5:C:88:CYS:SG	5:C:91:HIS:C	3.03	0.42
6:D:20:GLU:OE2	6:D:20:GLU:HA	2.19	0.42
6:D:39:ASN:ND2	6:D:41:GLN:NE2	2.60	0.42
6:D:118:THR:O	6:D:118:THR:HG22	2.20	0.42
6:D:179:GLN:HA	6:D:179:GLN:NE2	2.33	0.42
7:E:136:ASN:OD1	7:E:137:GLU:N	2.52	0.42
8:F:94:LEU:HD21	8:F:122:MET:HA	2.02	0.42
8:F:118:LEU:O	8:F:118:LEU:HD12	2.20	0.42
10:H:42:ILE:HG12	10:H:95:TYR:CE1	2.55	0.42
11:I:2:THR:O	11:I:4:PHE:N	2.52	0.42
12:J:7:CYS:SG	12:J:49:MET:CE	3.05	0.42
13:K:88:LYS:O	13:K:91:CYS:HB2	2.19	0.42
3:A:90:VAL:HG12	3:A:91:PHE:N	2.35	0.42
3:A:870:GLU:HB2	7:E:204:THR:HG21	2.02	0.42
3:A:873:MET:C	3:A:1058:VAL:CG2	2.93	0.42
3:A:1059:HIS:ND1	8:F:86:THR:HA	2.33	0.42
3:A:1339:LEU:HD13	7:E:147:HIS:CD2	2.54	0.42
4:B:31:TRP:CE3	4:B:34:ILE:HD12	2.54	0.42
4:B:69:LEU:HD13	4:B:432:MET:HE1	2.02	0.42
4:B:492:LEU:HD13	4:B:812:LEU:HD23	2.02	0.42
4:B:854:LEU:HB3	4:B:856:PHE:HE1	1.85	0.42
4:B:860:MET:HE3	4:B:860:MET:HB3	1.87	0.42
4:B:911:ILE:HG22	4:B:966:VAL:HG21	2.02	0.42
5:C:250:THR:O	5:C:253:LYS:N	2.53	0.42
6:D:7:THR:HG21	6:D:32:GLU:CD	2.43	0.42
6:D:7:THR:O	6:D:9:GLN:N	2.52	0.42
8:F:116:ASP:C	8:F:116:ASP:OD1	2.62	0.42
10:H:102:TYR:N	10:H:102:TYR:HD2	2.16	0.42
11:I:13:MET:HG3	11:I:14:LEU:N	2.34	0.42
12:J:13:VAL:C	12:J:14:VAL:HG23	2.44	0.42
3:A:114:LEU:O	3:A:115:LEU:HG	2.19	0.42
3:A:354:SER:O	3:A:469:ARG:HA	2.19	0.42
3:A:367:PRO:HA	3:A:463:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:605:MET:HG2	3:A:621:THR:HG21	2.01	0.42
3:A:664:THR:CG2	3:A:665:GLY:N	2.82	0.42
3:A:883:LEU:HD11	3:A:1017:LEU:HD11	2.02	0.42
3:A:940:ARG:HG2	3:A:940:ARG:NH1	2.34	0.42
3:A:1150:SER:O	3:A:1151:GLU:HG3	2.20	0.42
3:A:1154:TYR:HD1	3:A:1191:TRP:CH2	2.38	0.42
3:A:1219:THR:CB	3:A:1271:ILE:HD11	2.50	0.42
3:A:1279:ILE:HD11	3:A:1316:VAL:CG2	2.49	0.42
3:A:1297:GLU:H	3:A:1297:GLU:HG3	1.56	0.42
4:B:234:ILE:O	4:B:261:ARG:NH2	2.53	0.42
4:B:293:PRO:HG2	4:B:296:GLU:HB3	2.02	0.42
4:B:461:LEU:N	4:B:461:LEU:HD12	2.35	0.42
4:B:611:PRO:CB	4:B:685:LEU:HD21	2.50	0.42
4:B:828:ALA:HB2	4:B:1085:ILE:HG23	2.01	0.42
4:B:1070:GLU:OE1	12:J:44:TYR:OH	2.37	0.42
5:C:46:ILE:HD13	5:C:157:CYS:SG	2.60	0.42
5:C:66:ARG:CZ	12:J:2:ILE:CG2	2.98	0.42
5:C:93:ASP:OD1	5:C:122:SER:HB2	2.20	0.42
6:D:27:LEU:HD22	6:D:173:HIS:CD2	2.54	0.42
6:D:33:PHE:CE2	9:G:80:LYS:NZ	2.68	0.42
8:F:143:PHE:C	8:F:143:PHE:CD1	2.98	0.42
9:G:21:ARG:HA	9:G:21:ARG:HD3	1.79	0.42
10:H:107:VAL:HG21	10:H:126:GLU:OE2	2.20	0.42
11:I:105:SER:O	11:I:106:CYS:CB	2.68	0.42
13:K:55:LYS:HB2	13:K:81:TYR:HE1	1.83	0.42
13:K:83:PRO:O	13:K:84:LYS:C	2.63	0.42
3:A:349:ALA:C	4:B:1128:LEU:CD1	2.93	0.42
3:A:370:ILE:O	3:A:373:THR:N	2.45	0.42
3:A:532:ARG:HD3	3:A:749:ALA:HB2	2.02	0.42
3:A:867:ILE:HD12	3:A:867:ILE:N	2.32	0.42
3:A:979:SER:HG	3:A:980:ASP:H	1.66	0.42
3:A:1074:GLU:HB3	3:A:1075:PRO:CD	2.50	0.42
3:A:1120:LEU:HD11	3:A:1305:VAL:HA	2.01	0.42
3:A:1226:VAL:HG22	3:A:1240:CYS:CB	2.49	0.42
3:A:1260:LEU:CG	3:A:1260:LEU:O	2.68	0.42
3:A:1348:LEU:HD21	3:A:1375:MET:SD	2.60	0.42
3:A:1437:GLY:HA3	8:F:88:TYR:CD2	2.55	0.42
3:A:1441:PHE:CZ	8:F:89:GLU:HA	2.55	0.42
3:A:1449:SER:C	3:A:1451:VAL:H	2.28	0.42
4:B:222:ILE:O	4:B:240:ILE:HA	2.19	0.42
4:B:582:VAL:HG23	4:B:626:ILE:CB	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:603:LEU:HB3	4:B:609:ILE:HG13	2.01	0.42
4:B:1002:THR:HG21	4:B:1006:ILE:HD12	2.01	0.42
4:B:1186:ASP:OD1	4:B:1186:ASP:C	2.63	0.42
5:C:6:PRO:HB3	5:C:25:VAL:CG1	2.40	0.42
5:C:9:LYS:O	5:C:10:ILE:C	2.62	0.42
5:C:29:MET:HE2	13:K:98:LEU:HD23	2.01	0.42
5:C:174:ALA:O	12:J:10:CYS:HB2	2.19	0.42
5:C:191:TYR:CD2	5:C:201:TRP:CD1	3.00	0.42
5:C:241:ASP:C	5:C:245:VAL:HG23	2.44	0.42
9:G:39:THR:CG2	9:G:40:GLY:H	2.18	0.42
10:H:80:ARG:HA	10:H:81:PRO:HD3	1.87	0.42
10:H:83:GLN:O	10:H:85:GLY:N	2.51	0.42
3:A:383:TYR:CD2	3:A:383:TYR:N	2.88	0.41
3:A:404:TYR:CD2	3:A:414:ASP:HA	2.54	0.41
3:A:456:MET:HE1	3:A:477:PRO:HB2	2.02	0.41
3:A:494:SER:O	3:A:497:THR:N	2.53	0.41
3:A:500:GLU:O	3:A:504:LEU:HD13	2.20	0.41
3:A:699:ALA:O	3:A:700:ASN:HB3	2.20	0.41
3:A:873:MET:C	3:A:1058:VAL:HG23	2.45	0.41
3:A:875:ALA:HB2	3:A:1366:ARG:HD2	2.02	0.41
4:B:22:SER:HA	4:B:654:ARG:CG	2.50	0.41
4:B:60:GLN:NE2	4:B:94:LYS:HA	2.31	0.41
4:B:376:PHE:HB3	4:B:586:TRP:CZ3	2.55	0.41
4:B:736:THR:O	4:B:736:THR:HG22	2.20	0.41
4:B:794:ASN:C	4:B:795:ILE:HD12	2.44	0.41
4:B:806:THR:HG22	4:B:808:ALA:CB	2.50	0.41
4:B:839:MET:HG3	4:B:1010:LEU:CD1	2.50	0.41
4:B:841:MET:SD	4:B:846:ILE:HD11	2.59	0.41
4:B:1106:ARG:HD2	4:B:1125:ASP:O	2.20	0.41
5:C:77:ILE:HD13	5:C:77:ILE:HA	1.84	0.41
5:C:246:ARG:HA	5:C:249:ASP:HB3	2.02	0.41
7:E:122:LYS:C	7:E:123:LEU:HG	2.44	0.41
7:E:177:ARG:HD3	7:E:215:MET:CG	2.49	0.41
8:F:89:GLU:HB3	8:F:134:ILE:HD13	2.02	0.41
10:H:95:TYR:CE2	10:H:97:MET:CG	3.02	0.41
3:A:18:GLN:CB	4:B:1215:ARG:HG3	2.50	0.41
3:A:269:ILE:HG23	3:A:300:VAL:HG22	2.02	0.41
3:A:510:GLN:OE1	3:A:510:GLN:HA	2.19	0.41
3:A:567:LYS:HD3	10:H:95:TYR:HA	2.02	0.41
3:A:714:PHE:HE2	3:A:792:TYR:HD2	1.67	0.41
3:A:719:VAL:CG2	3:A:774:ARG:HD3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:822:GLU:HG3	4:B:513:GLN:NE2	2.35	0.41
3:A:857:ARG:HD3	3:A:861:GLY:O	2.20	0.41
3:A:870:GLU:HG2	7:E:208:TYR:CD1	2.55	0.41
3:A:1010:ALA:O	3:A:1013:ASP:HB2	2.19	0.41
3:A:1053:PHE:O	3:A:1055:ARG:N	2.53	0.41
3:A:1157:ASP:C	3:A:1159:ARG:H	2.28	0.41
4:B:458:LYS:O	4:B:459:TYR:C	2.63	0.41
4:B:593:PRO:O	4:B:594:ALA:C	2.63	0.41
4:B:761:HIS:HB2	4:B:1024:ALA:HB2	2.02	0.41
4:B:1208:MET:HA	4:B:1212:ILE:O	2.19	0.41
5:C:24:ASN:O	5:C:24:ASN:CG	2.62	0.41
5:C:45:ALA:O	5:C:159:ALA:HA	2.19	0.41
5:C:89:GLU:O	5:C:90:ASP:CB	2.68	0.41
5:C:187:LYS:HG3	5:C:219:PHE:CE1	2.54	0.41
6:D:8:PHE:HE1	6:D:37:GLN:HB2	1.86	0.41
6:D:156:ASP:HB3	6:D:159:THR:H	1.85	0.41
8:F:140:ASP:OD1	8:F:140:ASP:C	2.63	0.41
11:I:50:THR:CG2	11:I:51:ASN:N	2.83	0.41
3:A:48:ALA:O	3:A:49:LYS:HG2	2.20	0.41
3:A:182:VAL:CG2	3:A:201:VAL:HA	2.49	0.41
3:A:332:LYS:C	3:A:334:GLY:N	2.78	0.41
3:A:492:PRO:O	3:A:493:GLN:NE2	2.53	0.41
3:A:746:MET:CE	4:B:1018:PRO:CG	2.98	0.41
3:A:809:THR:OG1	3:A:812:GLU:HG3	2.21	0.41
3:A:1025:ARG:HG3	3:A:1025:ARG:NH1	2.34	0.41
3:A:1072:ILE:HG23	3:A:1356:ILE:HD11	2.02	0.41
3:A:1192:LEU:HG	3:A:1193:LEU:N	2.35	0.41
4:B:165:VAL:HG11	4:B:448:ILE:HD13	2.02	0.41
4:B:449:ASN:C	4:B:451:LYS:N	2.76	0.41
4:B:616:ILE:HG13	4:B:697:GLU:HA	2.03	0.41
4:B:700:SER:C	4:B:701:ILE:CG2	2.93	0.41
4:B:906:SER:O	4:B:907:GLY:O	2.38	0.41
4:B:1085:ILE:N	4:B:1085:ILE:CD1	2.79	0.41
5:C:239:PRO:O	5:C:241:ASP:N	2.53	0.41
6:D:139:LYS:O	6:D:143:ASN:ND2	2.50	0.41
7:E:29:PHE:C	7:E:30:ILE:HG13	2.43	0.41
8:F:101:ILE:HD13	8:F:120:ILE:CG2	2.51	0.41
9:G:1:MET:HG3	9:G:85:GLU:CD	2.44	0.41
10:H:43:ASN:CG	10:H:46:LEU:HG	2.45	0.41
12:J:16:ASP:O	12:J:18:TRP:N	2.54	0.41
13:K:55:LYS:CB	13:K:81:TYR:CE1	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:61:THR:HG22	14:L:63:ARG:HG2	2.01	0.41
3:A:34:LYS:CG	3:A:57:ARG:HH22	2.33	0.41
3:A:532:ARG:O	3:A:535:THR:HB	2.20	0.41
3:A:695:LYS:C	3:A:697:ALA:N	2.77	0.41
3:A:965:GLN:O	3:A:968:GLN:HB2	2.20	0.41
3:A:1209:MET:CE	3:A:1236:LEU:HB3	2.50	0.41
3:A:1263:ILE:O	3:A:1267:MET:HG3	2.20	0.41
3:A:1450:LEU:CD1	8:F:108:PHE:CZ	3.04	0.41
4:B:806:THR:HG22	4:B:808:ALA:HB3	2.02	0.41
4:B:1096:ARG:CG	4:B:1097:HIS:N	2.82	0.41
4:B:1207:LEU:HD23	4:B:1207:LEU:HA	1.93	0.41
5:C:94:LYS:HE3	5:C:94:LYS:HB2	1.76	0.41
6:D:38:ILE:HG22	6:D:39:ASN:O	2.20	0.41
6:D:154:PHE:HB2	6:D:160:VAL:HG22	2.02	0.41
7:E:164:LEU:HD21	7:E:211:TYR:CG	2.54	0.41
8:F:82:THR:HG23	8:F:83:PRO:HD2	2.03	0.41
3:A:693:VAL:O	3:A:693:VAL:HG12	2.20	0.41
3:A:929:LEU:HD23	3:A:983:ILE:HG21	2.02	0.41
3:A:1289:ARG:HH12	3:A:1326:ARG:NH1	2.18	0.41
4:B:27:ALA:C	4:B:29:ASP:H	2.29	0.41
4:B:259:TYR:HD1	4:B:259:TYR:H	1.68	0.41
4:B:654:ARG:N	4:B:657:HIS:HD2	2.05	0.41
4:B:990:ILE:HG22	4:B:991:GLY:N	2.36	0.41
4:B:1085:ILE:HG22	4:B:1086:PHE:N	2.35	0.41
4:B:1167:GLY:CA	4:B:1217:TYR:HE1	2.34	0.41
5:C:17:ASN:C	5:C:18:VAL:HG23	2.45	0.41
5:C:168:ALA:O	5:C:170:TRP:N	2.54	0.41
8:F:119:ARG:NH1	8:F:119:ARG:CG	2.83	0.41
9:G:65:ASP:OD2	9:G:67:SER:HB2	2.20	0.41
11:I:100:PHE:HD1	11:I:100:PHE:N	2.18	0.41
13:K:27:ALA:HB1	13:K:28:PRO:HD2	2.03	0.41
14:L:55:ILE:HG12	14:L:55:ILE:H	1.45	0.41
3:A:172:PRO:HB3	3:A:185:TRP:CD2	2.55	0.41
3:A:324:SER:O	3:A:325:ILE:C	2.63	0.41
3:A:412:ARG:HH21	4:B:1108:ARG:NH1	2.17	0.41
3:A:1152:ILE:HG13	11:I:44:TYR:HB3	2.03	0.41
4:B:21:GLU:O	4:B:22:SER:O	2.38	0.41
4:B:604:ARG:C	4:B:606:LYS:N	2.78	0.41
4:B:1106:ARG:HD3	4:B:1126:GLY:C	2.46	0.41
5:C:217:ASP:HA	5:C:218:PRO:HD3	1.85	0.41
5:C:252:GLN:HE21	13:K:95:ILE:HG23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:39:THR:CG2	9:G:41:LYS:H	2.29	0.41
9:G:99:PHE:C	9:G:99:PHE:HD1	2.27	0.41
10:H:33:GLN:C	10:H:35:GLN:H	2.28	0.41
11:I:54:GLU:HB3	11:I:100:PHE:CE2	2.55	0.41
3:A:116:ASP:O	3:A:117:GLU:C	2.62	0.41
3:A:404:TYR:CE2	3:A:414:ASP:HA	2.56	0.41
3:A:474:VAL:HG22	3:A:474:VAL:O	2.21	0.41
3:A:684:ALA:O	3:A:687:LYS:HB2	2.21	0.41
3:A:958:VAL:O	3:A:958:VAL:HG12	2.20	0.41
4:B:23:ALA:H	4:B:654:ARG:HD2	1.86	0.41
4:B:313:MET:HE2	4:B:390:LEU:HD21	2.03	0.41
4:B:464:GLY:O	4:B:477:ALA:HA	2.21	0.41
4:B:864:LYS:HB2	4:B:872:GLU:OE1	2.21	0.41
4:B:1033:LYS:NZ	4:B:1070:GLU:OE1	2.48	0.41
4:B:1197:PRO:C	4:B:1199:ALA:N	2.76	0.41
6:D:13:ARG:CA	6:D:17:LYS:NZ	2.83	0.41
6:D:48:ILE:CG2	9:G:4:ILE:HB	2.51	0.41
7:E:17:ARG:O	7:E:21:GLU:HG3	2.21	0.41
7:E:30:ILE:HG22	7:E:31:THR:N	2.35	0.41
7:E:114:ASN:O	7:E:115:ASN:CB	2.63	0.41
9:G:23:LYS:HG3	9:G:56:ILE:CD1	2.50	0.41
10:H:61:SER:O	10:H:62:SER:CB	2.64	0.41
13:K:5:ASP:O	13:K:6:ARG:C	2.63	0.41
3:A:42:ASP:O	3:A:44:THR:N	2.41	0.41
3:A:335:ARG:HE	3:A:335:ARG:HB2	1.58	0.41
3:A:666:ILE:HD11	4:B:1086:PHE:CE1	2.55	0.41
3:A:667:GLY:HA3	5:C:192:TRP:HH2	1.85	0.41
3:A:1019:CYS:O	3:A:1022:LEU:HB3	2.21	0.41
3:A:1115:SER:HB3	3:A:1330:ASN:HD21	1.86	0.41
3:A:1349:TYR:CD2	3:A:1349:TYR:C	2.98	0.41
4:B:307:ASP:O	4:B:309:GLN:N	2.54	0.41
4:B:595:ARG:O	4:B:596:LEU:C	2.63	0.41
6:D:63:LEU:O	6:D:129:LEU:HD11	2.21	0.41
7:E:168:TYR:CB	7:E:170:LEU:HG	2.50	0.41
9:G:59:GLY:CA	9:G:70:PHE:CD2	3.02	0.41
10:H:31:THR:O	10:H:31:THR:HG22	2.19	0.41
10:H:98:TYR:C	10:H:118:PHE:HD2	2.29	0.41
3:A:43:GLU:HB2	3:A:46:THR:HB	2.03	0.41
3:A:102:VAL:O	3:A:105:CYS:HB2	2.21	0.41
3:A:224:PHE:CE2	3:A:234:MET:HE2	2.55	0.41
3:A:385:ILE:HG22	3:A:386:ASP:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:399:HIS:CG	3:A:400:PRO:N	2.88	0.41
3:A:608:ILE:HD12	3:A:613:ILE:HD11	2.03	0.41
3:A:784:LEU:HB3	3:A:785:PRO:HD2	2.03	0.41
3:A:866:PHE:HE1	7:E:211:TYR:H	1.68	0.41
3:A:899:VAL:CG2	3:A:1029:ARG:HG2	2.51	0.41
3:A:1101:LEU:HD11	3:A:1105:LEU:HD11	2.02	0.41
3:A:1126:ALA:O	3:A:1128:GLN:N	2.54	0.41
3:A:1153:TYR:CD2	3:A:1163:ILE:HD11	2.55	0.41
3:A:1193:LEU:HD12	3:A:1193:LEU:C	2.46	0.41
3:A:1214:GLU:O	3:A:1218:GLN:HG2	2.21	0.41
4:B:211:VAL:HG23	4:B:483:LEU:HB2	2.03	0.41
4:B:284:ILE:HG23	4:B:324:ILE:HD12	2.03	0.41
4:B:487:THR:H	4:B:490:SER:HB3	1.85	0.41
4:B:619:ILE:HD12	11:I:65:ASP:HB2	2.02	0.41
4:B:711:GLU:HB2	4:B:712:PRO:CD	2.51	0.41
4:B:789:MET:HE2	4:B:953:LEU:CD2	2.43	0.41
4:B:890:TYR:CZ	4:B:910:VAL:HG21	2.55	0.41
4:B:1159:ARG:HD2	4:B:1159:ARG:C	2.46	0.41
5:C:33:LEU:O	5:C:37:MET:HG3	2.21	0.41
5:C:221:TYR:CD1	5:C:222:LYS:HG3	2.56	0.41
7:E:114:ASN:HD22	7:E:114:ASN:HA	1.62	0.41
7:E:116:ILE:CG2	7:E:120:ALA:HB3	2.50	0.41
8:F:82:THR:HA	8:F:83:PRO:HD3	1.80	0.41
8:F:103:MET:CE	9:G:65:ASP:HB2	2.50	0.41
9:G:15:PRO:O	9:G:18:PHE:HB2	2.21	0.41
9:G:66:GLY:O	9:G:67:SER:C	2.63	0.41
9:G:102:GLN:HG3	9:G:106:MET:O	2.21	0.41
9:G:114:LEU:HD12	9:G:114:LEU:HA	1.96	0.41
11:I:86:PHE:CE1	11:I:100:PHE:HB2	2.55	0.41
13:K:46:ILE:O	13:K:46:ILE:HG22	2.20	0.41
3:A:207:ILE:CG2	3:A:211:PHE:HE1	2.33	0.41
3:A:244:PRO:O	3:A:246:VAL:N	2.53	0.41
3:A:298:PHE:HD2	3:A:299:HIS:CD2	2.39	0.41
3:A:306:ASN:HB2	3:A:324:SER:HB3	2.02	0.41
3:A:526:ASP:O	3:A:527:THR:C	2.64	0.41
3:A:709:THR:HB	3:A:712:GLU:H	1.86	0.41
3:A:781:ASP:O	3:A:789:LYS:HA	2.21	0.41
3:A:852:TYR:CD2	3:A:1060:PRO:CB	3.03	0.41
3:A:898:ARG:O	3:A:1029:ARG:NH1	2.54	0.41
3:A:899:VAL:CG2	3:A:908:LEU:HD21	2.51	0.41
4:B:555:ILE:HG22	4:B:556:THR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:622:LYS:HE2	11:I:59:VAL:CG2	2.42	0.41
4:B:693:ILE:HG22	4:B:694:ASP:O	2.20	0.41
4:B:818:PRO:HB2	4:B:1091:TYR:OH	2.21	0.41
4:B:1000:PRO:O	4:B:1000:PRO:HG2	2.21	0.41
4:B:1132:GLU:O	4:B:1135:ARG:HB3	2.20	0.41
5:C:167:HIS:CD2	5:C:168:ALA:H	2.39	0.41
5:C:193:TYR:C	5:C:193:TYR:CD1	2.99	0.41
6:D:176:GLU:O	6:D:178:ALA:N	2.54	0.41
10:H:56:THR:HB	10:H:145:ARG:HG2	2.02	0.41
11:I:15:TYR:O	11:I:28:GLU:HG2	2.20	0.41
11:I:58:VAL:HG12	11:I:58:VAL:O	2.21	0.41
13:K:78:THR:O	13:K:81:TYR:HB3	2.21	0.41
2:T:12:G:C2'	2:T:13:U:O5'	2.69	0.40
3:A:207:ILE:O	3:A:208:LEU:C	2.64	0.40
3:A:497:THR:HG23	4:B:1146:PHE:HD1	1.85	0.40
3:A:1025:ARG:HG3	3:A:1025:ARG:HH11	1.85	0.40
4:B:46:GLN:CG	4:B:47:GLN:H	2.32	0.40
4:B:175:ARG:HG2	4:B:175:ARG:HH11	1.87	0.40
4:B:542:MET:CG	4:B:747:MET:HB3	2.51	0.40
4:B:681:TRP:O	4:B:683:SER:N	2.54	0.40
4:B:826:ALA:O	4:B:1011:ILE:HA	2.21	0.40
4:B:899:ILE:HG22	4:B:903:VAL:CG2	2.50	0.40
5:C:82:TYR:CD2	5:C:161:LYS:HB3	2.55	0.40
5:C:174:ALA:O	12:J:10:CYS:O	2.39	0.40
5:C:259:LEU:CD1	13:K:91:CYS:HB2	2.51	0.40
6:D:46:GLU:O	6:D:47:LEU:C	2.65	0.40
7:E:2:ASP:O	7:E:3:GLN:C	2.65	0.40
9:G:7:LEU:CB	9:G:74:TYR:CE2	2.97	0.40
3:A:84:ILE:HD11	3:A:270:LEU:HD22	2.02	0.40
3:A:108:MET:SD	3:A:108:MET:N	2.94	0.40
3:A:241:VAL:HG13	3:A:266:LEU:CD1	2.51	0.40
3:A:503:GLN:OE1	8:F:90:ARG:NH2	2.48	0.40
3:A:738:LYS:HB2	3:A:740:LEU:CG	2.45	0.40
3:A:821:ARG:HH11	3:A:821:ARG:CB	2.27	0.40
3:A:874:ASP:CA	3:A:1058:VAL:HG22	2.51	0.40
3:A:961:ARG:HG3	3:A:961:ARG:NH1	2.35	0.40
3:A:1389:PHE:C	3:A:1391:ARG:H	2.28	0.40
4:B:250:PHE:HD2	4:B:250:PHE:HA	1.69	0.40
4:B:388:CYS:O	4:B:391:ASP:N	2.51	0.40
4:B:552:MET:HA	4:B:555:ILE:HB	2.03	0.40
4:B:558:LEU:O	4:B:560:GLU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:728:ARG:HH12	4:B:1047:PHE:HB3	1.86	0.40
4:B:732:SER:HB2	4:B:734:HIS:CD2	2.56	0.40
4:B:950:ASP:O	4:B:951:GLN:HB2	2.21	0.40
7:E:117:THR:C	7:E:119:SER:N	2.79	0.40
8:F:99:LEU:HD21	9:G:64:THR:O	2.21	0.40
9:G:82:PHE:CD1	9:G:82:PHE:N	2.89	0.40
9:G:111:THR:HG22	9:G:113:HIS:N	2.20	0.40
12:J:48:ARG:HH21	12:J:49:MET:HE1	1.86	0.40
13:K:95:ILE:O	13:K:98:LEU:HB2	2.21	0.40
14:L:40:LEU:HB3	14:L:41:SER:H	1.47	0.40
3:A:699:ALA:O	3:A:700:ASN:CB	2.69	0.40
3:A:1364:ASN:HD22	3:A:1365:TYR:N	2.19	0.40
4:B:258:LEU:O	4:B:258:LEU:CG	2.69	0.40
4:B:309:GLN:CD	11:I:52:ILE:HD11	2.45	0.40
4:B:311:LEU:O	4:B:314:LEU:N	2.51	0.40
4:B:324:ILE:CG2	4:B:325:GLN:N	2.82	0.40
4:B:376:PHE:CZ	4:B:569:TYR:HB3	2.56	0.40
4:B:377:PHE:O	4:B:378:LEU:C	2.63	0.40
4:B:446:LEU:HD23	4:B:446:LEU:N	2.36	0.40
4:B:610:ASN:HA	4:B:611:PRO:HD3	1.89	0.40
4:B:791:THR:O	4:B:792:MET:O	2.38	0.40
4:B:835:GLN:HE21	4:B:835:GLN:HB2	1.65	0.40
4:B:953:LEU:CD2	4:B:965:LYS:HB2	2.50	0.40
4:B:984:HIS:CD2	4:B:1025:HIS:HB2	2.56	0.40
4:B:1080:LYS:HD2	5:C:188:HIS:HB2	2.04	0.40
6:D:51:ASN:C	6:D:52:LEU:O	2.64	0.40
6:D:154:PHE:CE2	6:D:163:VAL:CG2	3.04	0.40
6:D:195:ILE:O	6:D:198:LEU:HG	2.21	0.40
7:E:134:THR:C	7:E:135:PHE:HD1	2.28	0.40
9:G:88:ASP:CB	9:G:144:ARG:HA	2.44	0.40
10:H:113:ALA:CB	10:H:125:LEU:O	2.70	0.40
12:J:47:ARG:HG2	12:J:47:ARG:HH11	1.85	0.40
14:L:58:LYS:O	14:L:58:LYS:CG	2.65	0.40
3:A:231:PRO:C	3:A:233:TRP:H	2.28	0.40
3:A:262:LEU:C	3:A:264:PHE:H	2.29	0.40
3:A:491:VAL:HG12	3:A:492:PRO:O	2.21	0.40
3:A:576:GLN:HG3	10:H:119:GLY:HA3	2.04	0.40
3:A:1001:ARG:O	3:A:1002:GLY:C	2.64	0.40
3:A:1209:MET:O	3:A:1210:GLY:C	2.64	0.40
3:A:1441:PHE:HB2	8:F:135:ARG:O	2.21	0.40
4:B:26:THR:O	4:B:29:ASP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:48:LEU:O	4:B:49:ASP:C	2.63	0.40
4:B:236:HIS:CE1	4:B:389:ALA:HA	2.57	0.40
4:B:382:ILE:O	4:B:385:LEU:HB3	2.21	0.40
4:B:680:THR:O	4:B:684:LEU:CD1	2.69	0.40
4:B:984:HIS:CG	4:B:1025:HIS:HB2	2.56	0.40
4:B:1159:ARG:HB3	4:B:1159:ARG:HH11	1.87	0.40
5:C:179:GLU:CG	5:C:180:TYR:N	2.84	0.40
6:D:24:ALA:HB3	6:D:26:THR:OG1	2.21	0.40
7:E:212:ARG:CG	7:E:212:ARG:HH11	2.34	0.40
9:G:112:LYS:NZ	9:G:120:THR:HA	2.37	0.40
10:H:100:THR:CG2	10:H:101:ALA:N	2.83	0.40
12:J:3:VAL:HA	12:J:4:PRO:HD3	1.92	0.40
13:K:29:ASN:O	13:K:76:GLN:HG3	2.21	0.40
2:T:12:G:HO2'	2:T:13:U:C4'	2.35	0.40
3:A:24:PRO:HD2	3:A:233:TRP:NE1	2.36	0.40
3:A:43:GLU:O	3:A:44:THR:CB	2.68	0.40
3:A:49:LYS:NZ	3:A:60:SER:HA	2.36	0.40
3:A:70:CYS:O	3:A:71:GLN:C	2.64	0.40
3:A:1097:GLY:HA2	3:A:1355:VAL:HG13	2.04	0.40
3:A:1291:VAL:HG13	3:A:1292:PRO:N	2.36	0.40
4:B:400:HIS:O	4:B:401:PHE:C	2.63	0.40
4:B:802:PRO:HG2	4:B:805:THR:HG22	2.03	0.40
4:B:1017:ILE:HD13	4:B:1017:ILE:HA	1.92	0.40
7:E:58:MET:O	7:E:59:SER:O	2.39	0.40
9:G:3:PHE:CE1	9:G:80:LYS:HE2	2.56	0.40
9:G:81:PRO:C	9:G:82:PHE:CD1	2.99	0.40
12:J:23:ASN:C	12:J:25:LEU:H	2.28	0.40
12:J:28:ASP:O	12:J:29:GLU:C	2.64	0.40
12:J:53:HIS:CD2	12:J:53:HIS:C	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	1412/1733 (82%)	1030 (73%)	249 (18%)	133 (9%)	0	8
4	B	1094/1224 (89%)	780 (71%)	214 (20%)	100 (9%)	0	8
5	C	264/318 (83%)	164 (62%)	64 (24%)	36 (14%)	0	3
6	D	174/221 (79%)	126 (72%)	30 (17%)	18 (10%)	0	6
7	E	212/215 (99%)	158 (74%)	36 (17%)	18 (8%)	0	9
8	F	86/155 (56%)	69 (80%)	9 (10%)	8 (9%)	0	8
9	G	169/171 (99%)	130 (77%)	33 (20%)	6 (4%)	2	22
10	H	131/146 (90%)	74 (56%)	36 (28%)	21 (16%)	0	2
11	I	114/122 (93%)	69 (60%)	30 (26%)	15 (13%)	0	3
12	J	63/70 (90%)	39 (62%)	10 (16%)	14 (22%)	0	1
13	K	110/120 (92%)	87 (79%)	15 (14%)	8 (7%)	1	11
14	L	44/70 (63%)	18 (41%)	10 (23%)	16 (36%)	0	0
All	All	3873/4565 (85%)	2744 (71%)	736 (19%)	393 (10%)	0	7

All (393) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	4	GLN
3	A	44	THR
3	A	48	ALA
3	A	54	ASN
3	A	57	ARG
3	A	58	LEU
3	A	62	ASP
3	A	65	LEU
3	A	66	LYS
3	A	70	CYS
3	A	74	MET
3	A	93	VAL
3	A	154	SER
3	A	167	CYS
3	A	223	GLY
3	A	250	ILE
3	A	255	SER
3	A	286	HIS
3	A	311	GLN
3	A	318	SER
3	A	335	ARG
3	A	399	HIS

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Mol	Chain	Res	Type
3	A	516	SER
3	A	517	ASN
3	A	536	LEU
3	A	567	LYS
3	A	597	LEU
3	A	619	LYS
3	A	626	ASN
3	A	666	ILE
3	A	780	VAL
3	A	968	GLN
3	A	986	ILE
3	A	1016	THR
3	A	1036	ARG
3	A	1115	SER
3	A	1116	LEU
3	A	1120	LEU
3	A	1122	PRO
3	A	1124	HIS
3	A	1127	ASP
3	A	1176	LEU
3	A	1212	VAL
3	A	1223	ASP
3	A	1233	ASP
3	A	1314	SER
3	A	1365	TYR
3	A	1378	GLN
3	A	1405	THR
4	B	22	SER
4	B	28	GLU
4	B	45	SER
4	B	108	VAL
4	B	186	GLU
4	B	206	ASN
4	B	258	LEU
4	B	266	ALA
4	B	367	LEU
4	B	467	GLY
4	B	643	ASP
4	B	709	ASP
4	B	731	VAL
4	B	792	MET
4	B	879	ARG

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Mol	Chain	Res	Type
4	B	881	ASN
4	B	907	GLY
4	B	958	GLN
4	B	1003	ALA
4	B	1041	GLU
4	B	1046	PRO
4	B	1069	PHE
4	B	1097	HIS
4	B	1156	ASP
4	B	1171	VAL
4	B	1175	LEU
4	B	1181	GLU
4	B	1182	CYS
4	B	1188	LYS
5	C	4	GLU
5	C	18	VAL
5	C	110	THR
5	C	132	PRO
5	C	149	LYS
5	C	156	THR
5	C	161	LYS
5	C	184	ASN
5	C	214	ASN
5	C	215	GLU
5	C	216	GLY
6	D	5	THR
6	D	8	PHE
6	D	20	GLU
6	D	131	GLU
6	D	199	ASN
7	E	3	GLN
7	E	45	LYS
7	E	59	SER
7	E	73	PRO
7	E	106	GLN
7	E	130	ALA
8	F	81	THR
9	G	63	PRO
10	H	21	ASN
10	H	62	SER
10	H	78	SER
10	H	128	ASN

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Mol	Chain	Res	Type
10	H	140	ALA
11	I	3	THR
11	I	57	GLY
11	I	106	CYS
12	J	2	ILE
12	J	28	ASP
12	J	32	GLU
12	J	41	LEU
12	J	64	ASN
13	K	109	TRP
13	K	110	ASN
13	K	111	LEU
14	L	50	ASP
14	L	59	ALA
3	A	42	ASP
3	A	59	GLY
3	A	61	ILE
3	A	71	GLN
3	A	76	GLU
3	A	117	GLU
3	A	128	ILE
3	A	253	ASN
3	A	257	ARG
3	A	283	GLY
3	A	312	PRO
3	A	322	VAL
3	A	331	GLY
3	A	332	LYS
3	A	419	LYS
3	A	543	LEU
3	A	592	ASP
3	A	649	ILE
3	A	753	GLY
3	A	765	VAL
3	A	888	GLY
3	A	969	GLN
3	A	1002	GLY
3	A	1281	ARG
3	A	1377	THR
3	A	1438	THR
4	B	46	GLN
4	B	58	THR

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Mol	Chain	Res	Type
4	B	65	GLU
4	B	100	PRO
4	B	115	GLN
4	B	261	ARG
4	B	282	ILE
4	B	345	LYS
4	B	543	SER
4	B	605	ARG
4	B	641	GLU
4	B	655	LYS
4	B	746	SER
4	B	751	VAL
4	B	831	SER
4	B	848	ARG
4	B	867	GLY
4	B	891	ASP
4	B	1065	GLN
4	B	1075	GLY
4	B	1155	SER
4	B	1186	ASP
5	C	78	GLU
5	C	141	GLY
5	C	142	VAL
5	C	213	PRO
5	C	231	ASN
6	D	9	GLN
6	D	12	ARG
6	D	16	LYS
6	D	19	GLU
6	D	21	GLU
6	D	30	GLY
6	D	52	LEU
6	D	192	LYS
7	E	36	GLU
7	E	44	ALA
7	E	74	ASP
7	E	76	GLY
7	E	192	ARG
7	E	206	GLY
8	F	69	LEU
8	F	70	LYS
8	F	150	GLU

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Mol	Chain	Res	Type
8	F	151	LEU
9	G	139	ILE
10	H	17	PRO
10	H	59	ILE
10	H	77	ARG
10	H	81	PRO
10	H	82	PRO
10	H	84	ALA
10	H	90	ALA
10	H	107	VAL
10	H	108	SER
11	I	11	ASN
11	I	59	VAL
11	I	95	THR
12	J	6	ARG
12	J	9	SER
12	J	14	VAL
12	J	17	LYS
12	J	29	GLU
12	J	33	GLY
13	K	15	GLY
14	L	53	HIS
14	L	60	ARG
3	A	67	CYS
3	A	169	ASN
3	A	219	PHE
3	A	263	THR
3	A	336	ILE
3	A	424	ILE
3	A	465	TYR
3	A	591	PHE
3	A	652	VAL
3	A	846	GLU
3	A	847	ASP
3	A	871	ASP
3	A	875	ALA
3	A	926	GLN
3	A	972	HIS
3	A	1054	LEU
3	A	1221	LYS
4	B	184	ALA
4	B	257	LYS

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Mol	Chain	Res	Type
4	B	259	TYR
4	B	264	SER
4	B	401	PHE
4	B	470	LYS
4	B	642	ASP
4	B	708	GLU
4	B	711	GLU
4	B	943	SER
4	B	1100	ASP
4	B	1178	ASN
4	B	1183	LYS
5	C	90	ASP
5	C	117	ASP
5	C	217	ASP
5	C	233	GLU
6	D	47	LEU
7	E	43	LYS
7	E	115	ASN
7	E	158	SER
8	F	128	LYS
9	G	20	PRO
9	G	118	ASP
9	G	154	VAL
10	H	52	GLN
10	H	63	LEU
10	H	64	ASN
10	H	92	ASP
11	I	9	ASP
11	I	78	CYS
11	I	91	ARG
11	I	107	SER
12	J	8	PHE
13	K	29	ASN
14	L	35	SER
14	L	37	LYS
3	A	69	THR
3	A	84	ILE
3	A	410	GLY
3	A	439	ASN
3	A	483	ASP
3	A	648	ASN
3	A	706	HIS

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Mol	Chain	Res	Type
3	A	775	ILE
3	A	789	LYS
3	A	1114	PRO
3	A	1136	SER
4	B	48	LEU
4	B	114	PRO
4	B	249	ARG
4	B	260	GLY
4	B	308	TRP
4	B	362	PRO
4	B	450	ALA
4	B	474	SER
4	B	483	LEU
4	B	559	SER
4	B	575	PRO
4	B	764	SER
4	B	880	THR
4	B	977	GLY
4	B	1017	ILE
4	B	1035	ALA
4	B	1074	ASN
4	B	1108	ARG
4	B	1144	ALA
4	B	1157	ALA
5	C	11	ARG
5	C	87	PHE
5	C	175	ALA
5	C	188	HIS
5	C	240	VAL
6	D	218	GLU
7	E	40	GLU
7	E	56	LYS
9	G	115	MET
10	H	32	THR
10	H	44	VAL
11	I	47	GLU
11	I	79	HIS
12	J	62	ARG
13	K	7	PHE
14	L	26	THR
14	L	28	LYS
14	L	40	LEU

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Mol	Chain	Res	Type
14	L	43	THR
14	L	45	ALA
3	A	35	ILE
3	A	43	GLU
3	A	55	ASP
3	A	113	LEU
3	A	130	ASP
3	A	164	ARG
3	A	317	LYS
3	A	605	MET
3	A	739	ASP
3	A	783	THR
3	A	891	ALA
3	A	1366	ARG
3	A	1392	SER
4	B	27	ALA
4	B	365	THR
4	B	383	ASN
4	B	513	GLN
4	B	551	PRO
4	B	705	MET
4	B	712	PRO
4	B	1045	SER
5	C	10	ILE
5	C	13	ALA
5	C	108	GLU
5	C	264	GLN
8	F	104	ASN
11	I	4	PHE
11	I	54	GLU
11	I	62	ILE
13	K	103	THR
14	L	41	SER
14	L	44	ASP
14	L	54	ARG
3	A	5	GLN
3	A	245	PRO
3	A	249	SER
3	A	830	LYS
3	A	958	VAL
3	A	1094	VAL
3	A	1123	GLY

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Mol	Chain	Res	Type
3	A	1454	MET
4	B	20	ASP
4	B	94	LYS
4	B	295	GLY
5	C	70	ILE
5	C	133	ILE
5	C	137	LYS
5	C	209	TYR
6	D	139	LYS
10	H	36	CYS
12	J	57	ILE
14	L	56	LEU
3	A	400	PRO
3	A	604	GLY
3	A	1164	PRO
4	B	1167	GLY
5	C	51	VAL
3	A	599	SER
3	A	1324	PRO
5	C	126	GLY
5	C	202	PRO
3	A	51	GLY
3	A	825	ILE
6	D	59	ILE
8	F	131	PRO
13	K	43	GLY
3	A	600	PRO
3	A	622	VAL
4	B	411	PRO
4	B	613	VAL
4	B	976	ILE
6	D	202	ILE
14	L	55	ILE
4	B	524	PRO
7	E	129	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	1245/1520 (82%)	1121 (90%)	124 (10%)	7	28
4	B	964/1061 (91%)	882 (92%)	82 (8%)	10	33
5	C	235/274 (86%)	214 (91%)	21 (9%)	9	32
6	D	160/200 (80%)	141 (88%)	19 (12%)	5	22
7	E	196/197 (100%)	185 (94%)	11 (6%)	19	45
8	F	78/137 (57%)	73 (94%)	5 (6%)	16	42
9	G	152/152 (100%)	139 (91%)	13 (9%)	10	33
10	H	119/128 (93%)	114 (96%)	5 (4%)	26	50
11	I	110/116 (95%)	98 (89%)	12 (11%)	6	25
12	J	60/65 (92%)	55 (92%)	5 (8%)	10	34
13	K	97/102 (95%)	85 (88%)	12 (12%)	4	21
14	L	40/57 (70%)	37 (92%)	3 (8%)	12	38
All	All	3456/4009 (86%)	3144 (91%)	312 (9%)	9	32

All (312) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	2	VAL
3	A	11	LEU
3	A	32	VAL
3	A	37	PHE
3	A	38	PRO
3	A	41	MET
3	A	54	ASN
3	A	62	ASP
3	A	67	CYS
3	A	93	VAL
3	A	108	MET
3	A	131	SER
3	A	221	SER
3	A	236	LEU
3	A	245	PRO
3	A	250	ILE
3	A	261	ASP
3	A	270	LEU
3	A	289	ILE
3	A	293	GLU

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Mol	Chain	Res	Type
3	A	302	THR
3	A	312	PRO
3	A	324	SER
3	A	326	ARG
3	A	335	ARG
3	A	337	ARG
3	A	345	VAL
3	A	381	THR
3	A	385	ILE
3	A	406	ILE
3	A	407	ARG
3	A	408	ASP
3	A	425	GLN
3	A	434	ARG
3	A	442	VAL
3	A	443	LEU
3	A	445	ASN
3	A	450	LEU
3	A	460	VAL
3	A	461	LYS
3	A	462	VAL
3	A	470	LEU
3	A	472	LEU
3	A	493	GLN
3	A	504	LEU
3	A	512	VAL
3	A	515	GLN
3	A	518	LYS
3	A	524	VAL
3	A	560	ILE
3	A	562	THR
3	A	565	ILE
3	A	576	GLN
3	A	616	VAL
3	A	618	GLU
3	A	622	VAL
3	A	629	LEU
3	A	635	ARG
3	A	664	THR
3	A	666	ILE
3	A	685	GLU
3	A	741	ASN

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Mol	Chain	Res	Type
3	A	768	GLN
3	A	779	PHE
3	A	786	HIS
3	A	821	ARG
3	A	827	THR
3	A	831	THR
3	A	834	THR
3	A	858	ASN
3	A	886	ILE
3	A	890	ASP
3	A	907	THR
3	A	919	ILE
3	A	929	LEU
3	A	940	ARG
3	A	941	LYS
3	A	969	GLN
3	A	992	ASP
3	A	1001	ARG
3	A	1006	ILE
3	A	1029	ARG
3	A	1035	TYR
3	A	1052	GLN
3	A	1067	LEU
3	A	1116	LEU
3	A	1122	PRO
3	A	1138	ILE
3	A	1152	ILE
3	A	1170	ILE
3	A	1176	LEU
3	A	1177	LEU
3	A	1193	LEU
3	A	1206	ASP
3	A	1240	CYS
3	A	1245	PRO
3	A	1264	GLU
3	A	1271	ILE
3	A	1291	VAL
3	A	1295	THR
3	A	1297	GLU
3	A	1309	ASP
3	A	1325	THR
3	A	1329	THR

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Mol	Chain	Res	Type
3	A	1332	PHE
3	A	1333	ILE
3	A	1336	MET
3	A	1359	ASP
3	A	1371	LEU
3	A	1372	VAL
3	A	1378	GLN
3	A	1386	ARG
3	A	1389	PHE
3	A	1393	ASN
3	A	1394	THR
3	A	1405	THR
3	A	1424	VAL
3	A	1428	VAL
3	A	1436	ILE
3	A	1442	ASP
3	A	1443	VAL
3	A	1444	MET
3	A	1445	ILE
3	A	1447	GLU
4	B	57	TYR
4	B	100	PRO
4	B	106	ASP
4	B	178	ASN
4	B	203	PHE
4	B	205	ILE
4	B	217	ARG
4	B	225	VAL
4	B	250	PHE
4	B	258	LEU
4	B	268	THR
4	B	283	VAL
4	B	298	LEU
4	B	323	VAL
4	B	324	ILE
4	B	365	THR
4	B	371	GLU
4	B	378	LEU
4	B	393	LYS
4	B	396	ASP
4	B	401	PHE
4	B	404	LYS

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Mol	Chain	Res	Type
4	B	427	ASP
4	B	429	PHE
4	B	466	TRP
4	B	482	VAL
4	B	485	ARG
4	B	487	THR
4	B	496	ARG
4	B	498	THR
4	B	502	ILE
4	B	516	ASN
4	B	555	ILE
4	B	557	PHE
4	B	582	VAL
4	B	591	ARG
4	B	603	LEU
4	B	628	THR
4	B	644	GLU
4	B	682	SER
4	B	724	ASP
4	B	737	THR
4	B	742	GLU
4	B	748	ILE
4	B	780	VAL
4	B	787	VAL
4	B	790	ASP
4	B	791	THR
4	B	811	TYR
4	B	835	GLN
4	B	839	MET
4	B	878	GLN
4	B	901	PRO
4	B	909	ASP
4	B	939	THR
4	B	944	THR
4	B	986	GLN
4	B	999	MET
4	B	1002	THR
4	B	1006	ILE
4	B	1010	LEU
4	B	1034	VAL
4	B	1046	PRO
4	B	1047	PHE

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Mol	Chain	Res	Type
4	B	1069	PHE
4	B	1095	LEU
4	B	1096	ARG
4	B	1098	MET
4	B	1099	VAL
4	B	1103	ILE
4	B	1108	ARG
4	B	1123	SER
4	B	1159	ARG
4	B	1169	MET
4	B	1170	THR
4	B	1176	ASN
4	B	1183	LYS
4	B	1191	ILE
4	B	1202	LEU
4	B	1212	ILE
4	B	1216	LEU
4	B	1220	ARG
5	C	22	LEU
5	C	23	SER
5	C	56	THR
5	C	57	VAL
5	C	58	LEU
5	C	72	LEU
5	C	75	MET
5	C	77	ILE
5	C	119	VAL
5	C	129	ILE
5	C	147	LEU
5	C	156	THR
5	C	163	ILE
5	C	166	GLU
5	C	193	TYR
5	C	209	TYR
5	C	233	GLU
5	C	238	ILE
5	C	240	VAL
5	C	259	LEU
5	C	266	ASP
6	D	3	VAL
6	D	13	ARG
6	D	17	LYS

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Mol	Chain	Res	Type
6	D	22	GLU
6	D	47	LEU
6	D	63	LEU
6	D	70	PHE
6	D	126	ILE
6	D	137	ASN
6	D	139	LYS
6	D	148	LEU
6	D	149	THR
6	D	152	SER
6	D	156	ASP
6	D	170	THR
6	D	182	SER
6	D	192	LYS
6	D	193	THR
6	D	208	GLU
7	E	40	GLU
7	E	60	PHE
7	E	74	ASP
7	E	78	LEU
7	E	104	ASN
7	E	114	ASN
7	E	132	ILE
7	E	149	LEU
7	E	165	LEU
7	E	175	LEU
7	E	207	ARG
8	F	79	ARG
8	F	90	ARG
8	F	99	LEU
8	F	153	VAL
8	F	155	LEU
9	G	1	MET
9	G	13	LEU
9	G	17	PHE
9	G	51	TYR
9	G	52	ASP
9	G	64	THR
9	G	74	TYR
9	G	78	VAL
9	G	80	LYS
9	G	88	ASP

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Mol	Chain	Res	Type
9	G	115	MET
9	G	126	ASN
9	G	171	ILE
10	H	17	PRO
10	H	42	ILE
10	H	91	ASP
10	H	102	TYR
10	H	130	ARG
11	I	8	ARG
11	I	15	TYR
11	I	34	TYR
11	I	75	CYS
11	I	78	CYS
11	I	84	VAL
11	I	85	PHE
11	I	86	PHE
11	I	94	ASP
11	I	101	PHE
11	I	104	LEU
11	I	106	CYS
12	J	41	LEU
12	J	43	ARG
12	J	44	TYR
12	J	46	CYS
12	J	57	ILE
13	K	1	MET
13	K	5	ASP
13	K	10	PHE
13	K	25	THR
13	K	34	THR
13	K	42	LEU
13	K	47	ARG
13	K	50	LEU
13	K	61	TYR
13	K	107	THR
13	K	111	LEU
13	K	112	GLN
14	L	27	LEU
14	L	51	CYS
14	L	55	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (114) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	5	GLN
3	A	54	ASN
3	A	64	ASN
3	A	71	GLN
3	A	83	HIS
3	A	169	ASN
3	A	209	ASN
3	A	213	HIS
3	A	225	ASN
3	A	253	ASN
3	A	299	HIS
3	A	339	ASN
3	A	394	ASN
3	A	435	HIS
3	A	479	ASN
3	A	525	GLN
3	A	603	ASN
3	A	631	HIS
3	A	660	ASN
3	A	723	ASN
3	A	736	ASN
3	A	741	ASN
3	A	742	ASN
3	A	745	GLN
3	A	757	ASN
3	A	768	GLN
3	A	786	HIS
3	A	838	GLN
3	A	851	HIS
3	A	858	ASN
3	A	877	HIS
3	A	903	ASN
3	A	926	GLN
3	A	935	GLN
3	A	969	GLN
3	A	994	GLN
3	A	1009	ASN
3	A	1040	GLN
3	A	1070	GLN
3	A	1130	GLN
3	A	1140	HIS
3	A	1188	GLN
3	A	1211	GLN

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Mol	Chain	Res	Type
3	A	1218	GLN
3	A	1265	ASN
3	A	1364	ASN
3	A	1432	GLN
4	B	60	GLN
4	B	121	ASN
4	B	178	ASN
4	B	215	GLN
4	B	236	HIS
4	B	350	GLN
4	B	363	HIS
4	B	366	GLN
4	B	449	ASN
4	B	465	ASN
4	B	513	GLN
4	B	515	HIS
4	B	516	ASN
4	B	518	HIS
4	B	538	ASN
4	B	706	GLN
4	B	744	HIS
4	B	821	GLN
4	B	842	ASN
4	B	951	GLN
4	B	957	ASN
4	B	975	GLN
4	B	1015	HIS
4	B	1025	HIS
4	B	1065	GLN
4	B	1097	HIS
4	B	1117	GLN
4	B	1179	GLN
4	B	1193	GLN
5	C	7	GLN
5	C	24	ASN
5	C	73	GLN
5	C	112	ASN
5	C	151	GLN
5	C	167	HIS
5	C	231	ASN
6	D	39	ASN
6	D	40	HIS

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Mol	Chain	Res	Type
6	D	41	GLN
6	D	137	ASN
6	D	173	HIS
6	D	179	GLN
7	E	101	GLN
7	E	104	ASN
7	E	114	ASN
7	E	147	HIS
8	F	104	ASN
9	G	53	ASN
9	G	57	GLN
9	G	96	GLN
9	G	97	HIS
9	G	122	ASN
9	G	126	ASN
9	G	158	HIS
10	H	64	ASN
10	H	133	ASN
10	H	137	GLN
11	I	12	ASN
11	I	46	HIS
11	I	60	GLN
11	I	90	GLN
11	I	108	HIS
12	J	64	ASN
13	K	29	ASN
13	K	44	ASN
13	K	65	HIS
13	K	76	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	P	8/16 (50%)	1 (12%)	0
2	T	9/17 (52%)	5 (55%)	2 (22%)
All	All	17/33 (51%)	6 (35%)	2 (11%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	P	9	G

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Mol	Chain	Res	Type
2	T	11	G
2	T	12	G
2	T	13	U
2	T	14	C
2	T	15	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	T	12	G
2	T	13	U

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

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

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	C	1
4	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	2:SER	C	3:GLU	N	3.04
1	B	337:ARG	C	338:GLY	N	2.61

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	P	9/16 (56%)	2.46	4 (44%) 0 1	194, 200, 200, 200	0
2	T	10/17 (58%)	3.07	8 (80%) 0 0	180, 190, 200, 200	0
3	A	1422/1733 (82%)	-0.07	19 (1%) 75 53	56, 116, 175, 200	0
4	B	1112/1224 (90%)	0.09	29 (2%) 57 39	57, 126, 188, 200	0
5	C	267/318 (83%)	-0.12	1 (0%) 88 74	74, 110, 158, 180	0
6	D	178/221 (80%)	0.12	6 (3%) 48 33	87, 133, 184, 198	0
7	E	214/215 (99%)	0.24	2 (0%) 81 60	90, 159, 197, 200	0
8	F	88/155 (56%)	-0.39	0 100 100	65, 91, 129, 140	0
9	G	171/171 (100%)	-0.03	1 (0%) 85 68	88, 112, 155, 163	0
10	H	135/146 (92%)	0.67	11 (8%) 18 17	139, 166, 190, 200	0
11	I	116/122 (95%)	0.37	1 (0%) 81 60	114, 163, 191, 200	0
12	J	65/70 (92%)	-0.07	0 100 100	79, 108, 146, 153	0
13	K	112/120 (93%)	-0.27	0 100 100	81, 114, 139, 167	0
14	L	46/70 (65%)	0.62	3 (6%) 25 21	111, 166, 194, 196	0
All	All	3945/4598 (85%)	0.05	85 (2%) 62 44	56, 123, 187, 200	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	D	3	VAL	6.7
1	P	8	A	6.6
2	T	6	C	5.9
3	A	1081	LEU	5.2
6	D	25	ALA	4.7
1	P	16	C	4.5
3	A	3	GLY	4.2
6	D	24	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
10	H	140	ALA	4.2
10	H	76	THR	4.0
3	A	1254	ALA	4.0
2	T	15	A	4.0
3	A	69	THR	4.0
2	T	11	G	3.9
3	A	1257	ASP	3.9
10	H	139	ASN	3.7
10	H	136	LYS	3.6
4	B	882	THR	3.6
4	B	917	PRO	3.3
3	A	197	PRO	3.3
3	A	1245	PRO	3.3
3	A	292	ALA	3.2
4	B	715	ALA	3.2
2	T	9	C	3.2
10	H	119	GLY	3.2
3	A	2	VAL	3.1
10	H	65	LEU	3.1
2	T	12	G	3.1
2	T	14	C	3.1
4	B	734	HIS	3.0
3	A	56	PRO	2.9
4	B	710	LEU	2.9
4	B	883	LEU	2.9
11	I	2	THR	2.8
3	A	760	GLN	2.8
10	H	86	ASP	2.8
4	B	934	LYS	2.8
3	A	51	GLY	2.8
4	B	933	SER	2.7
4	B	478	GLY	2.7
10	H	135	LEU	2.7
4	B	641	GLU	2.7
6	D	13	ARG	2.6
4	B	468	GLU	2.6
1	P	9	G	2.6
4	B	729	ILE	2.6
4	B	101	MET	2.6
4	B	577	ALA	2.5
14	L	25	ALA	2.4
4	B	601	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
4	B	70	ILE	2.4
2	T	10	U	2.4
4	B	730	ARG	2.4
10	H	137	GLN	2.4
4	B	615	MET	2.4
2	T	13	U	2.3
3	A	36	ARG	2.3
7	E	88	VAL	2.3
6	D	16	LYS	2.3
9	G	21	ARG	2.3
1	P	14	G	2.3
4	B	110	HIS	2.3
14	L	27	LEU	2.3
3	A	587	HIS	2.2
3	A	50	ILE	2.2
4	B	252	SER	2.2
6	D	4	SER	2.2
14	L	26	THR	2.2
4	B	251	ILE	2.2
4	B	471	LYS	2.2
10	H	90	ALA	2.2
5	C	2	SER	2.2
3	A	1187	GLN	2.1
3	A	250	ILE	2.1
4	B	880	THR	2.1
3	A	253	ASN	2.1
4	B	870	ILE	2.1
4	B	723	VAL	2.1
4	B	769	TYR	2.1
4	B	476	ARG	2.1
4	B	733	HIS	2.1
4	B	605	ARG	2.1
3	A	171	GLN	2.0
10	H	116	TYR	2.0
7	E	83	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	ZN	I	204	1/1	0.97	0.07	181,181,181,181	0
15	ZN	A	1506	1/1	0.99	0.04	121,121,121,121	0
15	ZN	L	105	1/1	0.99	0.06	155,155,155,155	0
16	MG	A	1	1/1	0.99	0.06	79,79,79,79	0
15	ZN	I	203	1/1	1.00	0.08	120,120,120,120	0
15	ZN	A	1508	1/1	1.00	0.05	83,83,83,83	0
15	ZN	J	101	1/1	1.00	0.03	100,100,100,100	0
15	ZN	B	1307	1/1	1.00	0.07	83,83,83,83	0
15	ZN	C	302	1/1	1.00	0.05	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.