



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:06 AM EDT

PDB ID : 2JA8 / pdb_00002ja8
Title : CPD lesion containing RNA Polymerase II elongation complex D
Authors : Brueckner, F.; Hennecke, U.; Carell, T.; Cramer, P.
Deposited on : 2006-11-23
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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

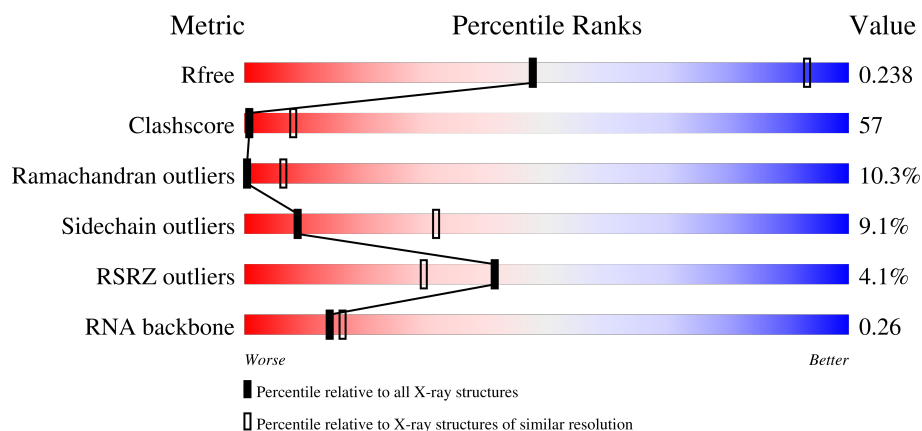
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	A	1733	
2	B	1224	
3	C	318	
4	D	221	

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	14	
14	P	11	
15	T	25	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	TT	T	19	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32000 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE II LARGEST SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1421	Total	C	N	O	S	0	0	0
			11186	7048	1958	2118	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II 140 KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1115	Total	C	N	O	S	0	0	0
			8866	5614	1553	1644	55			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KDA POLYPEPTIDE.

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

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 32KDA POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	177	Total	C	N	O	S	0	0	0
			1427	882	256	287	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 27 KDA POLYPEPTIDE.

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

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 23

KDA POLYPEPTIDE.

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

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE.

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

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE.

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

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9.

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

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10.

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

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE.

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

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	8	Total	C	N	O	P	0	0	0
			161	79	29	46	7			

- Molecule 14 is a RNA chain called 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*AP*UP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	10	Total	C	N	O	P	0	0	0
			209	95	38	67	9			

- Molecule 15 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*TP*TP*TTP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	19	Total	Br	C	N	O	P	0	0
			401	1	197	61	124	18		

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

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

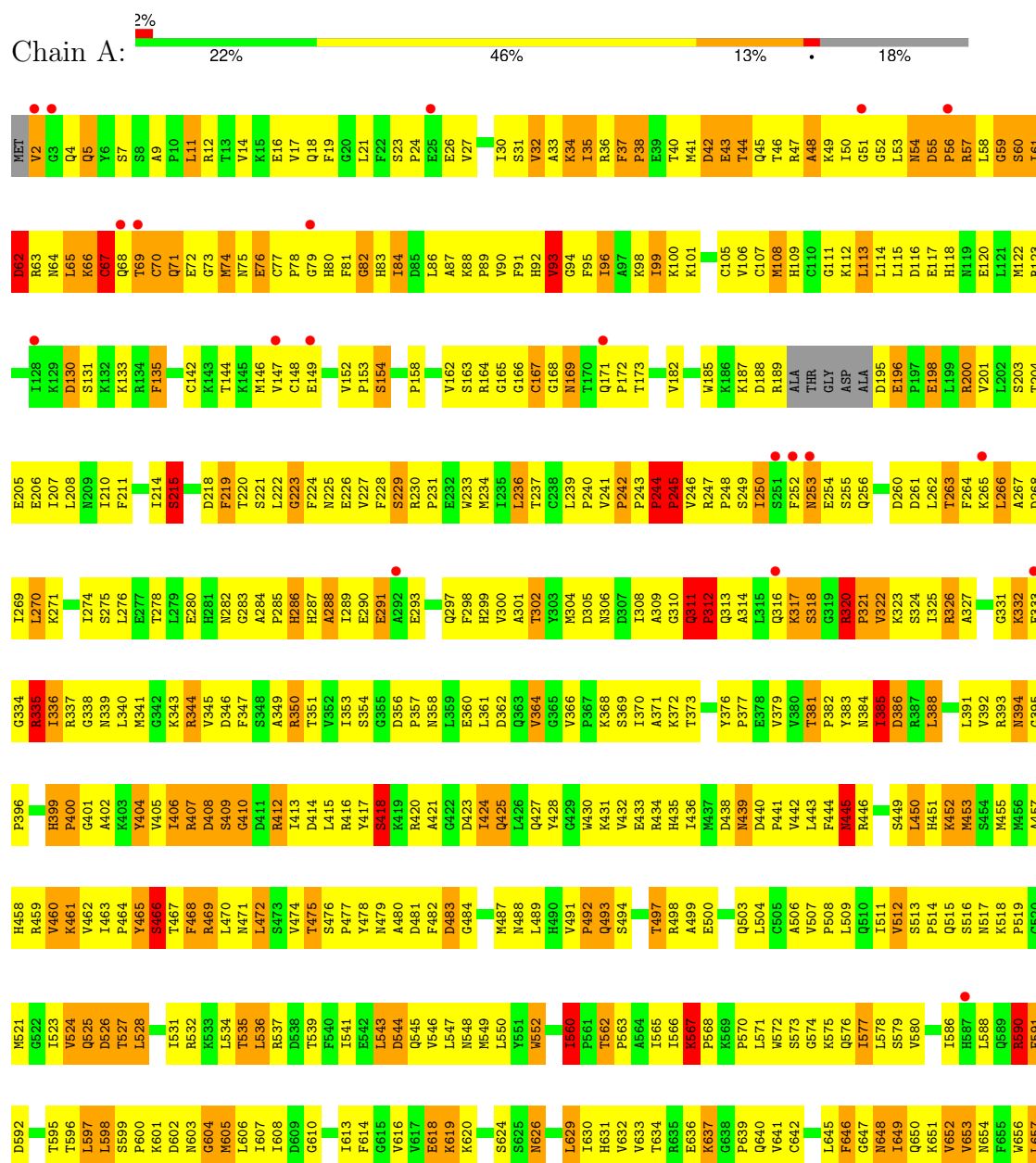
- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	8	Total	Zn	0	0
			8	8		

3 Residue-property plots

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

• Molecule 1: DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT

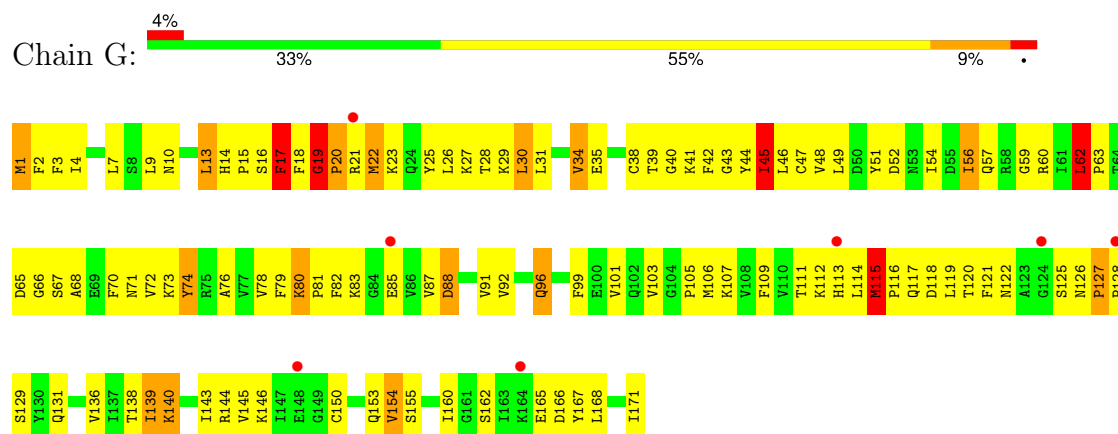




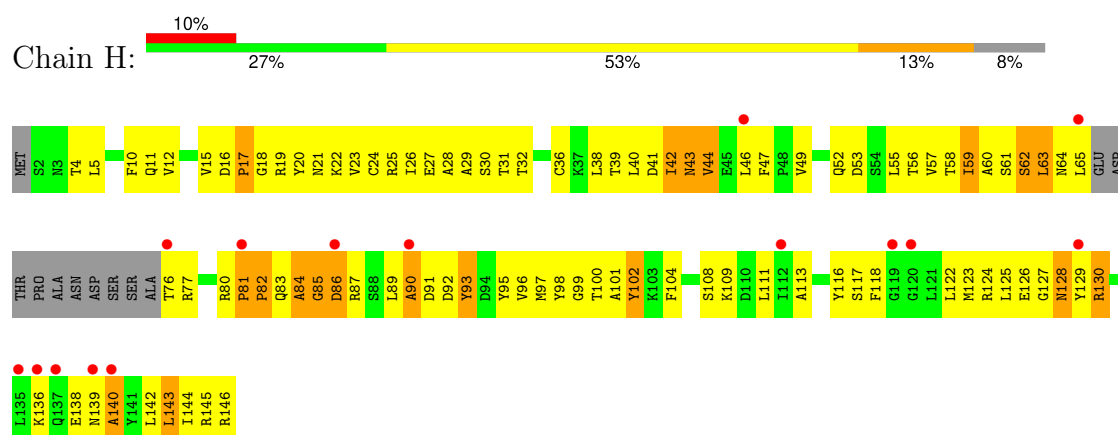
Chain D:



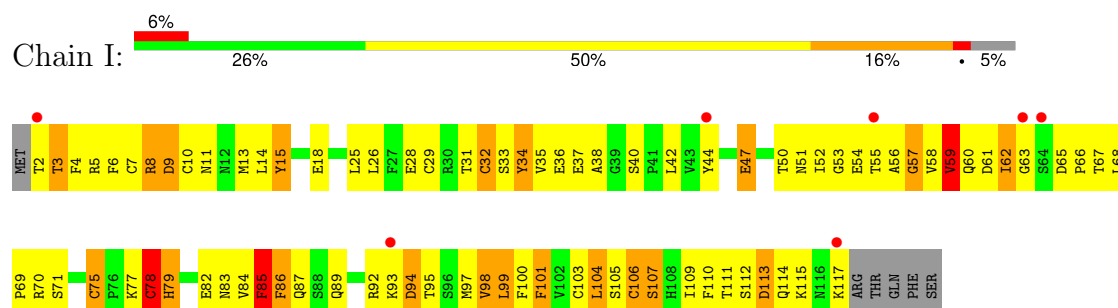
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II 19KDA POLYPEPTIDE



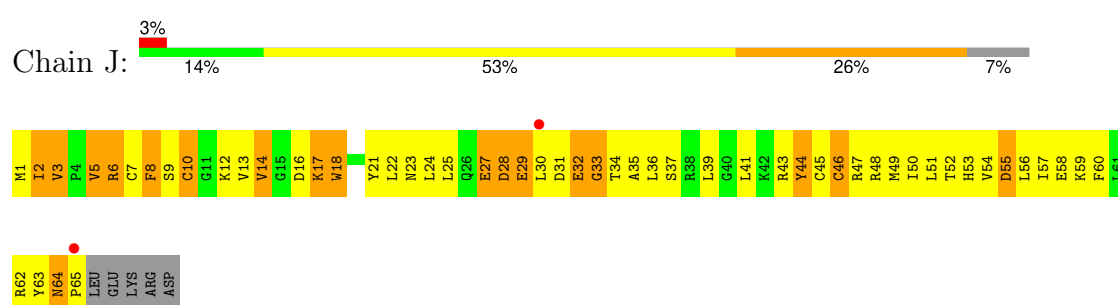
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III 14.5 KDA POLYPEPTIDE



• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT 9



• Molecule 10: DNA-DIRECTED RNA POLYMERASES I/II/III SUBUNIT 10



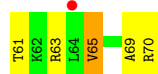
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II 13.6 KDA POLYPEPTIDE

Chain K: 

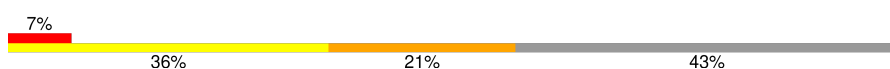


• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III 7.7 KDA POLYPEPTIDE

Chain L: 



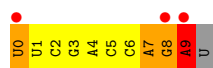
• Molecule 13: 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP *AP*GP*CP*T)-3'

Chain N: 



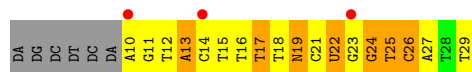
• Molecule 14: 5'-R(*UP*UP*CP*GP*AP*CP*CP*AP*GP*AP*UP)-3'

Chain P: 



• Molecule 15: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP *CP*TP*TP*TP*TP*TTP*CP *BRUP*GP*GP*TP*CP*AP*TP*T)-3'

Chain T: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.64Å 392.85Å 282.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 50.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-3.80) 99.1 (50.00-3.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 3.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.269 , 0.288 0.208 , 0.238	Depositor DCC
R_{free} test set	4685 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	110.0	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 81.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.015 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.023 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32000	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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: TT, ZN, MG, BRU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	0/11385	1.11	81/15393 (0.5%)
2	B	0.54	0/9037	1.06	59/12181 (0.5%)
3	C	0.60	0/2138	1.11	14/2896 (0.5%)
4	D	0.48	0/1437	1.09	12/1925 (0.6%)
5	E	0.49	0/1788	0.99	15/2406 (0.6%)
6	F	0.66	0/716	1.13	7/964 (0.7%)
7	G	0.57	0/1368	1.13	14/1844 (0.8%)
8	H	0.47	0/1102	1.04	8/1492 (0.5%)
9	I	0.45	0/962	1.07	8/1295 (0.6%)
10	J	0.58	0/541	1.04	2/727 (0.3%)
11	K	0.92	7/937 (0.7%)	1.32	12/1265 (0.9%)
12	L	0.51	0/366	0.91	0/485
13	N	0.63	0/180	1.17	3/276 (1.1%)
14	P	0.60	0/233	1.27	2/361 (0.6%)
15	T	0.61	0/380	1.29	6/580 (1.0%)
All	All	0.57	7/32570 (0.0%)	1.09	243/44090 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
15	T	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	113	THR	CA-C	11.90	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	113	THR	N-CA	8.38	1.58	1.46
11	K	112	GLN	CA-C	7.96	1.63	1.52
11	K	111	LEU	CA-C	6.71	1.61	1.52
11	K	112	GLN	N-CA	5.67	1.53	1.46
11	K	114	LEU	N-CA	5.43	1.56	1.46
11	K	112	GLN	C-N	5.06	1.39	1.33

All (243) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	113	THR	N-CA-C	21.65	136.81	108.24
1	A	242	PRO	CA-C-N	14.82	130.33	119.66
1	A	242	PRO	C-N-CA	14.82	130.33	119.66
2	B	1185	CYS	N-CA-C	-13.11	97.34	113.20
2	B	473	MET	N-CA-C	-11.45	98.97	113.16
4	D	26	THR	N-CA-C	-11.21	97.84	112.41
4	D	72	ARG	N-CA-C	-10.54	99.87	111.36
2	B	427	ASP	N-CA-C	-10.43	101.11	114.04
1	A	452	LYS	N-CA-C	-10.38	99.96	111.07
7	G	52	ASP	N-CA-C	10.04	122.31	111.36
3	C	41	ILE	CA-C-N	9.14	129.22	119.90
3	C	41	ILE	C-N-CA	9.14	129.22	119.90
2	B	111	ALA	N-CA-C	-8.65	95.21	108.96
1	A	288	ALA	N-CA-C	-8.64	100.76	112.94
1	A	266	LEU	N-CA-C	-8.45	102.01	111.14
2	B	296	GLU	N-CA-C	-8.22	102.69	112.89
11	K	111	LEU	N-CA-C	8.11	128.07	110.80
11	K	113	THR	CA-C-N	8.09	136.26	121.70
11	K	113	THR	C-N-CA	8.09	136.26	121.70
1	A	60	SER	N-CA-C	8.00	119.11	108.07
8	H	80	ARG	CA-C-N	7.92	128.54	120.38
8	H	80	ARG	C-N-CA	7.92	128.54	120.38
2	B	1009	ASP	N-CA-C	-7.88	104.18	113.88
7	G	62	LEU	CA-C-N	-7.84	110.04	119.84
7	G	62	LEU	C-N-CA	-7.84	110.04	119.84
3	C	38	ILE	N-CA-C	7.77	118.31	110.23
4	D	54	GLU	N-CA-C	-7.74	102.76	112.90
2	B	363	HIS	N-CA-C	-7.68	100.62	110.53
13	N	0	DT	O5'-C5'-C4'	7.65	122.28	110.80
1	A	1243	VAL	N-CA-C	7.59	119.27	108.42
1	A	344	ARG	N-CA-C	-7.54	98.34	110.32
1	A	861	GLY	N-CA-C	-7.53	104.65	115.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	173	ALA	N-CA-C	7.50	119.10	111.07
14	P	9	A	C2'-C3'-O3'	7.48	124.92	113.70
1	A	291	GLU	N-CA-C	-7.41	104.09	113.72
1	A	360	GLU	N-CA-C	-7.37	101.03	110.53
6	F	127	GLU	N-CA-C	-7.29	104.27	113.02
7	G	2	PHE	N-CA-C	-7.28	99.71	110.48
1	A	1261	LYS	N-CA-C	-7.27	105.32	114.56
7	G	22	MET	N-CA-C	-7.19	100.56	111.56
1	A	293	GLU	N-CA-C	-7.13	104.73	113.50
2	B	292	ILE	N-CA-C	7.09	121.53	112.67
4	D	38	ILE	N-CA-C	7.09	118.09	108.17
2	B	66	ASP	N-CA-C	-7.08	103.74	112.88
2	B	681	TRP	N-CA-C	-7.01	102.19	111.24
1	A	598	LEU	N-CA-C	-6.97	103.45	113.21
7	G	19	GLY	CA-C-N	6.94	128.51	119.84
7	G	19	GLY	C-N-CA	6.94	128.51	119.84
1	A	928	LEU	N-CA-C	-6.94	103.65	111.14
7	G	127	PRO	CA-C-N	6.93	126.97	119.90
7	G	127	PRO	C-N-CA	6.93	126.97	119.90
1	A	682	THR	N-CA-C	-6.90	104.84	113.18
5	E	173	SER	N-CA-C	6.85	118.83	111.36
2	B	472	ALA	N-CA-C	6.85	119.64	108.55
8	H	85	GLY	N-CA-C	-6.85	104.27	113.24
1	A	567	LYS	CA-C-N	-6.76	111.39	119.84
1	A	567	LYS	C-N-CA	-6.76	111.39	119.84
5	E	4	GLU	N-CA-C	6.75	118.29	111.07
2	B	292	ILE	CB-CA-C	-6.74	107.30	113.70
2	B	896	ASP	N-CA-C	-6.73	105.18	113.19
8	H	12	VAL	N-CA-C	6.72	117.13	108.12
1	A	513	SER	CA-C-N	6.72	126.35	119.56
1	A	513	SER	C-N-CA	6.72	126.35	119.56
15	T	29	DT	C4'-C3'-O3'	6.72	120.07	110.00
11	K	18	LYS	N-CA-C	-6.68	104.00	111.28
2	B	99	LYS	CA-C-N	6.64	128.14	119.84
2	B	99	LYS	C-N-CA	6.64	128.14	119.84
1	A	1422	ARG	N-CA-C	-6.62	104.92	114.12
2	B	1201	LYS	N-CA-C	-6.60	102.96	111.02
1	A	320	ARG	CA-C-N	6.60	128.09	119.84
1	A	320	ARG	C-N-CA	6.60	128.09	119.84
1	A	425	GLN	N-CA-C	-6.59	98.16	108.90
4	D	188	ALA	N-CA-C	-6.59	104.50	112.54
2	B	468	GLU	CB-CA-C	-6.57	107.14	116.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	171	LYS	N-CA-C	-6.51	99.59	109.95
9	I	85	PHE	N-CA-C	6.50	120.02	110.59
2	B	1142	GLY	N-CA-C	-6.46	106.77	115.36
3	C	39	ALA	N-CA-C	6.44	123.07	114.12
1	A	729	ALA	N-CA-C	-6.37	104.26	111.14
2	B	112	LEU	N-CA-C	6.35	120.63	109.96
1	A	698	GLN	N-CA-C	-6.35	105.82	112.93
1	A	539	THR	N-CA-C	6.34	119.04	108.96
15	T	17	DT	C4'-C3'-O3'	6.33	119.50	110.00
1	A	982	THR	N-CA-C	-6.32	100.27	110.32
2	B	1045	SER	CA-C-N	6.29	127.70	119.84
2	B	1045	SER	C-N-CA	6.29	127.70	119.84
2	B	361	LEU	CA-C-N	6.28	127.68	119.84
2	B	361	LEU	C-N-CA	6.28	127.68	119.84
1	A	1262	LYS	N-CA-C	-6.23	104.38	112.23
1	A	466	SER	N-CA-C	6.21	124.02	110.80
2	B	771	SER	N-CA-C	-6.20	104.28	112.72
9	I	32	CYS	N-CA-C	-6.20	102.80	108.75
5	E	63	ASN	CA-C-N	6.17	126.50	119.83
5	E	63	ASN	C-N-CA	6.17	126.50	119.83
5	E	149	LEU	N-CA-C	6.17	117.81	111.14
1	A	560	ILE	CA-C-N	6.16	126.10	119.76
1	A	560	ILE	C-N-CA	6.16	126.10	119.76
15	T	24	DG	C2'-C3'-O3'	-6.15	102.27	111.50
1	A	1376	THR	N-CA-C	6.14	120.62	111.96
2	B	1129	ARG	N-CA-C	6.11	118.36	108.34
13	N	7	DT	C4'-C3'-O3'	6.10	119.15	110.00
8	H	109	LYS	CB-CA-C	-6.09	109.53	116.54
3	C	96	SER	N-CA-C	6.09	118.03	108.96
1	A	1138	ILE	CB-CA-C	-6.05	106.56	111.71
4	D	16	LYS	N-CA-C	6.04	119.00	109.39
7	G	65	ASP	N-CA-C	-6.04	99.87	109.23
1	A	311	GLN	N-CA-C	6.04	123.16	109.81
1	A	227	VAL	N-CA-C	6.03	117.00	111.81
3	C	193	TYR	N-CA-C	6.03	117.36	108.86
1	A	983	ILE	N-CA-C	-6.03	103.60	112.04
2	B	805	THR	N-CA-C	6.03	117.36	108.86
2	B	628	THR	N-CA-C	-6.02	105.66	114.39
2	B	851	PHE	N-CA-C	6.00	119.91	112.47
1	A	82	GLY	N-CA-C	-5.99	102.92	111.42
11	K	84	LYS	N-CA-C	-5.99	103.93	111.11
2	B	1173	ALA	N-CA-C	5.98	117.94	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	864	ILE	N-CA-C	-5.95	107.01	112.96
1	A	1275	GLY	N-CA-C	5.95	120.50	112.17
7	G	129	SER	N-CA-C	5.95	117.25	108.86
1	A	1113	THR	CA-C-N	-5.94	112.41	119.84
1	A	1113	THR	C-N-CA	-5.94	112.41	119.84
1	A	436	ILE	N-CA-C	-5.92	101.94	109.58
7	G	30	LEU	N-CA-C	-5.89	103.84	111.02
1	A	56	PRO	N-CA-C	-5.89	100.34	112.47
2	B	555	ILE	N-CA-C	-5.88	105.98	111.45
1	A	173	THR	N-CA-C	-5.88	102.77	110.53
2	B	872	GLU	N-CA-C	-5.87	102.96	110.53
6	F	77	ASP	N-CA-C	-5.87	101.78	110.46
2	B	606	LYS	N-CA-C	-5.85	105.15	112.93
9	I	18	GLU	N-CA-C	5.82	118.38	108.90
1	A	468	PHE	N-CA-C	-5.75	101.14	109.59
1	A	1291	VAL	CA-C-N	5.75	127.02	119.84
1	A	1291	VAL	C-N-CA	5.75	127.02	119.84
1	A	1343	ALA	N-CA-C	-5.72	105.18	111.82
1	A	467	THR	N-CA-C	5.72	118.54	109.50
11	K	114	LEU	N-CA-C	5.72	127.00	111.00
2	B	213	ILE	N-CA-C	5.71	117.22	108.71
2	B	395	GLN	N-CA-C	-5.69	102.48	110.50
11	K	112	GLN	N-CA-C	5.68	122.90	110.80
2	B	1223	ASP	CB-CA-C	-5.68	109.03	115.79
1	A	1311	VAL	N-CA-C	5.67	117.00	107.18
5	E	177	ARG	N-CA-C	5.67	118.80	109.72
2	B	424	LEU	N-CA-C	-5.67	104.72	111.69
1	A	491	VAL	N-CA-C	5.64	114.16	107.73
1	A	158	PRO	N-CA-C	-5.63	107.10	114.03
1	A	646	PHE	N-CA-C	-5.62	104.17	111.02
1	A	229	SER	N-CA-C	5.61	116.58	107.32
2	B	837	ASP	N-CA-C	5.61	119.58	111.56
9	I	104	LEU	N-CA-C	-5.61	106.40	113.18
1	A	236	LEU	N-CA-C	5.58	117.79	109.25
8	H	63	LEU	N-CA-C	-5.56	105.64	113.20
2	B	192	LEU	N-CA-C	-5.55	106.50	113.72
2	B	535	LEU	N-CA-C	-5.55	104.74	112.45
1	A	67	CYS	N-CA-C	-5.54	99.00	110.80
1	A	227	VAL	CB-CA-C	-5.54	105.18	111.55
11	K	113	THR	CB-CA-C	-5.54	100.71	112.78
15	T	26	DC	C2'-C3'-O3'	-5.53	103.20	111.50
9	I	65	ASP	CA-C-N	5.53	125.19	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	65	ASP	C-N-CA	5.53	125.19	119.05
5	E	55	ARG	N-CA-C	5.51	117.09	111.14
10	J	3	VAL	CB-CA-C	-5.51	105.48	110.88
2	B	543	SER	N-CA-C	5.49	117.38	110.24
1	A	1064	VAL	N-CA-C	5.49	118.75	111.17
14	P	0	U	O5'-C5'-C4'	5.49	119.74	111.50
4	D	171	GLY	N-CA-C	-5.47	108.30	115.47
13	N	3	DG	C2'-C3'-O3'	5.46	119.69	111.50
1	A	244	PRO	N-CA-C	5.45	117.35	110.70
1	A	453	MET	N-CA-C	5.45	119.03	112.38
1	A	938	LYS	N-CA-C	-5.44	104.58	111.11
2	B	1172	ILE	N-CA-C	5.43	112.02	106.21
5	E	84	ASP	N-CA-C	-5.43	106.69	113.15
1	A	1403	GLU	N-CA-C	5.39	122.28	110.80
5	E	150	VAL	CA-C-N	5.36	125.56	120.31
5	E	150	VAL	C-N-CA	5.36	125.56	120.31
2	B	840	ILE	CB-CA-C	-5.35	103.65	110.98
1	A	1445	ILE	CB-CA-C	-5.33	104.48	111.25
1	A	590	ARG	N-CA-C	5.32	117.27	108.48
2	B	616	ILE	N-CA-C	5.32	115.51	107.75
5	E	6	GLU	N-CA-C	-5.31	105.16	111.69
4	D	66	ARG	N-CA-C	-5.31	104.40	112.04
7	G	45	ILE	N-CA-C	-5.29	100.96	108.58
9	I	68	LEU	CA-C-N	5.29	126.43	120.66
9	I	68	LEU	C-N-CA	5.29	126.43	120.66
2	B	574	SER	CA-C-N	5.28	126.44	119.84
2	B	574	SER	C-N-CA	5.28	126.44	119.84
2	B	545	ILE	N-CA-C	5.27	115.49	108.11
1	A	215	SER	N-CA-C	5.27	117.33	110.43
2	B	165	VAL	N-CA-C	5.25	116.04	108.48
2	B	208	SER	N-CA-C	5.25	118.28	110.52
2	B	413	LEU	N-CA-C	-5.25	105.56	111.28
15	T	25	DT	N1-C1'-C2'	5.24	121.36	113.50
1	A	552	TRP	N-CA-C	5.24	117.07	111.36
1	A	750	GLY	N-CA-C	-5.24	107.57	115.32
2	B	903	VAL	N-CA-C	5.23	120.22	109.34
10	J	5	VAL	N-CA-C	-5.23	101.99	108.89
3	C	91	HIS	N-CA-C	5.22	116.37	108.07
1	A	637	LYS	N-CA-C	5.22	116.65	111.07
2	B	964	VAL	N-CA-C	5.21	115.78	108.17
6	F	108	PHE	N-CA-C	5.21	118.76	112.93
8	H	129	TYR	N-CA-C	5.20	119.59	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	65	HIS	CA-C-N	5.18	126.32	119.84
11	K	65	HIS	C-N-CA	5.18	126.32	119.84
4	D	176	GLU	N-CA-C	-5.18	105.55	111.14
1	A	424	ILE	N-CA-C	5.17	120.09	109.34
2	B	392	ARG	N-CA-C	-5.15	107.66	114.04
4	D	169	SER	N-CA-C	-5.14	105.89	113.61
2	B	1104	HIS	N-CA-C	5.14	116.74	108.32
1	A	445	ASN	N-CA-C	5.13	116.32	108.52
3	C	200	GLU	N-CA-C	5.12	117.75	111.82
11	K	77	THR	N-CA-C	5.11	116.76	109.14
8	H	16	ASP	N-CA-C	5.11	118.39	107.91
1	A	237	THR	N-CA-C	-5.11	107.11	113.55
1	A	472	LEU	N-CA-C	5.11	116.70	111.03
4	D	15	LEU	N-CA-C	5.10	121.67	110.80
6	F	74	ILE	CA-C-N	5.10	125.03	119.78
6	F	74	ILE	C-N-CA	5.10	125.03	119.78
2	B	1099	VAL	N-CA-C	5.10	115.53	110.23
1	A	683	ILE	N-CA-C	-5.09	106.71	111.45
6	F	82	THR	CA-C-N	5.08	124.69	119.56
6	F	82	THR	C-N-CA	5.08	124.69	119.56
2	B	1078	GLY	N-CA-C	-5.07	108.12	115.27
1	A	1399	ARG	N-CA-C	-5.07	105.88	111.71
1	A	950	GLY	N-CA-C	-5.06	109.05	115.08
4	D	178	ALA	N-CA-C	-5.05	105.35	112.12
1	A	1010	ALA	N-CA-C	-5.05	105.85	111.36
2	B	570	VAL	CA-C-N	5.05	126.15	119.84
2	B	570	VAL	C-N-CA	5.05	126.15	119.84
3	C	5	GLY	CA-C-N	5.04	126.15	119.84
3	C	5	GLY	C-N-CA	5.04	126.15	119.84
2	B	773	MET	N-CA-C	-5.04	106.64	112.89
5	E	111	VAL	N-CA-C	5.04	114.54	106.88
3	C	201	TRP	CA-C-N	5.02	125.02	119.90
3	C	201	TRP	C-N-CA	5.02	125.02	119.90
5	E	52	ARG	CA-C-N	5.02	124.78	119.76
5	E	52	ARG	C-N-CA	5.02	124.78	119.76
1	A	440	ASP	N-CA-C	-5.01	99.52	109.10
7	G	56	ILE	CB-CA-C	-5.01	106.65	111.06
15	T	25	DT	C2'-C3'-O3'	-5.01	103.98	111.50
3	C	258	ILE	N-CA-C	-5.01	105.96	110.82
1	A	991	LYS	N-CA-C	-5.01	105.90	111.36
2	B	949	VAL	N-CA-C	-5.00	102.58	110.09
1	A	776	ALA	N-CA-C	5.00	117.79	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1299	VAL	N-CA-C	5.00	117.20	108.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	486	TYR	Sidechain
15	T	13	DA	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11186	0	11266	1404	0
2	B	8866	0	8898	1080	0
3	C	2101	0	2055	281	0
4	D	1427	0	1451	151	0
5	E	1752	0	1776	152	0
6	F	705	0	730	94	0
7	G	1340	0	1357	183	0
8	H	1084	0	1057	134	0
9	I	944	0	900	119	0
10	J	532	0	542	102	0
11	K	919	0	929	115	0
12	L	364	0	386	50	0
13	N	161	0	93	17	0
14	P	209	0	109	28	0
15	T	401	0	231	64	0
16	A	1	0	0	0	0
17	A	8	0	0	0	0
All	All	32000	0	31780	3662	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 57.

All (3662) 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)
1:A:53:LEU:HD23	1:A:54:ASN:N	1.61	1.13
1:A:855:THR:HG21	1:A:857:ARG:HE	1.10	1.11
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.34	1.10
7:G:14:HIS:CD2	7:G:16:SER:HB2	1.87	1.10
15:T:19:TT:H5R1	15:T:19:TT:C1'	1.83	1.09
1:A:1445:ILE:H	1:A:1445:ILE:HD12	1.16	1.09
15:T:17:DT:H2''	15:T:18:DT:H5'	1.32	1.08
2:B:343:ILE:HG23	2:B:347:LYS:HB2	1.16	1.08
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.36	1.08
15:T:19:TT:H5R1	15:T:19:TT:H1'	1.23	1.07
2:B:336:ARG:HG2	2:B:348:ARG:HD3	1.31	1.07
7:G:138:THR:HG22	7:G:139:ILE:H	1.20	1.07
15:T:17:DT:C2'	15:T:18:DT:H5'	1.83	1.06
1:A:34:LYS:HD3	1:A:57:ARG:HH22	0.92	1.04
11:K:111:LEU:C	11:K:112:GLN:HG2	1.76	1.04
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.17	1.03
1:A:40:THR:HG22	1:A:41:MET:HG3	1.39	1.03
2:B:882:THR:HG22	2:B:884:ARG:H	1.20	1.03
4:D:40:HIS:HB3	7:G:73:LYS:HZ3	1.23	1.02
1:A:913:LEU:HD12	1:A:914:GLU:H	1.24	1.02
1:A:58:LEU:HD12	1:A:59:GLY:H	1.23	1.01
1:A:53:LEU:HD23	1:A:54:ASN:H	0.84	1.01
2:B:589:VAL:HG12	2:B:590:HIS:H	1.24	1.01
1:A:1402:PHE:CE1	1:A:1403:GLU:HG3	1.94	1.01
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.42	1.01
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.96	1.00
3:C:166:GLU:HG3	11:K:10:PHE:HZ	1.27	1.00
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.38	1.00
1:A:34:LYS:HD3	1:A:57:ARG:NH2	1.77	1.00
1:A:1017:LEU:HB2	5:E:206:GLY:H	1.25	0.99
1:A:567:LYS:CG	1:A:568:PRO:HD2	1.91	0.98
1:A:53:LEU:CD2	1:A:54:ASN:H	1.74	0.98
2:B:65:GLU:HG3	2:B:66:ASP:H	1.27	0.98
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.43	0.98
3:C:43:THR:HG22	3:C:44:LEU:H	1.29	0.97
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.45	0.97
2:B:214:ALA:HB3	2:B:498:THR:HA	1.46	0.97
2:B:510:LYS:CG	2:B:511:PRO:HD3	1.94	0.96
10:J:1:MET:N	10:J:57:ILE:H	1.63	0.96
2:B:1187:ASN:O	2:B:1188:LYS:HB2	1.65	0.96
2:B:806:THR:HG22	2:B:808:ALA:H	1.29	0.96
1:A:709:THR:HG23	9:I:94:ASP:HA	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ARG:HH21	1:A:620:LYS:HB3	1.31	0.96
1:A:590:ARG:NH2	1:A:620:LYS:HB3	1.80	0.96
15:T:19:TT:H1'	15:T:19:TT:C5R	1.96	0.96
1:A:225:ASN:HD22	1:A:228:PHE:H	1.03	0.95
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.47	0.95
15:T:18:DT:C2'	15:T:19:TT:H5'1	1.94	0.95
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.06	0.95
2:B:516:ASN:HD22	2:B:516:ASN:N	1.64	0.94
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.48	0.94
4:D:144:THR:O	4:D:148:LEU:HB2	1.67	0.94
1:A:567:LYS:HB3	8:H:96:VAL:H	1.33	0.94
2:B:199:MET:HE2	2:B:492:LEU:HD23	1.49	0.94
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.28	0.94
2:B:502:ILE:H	2:B:502:ILE:HD12	1.31	0.94
9:I:8:ARG:HG3	9:I:34:TYR:HE1	1.30	0.94
10:J:1:MET:H1	10:J:57:ILE:N	1.65	0.94
15:T:17:DT:H2''	15:T:18:DT:C5'	1.97	0.94
1:A:34:LYS:HE3	1:A:57:ARG:HH12	1.30	0.94
2:B:168:GLY:H	2:B:450:ALA:HB1	1.32	0.94
11:K:110:ASN:O	11:K:111:LEU:HD23	1.68	0.94
2:B:486:TYR:OH	2:B:1096:ARG:HB3	1.66	0.93
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	1.65	0.93
15:T:19:TT:H5M1	15:T:21:DC:C5	2.03	0.93
1:A:58:LEU:HD21	1:A:243:PRO:HA	1.47	0.93
11:K:65:HIS:HD2	11:K:67:PHE:H	1.10	0.93
1:A:58:LEU:CD1	1:A:59:GLY:H	1.82	0.93
1:A:34:LYS:CD	1:A:57:ARG:HH22	1.82	0.93
1:A:754:SER:H	1:A:757:ASN:HD22	1.11	0.93
2:B:336:ARG:HH22	2:B:345:LYS:HE2	1.33	0.92
15:T:17:DT:C1'	15:T:18:DT:H5'	1.99	0.92
2:B:232:SER:HB3	2:B:261:ARG:HH21	1.32	0.92
3:C:66:ARG:NH1	10:J:2:ILE:HG21	1.82	0.92
3:C:6:PRO:HB3	3:C:25:VAL:HG12	1.50	0.92
1:A:524:VAL:HG12	1:A:525:GLN:H	1.32	0.92
3:C:6:PRO:HB3	3:C:25:VAL:CG1	1.99	0.92
1:A:254:GLU:HB2	2:B:935:ARG:HH12	1.34	0.92
2:B:515:HIS:H	2:B:518:HIS:HD2	1.16	0.92
6:F:111:LEU:HD12	6:F:111:LEU:H	1.35	0.91
1:A:115:LEU:HB2	1:A:122:MET:HE2	1.53	0.91
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.05	0.91
14:P:5:C:H2'	14:P:6:C:O4'	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.04	0.91
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.51	0.91
8:H:4:THR:HA	8:H:60:ALA:HB2	1.53	0.91
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.53	0.91
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.53	0.91
9:I:85:PHE:H	9:I:85:PHE:HD2	1.18	0.91
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.36	0.91
4:D:40:HIS:HB3	7:G:73:LYS:NZ	1.84	0.90
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.53	0.90
8:H:100:THR:HG23	8:H:138:GLU:HA	1.49	0.90
1:A:382:PRO:HB3	1:A:428:TYR:HE2	1.34	0.90
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.52	0.90
15:T:22:BRU:H2'	15:T:23:DG:C8	2.07	0.90
1:A:1094:VAL:HG12	1:A:1095:THR:H	1.34	0.90
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.53	0.90
1:A:855:THR:HG21	1:A:857:ARG:NE	1.86	0.90
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.02	0.89
2:B:549:THR:HG22	2:B:550:ASP:H	1.36	0.89
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.08	0.89
15:T:17:DT:H1'	15:T:18:DT:H5'	1.53	0.89
15:T:19:TT:H2R2	15:T:19:TT:H2'1	1.55	0.89
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.38	0.89
15:T:19:TT:H5R1	15:T:19:TT:C2'	2.02	0.88
15:T:15:DT:H1'	15:T:16:DT:H5'	1.53	0.88
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.56	0.88
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.03	0.88
1:A:901:LEU:H	1:A:926:GLN:NE2	1.71	0.88
2:B:842:ASN:ND2	2:B:845:SER:H	1.72	0.88
1:A:783:THR:HG21	1:A:815:PHE:CZ	2.08	0.88
2:B:824:ILE:HG22	2:B:1087:PHE:HE2	1.35	0.88
2:B:393:LYS:HA	2:B:393:LYS:HE3	1.56	0.88
1:A:534:LEU:O	1:A:574:GLY:HA3	1.74	0.87
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.54	0.87
1:A:58:LEU:HD11	1:A:243:PRO:HB3	1.56	0.87
2:B:1002:THR:HG21	2:B:1006:ILE:HD12	1.55	0.87
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.55	0.86
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.57	0.86
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.56	0.86
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.56	0.86
2:B:942:ARG:HH22	15:T:25:DT:P	1.98	0.86
2:B:510:LYS:HG2	2:B:511:PRO:HD3	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:THR:HG22	3:C:44:LEU:N	1.89	0.86
1:A:70:CYS:O	1:A:72:GLU:HG2	1.75	0.85
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.06	0.85
1:A:323:LYS:HZ3	14:P:1:U:H4'	1.39	0.85
1:A:646:PHE:O	1:A:650:GLN:HG3	1.76	0.85
2:B:343:ILE:HG21	2:B:348:ARG:HG3	1.58	0.85
5:E:19:VAL:O	5:E:23:VAL:HG23	1.76	0.85
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.11	0.85
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.76	0.85
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.57	0.85
6:F:86:THR:OG1	6:F:89:GLU:HG3	1.77	0.85
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.59	0.85
9:I:115:LYS:HD3	9:I:117:LYS:HE3	1.57	0.85
2:B:343:ILE:CG2	2:B:348:ARG:HG3	2.05	0.85
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.58	0.85
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.57	0.85
1:A:320:ARG:HH22	14:P:1:U:H1'	1.40	0.85
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.59	0.85
1:A:321:PRO:O	1:A:322:VAL:HB	1.76	0.84
2:B:46:GLN:HG3	2:B:47:GLN:H	1.41	0.84
11:K:65:HIS:CD2	11:K:67:PHE:H	1.94	0.84
4:D:22:GLU:H	4:D:22:GLU:CD	1.85	0.84
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.59	0.84
1:A:225:ASN:ND2	1:A:228:PHE:H	1.76	0.84
1:A:855:THR:CG2	1:A:857:ARG:HE	1.90	0.84
2:B:847:ASP:HB3	3:C:167:HIS:NE2	1.92	0.84
1:A:535:THR:HG21	1:A:616:VAL:HA	1.60	0.84
2:B:343:ILE:HG21	2:B:348:ARG:N	1.92	0.84
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.59	0.84
14:P:6:C:H2'	14:P:7:A:C8	2.12	0.84
2:B:98:THR:O	2:B:126:SER:HB2	1.78	0.84
6:F:69:LEU:HA	6:F:70:LYS:N	1.91	0.84
1:A:1424:VAL:HG13	1:A:1436:ILE:HD11	1.60	0.83
3:C:32:SER:O	3:C:36:VAL:HG23	1.78	0.83
1:A:215:SER:HB3	1:A:218:ASP:OD2	1.77	0.83
1:A:853:ASP:OD1	1:A:855:THR:HB	1.77	0.83
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.59	0.83
1:A:1094:VAL:HG12	1:A:1095:THR:N	1.93	0.83
1:A:58:LEU:HD12	1:A:59:GLY:N	1.94	0.83
1:A:913:LEU:HD12	1:A:914:GLU:N	1.94	0.83
1:A:1325:THR:O	5:E:148:GLU:HB2	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:ASN:HD22	1:A:744:LYS:H	1.27	0.82
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.14	0.82
1:A:709:THR:HG22	1:A:711:ARG:H	1.44	0.82
2:B:642:ASP:HA	2:B:649:LYS:HA	1.59	0.82
2:B:363:HIS:O	2:B:364:ILE:HB	1.76	0.82
1:A:903:ASN:HD22	1:A:904:THR:N	1.77	0.82
1:A:84:ILE:HD11	1:A:270:LEU:HD13	1.60	0.82
1:A:590:ARG:HG3	1:A:590:ARG:NH1	1.94	0.82
8:H:59:ILE:HG22	8:H:60:ALA:N	1.93	0.82
9:I:34:TYR:CD2	9:I:35:VAL:N	2.48	0.82
1:A:472:LEU:O	1:A:475:THR:HB	1.79	0.82
2:B:955:THR:HG22	2:B:956:THR:H	1.44	0.82
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.44	0.81
5:E:22:MET:HE3	5:E:26:ARG:HH21	1.45	0.81
9:I:105:SER:O	9:I:106:CYS:HB3	1.77	0.81
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.15	0.81
1:A:866:PHE:C	1:A:867:ILE:HD12	2.05	0.81
2:B:365:THR:HG23	2:B:367:LEU:H	1.45	0.81
4:D:47:LEU:HD11	7:G:3:PHE:CD2	2.14	0.81
11:K:47:ARG:HB3	11:K:47:ARG:NH1	1.96	0.81
2:B:336:ARG:HD3	2:B:348:ARG:HH11	1.46	0.81
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.62	0.81
7:G:80:LYS:HD3	7:G:80:LYS:H	1.45	0.81
7:G:80:LYS:HD3	7:G:80:LYS:N	1.96	0.81
15:T:18:DT:C3'	15:T:19:TT:H4'	2.11	0.81
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	1.96	0.81
7:G:128:PRO:O	7:G:138:THR:HG23	1.81	0.81
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.62	0.81
1:A:356:ASP:HB2	1:A:469:ARG:NH1	1.96	0.81
2:B:879:ARG:HH11	2:B:883:LEU:HD22	1.44	0.81
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.63	0.81
15:T:18:DT:H2''	15:T:19:TT:C5'	2.11	0.81
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.16	0.80
10:J:7:CYS:HB2	10:J:46:CYS:HB3	1.63	0.80
15:T:18:DT:H2'	15:T:19:TT:H5'1	1.62	0.80
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.16	0.80
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.63	0.80
1:A:743:VAL:O	1:A:747:VAL:HG23	1.82	0.80
5:E:192:ARG:HH11	5:E:192:ARG:HG3	1.45	0.80
3:C:244:VAL:O	3:C:248:ILE:HG13	1.82	0.80
2:B:189:LEU:O	2:B:192:LEU:N	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:467:GLY:H	2:B:475:SER:HB3	1.46	0.80
1:A:1116:LEU:N	1:A:1308:THR:HG22	1.97	0.80
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.64	0.80
9:I:34:TYR:HD2	9:I:35:VAL:N	1.80	0.80
1:A:767:GLN:NE2	1:A:774:ARG:HB3	1.96	0.79
10:J:64:ASN:HB3	10:J:65:PRO:CD	2.12	0.79
1:A:858:ASN:C	1:A:858:ASN:HD22	1.91	0.79
15:T:18:DT:H2''	15:T:19:TT:O5'	1.82	0.79
1:A:107:CYS:SG	1:A:171:GLN:HG2	2.21	0.79
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.45	0.79
1:A:886:ILE:HG22	1:A:887:GLY:N	1.96	0.79
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.63	0.79
15:T:18:DT:C2'	15:T:19:TT:C5'	2.60	0.79
1:A:567:LYS:HE3	8:H:46:LEU:HB2	1.64	0.79
2:B:171:PRO:HD2	2:B:457:LEU:HD13	1.62	0.79
2:B:467:GLY:N	2:B:475:SER:HB3	1.98	0.79
1:A:768:GLN:CG	1:A:816:HIS:HA	2.12	0.79
8:H:81:PRO:HB2	8:H:82:PRO:HD2	1.65	0.79
1:A:590:ARG:HG3	1:A:590:ARG:HH11	1.47	0.79
2:B:244:LEU:HD21	2:B:366:GLN:NE2	1.97	0.79
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.82	0.79
2:B:112:LEU:HD12	2:B:113:TYR:H	1.48	0.79
2:B:1202:LEU:O	2:B:1206:GLU:HG3	1.82	0.79
9:I:34:TYR:HE2	9:I:36:GLU:HB3	1.48	0.79
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.64	0.78
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.63	0.78
1:A:1030:ARG:HG3	1:A:1034:GLU:OE2	1.83	0.78
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.64	0.78
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.83	0.78
2:B:778:MET:HE3	2:B:1094:ARG:HD3	1.64	0.78
1:A:63:ARG:HA	1:A:74:MET:SD	2.24	0.78
1:A:1206:ASP:HB3	1:A:1274:ARG:HH12	1.47	0.78
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.66	0.78
2:B:613:VAL:HG13	2:B:627:PHE:O	1.83	0.78
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.65	0.78
2:B:580:VAL:HG22	2:B:624:LEU:HB3	1.66	0.78
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.18	0.78
3:C:174:ALA:HB2	3:C:235:VAL:HG22	1.65	0.78
1:A:34:LYS:CE	1:A:57:ARG:HH12	1.95	0.78
4:D:153:ARG:NH2	4:D:184:ALA:HA	1.99	0.78
8:H:59:ILE:HG22	8:H:60:ALA:H	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:MET:HE1	2:B:1135:ARG:NH1	1.98	0.78
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.66	0.78
5:E:213:ILE:HG12	5:E:214:CYS:H	1.48	0.78
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.49	0.78
2:B:882:THR:HG22	2:B:884:ARG:N	1.99	0.78
3:C:35:ARG:NH1	11:K:41:THR:H	1.80	0.78
7:G:111:THR:HG22	7:G:113:HIS:H	1.49	0.78
9:I:55:THR:HG21	9:I:109:ILE:HD13	1.66	0.78
1:A:1028:THR:O	1:A:1032:LEU:HD12	1.84	0.78
2:B:654:ARG:H	2:B:657:HIS:HD2	1.28	0.78
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.64	0.77
1:A:1341:ILE:HD12	1:A:1379:GLY:O	1.84	0.77
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.24	0.77
12:L:53:HIS:HB3	12:L:55:ILE:HD11	1.66	0.77
1:A:14:VAL:HG21	2:B:1216:LEU:HD13	1.66	0.77
1:A:528:LEU:O	1:A:531:ILE:HG22	1.84	0.77
1:A:596:THR:O	1:A:598:LEU:N	2.18	0.77
1:A:308:ILE:HG22	1:A:309:ALA:H	1.48	0.77
2:B:1095:LEU:H	2:B:1095:LEU:HD12	1.49	0.77
2:B:1224:PHE:HE2	5:E:171:LYS:HG3	1.49	0.77
6:F:82:THR:HG22	6:F:84:TYR:H	1.49	0.77
1:A:49:LYS:NZ	1:A:61:ILE:HG13	2.00	0.77
1:A:794:PRO:HG2	1:A:795:GLU:OE2	1.85	0.77
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.66	0.77
1:A:1036:ARG:HG2	1:A:1036:ARG:HH11	1.49	0.77
2:B:906:SER:O	2:B:941:LEU:HD23	1.85	0.77
2:B:65:GLU:HG3	2:B:66:ASP:N	1.97	0.77
12:L:32:ALA:HB3	12:L:55:ILE:HD12	1.67	0.77
1:A:836:TYR:CD1	15:T:18:DT:H5''	2.19	0.77
1:A:903:ASN:ND2	1:A:905:ASP:H	1.83	0.77
7:G:138:THR:HG22	7:G:139:ILE:N	1.99	0.77
13:N:5:DA:H1'	13:N:6:DC:O5'	1.85	0.77
1:A:269:ILE:HD13	1:A:300:VAL:HG22	1.67	0.76
1:A:323:LYS:NZ	14:P:1:U:H4'	1.99	0.76
2:B:340:ALA:HB2	2:B:343:ILE:HD12	1.67	0.76
2:B:737:THR:HG21	9:I:66:PRO:HA	1.67	0.76
4:D:40:HIS:CE1	4:D:41:GLN:HG3	2.21	0.76
14:P:9:A:N1	15:T:19:TT:O4T	2.17	0.76
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.48	0.76
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.16	0.76
2:B:821:GLN:HE22	2:B:851:PHE:HA	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:47:LEU:HD13	4:D:48:ILE:H	1.49	0.76
8:H:61:SER:O	8:H:62:SER:HB3	1.85	0.76
1:A:466:SER:O	2:B:1103:ILE:HD11	1.85	0.76
2:B:859:TYR:OH	2:B:941:LEU:HD12	1.85	0.76
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.68	0.76
1:A:106:VAL:HG13	1:A:112:LYS:O	1.85	0.76
2:B:114:PRO:HG2	2:B:115:GLN:H	1.51	0.76
13:N:3:DG:H1'	13:N:4:DT:H5'	1.68	0.76
1:A:1171:GLN:HA	1:A:1174:PHE:CE1	2.21	0.76
1:A:1372:VAL:O	1:A:1376:THR:HG22	1.84	0.76
2:B:44:VAL:HG11	2:B:199:MET:HG2	1.66	0.76
2:B:217:ARG:NE	2:B:405:ARG:HB2	2.01	0.76
3:C:213:PRO:O	3:C:214:ASN:HB2	1.84	0.76
4:D:176:GLU:C	4:D:178:ALA:H	1.94	0.76
1:A:1332:PHE:H	1:A:1332:PHE:HD2	1.32	0.76
3:C:73:GLN:HE21	3:C:75:MET:N	1.84	0.76
8:H:36:CYS:HA	8:H:126:GLU:O	1.84	0.76
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.66	0.75
1:A:982:THR:HB	1:A:985:ASP:H	1.49	0.75
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.48	0.75
2:B:708:GLU:O	2:B:710:LEU:N	2.20	0.75
6:F:90:ARG:HD3	6:F:155:LEU:HD11	1.67	0.75
2:B:510:LYS:HG3	2:B:511:PRO:HD3	1.67	0.75
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.68	0.75
1:A:657:LEU:O	1:A:657:LEU:HD12	1.86	0.75
1:A:885:THR:O	1:A:940:ARG:HD2	1.87	0.75
1:A:1329:THR:HG22	1:A:1331:SER:H	1.51	0.75
2:B:615:MET:C	2:B:616:ILE:HD12	2.12	0.75
4:D:130:LEU:C	4:D:132:GLN:H	1.94	0.75
1:A:666:ILE:HD12	1:A:667:GLY:H	1.51	0.75
1:A:230:ARG:H	1:A:233:TRP:HE3	1.35	0.75
1:A:351:THR:HB	2:B:1103:ILE:HD12	1.69	0.75
1:A:385:ILE:HG22	1:A:386:ASP:N	2.01	0.75
1:A:512:VAL:HA	1:A:519:PRO:HA	1.68	0.75
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.22	0.75
1:A:1424:VAL:HG13	1:A:1436:ILE:CD1	2.16	0.75
3:C:73:GLN:HE21	3:C:75:MET:H	1.31	0.75
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.67	0.75
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.21	0.75
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.69	0.75
11:K:12:LEU:H	11:K:12:LEU:HD12	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.68	0.75
1:A:986:ILE:HG22	1:A:987:VAL:N	2.00	0.75
4:D:47:LEU:HD11	7:G:3:PHE:HD2	1.50	0.75
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.17	0.74
1:A:92:HIS:O	1:A:94:GLY:N	2.20	0.74
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.67	0.74
4:D:7:THR:HG21	4:D:32:GLU:CD	2.11	0.74
1:A:1387:HIS:CE1	13:N:4:DT:H4'	2.21	0.74
7:G:81:PRO:HG3	7:G:106:MET:SD	2.26	0.74
11:K:47:ARG:HH11	11:K:47:ARG:CB	1.98	0.74
7:G:39:THR:HG22	7:G:41:LYS:H	1.52	0.74
1:A:335:ARG:HA	1:A:339:ASN:HB2	1.68	0.74
1:A:754:SER:H	1:A:757:ASN:ND2	1.86	0.74
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.28	0.74
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.00	0.74
2:B:830:TYR:O	2:B:832:GLY:N	2.20	0.74
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.69	0.74
7:G:59:GLY:HA3	7:G:70:PHE:CD2	2.23	0.74
2:B:999:MET:HA	2:B:999:MET:HE3	1.70	0.74
2:B:189:LEU:HA	2:B:192:LEU:HD12	1.68	0.74
2:B:434:ARG:O	2:B:437:GLU:HB2	1.86	0.74
2:B:515:HIS:HD2	2:B:517:THR:H	1.35	0.74
2:B:526:GLU:HG2	2:B:538:ASN:HD22	1.52	0.74
12:L:30:ILE:O	12:L:56:LEU:HA	1.87	0.74
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.23	0.74
2:B:549:THR:H	2:B:628:THR:HG23	1.52	0.74
3:C:43:THR:CG2	3:C:44:LEU:H	2.01	0.74
5:E:157:SER:OG	5:E:160:GLU:HG3	1.87	0.74
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.70	0.74
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.03	0.74
1:A:798:GLY:HA2	1:A:815:PHE:CD1	2.22	0.73
7:G:14:HIS:ND1	7:G:15:PRO:HD2	2.03	0.73
2:B:1138:MET:HA	2:B:1138:MET:HE3	1.68	0.73
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.69	0.73
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.87	0.73
2:B:1180:PHE:HB3	2:B:1191:ILE:HD12	1.68	0.73
12:L:38:LEU:O	12:L:39:SER:HB3	1.88	0.73
2:B:332:ASP:O	2:B:336:ARG:HG3	1.86	0.73
4:D:153:ARG:HB3	4:D:154:PHE:CE1	2.23	0.73
7:G:39:THR:HG22	7:G:40:GLY:H	1.54	0.73
1:A:35:ILE:HG22	1:A:35:ILE:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:HA	1:A:74:MET:CE	2.19	0.73
3:C:33:LEU:HG	3:C:37:MET:HE2	1.69	0.73
7:G:14:HIS:HD2	7:G:16:SER:HB2	1.49	0.73
3:C:166:GLU:HG3	11:K:10:PHE:CZ	2.18	0.73
1:A:53:LEU:HD22	1:A:54:ASN:HD22	1.54	0.73
1:A:384:ASN:OD1	1:A:388:LEU:HD12	1.89	0.73
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.71	0.73
4:D:66:ARG:HD2	4:D:133:THR:HB	1.71	0.73
1:A:254:GLU:HB2	2:B:935:ARG:NH1	2.03	0.73
2:B:232:SER:HB3	2:B:261:ARG:NH2	2.04	0.73
1:A:249:SER:O	1:A:250:ILE:HG13	1.87	0.73
1:A:567:LYS:HB3	8:H:96:VAL:N	2.03	0.73
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.24	0.72
3:C:47:ASP:HA	12:L:69:ALA:CB	2.19	0.72
1:A:845:LEU:HB3	1:A:848:ILE:HD12	1.71	0.72
2:B:589:VAL:HG12	2:B:590:HIS:N	2.03	0.72
4:D:130:LEU:O	4:D:132:GLN:N	2.21	0.72
1:A:1436:ILE:O	1:A:1437:GLY:C	2.33	0.72
3:C:167:HIS:HD2	3:C:168:ALA:N	1.85	0.72
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.71	0.72
1:A:67:CYS:O	1:A:70:CYS:HB3	1.89	0.72
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	1.89	0.72
3:C:174:ALA:HB2	3:C:235:VAL:CG2	2.19	0.72
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.70	0.72
2:B:336:ARG:NH2	2:B:345:LYS:HG2	2.05	0.72
2:B:879:ARG:NH1	2:B:883:LEU:HD22	2.03	0.72
5:E:157:SER:C	5:E:159:ASP:H	1.97	0.72
9:I:111:THR:HG22	9:I:112:SER:N	2.04	0.72
1:A:903:ASN:HD22	1:A:903:ASN:C	1.96	0.72
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.71	0.72
11:K:18:LYS:HZ3	11:K:38:GLU:HG2	1.54	0.72
1:A:62:ASP:HB3	1:A:64:ASN:ND2	2.05	0.72
1:A:537:ARG:HD2	8:H:20:TYR:HE1	1.55	0.72
2:B:343:ILE:CG2	2:B:347:LYS:HB2	2.07	0.72
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.24	0.72
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.71	0.72
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.19	0.72
4:D:29:LEU:HD22	7:G:82:PHE:CE2	2.25	0.72
1:A:58:LEU:HD13	1:A:80:HIS:O	1.90	0.72
2:B:336:ARG:CG	2:B:348:ARG:HD3	2.15	0.72
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1197:PRO:HG2	2:B:1200:ALA:HB2	1.72	0.72
2:B:217:ARG:HD2	2:B:217:ARG:C	2.15	0.72
15:T:24:DG:H2''	15:T:25:DT:O5'	1.89	0.72
1:A:68:GLN:C	1:A:70:CYS:H	1.97	0.72
1:A:69:THR:C	1:A:71:GLN:H	1.96	0.72
2:B:1087:PHE:HD2	2:B:1088:GLY:N	1.86	0.72
1:A:384:ASN:O	1:A:385:ILE:C	2.33	0.71
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.71	0.71
5:E:22:MET:CE	5:E:26:ARG:HH21	2.02	0.71
1:A:567:LYS:HD3	8:H:95:TYR:CD2	2.24	0.71
4:D:134:THR:HG22	4:D:136:GLY:H	1.55	0.71
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.54	0.71
1:A:325:ILE:HG21	2:B:1210:MET:HG3	1.72	0.71
1:A:858:ASN:ND2	1:A:860:LEU:H	1.88	0.71
2:B:516:ASN:HD22	2:B:516:ASN:H	1.37	0.71
14:P:5:C:O2'	14:P:6:C:H5'	1.91	0.71
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.31	0.71
1:A:1171:GLN:HA	1:A:1174:PHE:CD1	2.26	0.71
2:B:815:ARG:HD3	2:B:1041:GLU:OE2	1.91	0.71
13:N:6:DC:H2''	13:N:7:DT:OP2	1.89	0.71
15:T:19:TT:H2R2	15:T:19:TT:C2'	2.19	0.71
2:B:336:ARG:HH22	2:B:345:LYS:CE	2.03	0.71
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.72	0.71
2:B:35:SER:HA	2:B:811:TYR:HE2	1.56	0.71
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.73	0.71
2:B:336:ARG:HD3	2:B:348:ARG:NH1	2.05	0.71
2:B:515:HIS:H	2:B:518:HIS:CD2	2.04	0.71
3:C:208:GLU:O	3:C:210:GLU:N	2.24	0.71
8:H:56:THR:HB	8:H:145:ARG:HG2	1.72	0.71
1:A:254:GLU:CB	2:B:935:ARG:HH12	2.04	0.71
1:A:960:ILE:O	1:A:963:ILE:HG22	1.89	0.71
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.20	0.71
2:B:807:ARG:HG2	2:B:1045:SER:OG	1.89	0.71
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.54	0.71
1:A:382:PRO:HB3	1:A:428:TYR:CE2	2.23	0.71
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.05	0.71
10:J:43:ARG:HG3	10:J:45:CYS:SG	2.30	0.71
10:J:64:ASN:HD22	10:J:65:PRO:HD3	1.55	0.71
2:B:953:LEU:CD2	2:B:965:LYS:HB2	2.20	0.71
2:B:955:THR:HG22	2:B:956:THR:N	2.05	0.71
3:C:35:ARG:NH1	11:K:41:THR:N	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:186:LEU:HD21	3:C:224:GLN:O	1.90	0.71
1:A:69:THR:O	1:A:71:GLN:N	2.23	0.70
1:A:326:ARG:HH22	1:A:1407:GLU:HG3	1.53	0.70
1:A:1348:LEU:HG	1:A:1372:VAL:CG2	2.21	0.70
1:A:1437:GLY:O	1:A:1439:GLY:N	2.23	0.70
4:D:134:THR:HG22	4:D:135:GLY:N	2.06	0.70
6:F:103:MET:HE2	7:G:66:GLY:H	1.56	0.70
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.71	0.70
2:B:359:GLU:O	2:B:362:PRO:HD3	1.92	0.70
1:A:546:VAL:O	1:A:550:LEU:HG	1.92	0.70
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.55	0.70
5:E:117:THR:HG22	5:E:119:SER:H	1.56	0.70
9:I:111:THR:HG22	9:I:112:SER:H	1.56	0.70
1:A:567:LYS:CB	8:H:95:TYR:HA	2.21	0.70
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.55	0.70
3:C:226:ASP:O	3:C:227:THR:HB	1.90	0.70
8:H:40:LEU:CD1	8:H:123:MET:HB2	2.22	0.70
10:J:1:MET:H1	10:J:57:ILE:H	0.80	0.70
15:T:18:DT:O3'	15:T:19:TT:H4'	1.90	0.70
1:A:18:GLN:HB2	2:B:1215:ARG:HB2	1.73	0.70
1:A:34:LYS:HB2	1:A:36:ARG:HH21	1.57	0.70
2:B:1172:ILE:HG22	2:B:1172:ILE:O	1.90	0.70
7:G:39:THR:HG22	7:G:40:GLY:N	2.06	0.70
1:A:55:ASP:N	1:A:56:PRO:HD3	2.04	0.70
1:A:58:LEU:HD11	1:A:243:PRO:CB	2.21	0.70
10:J:7:CYS:CB	10:J:46:CYS:HB3	2.21	0.70
1:A:438:ASP:O	1:A:439:ASN:HB2	1.90	0.70
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.21	0.70
4:D:8:PHE:CE2	4:D:40:HIS:HA	2.25	0.70
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.25	0.70
1:A:1329:THR:HG22	1:A:1331:SER:N	2.06	0.70
1:A:1348:LEU:HG	1:A:1372:VAL:HG23	1.73	0.70
2:B:175:ARG:HG2	2:B:175:ARG:HH11	1.55	0.70
2:B:336:ARG:HG2	2:B:348:ARG:CD	2.17	0.70
1:A:265:LYS:N	1:A:265:LYS:HD2	2.06	0.70
1:A:1332:PHE:N	1:A:1332:PHE:CD2	2.60	0.70
2:B:557:PHE:C	2:B:557:PHE:CD2	2.70	0.70
11:K:61:TYR:C	11:K:61:TYR:CD2	2.69	0.70
1:A:34:LYS:H	1:A:57:ARG:NH2	1.90	0.70
1:A:50:ILE:C	1:A:52:GLY:H	2.00	0.70
8:H:123:MET:HG2	8:H:124:ARG:N	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:LYS:HB3	1:A:641:VAL:HG11	1.73	0.69
2:B:38:PHE:HD1	2:B:811:TYR:CD2	2.09	0.69
1:A:996:ASN:O	1:A:998:LEU:HD12	1.91	0.69
1:A:1035:TYR:O	1:A:1037:LEU:N	2.25	0.69
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.74	0.69
2:B:336:ARG:CD	2:B:348:ARG:HH11	2.04	0.69
2:B:824:ILE:CG2	2:B:1087:PHE:HE2	2.05	0.69
2:B:1069:PHE:H	2:B:1069:PHE:HD1	1.39	0.69
4:D:40:HIS:CB	7:G:73:LYS:NZ	2.54	0.69
4:D:34:GLN:O	4:D:47:LEU:HD23	1.92	0.69
6:F:90:ARG:HD3	6:F:155:LEU:CD1	2.22	0.69
6:F:111:LEU:HD12	6:F:111:LEU:N	2.06	0.69
12:L:53:HIS:HB3	12:L:55:ILE:CD1	2.22	0.69
1:A:347:PHE:H	2:B:1107:ALA:HA	1.57	0.69
1:A:471:ASN:OD1	1:A:472:LEU:N	2.25	0.69
15:T:26:DC:H2''	15:T:27:DA:H5'	1.74	0.69
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.74	0.69
8:H:100:THR:OG1	8:H:138:GLU:HG3	1.92	0.69
2:B:847:ASP:HB3	3:C:167:HIS:HE2	1.54	0.69
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.75	0.69
1:A:114:LEU:HD13	1:A:171:GLN:HE22	1.56	0.69
2:B:745:PRO:O	2:B:748:ILE:HG12	1.93	0.69
2:B:842:ASN:HD22	2:B:845:SER:CB	2.06	0.69
2:B:857:ARG:HD2	2:B:945:GLU:OE1	1.93	0.69
4:D:213:GLU:O	4:D:217:LEU:HG	1.93	0.69
1:A:265:LYS:NZ	1:A:322:VAL:HG22	2.08	0.69
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.74	0.69
1:A:701:LEU:HA	9:I:115:LYS:HE3	1.75	0.69
1:A:836:TYR:HD1	15:T:18:DT:H5''	1.57	0.69
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.73	0.69
2:B:411:PRO:O	2:B:414:ALA:HB3	1.93	0.69
2:B:642:ASP:O	2:B:644:GLU:N	2.26	0.69
2:B:975:GLN:HG2	2:B:976:ILE:H	1.58	0.69
2:B:1115:THR:O	2:B:1116:ARG:HB2	1.92	0.69
7:G:23:LYS:HG3	7:G:56:ILE:HD11	1.75	0.69
10:J:14:VAL:O	10:J:14:VAL:HG12	1.92	0.69
1:A:19:PHE:O	1:A:1416:ALA:HA	1.93	0.69
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.08	0.69
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.57	0.69
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.23	0.69
8:H:4:THR:HA	8:H:60:ALA:CB	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.28	0.69
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.28	0.69
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.74	0.69
1:A:1332:PHE:HD2	1:A:1332:PHE:N	1.90	0.69
2:B:247:GLY:C	2:B:249:ARG:H	1.99	0.69
7:G:23:LYS:HG3	7:G:56:ILE:CD1	2.23	0.69
15:T:18:DT:H3'	15:T:19:TT:H4'	1.73	0.69
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.75	0.68
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.08	0.68
11:K:6:ARG:O	11:K:9:LEU:HG	1.93	0.68
1:A:69:THR:C	1:A:71:GLN:N	2.49	0.68
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.28	0.68
1:A:1029:ARG:HH11	1:A:1029:ARG:HG3	1.58	0.68
2:B:180:TYR:HD1	2:B:180:TYR:H	1.41	0.68
2:B:1006:ILE:HD13	10:J:44:TYR:CE2	2.28	0.68
1:A:549:MET:SD	1:A:577:ILE:HD11	2.33	0.68
1:A:856:THR:HB	1:A:865:GLN:HB2	1.75	0.68
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.75	0.68
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.19	0.68
11:K:53:ASP:OD1	11:K:55:LYS:HB2	1.93	0.68
1:A:1445:ILE:HG12	7:G:18:PHE:CE2	2.28	0.68
2:B:1223:ASP:O	2:B:1224:PHE:HB2	1.92	0.68
4:D:33:PHE:CE1	7:G:80:LYS:HE3	2.29	0.68
6:F:76:LYS:O	6:F:79:ARG:HD3	1.94	0.68
2:B:39:ARG:HH21	2:B:665:GLU:CD	2.01	0.68
2:B:542:MET:HE3	2:B:636:PRO:HG3	1.75	0.68
8:H:102:TYR:OH	8:H:122:LEU:HD22	1.94	0.68
1:A:1057:VAL:HG12	1:A:1058:VAL:H	1.59	0.68
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.74	0.68
4:D:118:THR:HB	4:D:121:LYS:HB2	1.76	0.68
4:D:189:ASP:O	4:D:193:THR:HB	1.92	0.68
5:E:78:LEU:HD21	5:E:80:VAL:HG23	1.76	0.68
1:A:353:ILE:CD1	1:A:487:MET:HE2	2.23	0.68
1:A:537:ARG:HD2	8:H:20:TYR:CE1	2.29	0.68
2:B:121:ASN:HA	2:B:207:GLY:CA	2.23	0.68
2:B:863:GLU:OE2	2:B:873:THR:HA	1.94	0.68
2:B:882:THR:HB	2:B:934:LYS:O	1.94	0.68
6:F:103:MET:O	6:F:104:ASN:HB2	1.93	0.68
11:K:31:VAL:HG12	11:K:32:VAL:N	2.09	0.68
15:T:19:TT:H2'1	15:T:19:TT:C2R	2.23	0.68
2:B:516:ASN:N	2:B:516:ASN:ND2	2.35	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:263:THR:C	3:C:265:MET:H	2.02	0.68
5:E:198:ILE:HD11	5:E:212:ARG:HG3	1.74	0.68
8:H:84:ALA:CA	8:H:87:ARG:HB2	2.22	0.68
1:A:552:TRP:HE3	1:A:651:LYS:HB3	1.60	0.68
2:B:232:SER:CB	2:B:261:ARG:HH21	2.06	0.68
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.24	0.68
1:A:58:LEU:HD21	1:A:243:PRO:CA	2.23	0.67
2:B:1099:VAL:CG1	2:B:1100:ASP:N	2.56	0.67
8:H:130:ARG:H	8:H:130:ARG:HD2	1.59	0.67
1:A:42:ASP:HB3	1:A:45:GLN:H	1.59	0.67
10:J:1:MET:H3	10:J:56:LEU:N	1.91	0.67
10:J:23:ASN:C	10:J:25:LEU:H	1.99	0.67
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.75	0.67
2:B:351:TYR:O	2:B:355:ILE:HG13	1.95	0.67
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.59	0.67
3:C:35:ARG:HH12	11:K:41:THR:H	1.40	0.67
3:C:232:VAL:HG21	3:C:244:VAL:HG22	1.77	0.67
6:F:130:ILE:O	6:F:148:VAL:HG21	1.93	0.67
7:G:13:LEU:CD2	7:G:17:PHE:HB2	2.19	0.67
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.25	0.67
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.29	0.67
1:A:901:LEU:H	1:A:926:GLN:HE21	1.40	0.67
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	1.75	0.67
1:A:1120:LEU:HD12	1:A:1120:LEU:N	2.09	0.67
2:B:953:LEU:HD23	2:B:953:LEU:O	1.94	0.67
5:E:153:HIS:HB3	5:E:196:VAL:CG1	2.24	0.67
1:A:34:LYS:HE3	1:A:57:ARG:NH1	2.08	0.67
2:B:871:THR:HG22	2:B:872:GLU:O	1.94	0.67
2:B:1174:LYS:O	2:B:1176:ASN:N	2.28	0.67
3:C:56:THR:HG22	3:C:57:VAL:H	1.60	0.67
5:E:94:LYS:CE	5:E:98:ILE:HD11	2.23	0.67
8:H:143:LEU:HD12	8:H:143:LEU:N	2.08	0.67
15:T:19:TT:H5M1	15:T:21:DC:C4	2.29	0.67
1:A:253:ASN:HB3	2:B:935:ARG:CZ	2.25	0.67
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.75	0.67
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.77	0.67
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.76	0.67
9:I:8:ARG:CG	9:I:34:TYR:HE1	2.06	0.67
9:I:61:ASP:C	9:I:63:GLY:H	2.03	0.67
1:A:407:ARG:HB3	1:A:430:TRP:CE2	2.29	0.67
1:A:450:LEU:H	1:A:450:LEU:HD12	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:22:MET:HE3	5:E:26:ARG:HE	1.60	0.67
1:A:527:THR:CG2	1:A:650:GLN:HA	2.25	0.67
1:A:844:ALA:C	1:A:845:LEU:HD23	2.20	0.67
5:E:48:ASP:CG	5:E:49:SER:H	2.03	0.67
5:E:192:ARG:HG3	5:E:192:ARG:NH1	2.09	0.67
11:K:67:PHE:C	11:K:68:PHE:HD2	2.03	0.67
1:A:265:LYS:HZ3	1:A:322:VAL:HG22	1.60	0.67
2:B:563:MET:HE3	2:B:580:VAL:HB	1.77	0.67
8:H:58:THR:HG22	8:H:59:ILE:H	1.60	0.67
1:A:252:PHE:O	1:A:253:ASN:HB2	1.95	0.66
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.25	0.66
2:B:516:ASN:H	2:B:516:ASN:ND2	1.92	0.66
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.31	0.66
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.78	0.66
1:A:1450:LEU:O	1:A:1450:LEU:HG	1.96	0.66
2:B:1085:ILE:N	2:B:1085:ILE:HD12	2.10	0.66
8:H:41:ASP:O	8:H:42:ILE:HG13	1.95	0.66
1:A:881:GLN:NE2	1:A:958:VAL:O	2.28	0.66
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.24	0.66
2:B:1106:ARG:NH1	2:B:1110:PRO:HG2	2.11	0.66
3:C:43:THR:CG2	3:C:44:LEU:N	2.58	0.66
3:C:167:HIS:CD2	3:C:168:ALA:N	2.64	0.66
6:F:109:VAL:HG11	6:F:123:LYS:HD3	1.78	0.66
9:I:75:CYS:SG	9:I:79:HIS:N	2.68	0.66
11:K:111:LEU:C	11:K:112:GLN:CG	2.59	0.66
15:T:18:DT:H2''	15:T:19:TT:H5'1	1.72	0.66
1:A:1279:ILE:HG22	1:A:1279:ILE:O	1.96	0.66
2:B:378:LEU:O	2:B:382:ILE:HG13	1.95	0.66
2:B:464:GLY:HA2	2:B:479:VAL:O	1.96	0.66
8:H:44:VAL:O	8:H:44:VAL:HG12	1.96	0.66
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.78	0.66
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.64	0.66
2:B:18:PHE:N	2:B:19:GLU:N	2.44	0.66
2:B:825:VAL:CG1	2:B:826:ALA:N	2.58	0.66
1:A:896:ARG:NH2	1:A:1030:ARG:HH21	1.93	0.66
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.11	0.66
2:B:794:ASN:O	2:B:795:ILE:HD12	1.95	0.66
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.31	0.66
4:D:176:GLU:O	4:D:178:ALA:N	2.29	0.66
11:K:46:ILE:O	11:K:46:ILE:HG22	1.96	0.66
2:B:224:GLN:O	2:B:238:ALA:HA	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.77	0.66
1:A:84:ILE:O	1:A:84:ILE:HG23	1.96	0.66
1:A:356:ASP:HB2	1:A:469:ARG:HH11	1.60	0.66
2:B:842:ASN:ND2	2:B:845:SER:OG	2.29	0.66
10:J:64:ASN:ND2	10:J:65:PRO:HD3	2.11	0.66
14:P:1:U:O2'	14:P:2:C:H5'	1.96	0.66
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.26	0.65
2:B:1197:PRO:HG2	2:B:1200:ALA:CB	2.25	0.65
1:A:728:LYS:O	1:A:732:LEU:HG	1.97	0.65
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	2.11	0.65
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.78	0.65
2:B:824:ILE:HG22	2:B:1087:PHE:CE2	2.26	0.65
1:A:982:THR:H	1:A:985:ASP:HB2	1.61	0.65
1:A:984:LYS:O	1:A:988:LEU:HB2	1.97	0.65
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.11	0.65
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.44	0.65
2:B:1069:PHE:HA	2:B:1085:ILE:O	1.96	0.65
3:C:66:ARG:NH2	10:J:3:VAL:O	2.29	0.65
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.08	0.65
1:A:164:ARG:HG3	1:A:165:GLY:N	2.11	0.65
1:A:320:ARG:NH2	14:P:1:U:O2'	2.29	0.65
1:A:335:ARG:NH1	2:B:1202:LEU:HD13	2.11	0.65
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.78	0.65
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.12	0.65
2:B:770:GLN:CD	2:B:983:ARG:HA	2.21	0.65
1:A:224:PHE:CZ	1:A:234:MET:HE2	2.32	0.65
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.27	0.65
2:B:35:SER:O	2:B:39:ARG:HG3	1.97	0.65
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.79	0.65
3:C:167:HIS:HD2	3:C:168:ALA:H	1.43	0.65
8:H:11:GLN:HA	8:H:53:ASP:O	1.96	0.65
10:J:48:ARG:HE	10:J:49:MET:CE	2.10	0.65
11:K:114:LEU:HD13	11:K:114:LEU:C	2.20	0.65
1:A:714:PHE:O	1:A:718:VAL:HG23	1.97	0.65
1:A:1005:GLU:O	1:A:1009:ASN:HB2	1.97	0.65
2:B:850:LEU:HD12	2:B:851:PHE:N	2.11	0.65
4:D:71:LYS:HA	4:D:74:GLN:HB2	1.78	0.65
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.26	0.65
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.77	0.65
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.79	0.65
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:89:LEU:HB3	8:H:91:ASP:OD1	1.97	0.65
1:A:547:LEU:HD22	11:K:58:PHE:HD1	1.60	0.65
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.11	0.64
2:B:770:GLN:HG2	2:B:983:ARG:O	1.97	0.64
2:B:782:LEU:HD12	2:B:788:ARG:HH11	1.62	0.64
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.78	0.64
4:D:47:LEU:HD13	4:D:48:ILE:N	2.11	0.64
4:D:192:LYS:HE3	4:D:204:ASP:OD1	1.97	0.64
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.79	0.64
1:A:450:LEU:HD12	1:A:450:LEU:N	2.13	0.64
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.33	0.64
1:A:1445:ILE:HD12	1:A:1445:ILE:N	1.98	0.64
2:B:589:VAL:CG1	2:B:590:HIS:H	2.07	0.64
5:E:153:HIS:HB3	5:E:196:VAL:HG11	1.77	0.64
15:T:13:DA:H1'	15:T:14:DC:H5'	1.78	0.64
1:A:105:CYS:O	1:A:114:LEU:HG	1.97	0.64
1:A:591:PHE:HA	1:A:595:THR:HG21	1.80	0.64
1:A:979:SER:OG	1:A:980:ASP:N	2.29	0.64
2:B:185:THR:H	2:B:188:ASP:HB2	1.62	0.64
2:B:467:GLY:H	2:B:475:SER:CB	2.10	0.64
2:B:744:HIS:HD2	2:B:746:SER:OG	1.80	0.64
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.78	0.64
6:F:111:LEU:C	6:F:113:GLY:H	2.05	0.64
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.45	0.64
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.27	0.64
1:A:265:LYS:HE2	1:A:322:VAL:CG1	2.27	0.64
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.97	0.64
2:B:776:GLN:HE22	14:P:8:G:H5'	1.62	0.64
2:B:1161:HIS:NE2	2:B:1175:LEU:HD21	2.11	0.64
3:C:183:TRP:O	3:C:185:LYS:N	2.30	0.64
5:E:46:TYR:CD2	5:E:58:MET:HG2	2.32	0.64
1:A:35:ILE:HA	1:A:52:GLY:O	1.97	0.64
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.33	0.64
1:A:1006:ILE:HD12	5:E:163:GLU:HG3	1.78	0.64
2:B:918:ILE:HB	2:B:935:ARG:HD2	1.80	0.64
5:E:9:ILE:HD11	5:E:53:PRO:HD3	1.78	0.64
7:G:127:PRO:HG2	7:G:138:THR:HG21	1.79	0.64
1:A:1094:VAL:CG1	1:A:1095:THR:H	2.06	0.64
1:A:1134:ILE:O	1:A:1138:ILE:HG13	1.98	0.64
2:B:745:PRO:O	2:B:747:MET:N	2.31	0.64
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.80	0.64
5:E:22:MET:HE3	5:E:26:ARG:NH2	2.12	0.64
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.61	0.64
1:A:853:ASP:OD1	1:A:855:THR:CB	2.45	0.64
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	1.98	0.64
3:C:133:ILE:HD11	3:C:237:SER:HA	1.80	0.64
5:E:177:ARG:C	5:E:212:ARG:HD3	2.22	0.64
1:A:254:GLU:O	1:A:256:GLN:N	2.30	0.64
1:A:388:LEU:O	1:A:392:VAL:HG23	1.98	0.64
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.28	0.64
1:A:1444:MET:CG	7:G:60:ARG:HA	2.28	0.64
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.28	0.64
2:B:842:ASN:O	2:B:846:ILE:HG13	1.98	0.64
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.79	0.64
6:F:93:ILE:HD11	6:F:134:ILE:CD1	2.26	0.64
6:F:99:LEU:O	6:F:103:MET:HG2	1.97	0.64
8:H:81:PRO:CB	8:H:82:PRO:CD	2.75	0.64
12:L:47:ARG:HH21	12:L:54:ARG:HH21	1.44	0.64
1:A:34:LYS:CE	1:A:57:ARG:NH1	2.61	0.64
1:A:55:ASP:C	1:A:57:ARG:H	2.04	0.64
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.33	0.64
2:B:860:MET:HG2	2:B:861:ASP:H	1.63	0.64
2:B:806:THR:HG22	2:B:808:ALA:N	2.07	0.63
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.33	0.63
15:T:22:BRU:C2'	15:T:23:DG:O4'	2.46	0.63
1:A:144:THR:O	1:A:146:MET:HG3	1.98	0.63
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.28	0.63
2:B:339:THR:O	2:B:339:THR:HG22	1.98	0.63
2:B:601:ARG:O	2:B:605:ARG:HG3	1.98	0.63
2:B:637:LEU:O	2:B:690:VAL:HG13	1.99	0.63
2:B:745:PRO:C	2:B:747:MET:H	2.06	0.63
2:B:1072:MET:HE1	2:B:1085:ILE:HB	1.80	0.63
3:C:133:ILE:CD1	3:C:237:SER:HA	2.28	0.63
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.79	0.63
1:A:477:PRO:CG	1:A:521:MET:HG2	2.29	0.63
1:A:675:THR:O	1:A:679:ILE:HG13	1.98	0.63
1:A:832:ALA:O	1:A:833:GLU:C	2.42	0.63
2:B:211:VAL:O	2:B:480:SER:HA	1.99	0.63
2:B:336:ARG:HH21	2:B:345:LYS:HG2	1.63	0.63
2:B:1084:GLN:N	2:B:1084:GLN:NE2	2.46	0.63
4:D:52:LEU:C	4:D:54:GLU:H	2.05	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:28:ASP:O	10:J:30:LEU:HG	1.99	0.63
1:A:326:ARG:NH2	1:A:1407:GLU:HG3	2.13	0.63
1:A:535:THR:HG23	1:A:575:LYS:HE2	1.81	0.63
2:B:799:PRO:HB3	2:B:818:PRO:HG2	1.80	0.63
2:B:1165:ILE:HG22	2:B:1166:CYS:N	2.11	0.63
1:A:265:LYS:HD2	1:A:265:LYS:H	1.64	0.63
1:A:518:LYS:HE2	1:A:624:SER:O	1.97	0.63
1:A:528:LEU:C	1:A:528:LEU:HD12	2.23	0.63
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.80	0.63
2:B:121:ASN:HA	2:B:207:GLY:HA2	1.78	0.63
2:B:125:SER:HA	2:B:171:PRO:HA	1.80	0.63
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.28	0.63
2:B:957:ASN:O	2:B:959:ASP:N	2.31	0.63
4:D:52:LEU:O	4:D:54:GLU:N	2.32	0.63
1:A:598:LEU:HD22	8:H:25:ARG:NH1	2.14	0.63
2:B:542:MET:HE3	2:B:636:PRO:CG	2.28	0.63
5:E:114:ASN:O	5:E:115:ASN:HB3	1.97	0.63
6:F:69:LEU:CA	6:F:70:LYS:N	2.60	0.63
1:A:61:ILE:HG22	1:A:62:ASP:H	1.64	0.63
1:A:289:ILE:C	1:A:291:GLU:H	2.03	0.63
1:A:588:LEU:O	1:A:606:LEU:HA	1.99	0.63
1:A:714:PHE:HB2	9:I:97:MET:HE1	1.81	0.63
2:B:365:THR:HG23	2:B:367:LEU:HG	1.79	0.63
2:B:975:GLN:O	2:B:990:ILE:HD12	1.99	0.63
3:C:189:THR:HG22	3:C:190:ASP:N	2.14	0.63
7:G:17:PHE:N	7:G:17:PHE:CD2	2.66	0.63
8:H:93:TYR:HB3	8:H:144:ILE:O	1.99	0.63
1:A:321:PRO:O	1:A:322:VAL:CB	2.46	0.63
2:B:315:LYS:N	2:B:316:PRO:HD2	2.13	0.63
2:B:916:THR:O	2:B:935:ARG:HG3	1.99	0.63
4:D:7:THR:HB	7:G:42:PHE:CE2	2.34	0.63
6:F:138:LEU:HB3	6:F:139:PRO:HD2	1.80	0.63
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.14	0.62
2:B:705:MET:H	2:B:710:LEU:HD12	1.63	0.62
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.64	0.62
1:A:57:ARG:O	1:A:68:GLN:HG3	1.99	0.62
1:A:87:ALA:HB1	1:A:276:LEU:HD23	1.80	0.62
1:A:596:THR:C	1:A:598:LEU:H	2.05	0.62
1:A:648:ASN:O	1:A:649:ILE:C	2.41	0.62
6:F:99:LEU:C	6:F:99:LEU:HD12	2.24	0.62
9:I:34:TYR:CE2	9:I:36:GLU:HB3	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:GLY:O	1:A:732:LEU:N	2.32	0.62
1:A:979:SER:OG	1:A:981:LEU:HG	1.99	0.62
2:B:731:VAL:HG12	2:B:732:SER:H	1.64	0.62
4:D:159:THR:O	4:D:163:VAL:HG23	1.99	0.62
7:G:145:VAL:HG12	7:G:146:LYS:N	2.14	0.62
10:J:12:LYS:O	10:J:14:VAL:HG23	1.99	0.62
15:T:15:DT:C1'	15:T:16:DT:H5'	2.29	0.62
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.63	0.62
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.80	0.62
2:B:563:MET:CE	2:B:580:VAL:HB	2.29	0.62
2:B:1034:VAL:O	2:B:1037:LEU:N	2.30	0.62
3:C:100:THR:OG1	3:C:121:VAL:HG21	1.99	0.62
3:C:104:PHE:HD2	3:C:105:GLY:H	1.47	0.62
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.28	0.62
1:A:332:LYS:HG3	1:A:333:GLU:HG2	1.81	0.62
1:A:567:LYS:CB	1:A:568:PRO:CD	2.77	0.62
2:B:616:ILE:HD12	2:B:616:ILE:N	2.14	0.62
3:C:29:MET:HE2	11:K:98:LEU:CD2	2.29	0.62
3:C:35:ARG:HH11	11:K:41:THR:CA	2.12	0.62
6:F:77:ASP:C	6:F:79:ARG:H	2.06	0.62
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.79	0.62
10:J:16:ASP:OD1	10:J:17:LYS:HD2	1.99	0.62
1:A:341:MET:HE2	1:A:843:LYS:NZ	2.14	0.62
1:A:741:ASN:ND2	1:A:744:LYS:H	1.98	0.62
1:A:763:ALA:O	1:A:803:SER:HB3	2.00	0.62
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.29	0.62
1:A:1209:MET:SD	1:A:1236:LEU:HD22	2.39	0.62
1:A:1412:ALA:HA	1:A:1417:GLU:OE2	1.98	0.62
2:B:842:ASN:HB3	2:B:845:SER:OG	1.99	0.62
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.98	0.62
11:K:10:PHE:N	11:K:10:PHE:CD2	2.68	0.62
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.81	0.62
1:A:58:LEU:CG	1:A:59:GLY:H	2.11	0.62
1:A:524:VAL:HG12	1:A:525:GLN:N	2.12	0.62
1:A:1279:ILE:HD11	1:A:1316:VAL:HG21	1.80	0.62
2:B:465:ASN:HD22	2:B:465:ASN:N	1.98	0.62
3:C:29:MET:HE2	11:K:98:LEU:HD21	1.82	0.62
3:C:39:ALA:CA	3:C:164:ALA:HB3	2.30	0.62
5:E:39:LEU:O	5:E:42:PHE:HB3	2.00	0.62
6:F:97:ARG:O	6:F:101:ILE:HG13	1.99	0.62
2:B:525:ALA:O	2:B:768:THR:HA	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.29	0.62
3:C:112:ASN:HB2	3:C:114:TYR:CE1	2.34	0.62
3:C:253:LYS:O	3:C:256:ALA:HB3	2.00	0.62
4:D:8:PHE:CZ	4:D:40:HIS:HA	2.35	0.62
5:E:202:SER:OG	5:E:204:THR:HG22	2.00	0.62
6:F:90:ARG:HG3	6:F:91:ALA:N	2.14	0.62
1:A:53:LEU:CD2	1:A:54:ASN:HD22	2.13	0.62
1:A:482:PHE:C	1:A:484:GLY:H	2.07	0.62
1:A:997:LEU:HD13	1:A:1018:PHE:CE2	2.34	0.62
2:B:446:LEU:O	2:B:447:ALA:HB3	1.99	0.62
2:B:797:TYR:HE1	2:B:854:LEU:HD23	1.65	0.62
2:B:822:ASN:O	10:J:48:ARG:NH1	2.33	0.62
2:B:1182:CYS:O	2:B:1182:CYS:SG	2.57	0.62
13:N:5:DA:C2	15:T:13:DA:C2	2.88	0.62
1:A:384:ASN:CG	1:A:388:LEU:HD12	2.25	0.62
1:A:567:LYS:CE	8:H:46:LEU:HB2	2.29	0.62
1:A:1244:ARG:HB3	1:A:1245:PRO:HD2	1.80	0.62
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.34	0.62
2:B:751:VAL:HG13	2:B:812:LEU:HD22	1.80	0.62
1:A:107:CYS:N	1:A:114:LEU:HD21	2.15	0.61
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.30	0.61
2:B:36:ALA:HA	2:B:39:ARG:HD2	1.81	0.61
2:B:433:GLN:O	2:B:437:GLU:HG3	1.99	0.61
10:J:8:PHE:H	10:J:49:MET:CE	2.12	0.61
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.81	0.61
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.82	0.61
1:A:477:PRO:HG2	1:A:521:MET:HG2	1.82	0.61
1:A:901:LEU:N	1:A:926:GLN:NE2	2.47	0.61
2:B:464:GLY:O	2:B:477:ALA:HA	2.00	0.61
10:J:64:ASN:CB	10:J:65:PRO:HD3	2.30	0.61
2:B:336:ARG:NH2	2:B:345:LYS:HE2	2.10	0.61
2:B:498:THR:HB	2:B:537:LYS:O	2.00	0.61
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.82	0.61
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.29	0.61
10:J:44:TYR:HA	10:J:47:ARG:CB	2.30	0.61
1:A:1066:VAL:O	1:A:1070:GLN:HG3	2.01	0.61
2:B:168:GLY:N	2:B:450:ALA:HB1	2.12	0.61
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.31	0.61
2:B:622:LYS:CE	9:I:59:VAL:HG22	2.30	0.61
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.66	0.61
7:G:51:TYR:C	7:G:51:TYR:CD2	2.79	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:907:THR:CG2	1:A:908:LEU:N	2.63	0.61
1:A:971:PHE:CE2	1:A:1040:GLN:HG2	2.34	0.61
3:C:98:VAL:C	3:C:99:LEU:HD23	2.26	0.61
7:G:143:ILE:HG22	7:G:144:ARG:N	2.15	0.61
3:C:164:ALA:HA	3:C:167:HIS:O	2.00	0.61
1:A:450:LEU:HB3	1:A:838:GLN:NE2	2.15	0.61
1:A:746:MET:HE3	2:B:1018:PRO:HG2	1.83	0.61
2:B:278:GLN:HE22	2:B:337:ARG:HH21	1.47	0.61
2:B:520:GLY:H	2:B:748:ILE:HG22	1.64	0.61
3:C:69:LEU:N	3:C:69:LEU:HD12	2.16	0.61
3:C:104:PHE:HD2	3:C:105:GLY:N	1.99	0.61
3:C:142:VAL:H	10:J:16:ASP:HB3	1.66	0.61
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.82	0.61
8:H:42:ILE:HG23	8:H:95:TYR:HE1	1.64	0.61
8:H:91:ASP:C	8:H:93:TYR:H	2.08	0.61
1:A:382:PRO:HD3	1:A:428:TYR:HD2	1.65	0.61
3:C:34:ARG:O	3:C:38:ILE:HG13	2.01	0.61
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.16	0.61
2:B:1177:HIS:HB2	2:B:1179:GLN:HE21	1.65	0.61
3:C:20:PHE:HE1	3:C:22:LEU:HD12	1.66	0.61
3:C:77:ILE:HG23	3:C:161:LYS:HE3	1.81	0.61
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.83	0.61
5:E:29:PHE:O	5:E:30:ILE:HG13	2.00	0.61
8:H:25:ARG:HA	8:H:41:ASP:HA	1.83	0.61
8:H:47:PHE:CD2	8:H:95:TYR:HD1	2.19	0.61
1:A:427:GLN:HG3	1:A:430:TRP:CE2	2.34	0.60
1:A:590:ARG:HH11	1:A:590:ARG:CG	2.10	0.60
2:B:811:TYR:N	2:B:811:TYR:CD1	2.68	0.60
2:B:1084:GLN:NE2	2:B:1084:GLN:H	1.99	0.60
6:F:103:MET:CE	7:G:66:GLY:H	2.13	0.60
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.24	0.60
13:N:1:DA:H2''	13:N:2:DA:OP2	2.00	0.60
1:A:320:ARG:NH2	14:P:1:U:H1'	2.15	0.60
1:A:997:LEU:HD13	1:A:1018:PHE:HE2	1.66	0.60
2:B:557:PHE:C	2:B:557:PHE:HD2	2.09	0.60
2:B:882:THR:CG2	2:B:884:ARG:HB2	2.31	0.60
4:D:5:THR:O	4:D:5:THR:HG23	2.01	0.60
8:H:128:ASN:CG	8:H:128:ASN:O	2.44	0.60
10:J:7:CYS:SG	10:J:49:MET:HE3	2.40	0.60
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.36	0.60
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:PHE:O	1:A:96:ILE:C	2.44	0.60
1:A:596:THR:C	1:A:598:LEU:N	2.58	0.60
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.83	0.60
1:A:1095:THR:O	1:A:1096:SER:HB2	1.99	0.60
13:N:0:DT:H2''	13:N:1:DA:O5'	2.01	0.60
1:A:98:LYS:O	1:A:99:ILE:C	2.44	0.60
1:A:500:GLU:OE1	2:B:1143:ALA:C	2.44	0.60
1:A:886:ILE:CG2	1:A:887:GLY:N	2.64	0.60
2:B:100:PRO:HD2	2:B:180:TYR:HE1	1.66	0.60
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.49	0.60
3:C:147:LEU:N	3:C:147:LEU:HD23	2.16	0.60
10:J:1:MET:N	10:J:56:LEU:N	2.48	0.60
1:A:714:PHE:CB	9:I:97:MET:HE1	2.31	0.60
2:B:112:LEU:HD12	2:B:113:TYR:N	2.15	0.60
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.41	0.60
11:K:65:HIS:HD2	11:K:67:PHE:N	1.92	0.60
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.83	0.60
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.36	0.60
1:A:663:SER:OG	1:A:664:THR:N	2.33	0.60
1:A:694:THR:O	1:A:698:GLN:HG3	2.00	0.60
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.36	0.60
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.82	0.60
5:E:78:LEU:HD23	5:E:78:LEU:C	2.26	0.60
6:F:79:ARG:HG3	6:F:144:GLU:OE1	2.02	0.60
6:F:130:ILE:O	6:F:148:VAL:CG2	2.49	0.60
7:G:153:GLN:HG2	7:G:154:VAL:HG23	1.83	0.60
9:I:86:PHE:CE1	9:I:100:PHE:HB2	2.36	0.60
11:K:42:LEU:O	11:K:46:ILE:HG13	2.02	0.60
1:A:541:ILE:HD13	1:A:549:MET:CE	2.21	0.60
1:A:730:GLY:C	1:A:732:LEU:H	2.09	0.60
1:A:1333:ILE:O	1:A:1337:GLU:HG3	2.02	0.60
3:C:165:LYS:O	11:K:6:ARG:NH1	2.35	0.60
4:D:137:ASN:C	4:D:137:ASN:HD22	2.10	0.60
8:H:83:GLN:C	8:H:85:GLY:H	2.09	0.60
1:A:351:THR:HB	2:B:1103:ILE:CD1	2.32	0.60
1:A:382:PRO:CB	1:A:428:TYR:HE2	2.12	0.60
1:A:783:THR:HG22	1:A:784:LEU:HG	1.84	0.60
1:A:821:ARG:HD2	1:A:825:ILE:HD11	1.83	0.60
1:A:1289:ARG:HD2	1:A:1303:GLU:OE2	2.02	0.60
2:B:515:HIS:CD2	2:B:517:THR:H	2.17	0.60
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1176:ASN:C	2:B:1178:ASN:H	2.08	0.60
8:H:82:PRO:C	8:H:84:ALA:H	2.09	0.60
1:A:268:ASP:HB3	1:A:299:HIS:ND1	2.17	0.60
1:A:901:LEU:HA	1:A:907:THR:OG1	2.02	0.60
2:B:798:TYR:HE2	3:C:62:PHE:CZ	2.20	0.60
2:B:1001:PHE:CD2	3:C:34:ARG:NH2	2.70	0.60
3:C:100:THR:HG22	3:C:101:LEU:N	2.16	0.60
4:D:138:ASN:OD1	4:D:141:LEU:HB2	2.02	0.60
5:E:157:SER:C	5:E:159:ASP:N	2.57	0.60
7:G:1:MET:SD	7:G:79:PHE:CD1	2.95	0.60
11:K:68:PHE:N	11:K:68:PHE:CD2	2.67	0.60
15:T:22:BRU:H2'	15:T:23:DG:O4'	2.01	0.60
5:E:55:ARG:C	5:E:57:MET:H	2.08	0.60
7:G:80:LYS:O	7:G:80:LYS:HG2	2.02	0.60
12:L:32:ALA:HB3	12:L:55:ILE:CD1	2.31	0.60
1:A:12:ARG:HD2	2:B:1218:THR:HB	1.84	0.59
1:A:78:PRO:HA	2:B:1201:LYS:HZ2	1.67	0.59
1:A:311:GLN:O	1:A:312:PRO:C	2.45	0.59
1:A:1017:LEU:HB3	5:E:205:SER:HA	1.83	0.59
2:B:880:THR:O	2:B:881:ASN:HB2	2.01	0.59
3:C:2:SER:N	3:C:3:GLU:N	2.50	0.59
3:C:66:ARG:NH2	10:J:5:VAL:HG23	2.15	0.59
5:E:35:VAL:C	5:E:37:LEU:H	2.10	0.59
7:G:119:LEU:HD12	7:G:131:GLN:O	2.01	0.59
1:A:384:ASN:O	1:A:386:ASP:N	2.34	0.59
1:A:463:ILE:HD12	1:A:469:ARG:HD2	1.84	0.59
1:A:1120:LEU:HD13	1:A:1304:TRP:O	2.01	0.59
1:A:1451:VAL:O	1:A:1454:MET:HG2	2.02	0.59
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.32	0.59
2:B:542:MET:HE2	2:B:743:ILE:HG13	1.84	0.59
2:B:603:LEU:HD13	2:B:608:ASP:HB2	1.83	0.59
2:B:995:ARG:HH12	3:C:165:LYS:HG2	1.66	0.59
3:C:66:ARG:CZ	10:J:2:ILE:HG21	2.31	0.59
3:C:147:LEU:HD12	3:C:151:GLN:O	2.02	0.59
7:G:49:LEU:HG	7:G:76:ALA:HA	1.82	0.59
8:H:127:GLY:O	8:H:128:ASN:HB2	2.02	0.59
15:T:22:BRU:H2'	15:T:23:DG:H8	1.62	0.59
1:A:720:ARG:O	1:A:724:GLU:HB2	2.02	0.59
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.02	0.59
15:T:17:DT:C2'	15:T:18:DT:C5'	2.65	0.59
1:A:590:ARG:O	1:A:591:PHE:HB2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:THR:H	1:A:812:GLU:HB2	1.66	0.59
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.32	0.59
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.83	0.59
2:B:899:ILE:HD13	2:B:905:VAL:HG11	1.82	0.59
2:B:980:PHE:HD2	2:B:1094:ARG:HA	1.68	0.59
2:B:1079:LYS:HA	3:C:27:LEU:HD21	1.83	0.59
2:B:1106:ARG:HD3	2:B:1126:GLY:C	2.27	0.59
5:E:94:LYS:HE2	5:E:98:ILE:CD1	2.30	0.59
8:H:40:LEU:HD12	8:H:122:LEU:O	2.03	0.59
1:A:23:SER:HA	1:A:233:TRP:CD1	2.38	0.59
1:A:49:LYS:HZ3	1:A:61:ILE:HG13	1.67	0.59
1:A:405:VAL:HG22	1:A:432:VAL:HG13	1.85	0.59
1:A:738:LYS:HD2	1:A:740:LEU:HD21	1.84	0.59
1:A:1261:LYS:O	1:A:1264:GLU:HB3	2.03	0.59
2:B:34:ILE:HD13	2:B:747:MET:HE2	1.84	0.59
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.66	0.59
2:B:579:ARG:HG2	2:B:579:ARG:HH11	1.66	0.59
2:B:603:LEU:HD12	2:B:609:ILE:HG13	1.82	0.59
2:B:942:ARG:NH2	15:T:25:DT:P	2.75	0.59
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.35	0.59
7:G:99:PHE:CE2	7:G:115:MET:HE2	2.38	0.59
1:A:665:GLY:O	1:A:667:GLY:N	2.35	0.59
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.84	0.59
2:B:185:THR:H	2:B:188:ASP:CB	2.14	0.59
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.84	0.59
2:B:731:VAL:HG12	2:B:732:SER:N	2.17	0.59
10:J:44:TYR:H	10:J:44:TYR:HD2	1.48	0.59
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.83	0.59
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.18	0.59
2:B:616:ILE:HG13	2:B:697:GLU:HA	1.85	0.59
3:C:179:GLU:HG2	3:C:180:TYR:N	2.17	0.59
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.67	0.59
10:J:36:LEU:HD22	10:J:41:LEU:HD12	1.83	0.59
1:A:1107:VAL:HG12	1:A:1107:VAL:O	2.02	0.59
1:A:1385:THR:O	1:A:1387:HIS:N	2.36	0.59
2:B:1005:GLY:HA2	3:C:176:ILE:O	2.02	0.59
3:C:124:LEU:O	3:C:127:ARG:HG2	2.03	0.59
15:T:26:DC:H2''	15:T:27:DA:C5'	2.32	0.59
1:A:765:VAL:HG23	1:A:802:ASN:O	2.03	0.59
1:A:873:MET:C	1:A:1058:VAL:HG23	2.27	0.59
1:A:1224:LEU:HD12	1:A:1241:ARG:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:872:GLU:CD	2:B:914:LYS:HE2	2.28	0.59
4:D:13:ARG:HB2	4:D:17:LYS:HZ2	1.67	0.59
5:E:15:ALA:O	5:E:19:VAL:HG23	2.03	0.59
8:H:43:ASN:OD1	8:H:46:LEU:HG	2.03	0.59
1:A:75:ASN:O	1:A:76:GLU:CB	2.51	0.59
2:B:57:TYR:N	2:B:57:TYR:HD1	2.01	0.59
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.85	0.59
2:B:483:LEU:HD11	2:B:491:THR:CG2	2.33	0.59
1:A:1076:ALA:HA	1:A:1079:MET:HE2	1.85	0.58
2:B:431:TYR:CZ	2:B:447:ALA:HB2	2.38	0.58
2:B:594:ALA:HA	2:B:617:ARG:NH1	2.18	0.58
2:B:745:PRO:C	2:B:747:MET:N	2.60	0.58
5:E:156:LEU:HD12	5:E:195:VAL:HB	1.84	0.58
8:H:15:VAL:HG22	8:H:26:ILE:HG12	1.85	0.58
10:J:32:GLU:CD	10:J:32:GLU:H	2.10	0.58
1:A:42:ASP:C	1:A:44:THR:H	2.09	0.58
1:A:630:ILE:HD13	1:A:646:PHE:CZ	2.38	0.58
1:A:695:LYS:C	1:A:697:ALA:H	2.10	0.58
1:A:914:GLU:HB2	1:A:979:SER:O	2.03	0.58
2:B:1039:GLY:HA2	10:J:51:LEU:HD22	1.84	0.58
5:E:157:SER:HG	5:E:160:GLU:HG3	1.68	0.58
7:G:1:MET:SD	7:G:1:MET:O	2.61	0.58
10:J:64:ASN:CB	10:J:65:PRO:CD	2.81	0.58
1:A:33:ALA:HA	1:A:57:ARG:NH2	2.18	0.58
1:A:666:ILE:CD1	1:A:667:GLY:H	2.17	0.58
1:A:1116:LEU:HB2	1:A:1329:THR:OG1	2.03	0.58
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.03	0.58
8:H:38:LEU:HD12	8:H:124:ARG:O	2.03	0.58
15:T:14:DC:H1'	15:T:15:DT:H5'	1.86	0.58
1:A:444:PHE:HB2	1:A:458:HIS:HD2	1.68	0.58
2:B:225:VAL:HA	2:B:237:VAL:O	2.03	0.58
2:B:343:ILE:HG22	2:B:345:LYS:H	1.66	0.58
4:D:160:VAL:O	4:D:164:ILE:HG13	2.03	0.58
1:A:982:THR:O	1:A:985:ASP:HB2	2.04	0.58
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.33	0.58
2:B:57:TYR:N	2:B:57:TYR:CD1	2.70	0.58
2:B:309:GLN:OE1	9:I:52:ILE:HD11	2.04	0.58
2:B:864:LYS:N	2:B:872:GLU:OE1	2.37	0.58
5:E:178:ILE:HG22	5:E:213:ILE:O	2.04	0.58
6:F:111:LEU:H	6:F:111:LEU:CD1	2.13	0.58
1:A:224:PHE:HD2	1:A:229:SER:O	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:O	1:A:401:GLY:N	2.36	0.58
1:A:444:PHE:CB	1:A:458:HIS:HD2	2.15	0.58
2:B:344:LYS:O	2:B:345:LYS:HB2	2.03	0.58
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.85	0.58
4:D:53:SER:HB3	4:D:153:ARG:H	1.67	0.58
4:D:66:ARG:O	4:D:70:PHE:HB2	2.04	0.58
7:G:48:VAL:HG13	7:G:74:TYR:HD1	1.68	0.58
1:A:34:LYS:HB3	1:A:36:ARG:HE	1.69	0.58
1:A:49:LYS:HZ1	1:A:61:ILE:N	2.01	0.58
1:A:783:THR:HG21	1:A:815:PHE:CE2	2.39	0.58
1:A:964:ILE:O	1:A:967:ALA:N	2.37	0.58
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.33	0.58
1:A:1402:PHE:CD1	1:A:1403:GLU:HG3	2.38	0.58
2:B:990:ILE:HG22	2:B:991:GLY:N	2.19	0.58
2:B:1084:GLN:H	2:B:1084:GLN:HE21	1.50	0.58
2:B:1159:ARG:HE	2:B:1193:GLN:HE21	1.51	0.58
5:E:23:VAL:O	5:E:28:TYR:HB2	2.04	0.58
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.34	0.58
12:L:31:CYS:HB3	12:L:34:CYS:C	2.28	0.58
1:A:606:LEU:HB3	1:A:614:PHE:CE2	2.39	0.58
2:B:310:MET:HE1	2:B:387:LEU:CD1	2.33	0.58
2:B:830:TYR:O	2:B:831:SER:C	2.47	0.58
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.86	0.58
9:I:25:LEU:HB3	9:I:38:ALA:HB2	1.84	0.58
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.85	0.58
1:A:475:THR:CG2	1:A:476:SER:N	2.66	0.58
1:A:492:PRO:O	1:A:493:GLN:NE2	2.36	0.58
1:A:1001:ARG:O	1:A:1002:GLY:O	2.22	0.58
2:B:778:MET:CE	2:B:1094:ARG:CD	2.82	0.58
2:B:1159:ARG:HB3	2:B:1159:ARG:NH1	2.18	0.58
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.34	0.58
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.85	0.58
10:J:23:ASN:C	10:J:25:LEU:N	2.61	0.58
11:K:111:LEU:O	11:K:112:GLN:HG2	2.03	0.58
15:T:19:TT:H5R1	15:T:19:TT:H2'1	1.83	0.58
1:A:224:PHE:HZ	1:A:234:MET:HE2	1.68	0.58
2:B:265:SER:O	2:B:266:ALA:HB3	2.04	0.58
3:C:184:ASN:ND2	3:C:187:LYS:HA	2.19	0.58
4:D:53:SER:HB3	4:D:152:SER:CB	2.33	0.58
6:F:75:PRO:O	6:F:77:ASP:O	2.22	0.58
1:A:58:LEU:CG	1:A:59:GLY:N	2.66	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:ALA:CB	1:A:701:LEU:HG	2.34	0.57
1:A:1017:LEU:HB2	5:E:206:GLY:N	2.07	0.57
1:A:1305:VAL:HG12	1:A:1306:LEU:N	2.19	0.57
3:C:214:ASN:HB3	3:C:217:ASP:OD2	2.03	0.57
4:D:51:ASN:O	4:D:52:LEU:O	2.22	0.57
5:E:163:GLU:O	5:E:164:LEU:C	2.47	0.57
5:E:207:ARG:CB	5:E:207:ARG:HH11	2.16	0.57
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.29	0.57
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.03	0.57
2:B:229:ALA:CB	2:B:231:PRO:HD2	2.34	0.57
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.69	0.57
2:B:1033:LYS:NZ	2:B:1070:GLU:OE1	2.36	0.57
4:D:167:LEU:HB3	4:D:177:VAL:HG13	1.85	0.57
7:G:3:PHE:CE1	7:G:80:LYS:HE2	2.38	0.57
12:L:39:SER:O	12:L:40:LEU:HG	2.03	0.57
1:A:471:ASN:O	1:A:474:VAL:HG12	2.04	0.57
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.67	0.57
2:B:792:MET:HG3	2:B:855:PHE:HE1	1.69	0.57
2:B:910:VAL:HG12	2:B:912:ILE:H	1.69	0.57
4:D:134:THR:CG2	4:D:135:GLY:N	2.66	0.57
5:E:213:ILE:HG12	5:E:214:CYS:N	2.19	0.57
1:A:699:ALA:HB1	1:A:701:LEU:HG	1.85	0.57
1:A:754:SER:N	1:A:757:ASN:HD22	1.92	0.57
1:A:1369:ALA:O	1:A:1370:LEU:C	2.46	0.57
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.86	0.57
3:C:263:THR:C	3:C:265:MET:N	2.63	0.57
1:A:37:PHE:N	1:A:37:PHE:CD1	2.72	0.57
1:A:567:LYS:CG	1:A:568:PRO:CD	2.76	0.57
1:A:1373:ASP:HA	1:A:1376:THR:CG2	2.34	0.57
2:B:486:TYR:CZ	2:B:1096:ARG:HB3	2.39	0.57
2:B:996:ARG:NH2	3:C:175:ALA:HA	2.20	0.57
4:D:18:VAL:HG13	4:D:18:VAL:O	2.05	0.57
7:G:145:VAL:CG1	7:G:146:LYS:N	2.67	0.57
9:I:103:CYS:HB3	9:I:106:CYS:SG	2.45	0.57
14:P:4:A:O2'	14:P:5:C:H5'	2.05	0.57
1:A:42:ASP:HB3	1:A:45:GLN:N	2.19	0.57
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.86	0.57
1:A:709:THR:HG21	9:I:93:LYS:O	2.05	0.57
1:A:903:ASN:ND2	1:A:903:ASN:C	2.63	0.57
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.86	0.57
2:B:580:VAL:HG22	2:B:624:LEU:CB	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:654:ARG:C	2:B:656:GLY:H	2.11	0.57
2:B:769:TYR:C	2:B:771:SER:N	2.62	0.57
2:B:1159:ARG:HD3	2:B:1193:GLN:CG	2.35	0.57
2:B:1219:ASP:OD1	2:B:1219:ASP:O	2.23	0.57
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.86	0.57
5:E:124:VAL:HB	5:E:125:PRO:HD3	1.87	0.57
12:L:58:LYS:O	12:L:58:LYS:HG2	2.03	0.57
1:A:1111:MET:HE1	1:A:1330:ASN:OD1	2.05	0.57
1:A:1116:LEU:HB3	1:A:1308:THR:HG21	1.87	0.57
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.45	0.57
2:B:1023:VAL:O	2:B:1026:LEU:N	2.38	0.57
4:D:4:SER:OG	4:D:5:THR:N	2.34	0.57
1:A:58:LEU:CD1	1:A:243:PRO:HB3	2.33	0.57
1:A:699:ALA:O	1:A:700:ASN:HB3	2.04	0.57
1:A:1332:PHE:CE1	1:A:1348:LEU:HD13	2.39	0.57
2:B:332:ASP:OD1	2:B:336:ARG:NE	2.38	0.57
2:B:340:ALA:CB	2:B:343:ILE:HD12	2.35	0.57
7:G:154:VAL:HG12	7:G:155:SER:N	2.20	0.57
1:A:1226:VAL:HG13	1:A:1240:CYS:HB3	1.87	0.57
2:B:434:ARG:HA	2:B:437:GLU:CD	2.29	0.57
2:B:496:ARG:HB3	2:B:496:ARG:HH11	1.69	0.57
2:B:744:HIS:HD2	2:B:746:SER:CB	2.16	0.57
2:B:874:PHE:HA	2:B:913:GLY:O	2.05	0.57
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.18	0.57
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.87	0.57
4:D:4:SER:O	4:D:5:THR:HB	2.03	0.57
1:A:35:ILE:HD12	1:A:241:VAL:HG21	1.85	0.57
1:A:840:ARG:O	1:A:841:LEU:C	2.47	0.57
1:A:1095:THR:OG1	1:A:1113:THR:HB	2.05	0.57
1:A:1127:ASP:HB3	1:A:1130:GLN:CB	2.34	0.57
10:J:44:TYR:HA	10:J:47:ARG:HB3	1.87	0.57
1:A:406:ILE:HG13	1:A:431:LYS:HB2	1.87	0.56
1:A:600:PRO:HG2	1:A:601:LYS:H	1.70	0.56
1:A:709:THR:HB	1:A:712:GLU:HG3	1.87	0.56
2:B:176:SER:O	2:B:182:SER:HB3	2.04	0.56
2:B:386:LEU:O	2:B:388:CYS:N	2.37	0.56
3:C:11:ARG:HD3	3:C:209:TYR:CE2	2.39	0.56
3:C:212:PRO:CB	3:C:213:PRO:HD2	2.35	0.56
4:D:130:LEU:C	4:D:132:GLN:N	2.62	0.56
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.86	0.56
7:G:88:ASP:OD2	7:G:88:ASP:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:15:TYR:N	9:I:15:TYR:CD1	2.73	0.56
11:K:47:ARG:O	11:K:47:ARG:HD2	2.05	0.56
1:A:774:ARG:O	1:A:775:ILE:C	2.47	0.56
1:A:853:ASP:OD1	1:A:855:THR:N	2.38	0.56
1:A:982:THR:N	1:A:985:ASP:HB2	2.20	0.56
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.05	0.56
1:A:1450:LEU:HD21	7:G:18:PHE:O	2.04	0.56
2:B:288:ALA:HA	2:B:331:LEU:HD12	1.87	0.56
3:C:20:PHE:CE1	3:C:22:LEU:HD12	2.40	0.56
3:C:241:ASP:O	3:C:245:VAL:HG23	2.05	0.56
6:F:81:THR:HG23	6:F:144:GLU:OE2	2.06	0.56
9:I:62:ILE:O	9:I:62:ILE:HG12	2.05	0.56
1:A:31:SER:OG	1:A:82:GLY:HA2	2.04	0.56
1:A:222:LEU:O	1:A:224:PHE:N	2.38	0.56
1:A:244:PRO:HG2	1:A:245:PRO:HD3	1.86	0.56
1:A:412:ARG:NH2	2:B:1108:ARG:NH1	2.54	0.56
1:A:525:GLN:HG3	2:B:835:GLN:HG2	1.86	0.56
1:A:709:THR:HG22	1:A:710:LEU:N	2.20	0.56
1:A:711:ARG:NH2	9:I:87:GLN:OE1	2.39	0.56
1:A:866:PHE:O	1:A:867:ILE:HD12	2.06	0.56
1:A:869:GLY:O	5:E:204:THR:HG21	2.04	0.56
1:A:1072:ILE:O	1:A:1075:PRO:HD2	2.05	0.56
1:A:1279:ILE:CD1	1:A:1316:VAL:HG21	2.35	0.56
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.45	0.56
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.36	0.56
2:B:295:GLY:H	2:B:298:LEU:HD23	1.69	0.56
2:B:640:VAL:O	2:B:641:GLU:C	2.47	0.56
2:B:1006:ILE:HG22	10:J:45:CYS:HB3	1.87	0.56
2:B:1155:SER:OG	2:B:1156:ASP:N	2.37	0.56
3:C:33:LEU:O	3:C:34:ARG:C	2.48	0.56
5:E:168:TYR:HB2	5:E:170:LEU:HG	1.86	0.56
6:F:89:GLU:OE2	6:F:134:ILE:HG21	2.05	0.56
7:G:114:LEU:HG	7:G:162:SER:HB3	1.87	0.56
8:H:62:SER:C	8:H:64:ASN:H	2.13	0.56
9:I:2:THR:O	9:I:3:THR:C	2.47	0.56
9:I:82:GLU:O	9:I:104:LEU:HG	2.05	0.56
1:A:968:GLN:O	1:A:970:THR:N	2.38	0.56
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.04	0.56
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.41	0.56
2:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.87	0.56
2:B:1050:ILE:HG22	2:B:1051:THR:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:LEU:HD21	10:J:57:ILE:HD12	1.88	0.56
3:C:77:ILE:O	3:C:79:GLN:N	2.39	0.56
3:C:174:ALA:O	3:C:175:ALA:HB2	2.04	0.56
8:H:61:SER:O	8:H:62:SER:CB	2.54	0.56
10:J:44:TYR:CD2	10:J:44:TYR:N	2.73	0.56
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.88	0.56
1:A:168:GLY:O	1:A:169:ASN:C	2.47	0.56
1:A:626:ASN:O	1:A:631:HIS:CD2	2.59	0.56
1:A:974:ASP:C	1:A:976:THR:H	2.13	0.56
1:A:1124:HIS:HB3	1:A:1130:GLN:HG2	1.87	0.56
2:B:344:LYS:O	2:B:345:LYS:CB	2.53	0.56
2:B:831:SER:HB3	2:B:994:TYR:OH	2.05	0.56
4:D:191:ALA:C	4:D:193:THR:H	2.12	0.56
8:H:113:ALA:HB2	8:H:126:GLU:HG3	1.88	0.56
9:I:55:THR:CG2	9:I:58:VAL:HG21	2.36	0.56
9:I:92:ARG:HB3	9:I:95:THR:OG1	2.05	0.56
12:L:58:LYS:O	12:L:59:ALA:O	2.24	0.56
1:A:867:ILE:HG22	1:A:872:GLY:N	2.21	0.56
1:A:1376:THR:O	1:A:1377:THR:C	2.48	0.56
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.87	0.56
2:B:449:ASN:C	2:B:451:LYS:H	2.13	0.56
2:B:758:PHE:CE1	2:B:1027:ILE:CG2	2.88	0.56
2:B:776:GLN:O	2:B:1095:LEU:HA	2.06	0.56
6:F:99:LEU:O	6:F:99:LEU:HD12	2.05	0.56
7:G:111:THR:HG22	7:G:113:HIS:N	2.17	0.56
8:H:39:THR:O	8:H:123:MET:HA	2.06	0.56
8:H:100:THR:HG22	8:H:101:ALA:N	2.20	0.56
10:J:44:TYR:HD2	10:J:44:TYR:N	2.03	0.56
14:P:3:G:H2'	14:P:4:A:C8	2.41	0.56
1:A:89:PRO:HB2	1:A:204:THR:HG22	1.87	0.56
1:A:528:LEU:O	1:A:528:LEU:HD12	2.05	0.56
1:A:806:ARG:HH12	2:B:729:ILE:CD1	2.18	0.56
2:B:521:LEU:HD13	2:B:633:VAL:HB	1.86	0.56
2:B:789:MET:HE2	2:B:953:LEU:HD22	1.87	0.56
3:C:176:ILE:HG22	3:C:177:GLU:N	2.21	0.56
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.86	0.56
2:B:337:ARG:C	2:B:338:GLY:N	2.64	0.56
2:B:343:ILE:HG21	2:B:348:ARG:H	1.70	0.56
2:B:357:GLN:O	2:B:366:GLN:HA	2.04	0.56
2:B:388:CYS:C	2:B:390:LEU:H	2.13	0.56
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:658:ILE:HG22	2:B:659:ALA:N	2.21	0.56
2:B:1002:THR:HG23	2:B:1006:ILE:HG13	1.88	0.56
10:J:36:LEU:O	10:J:39:LEU:N	2.37	0.56
14:P:7:A:H2'	14:P:8:G:C1'	2.36	0.56
1:A:55:ASP:CG	1:A:55:ASP:O	2.46	0.56
1:A:442:VAL:HB	1:A:489:LEU:HD11	1.87	0.56
1:A:590:ARG:HB3	1:A:605:MET:N	2.20	0.56
1:A:1387:HIS:NE2	13:N:4:DT:H5''	2.21	0.56
1:A:1410:PHE:HA	2:B:1212:ILE:CD1	2.35	0.56
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.88	0.56
2:B:466:TRP:HA	2:B:466:TRP:CE3	2.41	0.56
2:B:705:MET:H	2:B:710:LEU:CD1	2.19	0.56
2:B:843:GLN:O	2:B:846:ILE:HB	2.06	0.56
2:B:882:THR:HG21	2:B:935:ARG:HA	1.87	0.56
5:E:105:PHE:O	5:E:106:GLN:HB2	2.06	0.56
8:H:61:SER:HB2	8:H:139:ASN:HB3	1.87	0.56
1:A:2:VAL:HG21	2:B:1157:ALA:C	2.31	0.56
1:A:920:LEU:HD23	1:A:921:GLY:N	2.20	0.56
1:A:929:LEU:HD23	1:A:983:ILE:HG21	1.88	0.56
1:A:942:PHE:HD2	1:A:943:LEU:HD23	1.70	0.56
4:D:17:LYS:CA	4:D:17:LYS:HE3	2.35	0.56
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.87	0.56
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.86	0.55
1:A:108:MET:N	1:A:108:MET:SD	2.79	0.55
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.87	0.55
1:A:446:ARG:HB2	1:A:487:MET:SD	2.47	0.55
1:A:730:GLY:C	1:A:732:LEU:N	2.62	0.55
1:A:1397:LEU:HB2	1:A:1426:GLU:OE1	2.05	0.55
2:B:53:GLN:HG2	2:B:547:VAL:CG2	2.35	0.55
2:B:360:PHE:C	2:B:360:PHE:CD2	2.84	0.55
2:B:1166:CYS:SG	2:B:1166:CYS:O	2.63	0.55
4:D:47:LEU:HD11	7:G:3:PHE:CE2	2.40	0.55
7:G:81:PRO:HB3	7:G:106:MET:HE1	1.87	0.55
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.33	0.55
1:A:302:THR:HA	1:A:305:ASP:O	2.05	0.55
1:A:449:SER:O	2:B:1133:MET:HB3	2.06	0.55
1:A:883:LEU:HD11	1:A:1017:LEU:HD11	1.87	0.55
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.35	0.55
1:A:1377:THR:O	1:A:1379:GLY:N	2.39	0.55
2:B:51:PHE:O	2:B:54:PHE:HB3	2.06	0.55
2:B:114:PRO:O	2:B:116:GLU:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.36	0.55
2:B:472:ALA:C	2:B:474:SER:H	2.14	0.55
3:C:18:VAL:O	3:C:20:PHE:HD2	1.90	0.55
6:F:118:LEU:O	6:F:122:MET:HG3	2.06	0.55
8:H:89:LEU:C	8:H:91:ASP:H	2.13	0.55
9:I:106:CYS:O	9:I:107:SER:HB2	2.07	0.55
11:K:110:ASN:O	11:K:111:LEU:CD2	2.50	0.55
1:A:42:ASP:HB3	1:A:45:GLN:HA	1.88	0.55
1:A:785:PRO:HG2	1:A:786:HIS:HD2	1.71	0.55
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.41	0.55
1:A:1444:MET:HE1	6:F:135:ARG:CB	2.34	0.55
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.41	0.55
4:D:52:LEU:HD21	4:D:147:TYR:HE2	1.71	0.55
6:F:89:GLU:HB3	6:F:134:ILE:CD1	2.35	0.55
7:G:1:MET:SD	7:G:1:MET:C	2.89	0.55
7:G:83:LYS:HE2	7:G:150:CYS:H	1.72	0.55
8:H:4:THR:CA	8:H:60:ALA:HB2	2.32	0.55
8:H:64:ASN:O	8:H:65:LEU:HB2	2.05	0.55
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.36	0.55
15:T:10:DA:H2"	15:T:11:DG:OP2	2.06	0.55
1:A:23:SER:O	1:A:24:PRO:C	2.48	0.55
1:A:60:SER:C	1:A:61:ILE:HG13	2.29	0.55
1:A:364:VAL:O	1:A:364:VAL:HG13	2.06	0.55
1:A:595:THR:O	1:A:596:THR:HG23	2.05	0.55
1:A:852:TYR:CD2	1:A:1060:PRO:CB	2.89	0.55
1:A:1076:ALA:HA	1:A:1079:MET:CE	2.36	0.55
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.40	0.55
4:D:128:VAL:O	4:D:132:GLN:HG3	2.06	0.55
7:G:47:CYS:O	7:G:76:ALA:HB1	2.06	0.55
9:I:86:PHE:HE1	9:I:100:PHE:HB2	1.71	0.55
10:J:8:PHE:H	10:J:49:MET:HE3	1.72	0.55
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.88	0.55
1:A:42:ASP:HB3	1:A:45:GLN:CA	2.36	0.55
1:A:61:ILE:O	1:A:63:ARG:N	2.40	0.55
1:A:64:ASN:O	1:A:65:LEU:C	2.50	0.55
1:A:341:MET:HE2	1:A:843:LYS:HZ3	1.70	0.55
1:A:427:GLN:HB2	1:A:430:TRP:CD1	2.42	0.55
1:A:670:ILE:HG23	1:A:805:LEU:HD21	1.86	0.55
1:A:742:ASN:O	1:A:745:GLN:HB2	2.05	0.55
1:A:896:ARG:NH2	1:A:1030:ARG:NH2	2.54	0.55
1:A:1114:PRO:O	1:A:1115:SER:O	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.89	0.55
4:D:7:THR:O	4:D:9:GLN:N	2.40	0.55
6:F:69:LEU:N	6:F:70:LYS:CA	2.69	0.55
6:F:125:LEU:HG	6:F:125:LEU:O	2.07	0.55
6:F:143:PHE:C	6:F:143:PHE:CD1	2.85	0.55
8:H:55:LEU:HD22	8:H:144:ILE:CG2	2.36	0.55
1:A:316:GLN:O	1:A:317:LYS:C	2.49	0.55
1:A:919:ILE:O	1:A:920:LEU:C	2.50	0.55
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.42	0.55
2:B:466:TRP:O	2:B:468:GLU:N	2.39	0.55
2:B:1002:THR:HG21	2:B:1006:ILE:CD1	2.30	0.55
3:C:167:HIS:CD2	3:C:168:ALA:H	2.23	0.55
9:I:52:ILE:HG13	9:I:52:ILE:O	2.06	0.55
11:K:47:ARG:HD2	11:K:47:ARG:C	2.32	0.55
11:K:69:ALA:O	11:K:70:ARG:HB3	2.06	0.55
1:A:17:VAL:HA	2:B:1215:ARG:O	2.06	0.55
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.32	0.55
1:A:608:ILE:C	1:A:610:GLY:N	2.63	0.55
1:A:858:ASN:C	1:A:858:ASN:ND2	2.59	0.55
2:B:729:ILE:O	2:B:729:ILE:HG22	2.04	0.55
2:B:792:MET:HA	2:B:856:PHE:O	2.06	0.55
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.06	0.55
2:B:1087:PHE:HD2	2:B:1088:GLY:H	1.50	0.55
3:C:243:VAL:O	3:C:243:VAL:HG12	2.05	0.55
7:G:10:ASN:OD1	7:G:71:ASN:HA	2.07	0.55
7:G:20:PRO:HG2	7:G:21:ARG:H	1.70	0.55
15:T:17:DT:HI'	15:T:18:DT:C5'	2.33	0.55
1:A:14:VAL:CG2	2:B:1216:LEU:HD13	2.34	0.55
1:A:68:GLN:O	1:A:70:CYS:N	2.39	0.55
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.88	0.55
1:A:687:LYS:O	1:A:690:VAL:HB	2.06	0.55
1:A:960:ILE:O	1:A:961:ARG:C	2.50	0.55
1:A:1039:LYS:HE3	1:A:1043:ASP:OD2	2.07	0.55
1:A:1151:GLU:HA	9:I:44:TYR:O	2.07	0.55
1:A:1215:ARG:HA	1:A:1218:GLN:HG2	1.89	0.55
1:A:1450:LEU:HD11	6:F:108:PHE:CZ	2.41	0.55
2:B:44:VAL:O	2:B:45:SER:C	2.49	0.55
2:B:130:VAL:HB	2:B:167:ILE:CD1	2.36	0.55
2:B:1102:LYS:O	2:B:1103:ILE:C	2.49	0.55
3:C:90:ASP:O	3:C:91:HIS:HB3	2.05	0.55
6:F:85:MET:HE2	6:F:93:ILE:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:48:ARG:HD2	10:J:49:MET:N	2.21	0.55
14:P:6:C:H2'	14:P:7:A:H8	1.68	0.55
1:A:343:LYS:NZ	2:B:1151:LEU:O	2.40	0.55
1:A:432:VAL:O	1:A:433:GLU:C	2.49	0.55
2:B:310:MET:CE	2:B:387:LEU:HD12	2.37	0.55
2:B:1077:THR:HG22	11:K:44:ASN:HD21	1.71	0.55
4:D:24:ALA:C	4:D:26:THR:H	2.15	0.55
5:E:13:TRP:O	5:E:16:PHE:HB3	2.07	0.55
9:I:61:ASP:C	9:I:63:GLY:N	2.63	0.55
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.42	0.55
1:A:47:ARG:HH12	1:A:254:GLU:HG2	1.72	0.55
1:A:1364:ASN:HD22	1:A:1365:TYR:N	2.05	0.55
2:B:129:PHE:HA	2:B:165:VAL:O	2.07	0.55
2:B:343:ILE:CG2	2:B:348:ARG:N	2.66	0.55
2:B:654:ARG:H	2:B:657:HIS:CD2	2.17	0.55
4:D:7:THR:HB	7:G:42:PHE:HE2	1.72	0.55
1:A:130:ASP:O	1:A:131:SER:C	2.50	0.54
1:A:548:ASN:HA	11:K:60:ALA:HB1	1.89	0.54
1:A:1120:LEU:N	1:A:1120:LEU:CD1	2.69	0.54
2:B:758:PHE:HE1	2:B:1027:ILE:HG22	1.72	0.54
2:B:911:ILE:O	2:B:912:ILE:HG13	2.07	0.54
3:C:189:THR:HG22	3:C:190:ASP:H	1.71	0.54
7:G:18:PHE:HA	7:G:22:MET:CE	2.36	0.54
1:A:50:ILE:C	1:A:52:GLY:N	2.65	0.54
1:A:182:VAL:HG22	1:A:201:VAL:HA	1.89	0.54
1:A:265:LYS:HE2	1:A:322:VAL:HG11	1.89	0.54
1:A:853:ASP:OD1	1:A:853:ASP:C	2.50	0.54
1:A:1308:THR:HG23	1:A:1309:ASP:N	2.22	0.54
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.07	0.54
1:A:1424:VAL:CG1	1:A:1436:ILE:HD11	2.34	0.54
2:B:847:ASP:C	2:B:849:GLY:H	2.14	0.54
3:C:97:VAL:HG12	3:C:99:LEU:CD2	2.37	0.54
4:D:48:ILE:HG21	7:G:4:ILE:HB	1.89	0.54
4:D:63:LEU:HD13	4:D:133:THR:OG1	2.07	0.54
9:I:50:THR:HG22	9:I:52:ILE:H	1.72	0.54
10:J:48:ARG:HE	10:J:49:MET:HE2	1.72	0.54
1:A:1343:ALA:HB2	5:E:150:VAL:HG22	1.88	0.54
1:A:1445:ILE:HD11	7:G:68:ALA:HB1	1.90	0.54
2:B:38:PHE:CD1	2:B:811:TYR:CD2	2.94	0.54
2:B:834:ASN:HA	2:B:838:SER:O	2.06	0.54
2:B:1165:ILE:HG12	4:D:17:LYS:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:64:VAL:C	4:D:66:ARG:H	2.14	0.54
4:D:185:CYS:HB2	4:D:211:LEU:HD22	1.88	0.54
1:A:44:THR:O	1:A:45:GLN:HB2	2.07	0.54
1:A:527:THR:HG23	1:A:650:GLN:HA	1.89	0.54
2:B:129:PHE:HE2	2:B:166:PHE:HD1	1.56	0.54
2:B:496:ARG:NH1	2:B:539:LEU:HB2	2.22	0.54
2:B:542:MET:HG2	2:B:747:MET:HB3	1.89	0.54
2:B:841:MET:O	2:B:993:THR:HA	2.08	0.54
2:B:879:ARG:HH11	2:B:883:LEU:CD2	2.17	0.54
2:B:1187:ASN:O	2:B:1188:LYS:CB	2.49	0.54
7:G:143:ILE:CG2	7:G:144:ARG:N	2.71	0.54
8:H:116:TYR:HE2	8:H:140:ALA:CB	2.19	0.54
9:I:101:PHE:N	9:I:101:PHE:CD1	2.76	0.54
1:A:18:GLN:CB	2:B:1215:ARG:HB2	2.38	0.54
1:A:306:ASN:HB2	1:A:324:SER:HB3	1.90	0.54
2:B:287:ARG:NH1	2:B:324:ILE:O	2.41	0.54
2:B:305:VAL:O	2:B:305:VAL:HG12	2.07	0.54
2:B:865:LYS:NZ	2:B:869:SER:HA	2.23	0.54
7:G:26:LEU:O	7:G:27:LYS:C	2.50	0.54
1:A:340:LEU:HD21	2:B:1200:ALA:N	2.23	0.54
1:A:814:PHE:O	1:A:817:ALA:HB3	2.08	0.54
2:B:372:SER:O	2:B:376:PHE:HD1	1.90	0.54
2:B:1159:ARG:HD2	2:B:1159:ARG:C	2.33	0.54
3:C:100:THR:HG22	3:C:101:LEU:H	1.71	0.54
14:P:7:A:H2'	14:P:8:G:O4'	2.08	0.54
1:A:381:THR:HG21	1:A:383:TYR:CD1	2.43	0.54
1:A:401:GLY:C	1:A:435:HIS:CD2	2.86	0.54
2:B:25:ILE:HD11	2:B:653:VAL:O	2.08	0.54
2:B:479:VAL:O	2:B:480:SER:HB3	2.07	0.54
3:C:70:ILE:HD11	3:C:144:ILE:CG1	2.38	0.54
6:F:69:LEU:N	6:F:70:LYS:N	2.56	0.54
7:G:15:PRO:O	7:G:16:SER:C	2.50	0.54
7:G:111:THR:HB	7:G:114:LEU:HB2	1.90	0.54
8:H:58:THR:HG22	8:H:59:ILE:N	2.22	0.54
1:A:4:GLN:O	1:A:5:GLN:HB2	2.07	0.54
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.29	0.54
2:B:687:GLU:O	2:B:689:LEU:HG	2.08	0.54
2:B:705:MET:N	2:B:710:LEU:HD12	2.23	0.54
2:B:850:LEU:HD12	2:B:851:PHE:H	1.72	0.54
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.38	0.54
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1001:PHE:CE2	3:C:34:ARG:CZ	2.90	0.54
2:B:1023:VAL:O	2:B:1026:LEU:HB2	2.08	0.54
3:C:235:VAL:HG13	10:J:13:VAL:CG2	2.37	0.54
5:E:55:ARG:C	5:E:57:MET:N	2.61	0.54
1:A:71:GLN:O	1:A:73:GLY:N	2.37	0.54
1:A:1336:MET:HE3	1:A:1381:LEU:HG	1.90	0.54
1:A:1364:ASN:O	1:A:1365:TYR:C	2.51	0.54
2:B:63:ILE:O	2:B:67:SER:HB3	2.08	0.54
2:B:942:ARG:NH2	15:T:25:DT:OP2	2.39	0.54
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.08	0.54
9:I:26:LEU:CD2	9:I:37:GLU:HA	2.33	0.54
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.41	0.54
11:K:31:VAL:CG1	11:K:32:VAL:N	2.71	0.54
1:A:164:ARG:HG3	1:A:165:GLY:H	1.72	0.54
1:A:535:THR:CG2	1:A:616:VAL:HA	2.35	0.54
1:A:787:PHE:CE1	1:A:796:SER:HA	2.43	0.54
1:A:821:ARG:HB2	1:A:821:ARG:NH1	2.18	0.54
1:A:857:ARG:NH1	6:F:139:PRO:HB2	2.23	0.54
1:A:863:VAL:HG11	1:A:866:PHE:CD2	2.42	0.54
1:A:966:ASN:O	1:A:967:ALA:C	2.51	0.54
1:A:1162:VAL:O	1:A:1162:VAL:HG12	2.06	0.54
1:A:1171:GLN:HA	1:A:1174:PHE:HE1	1.71	0.54
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.15	0.54
2:B:217:ARG:HD2	2:B:217:ARG:O	2.07	0.54
2:B:502:ILE:H	2:B:502:ILE:CD1	2.07	0.54
2:B:860:MET:HG2	2:B:861:ASP:N	2.23	0.54
3:C:254:LYS:C	3:C:256:ALA:H	2.16	0.54
11:K:47:ARG:HD3	11:K:59:ALA:O	2.07	0.54
11:K:55:LYS:HB2	11:K:81:TYR:HE1	1.73	0.54
1:A:187:LYS:HE3	1:A:198:GLU:OE2	2.08	0.53
1:A:500:GLU:OE2	2:B:1145:SER:HB2	2.08	0.53
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.22	0.53
1:A:1369:ALA:O	1:A:1372:VAL:HG12	2.08	0.53
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.89	0.53
2:B:843:GLN:O	2:B:844:SER:C	2.50	0.53
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.90	0.53
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.43	0.53
3:C:208:GLU:C	3:C:210:GLU:H	2.15	0.53
4:D:135:GLY:C	4:D:137:ASN:H	2.15	0.53
1:A:590:ARG:HB2	1:A:605:MET:HB3	1.90	0.53
1:A:1259:MET:C	1:A:1261:LYS:H	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1313:LEU:O	1:A:1315:GLU:N	2.41	0.53
2:B:327:ARG:O	2:B:331:LEU:HD13	2.07	0.53
2:B:386:LEU:O	2:B:387:LEU:C	2.50	0.53
2:B:582:VAL:HG23	2:B:626:ILE:HB	1.90	0.53
2:B:1189:ILE:HG22	2:B:1190:ASP:N	2.22	0.53
3:C:73:GLN:HB3	3:C:131:HIS:H	1.73	0.53
11:K:52:ASN:O	11:K:53:ASP:C	2.51	0.53
1:A:886:ILE:HG13	1:A:943:LEU:HD12	1.89	0.53
2:B:1077:THR:HG22	11:K:44:ASN:ND2	2.23	0.53
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.23	0.53
7:G:138:THR:CG2	7:G:139:ILE:H	2.00	0.53
11:K:109:TRP:O	11:K:111:LEU:N	2.39	0.53
12:L:32:ALA:CB	12:L:55:ILE:HD12	2.39	0.53
1:A:761:MET:HA	1:A:804:TYR:HB2	1.89	0.53
1:A:958:VAL:O	1:A:958:VAL:HG12	2.08	0.53
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.42	0.53
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.43	0.53
2:B:1182:CYS:O	2:B:1183:LYS:C	2.51	0.53
3:C:177:GLU:HG3	3:C:231:ASN:HD22	1.73	0.53
11:K:55:LYS:CB	11:K:81:TYR:HE1	2.21	0.53
1:A:1059:HIS:O	1:A:1060:PRO:C	2.52	0.53
1:A:1120:LEU:CD1	1:A:1120:LEU:H	2.21	0.53
4:D:192:LYS:HB3	4:D:192:LYS:HZ3	1.73	0.53
4:D:198:LEU:O	4:D:200:ASN:N	2.42	0.53
5:E:207:ARG:NH1	5:E:207:ARG:HB2	2.23	0.53
7:G:35:GLU:OE2	7:G:48:VAL:HG23	2.08	0.53
1:A:53:LEU:CD2	1:A:54:ASN:N	2.51	0.53
1:A:90:VAL:HG13	1:A:297:GLN:HA	1.90	0.53
1:A:666:ILE:HD12	1:A:666:ILE:N	2.23	0.53
1:A:816:HIS:CD2	2:B:764:SER:HB2	2.43	0.53
1:A:982:THR:HB	1:A:985:ASP:N	2.23	0.53
2:B:34:ILE:O	2:B:35:SER:C	2.52	0.53
2:B:412:LEU:HB3	2:B:466:TRP:CZ2	2.43	0.53
4:D:59:ILE:O	4:D:60:LYS:C	2.50	0.53
4:D:156:ASP:C	4:D:158:GLU:H	2.15	0.53
7:G:91:VAL:HB	7:G:139:ILE:O	2.08	0.53
1:A:351:THR:HG21	2:B:1103:ILE:HG13	1.91	0.53
1:A:420:ARG:O	1:A:421:ALA:C	2.50	0.53
1:A:446:ARG:CD	1:A:480:ALA:HB2	2.39	0.53
1:A:1341:ILE:HG23	1:A:1342:GLU:H	1.74	0.53
2:B:408:LEU:HG	2:B:409:ALA:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:769:TYR:C	2:B:771:SER:H	2.16	0.53
4:D:56:ARG:HD3	4:D:149:THR:HA	1.91	0.53
1:A:288:ALA:HA	1:A:291:GLU:OE2	2.09	0.53
1:A:407:ARG:HG2	1:A:430:TRP:CZ3	2.44	0.53
1:A:478:TYR:O	1:A:479:ASN:HB3	2.08	0.53
1:A:603:ASN:O	1:A:604:GLY:C	2.51	0.53
2:B:343:ILE:CB	2:B:348:ARG:HG3	2.37	0.53
2:B:1166:CYS:O	2:B:1168:LEU:N	2.41	0.53
2:B:1180:PHE:O	2:B:1181:GLU:O	2.27	0.53
3:C:239:PRO:HB2	3:C:241:ASP:OD1	2.08	0.53
4:D:53:SER:HB3	4:D:152:SER:HB2	1.91	0.53
6:F:124:GLU:HB3	6:F:130:ILE:HG12	1.90	0.53
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.74	0.53
2:B:54:PHE:O	2:B:58:THR:HB	2.09	0.53
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.39	0.53
2:B:1162:ILE:C	2:B:1171:VAL:HG21	2.34	0.53
3:C:120:ILE:HD13	3:C:124:LEU:HD21	1.91	0.53
3:C:215:GLU:O	3:C:216:GLY:C	2.51	0.53
7:G:117:GLN:C	7:G:119:LEU:H	2.17	0.53
9:I:111:THR:CG2	9:I:112:SER:N	2.72	0.53
9:I:112:SER:O	9:I:114:GLN:N	2.42	0.53
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.73	0.53
14:P:1:U:H2'	14:P:2:C:C6	2.43	0.53
15:T:22:BRU:H2''	15:T:23:DG:O4'	2.09	0.53
1:A:353:ILE:HD12	1:A:470:LEU:HD21	1.91	0.53
1:A:645:LEU:HD11	1:A:649:ILE:HD11	1.91	0.53
1:A:1153:TYR:CE1	9:I:42:LEU:HD13	2.44	0.53
1:A:1444:MET:HG2	7:G:60:ARG:HA	1.91	0.53
2:B:756:ILE:O	2:B:759:PRO:HD3	2.08	0.53
2:B:839:MET:CE	2:B:1010:LEU:HD21	2.38	0.53
3:C:82:TYR:O	3:C:83:SER:C	2.51	0.53
4:D:208:GLU:O	4:D:212:LYS:HG3	2.08	0.53
6:F:86:THR:HG23	6:F:89:GLU:OE1	2.09	0.53
7:G:44:TYR:CD2	7:G:105:PRO:HB2	2.44	0.53
13:N:0:DT:H1'	13:N:1:DA:H5'	1.90	0.53
1:A:71:GLN:C	1:A:73:GLY:H	2.16	0.52
1:A:282:ASN:O	1:A:284:ALA:N	2.42	0.52
1:A:427:GLN:O	1:A:428:TYR:C	2.52	0.52
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.42	0.52
1:A:600:PRO:C	1:A:602:ASP:H	2.16	0.52
1:A:828:ALA:HB1	2:B:530:GLY:HA2	1.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1214:GLU:O	1:A:1218:GLN:HG2	2.10	0.52
2:B:412:LEU:HB3	2:B:466:TRP:HZ2	1.74	0.52
3:C:87:PHE:H	3:C:87:PHE:HD1	1.56	0.52
4:D:19:GLU:O	4:D:21:GLU:N	2.42	0.52
8:H:123:MET:HE1	8:H:142:LEU:HD11	1.90	0.52
9:I:99:LEU:O	9:I:111:THR:HG23	2.09	0.52
9:I:115:LYS:CD	9:I:117:LYS:HE3	2.35	0.52
11:K:60:ALA:O	11:K:73:LEU:HD12	2.09	0.52
14:P:8:G:H8	14:P:8:G:OP2	1.91	0.52
1:A:19:PHE:HB3	1:A:1413:GLY:HA2	1.90	0.52
1:A:341:MET:CE	2:B:1135:ARG:NH1	2.70	0.52
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.44	0.52
1:A:1187:GLN:O	1:A:1243:VAL:HG13	2.09	0.52
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.09	0.52
2:B:683:SER:C	2:B:685:LEU:H	2.15	0.52
2:B:792:MET:HE2	2:B:857:ARG:NH2	2.24	0.52
2:B:954:VAL:O	12:L:55:ILE:O	2.28	0.52
2:B:1183:LYS:N	2:B:1183:LYS:CE	2.72	0.52
3:C:263:THR:O	3:C:265:MET:N	2.43	0.52
5:E:168:TYR:CB	5:E:170:LEU:HG	2.38	0.52
7:G:1:MET:O	7:G:3:PHE:CE1	2.63	0.52
7:G:138:THR:HG22	7:G:139:ILE:HG13	1.90	0.52
11:K:110:ASN:C	11:K:111:LEU:HG	2.34	0.52
1:A:54:ASN:HB3	1:A:247:ARG:HH22	1.74	0.52
1:A:89:PRO:HB2	1:A:204:THR:CG2	2.39	0.52
1:A:682:THR:HG23	1:A:728:LYS:HE3	1.91	0.52
1:A:963:ILE:HD13	1:A:1049:ILE:HG13	1.90	0.52
1:A:1377:THR:O	1:A:1378:GLN:C	2.52	0.52
2:B:95:ILE:HG13	2:B:129:PHE:O	2.08	0.52
2:B:102:VAL:CG2	2:B:112:LEU:HD22	2.39	0.52
2:B:546:SER:OG	2:B:631:GLY:N	2.39	0.52
4:D:29:LEU:HD22	7:G:82:PHE:CD2	2.44	0.52
5:E:78:LEU:HD23	5:E:79:TRP:N	2.24	0.52
1:A:108:MET:HB3	1:A:210:ILE:CD1	2.39	0.52
1:A:317:LYS:O	1:A:318:SER:HB3	2.09	0.52
1:A:618:GLU:O	1:A:619:LYS:C	2.52	0.52
1:A:722:LEU:HD22	1:A:799:PHE:CD1	2.44	0.52
2:B:223:VAL:HG21	2:B:380:TYR:HE2	1.75	0.52
2:B:459:TYR:C	2:B:459:TYR:CD2	2.88	0.52
2:B:525:ALA:O	2:B:768:THR:HG23	2.09	0.52
2:B:787:VAL:O	2:B:787:VAL:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:980:PHE:CD2	2:B:1094:ARG:HA	2.44	0.52
3:C:31:ASN:O	3:C:32:SER:C	2.51	0.52
6:F:94:LEU:HD21	6:F:122:MET:HA	1.92	0.52
7:G:51:TYR:O	7:G:54:ILE:HG13	2.10	0.52
7:G:115:MET:HB3	7:G:116:PRO:HD2	1.91	0.52
1:A:92:HIS:O	1:A:95:PHE:N	2.36	0.52
1:A:401:GLY:C	1:A:435:HIS:HD2	2.16	0.52
1:A:475:THR:HG23	1:A:476:SER:N	2.25	0.52
1:A:1095:THR:O	1:A:1096:SER:CB	2.57	0.52
2:B:274:PRO:O	2:B:275:TYR:HB2	2.09	0.52
2:B:657:HIS:CE1	2:B:689:LEU:HD11	2.45	0.52
2:B:1201:LYS:O	2:B:1204:PHE:HB2	2.09	0.52
3:C:76:ASP:OD2	3:C:128:ASN:N	2.41	0.52
7:G:79:PHE:CZ	7:G:106:MET:HE2	2.45	0.52
8:H:102:TYR:N	8:H:102:TYR:CD2	2.77	0.52
13:N:3:DG:C1'	13:N:4:DT:H5'	2.38	0.52
1:A:78:PRO:HA	2:B:1201:LYS:NZ	2.24	0.52
1:A:244:PRO:O	1:A:246:VAL:N	2.43	0.52
1:A:325:ILE:O	1:A:326:ARG:C	2.52	0.52
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.92	0.52
1:A:567:LYS:HE3	8:H:46:LEU:HD12	1.91	0.52
1:A:836:TYR:HB2	15:T:18:DT:H4'	1.92	0.52
1:A:838:GLN:O	1:A:842:VAL:HG23	2.09	0.52
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.74	0.52
3:C:66:ARG:NH1	3:C:144:ILE:O	2.43	0.52
3:C:254:LYS:C	3:C:256:ALA:N	2.67	0.52
11:K:40:HIS:O	11:K:41:THR:C	2.53	0.52
1:A:317:LYS:O	1:A:318:SER:CB	2.57	0.52
1:A:881:GLN:O	1:A:953:ASN:HA	2.10	0.52
1:A:1394:THR:CG2	1:A:1398:MET:SD	2.89	0.52
2:B:34:ILE:O	2:B:37:PHE:N	2.41	0.52
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.91	0.52
2:B:1095:LEU:HD12	2:B:1095:LEU:N	2.21	0.52
7:G:1:MET:HG3	7:G:85:GLU:OE2	2.10	0.52
8:H:4:THR:O	8:H:5:LEU:HD23	2.09	0.52
8:H:142:LEU:C	8:H:143:LEU:HD12	2.35	0.52
11:K:63:VAL:HG23	11:K:63:VAL:O	2.09	0.52
1:A:40:THR:HG22	1:A:41:MET:CG	2.28	0.52
1:A:541:ILE:HG21	1:A:549:MET:CE	2.39	0.52
1:A:956:LEU:HD23	1:A:957:PRO:HD2	1.92	0.52
1:A:1410:PHE:HA	2:B:1212:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:496:ARG:HH12	2:B:539:LEU:HB2	1.75	0.52
2:B:654:ARG:N	2:B:657:HIS:HD2	2.04	0.52
2:B:794:ASN:C	2:B:795:ILE:HD12	2.35	0.52
2:B:899:ILE:O	2:B:952:VAL:HG21	2.09	0.52
2:B:1022:THR:HG23	2:B:1022:THR:O	2.09	0.52
2:B:1064:TYR:O	2:B:1065:GLN:C	2.53	0.52
2:B:1099:VAL:HG12	2:B:1100:ASP:N	2.24	0.52
2:B:1177:HIS:O	2:B:1179:GLN:N	2.42	0.52
3:C:167:HIS:CD2	3:C:169:LYS:H	2.27	0.52
3:C:242:GLN:C	3:C:244:VAL:H	2.16	0.52
3:C:256:ALA:O	3:C:259:LEU:N	2.42	0.52
5:E:17:ARG:O	5:E:20:LYS:HB2	2.10	0.52
6:F:125:LEU:N	6:F:130:ILE:HD11	2.23	0.52
7:G:30:LEU:HD22	7:G:72:VAL:HG11	1.92	0.52
8:H:84:ALA:HA	8:H:87:ARG:CB	2.34	0.52
9:I:13:MET:HG3	9:I:14:LEU:N	2.23	0.52
1:A:30:ILE:HD11	2:B:1168:LEU:HD13	1.92	0.52
1:A:114:LEU:HD13	1:A:171:GLN:NE2	2.25	0.52
1:A:243:PRO:O	1:A:244:PRO:C	2.53	0.52
1:A:672:ASP:HB2	1:A:736:ASN:OD1	2.09	0.52
1:A:886:ILE:HG13	1:A:943:LEU:CD1	2.40	0.52
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.91	0.52
2:B:936:ASP:OD1	2:B:938:SER:N	2.39	0.52
2:B:1147:LEU:C	2:B:1147:LEU:HD23	2.35	0.52
4:D:53:SER:CB	4:D:153:ARG:H	2.22	0.52
11:K:55:LYS:HB3	11:K:81:TYR:CE1	2.45	0.52
1:A:58:LEU:CD1	1:A:80:HIS:H	2.23	0.52
1:A:67:CYS:O	1:A:68:GLN:HB2	2.09	0.52
1:A:1441:PHE:HZ	6:F:89:GLU:HA	1.74	0.52
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.75	0.52
2:B:388:CYS:C	2:B:390:LEU:N	2.67	0.52
3:C:256:ALA:C	3:C:258:ILE:N	2.68	0.52
5:E:177:ARG:HD3	5:E:215:MET:CG	2.40	0.52
7:G:3:PHE:CD1	7:G:80:LYS:NZ	2.68	0.52
8:H:26:ILE:HD13	8:H:49:VAL:HG11	1.92	0.52
9:I:61:ASP:O	9:I:63:GLY:N	2.43	0.52
11:K:18:LYS:NZ	11:K:38:GLU:HG2	2.23	0.52
11:K:55:LYS:CB	11:K:81:TYR:CE1	2.93	0.52
1:A:84:ILE:HG22	1:A:239:LEU:HB3	1.91	0.51
1:A:264:PHE:O	1:A:267:ALA:HB3	2.10	0.51
1:A:350:ARG:HB2	1:A:488:ASN:OD1	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:THR:CG2	1:A:383:TYR:H	2.23	0.51
1:A:605:MET:HE2	1:A:607:ILE:CG1	2.40	0.51
1:A:613:ILE:O	1:A:614:PHE:HB3	2.09	0.51
1:A:632:VAL:O	1:A:633:VAL:C	2.53	0.51
1:A:715:GLU:OE2	1:A:774:ARG:NH1	2.43	0.51
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.72	0.51
1:A:965:GLN:O	1:A:968:GLN:HB2	2.10	0.51
1:A:1118:VAL:HG12	1:A:1327:ILE:HG13	1.92	0.51
2:B:184:ALA:HB1	2:B:188:ASP:HB3	1.92	0.51
2:B:278:GLN:HG2	2:B:279:ASP:H	1.74	0.51
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.27	0.51
2:B:825:VAL:HG13	2:B:826:ALA:N	2.25	0.51
2:B:1162:ILE:HG22	2:B:1163:CYS:H	1.75	0.51
7:G:139:ILE:HG22	7:G:140:LYS:N	2.24	0.51
9:I:14:LEU:HA	9:I:28:GLU:O	2.10	0.51
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.40	0.51
1:A:822:GLU:HG3	2:B:513:GLN:NE2	2.26	0.51
2:B:343:ILE:CG2	2:B:348:ARG:H	2.22	0.51
3:C:83:SER:OG	3:C:160:LYS:HD3	2.10	0.51
3:C:146:LYS:C	3:C:147:LEU:HD23	2.36	0.51
4:D:17:LYS:HE3	4:D:17:LYS:HA	1.92	0.51
4:D:40:HIS:CB	7:G:73:LYS:HZ2	2.23	0.51
4:D:167:LEU:O	4:D:170:THR:OG1	2.24	0.51
5:E:61:GLN:HG2	5:E:62:ALA:N	2.24	0.51
1:A:107:CYS:H	1:A:114:LEU:HD21	1.74	0.51
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.91	0.51
1:A:211:PHE:HA	1:A:214:ILE:HG13	1.92	0.51
1:A:826:ASP:HB2	1:A:830:LYS:HD3	1.91	0.51
2:B:199:MET:HE2	2:B:492:LEU:CD2	2.30	0.51
2:B:278:GLN:NE2	2:B:337:ARG:HH21	2.08	0.51
2:B:281:PRO:O	2:B:283:VAL:N	2.43	0.51
2:B:693:ILE:HD13	2:B:701:ILE:HD13	1.93	0.51
3:C:226:ASP:O	3:C:227:THR:CB	2.58	0.51
4:D:29:LEU:HD13	7:G:82:PHE:CZ	2.45	0.51
1:A:72:GLU:OE2	2:B:1175:LEU:HB2	2.11	0.51
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.10	0.51
1:A:567:LYS:HB3	8:H:95:TYR:CA	2.38	0.51
1:A:738:LYS:HB2	1:A:740:LEU:HG	1.91	0.51
1:A:1409:LEU:HD13	2:B:1207:LEU:HD11	1.92	0.51
2:B:37:PHE:HD2	2:B:542:MET:SD	2.33	0.51
2:B:882:THR:O	2:B:883:LEU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.93	0.51
2:B:902:GLY:O	12:L:65:VAL:HG11	2.11	0.51
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.10	0.51
4:D:50:LEU:HD13	4:D:55:ALA:HA	1.93	0.51
13:N:0:DT:H71	13:N:1:DA:N6	2.24	0.51
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.40	0.51
1:A:982:THR:HG22	1:A:984:LYS:H	1.75	0.51
1:A:1453:TYR:O	1:A:1454:MET:HB3	2.10	0.51
2:B:37:PHE:CD1	2:B:41:LYS:HG3	2.45	0.51
2:B:483:LEU:CD1	2:B:491:THR:HG23	2.39	0.51
2:B:852:ARG:NH2	12:L:70:ARG:OXT	2.37	0.51
2:B:1109:GLY:O	2:B:1110:PRO:C	2.54	0.51
3:C:22:LEU:HD13	3:C:230:MET:HE3	1.92	0.51
3:C:56:THR:HG21	3:C:145:CYS:SG	2.51	0.51
6:F:123:LYS:O	6:F:124:GLU:C	2.54	0.51
7:G:16:SER:HB3	7:G:17:PHE:CD2	2.46	0.51
1:A:116:ASP:C	1:A:118:HIS:N	2.66	0.51
1:A:289:ILE:C	1:A:291:GLU:N	2.68	0.51
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.46	0.51
2:B:606:LYS:HD2	2:B:608:ASP:OD2	2.11	0.51
2:B:865:LYS:HZ3	2:B:869:SER:HA	1.75	0.51
3:C:238:ILE:HG22	3:C:243:VAL:HG23	1.92	0.51
1:A:527:THR:HG21	1:A:650:GLN:HA	1.91	0.51
1:A:626:ASN:O	1:A:631:HIS:HD2	1.93	0.51
1:A:834:THR:O	1:A:837:ILE:HB	2.10	0.51
2:B:226:PHE:HA	2:B:395:GLN:CG	2.40	0.51
2:B:383:ASN:O	2:B:384:ARG:C	2.53	0.51
4:D:156:ASP:C	4:D:158:GLU:N	2.69	0.51
5:E:22:MET:HE3	5:E:26:ARG:NE	2.24	0.51
8:H:58:THR:HB	8:H:143:LEU:HD13	1.93	0.51
1:A:332:LYS:HG3	1:A:333:GLU:N	2.26	0.51
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.41	0.51
1:A:921:GLY:O	1:A:922:ASP:C	2.52	0.51
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.41	0.51
2:B:434:ARG:HA	2:B:437:GLU:OE2	2.10	0.51
2:B:604:ARG:C	2:B:606:LYS:H	2.18	0.51
2:B:711:GLU:H	2:B:712:PRO:HD2	1.75	0.51
2:B:825:VAL:HG13	2:B:826:ALA:H	1.76	0.51
3:C:174:ALA:O	10:J:10:CYS:O	2.29	0.51
5:E:48:ASP:CG	5:E:49:SER:N	2.69	0.51
10:J:36:LEU:HA	10:J:39:LEU:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ILE:O	1:A:84:ILE:CG2	2.58	0.51
1:A:474:VAL:C	1:A:477:PRO:HD2	2.36	0.51
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.26	0.51
1:A:1323:ASP:C	1:A:1325:THR:H	2.18	0.51
2:B:27:ALA:O	2:B:29:ASP:N	2.44	0.51
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.43	0.51
2:B:616:ILE:HG13	2:B:697:GLU:HG3	1.92	0.51
2:B:763:GLN:C	2:B:765:PRO:HD2	2.36	0.51
2:B:896:ASP:OD2	12:L:58:LYS:HE3	2.11	0.51
3:C:77:ILE:HG22	3:C:78:GLU:N	2.26	0.51
8:H:40:LEU:HD22	8:H:123:MET:HE3	1.91	0.51
9:I:5:ARG:HD3	9:I:36:GLU:OE2	2.11	0.51
1:A:33:ALA:O	1:A:83:HIS:HD2	1.93	0.51
1:A:1362:TYR:HD1	1:A:1363:VAL:N	2.08	0.51
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.11	0.51
2:B:360:PHE:O	2:B:361:LEU:C	2.54	0.51
2:B:683:SER:C	2:B:685:LEU:N	2.62	0.51
2:B:955:THR:CG2	2:B:956:THR:H	2.19	0.51
4:D:177:VAL:O	4:D:177:VAL:HG12	2.11	0.51
5:E:9:ILE:CD1	5:E:53:PRO:HD3	2.40	0.51
7:G:18:PHE:HA	7:G:22:MET:HE3	1.93	0.51
10:J:27:GLU:C	10:J:29:GLU:H	2.17	0.51
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.93	0.51
1:A:7:SER:C	1:A:9:ALA:H	2.19	0.50
1:A:244:PRO:CB	1:A:245:PRO:HD3	2.41	0.50
1:A:366:VAL:HG21	1:A:460:VAL:HG22	1.93	0.50
1:A:652:VAL:O	1:A:653:VAL:C	2.55	0.50
2:B:123:THR:O	2:B:125:SER:N	2.44	0.50
2:B:190:TYR:CE1	2:B:196:PRO:HG3	2.45	0.50
2:B:552:MET:HA	2:B:555:ILE:HB	1.93	0.50
7:G:1:MET:O	7:G:3:PHE:CD1	2.65	0.50
11:K:68:PHE:HD2	11:K:68:PHE:N	2.08	0.50
1:A:284:ALA:O	1:A:286:HIS:N	2.36	0.50
1:A:464:PRO:O	1:A:465:TYR:O	2.29	0.50
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.42	0.50
2:B:43:LEU:HD13	2:B:812:LEU:HD23	1.93	0.50
2:B:737:THR:CG2	9:I:66:PRO:HA	2.38	0.50
2:B:792:MET:HE2	2:B:857:ARG:HH22	1.76	0.50
4:D:56:ARG:HA	4:D:148:LEU:HD13	1.93	0.50
5:E:205:SER:O	5:E:206:GLY:C	2.52	0.50
6:F:77:ASP:O	6:F:78:GLN:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:13:LEU:O	7:G:67:SER:HA	2.12	0.50
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.93	0.50
8:H:26:ILE:CD1	8:H:49:VAL:HG11	2.41	0.50
8:H:40:LEU:HD22	8:H:123:MET:CE	2.40	0.50
1:A:362:ASP:OD2	1:A:459:ARG:HD3	2.10	0.50
1:A:1135:ARG:HH21	1:A:1284:MET:HG3	1.77	0.50
2:B:654:ARG:O	2:B:656:GLY:N	2.45	0.50
2:B:955:THR:CG2	2:B:956:THR:N	2.74	0.50
2:B:1099:VAL:O	2:B:1101:ASP:N	2.44	0.50
5:E:35:VAL:O	5:E:37:LEU:N	2.44	0.50
7:G:79:PHE:HZ	7:G:106:MET:HE2	1.77	0.50
9:I:111:THR:CG2	9:I:112:SER:H	2.22	0.50
1:A:244:PRO:O	1:A:247:ARG:N	2.43	0.50
1:A:252:PHE:HB2	1:A:256:GLN:NE2	2.27	0.50
1:A:262:LEU:O	1:A:264:PHE:N	2.45	0.50
1:A:541:ILE:HG21	1:A:549:MET:HE1	1.92	0.50
1:A:710:LEU:N	1:A:710:LEU:HD12	2.27	0.50
1:A:786:HIS:N	1:A:786:HIS:CD2	2.79	0.50
1:A:981:LEU:HD21	1:A:1038:THR:C	2.36	0.50
1:A:1283:VAL:HG12	1:A:1284:MET:H	1.76	0.50
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	1.93	0.50
2:B:515:HIS:N	2:B:518:HIS:HD2	1.98	0.50
2:B:1020:ARG:HB2	2:B:1022:THR:HG22	1.93	0.50
2:B:1084:GLN:C	2:B:1085:ILE:HD12	2.37	0.50
2:B:1085:ILE:HG22	2:B:1086:PHE:N	2.27	0.50
3:C:89:GLU:O	3:C:90:ASP:HB3	2.11	0.50
3:C:179:GLU:HG2	3:C:180:TYR:H	1.77	0.50
4:D:51:ASN:O	4:D:54:GLU:HB3	2.10	0.50
8:H:17:PRO:HB3	8:H:24:CYS:HG	1.74	0.50
1:A:23:SER:HA	1:A:233:TRP:NE1	2.27	0.50
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.76	0.50
1:A:798:GLY:HA2	1:A:815:PHE:HD1	1.73	0.50
2:B:298:LEU:HD13	2:B:314:LEU:HD13	1.92	0.50
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.40	0.50
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.36	0.50
3:C:112:ASN:HD22	3:C:112:ASN:N	2.07	0.50
3:C:140:ASN:O	3:C:141:GLY:O	2.29	0.50
4:D:27:LEU:HD22	4:D:173:HIS:CD2	2.46	0.50
6:F:82:THR:HG22	6:F:84:TYR:N	2.23	0.50
6:F:114:GLU:OE2	6:F:119:ARG:HG2	2.12	0.50
7:G:22:MET:O	7:G:23:LYS:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LYS:NZ	1:A:57:ARG:NH1	2.60	0.50
1:A:42:ASP:C	1:A:44:THR:N	2.68	0.50
1:A:58:LEU:HD11	1:A:80:HIS:H	1.76	0.50
1:A:115:LEU:CB	1:A:122:MET:HE2	2.33	0.50
1:A:310:GLY:O	1:A:312:PRO:HD2	2.12	0.50
1:A:332:LYS:C	1:A:334:GLY:H	2.20	0.50
1:A:774:ARG:NH2	1:A:797:LYS:HG3	2.27	0.50
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.11	0.50
2:B:192:LEU:O	2:B:193:LYS:HB2	2.12	0.50
2:B:510:LYS:HG3	2:B:511:PRO:CD	2.38	0.50
2:B:549:THR:HG22	2:B:550:ASP:N	2.15	0.50
3:C:69:LEU:HD12	3:C:69:LEU:H	1.76	0.50
5:E:131:THR:HG21	5:E:191:LYS:NZ	2.26	0.50
7:G:88:ASP:HA	7:G:144:ARG:HA	1.92	0.50
7:G:96:GLN:HB3	7:G:121:PHE:CE2	2.47	0.50
1:A:55:ASP:HA	1:A:58:LEU:HB3	1.94	0.50
1:A:269:ILE:CD1	1:A:300:VAL:HA	2.41	0.50
1:A:350:ARG:HA	1:A:468:PHE:HE1	1.77	0.50
1:A:370:ILE:O	1:A:371:ALA:C	2.52	0.50
1:A:1341:ILE:CG2	1:A:1342:GLU:H	2.24	0.50
2:B:233:PRO:HG2	2:B:234:ILE:CD1	2.42	0.50
2:B:247:GLY:C	2:B:249:ARG:N	2.67	0.50
2:B:329:THR:O	2:B:332:ASP:HB3	2.12	0.50
2:B:497:ARG:NH2	2:B:775:LYS:NZ	2.59	0.50
6:F:69:LEU:N	6:F:70:LYS:HA	2.26	0.50
6:F:85:MET:HE1	6:F:148:VAL:HG12	1.93	0.50
1:A:95:PHE:CZ	1:A:1414:ALA:HB2	2.47	0.50
1:A:195:ASP:O	1:A:196:GLU:HB3	2.12	0.50
1:A:250:ILE:CD1	14:P:0:U:H1'	2.41	0.50
1:A:567:LYS:HG3	1:A:568:PRO:CD	2.39	0.50
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.94	0.50
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.92	0.50
2:B:746:SER:HB2	2:B:1046:PRO:HG2	1.93	0.50
3:C:22:LEU:HD13	3:C:230:MET:CE	2.42	0.50
12:L:55:ILE:O	12:L:56:LEU:HB2	2.11	0.50
1:A:58:LEU:HG	1:A:59:GLY:N	2.26	0.50
2:B:1033:LYS:NZ	2:B:1068:GLY:O	2.45	0.50
10:J:48:ARG:HH21	10:J:49:MET:HE1	1.77	0.50
15:T:19:TT:C5R	15:T:19:TT:H2'1	2.42	0.50
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.94	0.49
1:A:90:VAL:HG13	1:A:297:GLN:OE1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.12	0.49
2:B:122:LEU:O	2:B:206:ASN:HA	2.12	0.49
2:B:220:GLY:O	2:B:222:ILE:HG13	2.12	0.49
2:B:365:THR:HG23	2:B:367:LEU:N	2.21	0.49
2:B:549:THR:N	2:B:628:THR:HG23	2.25	0.49
2:B:899:ILE:CG2	2:B:903:VAL:HB	2.42	0.49
2:B:1060:ARG:C	2:B:1062:HIS:H	2.19	0.49
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.93	0.49
7:G:59:GLY:CA	7:G:70:PHE:CD2	2.94	0.49
12:L:36:SER:O	12:L:37:LYS:C	2.54	0.49
1:A:92:HIS:HD2	1:A:304:MET:HE1	1.77	0.49
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.93	0.49
1:A:409:SER:O	1:A:410:GLY:C	2.54	0.49
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.94	0.49
1:A:826:ASP:O	1:A:827:THR:C	2.52	0.49
1:A:867:ILE:CG2	1:A:872:GLY:N	2.75	0.49
1:A:1329:THR:CG2	1:A:1331:SER:H	2.22	0.49
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.93	0.49
2:B:549:THR:H	2:B:628:THR:CG2	2.22	0.49
2:B:800:GLN:O	2:B:801:LYS:C	2.55	0.49
3:C:74:SER:HB2	3:C:77:ILE:HG12	1.93	0.49
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.47	0.49
8:H:116:TYR:HE2	8:H:140:ALA:HB1	1.76	0.49
9:I:58:VAL:O	9:I:58:VAL:HG12	2.11	0.49
14:P:5:C:C2'	14:P:6:C:H5'	2.41	0.49
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.93	0.49
1:A:947:PHE:CD2	1:A:954:TRP:CE2	3.00	0.49
1:A:1211:GLN:O	1:A:1212:VAL:C	2.55	0.49
1:A:1291:VAL:HG13	1:A:1292:PRO:CD	2.42	0.49
2:B:19:GLU:O	2:B:20:ASP:C	2.55	0.49
2:B:792:MET:HG3	2:B:855:PHE:CE1	2.47	0.49
3:C:242:GLN:C	3:C:244:VAL:N	2.70	0.49
4:D:14:ARG:N	4:D:17:LYS:HZ3	2.10	0.49
4:D:40:HIS:CG	4:D:41:GLN:N	2.80	0.49
4:D:57:LEU:O	4:D:61:GLU:HB2	2.12	0.49
7:G:9:LEU:HD12	7:G:10:ASN:H	1.77	0.49
11:K:21:ILE:HG23	11:K:31:VAL:CG1	2.42	0.49
15:T:19:TT:H2'1	15:T:19:TT:C3R	2.42	0.49
1:A:767:GLN:HA	1:A:799:PHE:HA	1.94	0.49
1:A:1115:SER:OG	1:A:1116:LEU:N	2.45	0.49
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:658:ILE:CG2	2:B:662:MET:HE2	2.42	0.49
2:B:797:TYR:HE1	2:B:854:LEU:CD2	2.24	0.49
2:B:980:PHE:HE2	2:B:1094:ARG:HB2	1.78	0.49
3:C:123:ASN:HD21	3:C:125:MET:HA	1.78	0.49
3:C:168:ALA:C	3:C:170:TRP:N	2.68	0.49
3:C:254:LYS:O	3:C:256:ALA:N	2.45	0.49
5:E:29:PHE:C	5:E:30:ILE:HG13	2.37	0.49
5:E:55:ARG:O	5:E:57:MET:N	2.46	0.49
7:G:4:ILE:O	7:G:4:ILE:HG22	2.12	0.49
8:H:138:GLU:O	8:H:139:ASN:C	2.54	0.49
10:J:7:CYS:SG	10:J:8:PHE:N	2.85	0.49
11:K:12:LEU:HD12	11:K:12:LEU:N	2.22	0.49
12:L:34:CYS:O	12:L:36:SER:N	2.46	0.49
1:A:335:ARG:HH11	2:B:1202:LEU:HD13	1.76	0.49
1:A:507:VAL:HG13	1:A:521:MET:HE1	1.93	0.49
1:A:601:LYS:HB2	1:A:603:ASN:ND2	2.27	0.49
1:A:1118:VAL:HG23	1:A:1118:VAL:O	2.11	0.49
1:A:1213:GLY:O	1:A:1214:GLU:C	2.56	0.49
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.11	0.49
2:B:190:TYR:CE2	10:J:62:ARG:HB3	2.47	0.49
2:B:661:LEU:C	2:B:663:ALA:N	2.70	0.49
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.95	0.49
2:B:1184:GLY:C	2:B:1186:ASP:H	2.16	0.49
3:C:73:GLN:NE2	3:C:75:MET:N	2.57	0.49
3:C:241:ASP:OD1	3:C:242:GLN:N	2.39	0.49
4:D:176:GLU:HB3	4:D:198:LEU:HD21	1.94	0.49
6:F:119:ARG:HG3	6:F:119:ARG:NH1	2.26	0.49
8:H:18:GLY:O	8:H:19:ARG:HB2	2.12	0.49
9:I:84:VAL:HG13	9:I:84:VAL:O	2.13	0.49
12:L:38:LEU:O	12:L:39:SER:CB	2.60	0.49
1:A:93:VAL:HG21	1:A:301:ALA:O	2.13	0.49
1:A:534:LEU:O	1:A:534:LEU:HG	2.11	0.49
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.94	0.49
1:A:1017:LEU:CB	5:E:205:SER:HA	2.42	0.49
1:A:1139:GLU:O	1:A:1275:GLY:HA3	2.12	0.49
2:B:25:ILE:HD11	2:B:653:VAL:C	2.37	0.49
2:B:294:ASP:O	2:B:296:GLU:N	2.43	0.49
2:B:309:GLN:HG3	9:I:52:ILE:HD11	1.94	0.49
3:C:66:ARG:HH12	10:J:2:ILE:HG21	1.75	0.49
5:E:156:LEU:HD12	5:E:195:VAL:CG1	2.42	0.49
11:K:21:ILE:HG23	11:K:31:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:17:DT:H2''	15:T:18:DT:O5'	2.12	0.49
1:A:147:VAL:O	1:A:149:GLU:N	2.46	0.49
1:A:381:THR:HG23	1:A:383:TYR:H	1.78	0.49
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.43	0.49
1:A:658:LEU:HD13	2:B:831:SER:N	2.27	0.49
1:A:695:LYS:C	1:A:697:ALA:N	2.69	0.49
1:A:837:ILE:HA	1:A:840:ARG:HD3	1.95	0.49
1:A:1032:LEU:O	1:A:1036:ARG:HD3	2.12	0.49
2:B:259:TYR:HD1	2:B:259:TYR:H	1.60	0.49
2:B:310:MET:HE1	2:B:387:LEU:HD12	1.92	0.49
2:B:893:LEU:HD22	2:B:897:GLY:C	2.38	0.49
2:B:995:ARG:NH1	3:C:165:LYS:HG2	2.27	0.49
2:B:1068:GLY:O	2:B:1069:PHE:O	2.31	0.49
3:C:175:ALA:HB3	10:J:43:ARG:NH2	2.28	0.49
3:C:239:PRO:O	3:C:240:VAL:C	2.55	0.49
4:D:53:SER:HB3	4:D:152:SER:CA	2.42	0.49
7:G:117:GLN:C	7:G:119:LEU:N	2.71	0.49
10:J:56:LEU:O	10:J:57:ILE:C	2.54	0.49
1:A:166:GLY:O	1:A:167:CYS:CB	2.60	0.49
1:A:260:ASP:O	1:A:261:ASP:C	2.56	0.49
1:A:825:ILE:O	1:A:826:ASP:C	2.55	0.49
1:A:1029:ARG:HG3	1:A:1029:ARG:NH1	2.24	0.49
1:A:1342:GLU:OE2	5:E:212:ARG:NH1	2.45	0.49
1:A:1389:PHE:CD1	1:A:1389:PHE:C	2.90	0.49
2:B:46:GLN:CG	2:B:47:GLN:H	2.20	0.49
2:B:758:PHE:N	2:B:759:PRO:CD	2.76	0.49
2:B:1010:LEU:HD23	2:B:1092:TYR:CD1	2.47	0.49
2:B:1084:GLN:N	2:B:1084:GLN:HE21	2.10	0.49
3:C:129:ILE:HG23	3:C:130:GLY:N	2.26	0.49
3:C:161:LYS:O	3:C:170:TRP:NE1	2.46	0.49
6:F:77:ASP:C	6:F:79:ARG:N	2.70	0.49
1:A:50:ILE:O	1:A:52:GLY:N	2.45	0.49
1:A:699:ALA:O	1:A:700:ASN:CB	2.60	0.49
1:A:829:VAL:C	1:A:831:THR:H	2.20	0.49
1:A:894:GLU:HG3	1:A:933:TYR:OH	2.12	0.49
1:A:996:ASN:C	1:A:998:LEU:HD12	2.36	0.49
1:A:1334:ASP:O	1:A:1336:MET:N	2.46	0.49
1:A:1389:PHE:CD1	1:A:1390:ASN:N	2.81	0.49
1:A:1446:ASP:HB2	6:F:133:VAL:CG2	2.43	0.49
2:B:23:ALA:H	2:B:654:ARG:HB3	1.78	0.49
2:B:180:TYR:CD1	2:B:180:TYR:N	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:801:LYS:O	10:J:52:THR:HG23	2.13	0.49
2:B:841:MET:HE1	2:B:980:PHE:CE1	2.48	0.49
2:B:843:GLN:O	2:B:846:ILE:N	2.45	0.49
2:B:1099:VAL:C	2:B:1101:ASP:H	2.21	0.49
3:C:191:TYR:CD2	3:C:201:TRP:CD1	3.01	0.49
10:J:27:GLU:O	10:J:29:GLU:N	2.40	0.49
1:A:18:GLN:HB3	2:B:1215:ARG:HG3	1.94	0.49
1:A:577:ILE:HG13	1:A:578:LEU:N	2.27	0.49
1:A:901:LEU:HD22	1:A:919:ILE:HG21	1.95	0.49
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.78	0.49
2:B:222:ILE:O	2:B:240:ILE:HA	2.13	0.49
2:B:1084:GLN:OE1	3:C:189:THR:CG2	2.61	0.49
2:B:1142:GLY:HA3	6:F:88:TYR:HE2	1.77	0.49
2:B:1214:PRO:O	2:B:1214:PRO:HG2	2.13	0.49
3:C:77:ILE:C	3:C:79:GLN:H	2.21	0.49
4:D:173:HIS:ND1	4:D:174:PRO:HD2	2.28	0.49
5:E:124:VAL:HG13	5:E:132:ILE:CB	2.41	0.49
1:A:71:GLN:C	1:A:73:GLY:N	2.71	0.48
1:A:577:ILE:O	1:A:578:LEU:C	2.52	0.48
1:A:829:VAL:C	1:A:831:THR:N	2.68	0.48
1:A:862:ASN:O	1:A:864:ILE:HG13	2.12	0.48
1:A:958:VAL:HG22	1:A:1052:GLN:HB3	1.95	0.48
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.95	0.48
2:B:167:ILE:HG22	2:B:453:ILE:CD1	2.42	0.48
2:B:591:ARG:O	2:B:592:ASN:C	2.55	0.48
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.94	0.48
2:B:863:GLU:O	2:B:961:LEU:HD22	2.12	0.48
2:B:910:VAL:HG12	2:B:911:ILE:N	2.28	0.48
3:C:35:ARG:HH11	11:K:41:THR:N	2.10	0.48
3:C:190:ASP:O	3:C:191:TYR:C	2.55	0.48
3:C:245:VAL:HA	3:C:248:ILE:HD12	1.94	0.48
5:E:136:ASN:OD1	5:E:137:GLU:N	2.46	0.48
9:I:60:GLN:NE2	9:I:107:SER:OG	2.46	0.48
11:K:67:PHE:C	11:K:68:PHE:CD2	2.89	0.48
12:L:31:CYS:SG	12:L:34:CYS:N	2.84	0.48
1:A:388:LEU:CD2	1:A:432:VAL:HB	2.43	0.48
1:A:710:LEU:HD12	1:A:710:LEU:H	1.78	0.48
1:A:961:ARG:HG2	1:A:965:GLN:HE21	1.78	0.48
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.95	0.48
1:A:1115:SER:HB3	1:A:1330:ASN:HD21	1.78	0.48
1:A:1219:THR:HG21	1:A:1271:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1349:TYR:CA	1:A:1372:VAL:HG21	2.43	0.48
2:B:33:VAL:O	2:B:36:ALA:HB3	2.13	0.48
2:B:203:PHE:N	2:B:203:PHE:CD1	2.81	0.48
2:B:344:LYS:O	2:B:345:LYS:HG3	2.13	0.48
2:B:799:PRO:CB	2:B:818:PRO:HG2	2.43	0.48
2:B:978:ASP:O	2:B:989:THR:HB	2.12	0.48
2:B:1070:GLU:OE1	10:J:44:TYR:OH	2.30	0.48
2:B:1095:LEU:H	2:B:1095:LEU:CD1	2.16	0.48
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.94	0.48
5:E:10:SER:O	5:E:14:ARG:HG3	2.11	0.48
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.95	0.48
9:I:69:PRO:HB2	9:I:85:PHE:CE2	2.48	0.48
1:A:35:ILE:CD1	1:A:241:VAL:HG11	2.42	0.48
1:A:300:VAL:O	1:A:300:VAL:HG12	2.11	0.48
1:A:767:GLN:HE21	1:A:774:ARG:HB3	1.74	0.48
1:A:847:ASP:HB3	1:A:1398:MET:HE1	1.95	0.48
1:A:947:PHE:CD2	1:A:954:TRP:CZ2	3.02	0.48
1:A:1385:THR:C	1:A:1387:HIS:N	2.70	0.48
2:B:343:ILE:HB	2:B:348:ARG:HG3	1.95	0.48
2:B:1135:ARG:O	2:B:1136:ASP:C	2.56	0.48
2:B:1156:ASP:HB3	2:B:1197:PRO:HA	1.95	0.48
8:H:11:GLN:O	8:H:28:ALA:HB1	2.13	0.48
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.95	0.48
12:L:47:ARG:HH21	12:L:54:ARG:NH2	2.11	0.48
13:N:5:DA:H2"	13:N:6:DC:OP2	2.12	0.48
1:A:108:MET:SD	1:A:210:ILE:HD13	2.53	0.48
1:A:265:LYS:HZ3	1:A:322:VAL:HG13	1.78	0.48
1:A:701:LEU:HD23	9:I:115:LYS:HG3	1.95	0.48
1:A:718:VAL:O	1:A:721:PHE:HB2	2.12	0.48
1:A:913:LEU:CD1	1:A:914:GLU:N	2.71	0.48
2:B:363:HIS:O	2:B:364:ILE:CB	2.55	0.48
2:B:603:LEU:HB3	2:B:609:ILE:HG13	1.93	0.48
2:B:604:ARG:O	2:B:606:LYS:N	2.46	0.48
2:B:758:PHE:CE2	2:B:1044:ALA:CA	2.92	0.48
2:B:1007:VAL:HG22	2:B:1008:PRO:CD	2.41	0.48
3:C:107:SER:C	3:C:109:SER:H	2.21	0.48
7:G:80:LYS:N	7:G:80:LYS:CD	2.73	0.48
8:H:123:MET:HE1	8:H:142:LEU:CD1	2.43	0.48
1:A:936:LEU:O	1:A:939:ASP:HB2	2.13	0.48
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.78	0.48
1:A:1299:VAL:CG1	1:A:1300:LYS:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:PHE:HE1	2:B:41:LYS:CD	2.26	0.48
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.96	0.48
2:B:810:GLU:HB3	2:B:811:TYR:CE1	2.48	0.48
2:B:899:ILE:HD13	2:B:905:VAL:CG1	2.43	0.48
3:C:209:TYR:H	3:C:209:TYR:HD1	1.58	0.48
5:E:161:LYS:C	5:E:163:GLU:N	2.69	0.48
7:G:20:PRO:CG	7:G:21:ARG:H	2.26	0.48
1:A:399:HIS:CB	1:A:400:PRO:CD	2.88	0.48
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.95	0.48
1:A:535:THR:HG22	1:A:536:LEU:N	2.27	0.48
1:A:1225:PHE:CE2	1:A:1227:ILE:HD11	2.49	0.48
2:B:128:LEU:HB2	2:B:168:GLY:O	2.13	0.48
2:B:197:PHE:HZ	2:B:816:GLU:HG2	1.78	0.48
2:B:769:TYR:O	2:B:771:SER:N	2.47	0.48
2:B:814:PHE:C	2:B:816:GLU:N	2.69	0.48
7:G:99:PHE:CD1	7:G:99:PHE:C	2.91	0.48
9:I:71:SER:OG	9:I:83:ASN:HB2	2.13	0.48
1:A:504:LEU:HD12	1:A:504:LEU:N	2.28	0.48
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.84	0.48
1:A:1030:ARG:NH1	1:A:1035:TYR:OH	2.47	0.48
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.29	0.48
2:B:213:ILE:O	2:B:215:GLN:HG2	2.13	0.48
2:B:244:LEU:C	2:B:246:LYS:N	2.68	0.48
2:B:281:PRO:O	2:B:282:ILE:C	2.56	0.48
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.78	0.48
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.44	0.48
2:B:997:GLU:CD	2:B:997:GLU:H	2.22	0.48
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.49	0.48
3:C:88:CYS:SG	3:C:91:HIS:HA	2.53	0.48
6:F:85:MET:CE	6:F:93:ILE:HD12	2.44	0.48
7:G:20:PRO:HG2	7:G:21:ARG:N	2.28	0.48
8:H:63:LEU:HD22	8:H:90:ALA:HB3	1.96	0.48
9:I:85:PHE:CD2	9:I:85:PHE:N	2.68	0.48
1:A:92:HIS:O	1:A:93:VAL:C	2.56	0.48
1:A:701:LEU:HD23	9:I:115:LYS:CG	2.44	0.48
1:A:844:ALA:O	1:A:845:LEU:HD23	2.13	0.48
1:A:852:TYR:HA	1:A:1060:PRO:HB3	1.96	0.48
1:A:863:VAL:HG11	1:A:866:PHE:CE2	2.49	0.48
7:G:17:PHE:C	7:G:19:GLY:H	2.20	0.48
10:J:34:THR:O	10:J:35:ALA:C	2.56	0.48
1:A:218:ASP:O	1:A:219:PHE:O	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:MET:CE	1:A:843:LYS:HZ3	2.27	0.48
1:A:353:ILE:HB	1:A:470:LEU:CD2	2.43	0.48
1:A:666:ILE:HD12	1:A:667:GLY:N	2.25	0.48
1:A:795:GLU:CD	1:A:795:GLU:H	2.22	0.48
1:A:954:TRP:HB3	1:A:955:PRO:HD2	1.95	0.48
1:A:1036:ARG:HG2	1:A:1036:ARG:NH1	2.21	0.48
1:A:1373:ASP:O	1:A:1376:THR:HG23	2.14	0.48
1:A:1385:THR:O	1:A:1386:ARG:C	2.57	0.48
2:B:175:ARG:HG2	2:B:175:ARG:NH1	2.27	0.48
2:B:575:PRO:HG2	2:B:576:ASP:H	1.79	0.48
2:B:970:THR:HG22	2:B:971:THR:N	2.28	0.48
6:F:121:ALA:O	6:F:122:MET:C	2.57	0.48
7:G:122:ASN:ND2	7:G:125:SER:HB3	2.29	0.48
1:A:21:LEU:HG	1:A:1413:GLY:O	2.14	0.48
1:A:130:ASP:O	1:A:133:LYS:N	2.38	0.48
1:A:608:ILE:C	1:A:610:GLY:H	2.22	0.48
1:A:1325:THR:O	1:A:1325:THR:CG2	2.61	0.48
1:A:1387:HIS:CE1	13:N:4:DT:H5"	2.48	0.48
1:A:1445:ILE:N	1:A:1445:ILE:CD1	2.68	0.48
1:A:1446:ASP:HB2	6:F:133:VAL:HG23	1.96	0.48
2:B:189:LEU:O	2:B:190:TYR:C	2.55	0.48
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.48	0.48
2:B:259:TYR:N	2:B:259:TYR:CD1	2.82	0.48
2:B:446:LEU:O	2:B:447:ALA:CB	2.62	0.48
2:B:515:HIS:CD2	2:B:517:THR:HG23	2.49	0.48
2:B:653:VAL:HG22	2:B:689:LEU:HD13	1.95	0.48
2:B:899:ILE:HD12	2:B:911:ILE:HG23	1.95	0.48
2:B:992:ILE:HD11	11:K:66:PRO:HB2	1.96	0.48
3:C:235:VAL:HG13	10:J:13:VAL:HG23	1.95	0.48
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.95	0.48
5:E:180:ARG:NH2	5:E:192:ARG:HB2	2.25	0.48
8:H:111:LEU:HD23	8:H:127:GLY:O	2.14	0.48
10:J:23:ASN:O	10:J:25:LEU:N	2.47	0.48
1:A:262:LEU:C	1:A:264:PHE:N	2.69	0.47
1:A:789:LYS:HE3	9:I:67:THR:OG1	2.14	0.47
1:A:1377:THR:HA	5:E:212:ARG:HH21	1.79	0.47
1:A:1397:LEU:O	1:A:1400:CYS:HB3	2.13	0.47
2:B:30:SER:HB3	2:B:743:ILE:O	2.14	0.47
2:B:310:MET:O	2:B:313:MET:HB2	2.14	0.47
2:B:579:ARG:N	2:B:589:VAL:HG13	2.29	0.47
2:B:654:ARG:C	2:B:656:GLY:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1047:PHE:CD1	2:B:1047:PHE:N	2.76	0.47
2:B:1099:VAL:HG12	2:B:1100:ASP:H	1.79	0.47
3:C:31:ASN:O	3:C:34:ARG:HB3	2.14	0.47
7:G:35:GLU:CG	7:G:48:VAL:HG23	2.44	0.47
11:K:19:LEU:HD22	11:K:33:ILE:CG2	2.43	0.47
1:A:224:PHE:CE2	1:A:231:PRO:HA	2.49	0.47
1:A:466:SER:HB2	2:B:1099:VAL:HG11	1.96	0.47
1:A:506:ALA:C	1:A:508:PRO:HD2	2.39	0.47
2:B:118:ARG:HG2	2:B:204:ILE:HD13	1.94	0.47
2:B:185:THR:O	2:B:188:ASP:HB2	2.13	0.47
2:B:205:ILE:N	2:B:205:ILE:HD12	2.28	0.47
2:B:1050:ILE:HG22	2:B:1051:THR:H	1.79	0.47
2:B:1152:MET:HE1	2:B:1196:ILE:C	2.39	0.47
2:B:1202:LEU:HD22	2:B:1206:GLU:CD	2.39	0.47
3:C:114:TYR:CD2	3:C:140:ASN:HB2	2.49	0.47
11:K:5:ASP:O	11:K:6:ARG:C	2.57	0.47
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.95	0.47
1:A:399:HIS:CG	1:A:400:PRO:N	2.81	0.47
1:A:672:ASP:O	1:A:673:GLY:C	2.58	0.47
1:A:722:LEU:O	1:A:725:ALA:HB3	2.14	0.47
1:A:877:HIS:C	1:A:878:ILE:CG1	2.87	0.47
1:A:935:GLN:O	1:A:936:LEU:C	2.56	0.47
1:A:1127:ASP:O	1:A:1128:GLN:C	2.57	0.47
2:B:100:PRO:HD3	2:B:172:ILE:HD12	1.96	0.47
2:B:197:PHE:CZ	2:B:816:GLU:HG2	2.49	0.47
2:B:785:TYR:CD1	2:B:785:TYR:C	2.91	0.47
2:B:882:THR:CB	2:B:934:LYS:O	2.62	0.47
2:B:1031:LEU:HA	2:B:1055:ILE:HD13	1.96	0.47
2:B:1033:LYS:CE	2:B:1070:GLU:OE1	2.62	0.47
3:C:36:VAL:HG11	3:C:251:LEU:HB2	1.96	0.47
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.95	0.47
7:G:25:TYR:O	7:G:28:THR:HB	2.14	0.47
7:G:115:MET:CB	7:G:116:PRO:HD2	2.44	0.47
7:G:154:VAL:HG12	7:G:155:SER:H	1.79	0.47
8:H:26:ILE:CG2	8:H:27:GLU:N	2.77	0.47
1:A:43:GLU:O	1:A:44:THR:CB	2.61	0.47
1:A:500:GLU:O	1:A:504:LEU:HD13	2.14	0.47
1:A:735:VAL:O	1:A:735:VAL:HG12	2.14	0.47
1:A:770:VAL:HA	1:A:822:GLU:OE1	2.14	0.47
2:B:298:LEU:N	2:B:298:LEU:CD2	2.77	0.47
2:B:696:GLU:O	2:B:699:GLU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1099:VAL:HG13	2:B:1100:ASP:N	2.27	0.47
2:B:1110:PRO:HB2	2:B:1119:VAL:HG21	1.96	0.47
3:C:27:LEU:O	3:C:28:ALA:C	2.57	0.47
3:C:242:GLN:HB3	3:C:246:ARG:HG3	1.97	0.47
7:G:34:VAL:HG12	7:G:45:ILE:CG2	2.39	0.47
9:I:56:ALA:O	9:I:57:GLY:C	2.57	0.47
1:A:40:THR:C	1:A:41:MET:HG3	2.39	0.47
1:A:326:ARG:HG2	1:A:327:ALA:N	2.30	0.47
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.30	0.47
1:A:577:ILE:C	1:A:579:SER:N	2.69	0.47
1:A:1205:LYS:O	1:A:1206:ASP:C	2.57	0.47
2:B:579:ARG:HG2	2:B:579:ARG:NH1	2.29	0.47
2:B:841:MET:SD	2:B:846:ILE:HD11	2.54	0.47
6:F:79:ARG:HH22	6:F:150:GLU:CD	2.22	0.47
14:P:7:A:C2'	14:P:8:G:O4'	2.62	0.47
1:A:88:LYS:HE3	1:A:280:GLU:OE2	2.15	0.47
1:A:299:HIS:C	1:A:301:ALA:H	2.23	0.47
1:A:331:GLY:O	1:A:332:LYS:HB3	2.15	0.47
1:A:335:ARG:O	1:A:336:ILE:C	2.55	0.47
1:A:369:SER:HB2	11:K:2:ASN:OD1	2.15	0.47
1:A:867:ILE:HG22	1:A:872:GLY:H	1.79	0.47
1:A:871:ASP:O	1:A:873:MET:HE2	2.14	0.47
1:A:1166:ASP:OD2	1:A:1239:ARG:HD2	2.14	0.47
1:A:1356:ILE:HG22	1:A:1356:ILE:O	2.14	0.47
1:A:1437:GLY:O	1:A:1438:THR:C	2.58	0.47
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.96	0.47
2:B:386:LEU:O	2:B:389:ALA:N	2.47	0.47
2:B:705:MET:HA	2:B:705:MET:HE3	1.96	0.47
3:C:208:GLU:C	3:C:210:GLU:N	2.71	0.47
6:F:135:ARG:HD3	6:F:143:PHE:CD2	2.50	0.47
7:G:3:PHE:CG	7:G:80:LYS:NZ	2.73	0.47
9:I:33:SER:O	9:I:34:TYR:O	2.32	0.47
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.30	0.47
12:L:30:ILE:HG22	12:L:31:CYS:N	2.29	0.47
12:L:61:THR:HG22	12:L:63:ARG:HG2	1.96	0.47
1:A:41:MET:HB3	1:A:48:ALA:O	2.15	0.47
1:A:122:MET:O	1:A:123:ARG:C	2.58	0.47
1:A:298:PHE:O	1:A:301:ALA:HB3	2.13	0.47
1:A:339:ASN:O	1:A:343:LYS:HG2	2.14	0.47
1:A:350:ARG:HH11	1:A:350:ARG:HG3	1.79	0.47
1:A:402:ALA:CB	1:A:434:ARG:HA	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:LEU:HD11	6:F:91:ALA:HB1	1.95	0.47
1:A:565:ILE:O	1:A:570:PRO:HA	2.14	0.47
1:A:817:ALA:O	1:A:818:MET:C	2.56	0.47
1:A:888:GLY:O	1:A:940:ARG:NH2	2.48	0.47
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.97	0.47
1:A:964:ILE:O	1:A:965:GLN:C	2.57	0.47
1:A:982:THR:H	1:A:985:ASP:CB	2.27	0.47
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.13	0.47
1:A:1151:GLU:HB3	1:A:1153:TYR:HE1	1.79	0.47
1:A:1265:ASN:C	1:A:1267:MET:N	2.69	0.47
1:A:1313:LEU:HD23	1:A:1338:VAL:CB	2.45	0.47
1:A:1315:GLU:C	1:A:1317:MET:H	2.22	0.47
2:B:37:PHE:CD2	2:B:542:MET:SD	3.08	0.47
2:B:45:SER:O	2:B:46:GLN:C	2.57	0.47
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.15	0.47
2:B:597:MET:C	2:B:599:THR:H	2.22	0.47
2:B:653:VAL:HG23	2:B:689:LEU:HB3	1.97	0.47
2:B:658:ILE:HG22	2:B:662:MET:HE2	1.95	0.47
2:B:757:PRO:HG3	2:B:1028:GLU:OE2	2.14	0.47
2:B:839:MET:HB3	2:B:1012:ILE:HG22	1.96	0.47
2:B:847:ASP:C	2:B:849:GLY:N	2.71	0.47
2:B:950:ASP:O	2:B:951:GLN:HB2	2.15	0.47
3:C:73:GLN:NE2	3:C:75:MET:HB2	2.30	0.47
4:D:119:ARG:HG2	4:D:120:GLU:N	2.29	0.47
4:D:134:THR:CG2	4:D:135:GLY:H	2.26	0.47
4:D:191:ALA:O	4:D:193:THR:N	2.47	0.47
5:E:31:THR:O	5:E:35:VAL:HG23	2.13	0.47
5:E:84:ASP:O	5:E:86:PRO:HD3	2.15	0.47
6:F:86:THR:HG23	6:F:89:GLU:CD	2.39	0.47
6:F:88:TYR:N	6:F:88:TYR:CD1	2.83	0.47
7:G:29:LYS:O	7:G:30:LEU:C	2.54	0.47
8:H:55:LEU:HD22	8:H:144:ILE:HG21	1.96	0.47
8:H:93:TYR:CD1	8:H:93:TYR:N	2.82	0.47
10:J:32:GLU:O	10:J:33:GLY:C	2.57	0.47
11:K:52:ASN:O	11:K:54:ARG:N	2.48	0.47
11:K:89:ASN:O	11:K:92:ASN:N	2.48	0.47
1:A:37:PHE:N	1:A:37:PHE:HD1	2.13	0.47
1:A:325:ILE:HG22	2:B:1210:MET:HE2	1.96	0.47
1:A:534:LEU:HD13	1:A:656:TRP:CG	2.50	0.47
1:A:774:ARG:H	1:A:774:ARG:HG2	1.42	0.47
1:A:1105:LEU:HD22	1:A:1384:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.72	0.47
2:B:895:ASP:C	2:B:897:GLY:H	2.22	0.47
2:B:949:VAL:HG12	2:B:950:ASP:N	2.29	0.47
5:E:175:LEU:HD23	5:E:176:PRO:HD2	1.95	0.47
7:G:1:MET:SD	7:G:79:PHE:CE1	3.08	0.47
11:K:12:LEU:H	11:K:12:LEU:CD1	2.24	0.47
12:L:60:ARG:HG2	12:L:61:THR:H	1.80	0.47
1:A:42:ASP:HA	1:A:46:THR:O	2.15	0.47
1:A:53:LEU:O	1:A:54:ASN:C	2.57	0.47
1:A:853:ASP:O	1:A:854:ASN:HB2	2.15	0.47
1:A:901:LEU:N	1:A:926:GLN:HE21	2.08	0.47
2:B:431:TYR:CE2	2:B:447:ALA:HB2	2.50	0.47
2:B:582:VAL:HA	2:B:626:ILE:O	2.15	0.47
2:B:730:ARG:O	2:B:731:VAL:O	2.33	0.47
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.50	0.47
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.80	0.47
2:B:1107:ALA:O	2:B:1108:ARG:HG2	2.15	0.47
3:C:98:VAL:C	3:C:99:LEU:CD2	2.88	0.47
3:C:168:ALA:O	3:C:170:TRP:N	2.48	0.47
7:G:25:TYR:HE2	7:G:29:LYS:HD2	1.80	0.47
8:H:128:ASN:O	8:H:128:ASN:OD1	2.32	0.47
11:K:101:LEU:O	11:K:101:LEU:HD23	2.15	0.47
1:A:43:GLU:O	1:A:44:THR:HB	2.15	0.47
1:A:427:GLN:HB2	1:A:430:TRP:NE1	2.30	0.47
1:A:588:LEU:O	1:A:606:LEU:HD12	2.14	0.47
1:A:598:LEU:O	1:A:599:SER:C	2.58	0.47
1:A:665:GLY:O	1:A:666:ILE:C	2.58	0.47
1:A:920:LEU:HD23	1:A:920:LEU:C	2.40	0.47
1:A:1280:GLU:O	1:A:1281:ARG:O	2.33	0.47
1:A:1389:PHE:C	1:A:1391:ARG:H	2.22	0.47
1:A:1410:PHE:HD2	2:B:1212:ILE:HD12	1.80	0.47
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.51	0.47
2:B:458:LYS:O	2:B:459:TYR:C	2.58	0.47
2:B:461:LEU:N	2:B:461:LEU:HD12	2.29	0.47
7:G:23:LYS:HG3	7:G:56:ILE:HD12	1.96	0.47
7:G:66:GLY:O	7:G:67:SER:C	2.55	0.47
8:H:31:THR:O	8:H:31:THR:HG22	2.13	0.47
11:K:111:LEU:O	11:K:112:GLN:CG	2.62	0.47
1:A:278:THR:O	1:A:278:THR:HG22	2.15	0.46
1:A:698:GLN:HA	9:I:97:MET:O	2.14	0.46
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:7:THR:HG21	4:D:32:GLU:OE2	2.15	0.46
4:D:48:ILE:CG2	7:G:4:ILE:HB	2.45	0.46
4:D:51:ASN:C	4:D:52:LEU:O	2.56	0.46
4:D:64:VAL:C	4:D:66:ARG:N	2.73	0.46
7:G:39:THR:CG2	7:G:40:GLY:H	2.26	0.46
8:H:42:ILE:O	8:H:44:VAL:HG23	2.15	0.46
1:A:253:ASN:HB3	2:B:935:ARG:NH1	2.30	0.46
1:A:353:ILE:HG21	1:A:487:MET:CG	2.41	0.46
1:A:547:LEU:HD22	11:K:58:PHE:CE1	2.50	0.46
1:A:586:ILE:CD1	1:A:633:VAL:HG22	2.45	0.46
1:A:925:LEU:C	1:A:927:VAL:H	2.23	0.46
1:A:1027:ALA:O	1:A:1031:VAL:HG23	2.15	0.46
1:A:1072:ILE:HD11	1:A:1368:MET:HA	1.98	0.46
2:B:212:LEU:HD23	2:B:480:SER:HB2	1.97	0.46
2:B:823:ALA:O	2:B:825:VAL:N	2.48	0.46
2:B:865:LYS:HE2	2:B:871:THR:OG1	2.15	0.46
2:B:1115:THR:CG2	2:B:1117:GLN:HG3	2.45	0.46
8:H:4:THR:HG22	8:H:5:LEU:N	2.29	0.46
8:H:98:TYR:C	8:H:118:PHE:HD2	2.23	0.46
10:J:16:ASP:O	10:J:18:TRP:N	2.48	0.46
11:K:42:LEU:HD21	11:K:46:ILE:HD11	1.96	0.46
15:T:11:DG:H2"	15:T:12:DT:OP2	2.15	0.46
1:A:224:PHE:HZ	1:A:234:MET:CE	2.27	0.46
1:A:224:PHE:CE2	1:A:231:PRO:HG3	2.50	0.46
1:A:274:ILE:O	1:A:275:SER:C	2.57	0.46
1:A:438:ASP:OD1	1:A:461:LYS:HA	2.15	0.46
1:A:634:THR:HG1	1:A:642:CYS:HG	1.63	0.46
1:A:967:ALA:O	1:A:968:GLN:O	2.33	0.46
1:A:1175:SER:O	1:A:1176:LEU:HB2	2.15	0.46
1:A:1193:LEU:HD22	1:A:1260:LEU:HD11	1.97	0.46
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.96	0.46
1:A:1239:ARG:NH1	1:A:1239:ARG:HB3	2.30	0.46
2:B:46:GLN:HG3	2:B:47:GLN:N	2.18	0.46
2:B:185:THR:N	2:B:188:ASP:HB2	2.27	0.46
2:B:230:ALA:N	2:B:231:PRO:CD	2.78	0.46
2:B:263:GLY:O	2:B:264:SER:C	2.58	0.46
2:B:467:GLY:N	2:B:475:SER:CB	2.71	0.46
2:B:821:GLN:NE2	2:B:851:PHE:HA	2.23	0.46
2:B:861:ASP:OD1	2:B:862:GLN:N	2.48	0.46
2:B:957:ASN:O	2:B:958:GLN:C	2.58	0.46
3:C:47:ASP:HA	3:C:169:LYS:NZ	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:GLY:HA2	10:J:16:ASP:HB3	1.97	0.46
4:D:54:GLU:O	4:D:58:VAL:HG23	2.14	0.46
7:G:1:MET:O	7:G:1:MET:CE	2.64	0.46
9:I:98:VAL:HG11	9:I:113:ASP:OD1	2.15	0.46
1:A:261:ASP:O	1:A:264:PHE:HB2	2.15	0.46
1:A:393:ARG:O	1:A:395:GLY:N	2.49	0.46
1:A:499:ALA:O	1:A:503:GLN:HG2	2.15	0.46
1:A:842:VAL:O	1:A:843:LYS:C	2.57	0.46
1:A:845:LEU:O	1:A:846:GLU:C	2.58	0.46
1:A:871:ASP:OD2	1:A:873:MET:HB2	2.15	0.46
1:A:1219:THR:HG21	1:A:1271:ILE:HG13	1.97	0.46
2:B:39:ARG:CZ	2:B:665:GLU:HG2	2.45	0.46
2:B:547:VAL:HG12	2:B:612:GLU:OE2	2.14	0.46
2:B:683:SER:O	2:B:685:LEU:N	2.48	0.46
2:B:990:ILE:CG2	2:B:991:GLY:N	2.78	0.46
3:C:123:ASN:ND2	3:C:125:MET:SD	2.89	0.46
4:D:10:THR:HG23	4:D:10:THR:O	2.16	0.46
4:D:151:PHE:CD1	4:D:151:PHE:N	2.83	0.46
5:E:16:PHE:HZ	5:E:20:LYS:HE2	1.77	0.46
5:E:67:GLU:O	5:E:70:SER:HB3	2.15	0.46
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.97	0.46
11:K:10:PHE:CD1	11:K:11:LEU:CD2	2.99	0.46
1:A:34:LYS:HB3	1:A:36:ARG:NE	2.31	0.46
1:A:114:LEU:O	1:A:115:LEU:HG	2.14	0.46
1:A:167:CYS:O	1:A:167:CYS:SG	2.73	0.46
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.50	0.46
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.98	0.46
1:A:470:LEU:HD22	1:A:487:MET:CE	2.46	0.46
1:A:637:LYS:CB	1:A:641:VAL:HG11	2.45	0.46
1:A:699:ALA:HB2	9:I:114:GLN:CD	2.41	0.46
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.96	0.46
2:B:388:CYS:O	2:B:390:LEU:N	2.49	0.46
2:B:520:GLY:N	2:B:748:ILE:HG22	2.29	0.46
3:C:112:ASN:CB	3:C:114:TYR:CE1	2.98	0.46
3:C:152:GLU:OE2	3:C:154:LYS:HE3	2.15	0.46
3:C:236:GLY:O	3:C:237:SER:C	2.59	0.46
4:D:20:GLU:HA	4:D:20:GLU:OE2	2.14	0.46
4:D:22:GLU:CD	4:D:22:GLU:N	2.64	0.46
9:I:51:ASN:O	9:I:54:GLU:HG3	2.16	0.46
10:J:28:ASP:O	10:J:29:GLU:C	2.59	0.46
1:A:117:GLU:H	1:A:117:GLU:CD	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:ILE:H	1:A:560:ILE:HG12	1.46	0.46
1:A:596:THR:O	1:A:597:LEU:C	2.59	0.46
1:A:767:GLN:HB2	1:A:799:PHE:HD1	1.80	0.46
1:A:925:LEU:C	1:A:927:VAL:N	2.73	0.46
1:A:1053:PHE:O	1:A:1055:ARG:N	2.49	0.46
1:A:1157:ASP:C	1:A:1159:ARG:H	2.24	0.46
2:B:39:ARG:NH2	2:B:665:GLU:CG	2.76	0.46
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.46	0.46
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.97	0.46
3:C:87:PHE:CD1	3:C:87:PHE:N	2.84	0.46
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.96	0.46
3:C:115:SER:HB3	3:C:142:VAL:HB	1.98	0.46
3:C:175:ALA:HB3	10:J:43:ARG:HH22	1.81	0.46
4:D:153:ARG:C	4:D:154:PHE:CD1	2.93	0.46
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.79	0.46
5:E:42:PHE:CZ	5:E:58:MET:HE3	2.51	0.46
5:E:207:ARG:CB	5:E:207:ARG:NH1	2.78	0.46
7:G:138:THR:CG2	7:G:139:ILE:N	2.68	0.46
11:K:85:ASP:O	11:K:88:LYS:HB2	2.15	0.46
1:A:23:SER:CB	1:A:233:TRP:NE1	2.79	0.46
1:A:34:LYS:NZ	1:A:57:ARG:CZ	2.79	0.46
1:A:566:ILE:O	1:A:567:LYS:O	2.34	0.46
1:A:1010:ALA:O	1:A:1011:GLN:C	2.59	0.46
2:B:750:GLY:O	2:B:751:VAL:C	2.59	0.46
2:B:801:LYS:O	10:J:52:THR:CG2	2.64	0.46
2:B:859:TYR:OH	2:B:941:LEU:CD1	2.60	0.46
3:C:114:TYR:HB3	3:C:140:ASN:O	2.16	0.46
5:E:161:LYS:NZ	5:E:172:GLU:OE2	2.46	0.46
8:H:83:GLN:C	8:H:85:GLY:N	2.74	0.46
9:I:55:THR:HG22	9:I:58:VAL:CG2	2.45	0.46
9:I:59:VAL:C	9:I:61:ASP:H	2.22	0.46
9:I:115:LYS:HD3	9:I:117:LYS:CE	2.38	0.46
1:A:49:LYS:NZ	1:A:61:ILE:CG1	2.74	0.46
1:A:116:ASP:C	1:A:118:HIS:H	2.24	0.46
1:A:305:ASP:CG	1:A:326:ARG:HD2	2.41	0.46
1:A:719:VAL:C	1:A:721:PHE:N	2.73	0.46
1:A:835:GLY:HA3	15:T:19:TT:O1P	2.16	0.46
1:A:1152:ILE:HG13	9:I:44:TYR:HD2	1.81	0.46
1:A:1385:THR:O	1:A:1388:GLY:N	2.46	0.46
1:A:1418:LEU:HD12	1:A:1419:ASP:N	2.30	0.46
2:B:900:ALA:HB3	12:L:61:THR:OG1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.43	0.46
2:B:1023:VAL:O	2:B:1024:ALA:C	2.59	0.46
4:D:29:LEU:HB3	7:G:82:PHE:HE2	1.81	0.46
4:D:64:VAL:O	4:D:66:ARG:N	2.49	0.46
5:E:42:PHE:O	5:E:43:LYS:C	2.59	0.46
5:E:145:THR:HG21	5:E:187:TYR:CD2	2.50	0.46
7:G:106:MET:CG	7:G:107:LYS:N	2.77	0.46
10:J:21:TYR:CD2	10:J:21:TYR:C	2.94	0.46
1:A:77:CYS:C	1:A:78:PRO:O	2.55	0.46
1:A:172:PRO:HG3	1:A:185:TRP:CZ2	2.51	0.46
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.51	0.46
1:A:252:PHE:HB2	1:A:256:GLN:CD	2.41	0.46
1:A:494:SER:O	1:A:497:THR:N	2.49	0.46
1:A:849:MET:HE3	1:A:1061:GLY:C	2.40	0.46
1:A:883:LEU:CD2	1:A:1021:LEU:HB2	2.46	0.46
2:B:839:MET:HE3	2:B:1010:LEU:CD2	2.44	0.46
2:B:1110:PRO:HG3	2:B:1125:ASP:HB3	1.98	0.46
3:C:34:ARG:HA	3:C:37:MET:HE3	1.96	0.46
3:C:59:ALA:O	3:C:60:ASP:C	2.58	0.46
4:D:40:HIS:C	4:D:42:GLY:N	2.72	0.46
6:F:143:PHE:C	6:F:143:PHE:HD1	2.23	0.46
14:P:8:G:H2'	14:P:9:A:C8	2.51	0.46
1:A:18:GLN:O	2:B:1215:ARG:HG2	2.16	0.46
1:A:241:VAL:HG13	1:A:266:LEU:HD13	1.97	0.46
1:A:268:ASP:O	1:A:269:ILE:C	2.59	0.46
1:A:332:LYS:NZ	15:T:19:TT:H7C2	2.31	0.46
1:A:639:PRO:HG2	1:A:640:GLN:H	1.81	0.46
1:A:697:ALA:C	1:A:699:ALA:H	2.23	0.46
1:A:818:MET:HA	2:B:514:LEU:HB3	1.98	0.46
1:A:857:ARG:HG2	1:A:863:VAL:HA	1.98	0.46
1:A:1222:ASN:O	1:A:1223:ASP:HB3	2.16	0.46
1:A:1224:LEU:HD11	1:A:1240:CYS:HB2	1.97	0.46
1:A:1445:ILE:HD12	7:G:59:GLY:O	2.15	0.46
2:B:210:LYS:HG3	2:B:461:LEU:O	2.16	0.46
2:B:244:LEU:O	2:B:246:LYS:N	2.49	0.46
2:B:510:LYS:CG	2:B:511:PRO:CD	2.82	0.46
2:B:812:LEU:O	2:B:813:LYS:C	2.59	0.46
2:B:1045:SER:O	2:B:1046:PRO:O	2.34	0.46
3:C:112:ASN:HB2	3:C:114:TYR:HE1	1.80	0.46
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.51	0.46
6:F:147:SER:O	6:F:148:VAL:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.98	0.46
10:J:31:ASP:O	10:J:32:GLU:C	2.59	0.46
12:L:49:LYS:O	12:L:50:ASP:CB	2.63	0.46
1:A:244:PRO:HG2	1:A:245:PRO:CD	2.46	0.45
1:A:270:LEU:O	1:A:271:LYS:C	2.57	0.45
1:A:514:PRO:CB	1:A:875:ALA:HB3	2.47	0.45
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.49	0.45
1:A:715:GLU:O	1:A:716:ASP:C	2.59	0.45
1:A:846:GLU:OE1	1:A:1425:SER:OG	2.33	0.45
2:B:37:PHE:HE2	2:B:542:MET:HA	1.81	0.45
2:B:181:LEU:O	2:B:182:SER:C	2.59	0.45
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.30	0.45
2:B:1184:GLY:C	2:B:1186:ASP:N	2.68	0.45
3:C:41:ILE:HD11	3:C:247:GLY:CA	2.46	0.45
3:C:44:LEU:HD21	3:C:159:ALA:CB	2.46	0.45
3:C:73:GLN:NE2	3:C:74:SER:H	2.14	0.45
4:D:191:ALA:C	4:D:193:THR:N	2.74	0.45
12:L:40:LEU:HB3	12:L:41:SER:H	1.68	0.45
12:L:55:ILE:H	12:L:55:ILE:HG12	1.32	0.45
1:A:800:VAL:HA	1:A:812:GLU:OE2	2.16	0.45
1:A:874:ASP:O	1:A:876:ALA:N	2.49	0.45
1:A:1004:ASN:O	1:A:1008:GLN:HB2	2.16	0.45
1:A:1362:TYR:CD1	1:A:1362:TYR:C	2.92	0.45
1:A:1445:ILE:HG12	7:G:18:PHE:HE2	1.78	0.45
2:B:102:VAL:HG12	2:B:104:GLU:HG2	1.98	0.45
2:B:240:ILE:HG22	2:B:254:LEU:HB3	1.97	0.45
2:B:245:GLU:C	2:B:246:LYS:HG3	2.41	0.45
2:B:309:GLN:CD	9:I:52:ILE:HD11	2.41	0.45
2:B:798:TYR:CE2	3:C:62:PHE:CZ	3.04	0.45
3:C:167:HIS:ND1	12:L:70:ARG:HB3	2.31	0.45
4:D:119:ARG:HD3	4:D:221:TYR:CE2	2.51	0.45
7:G:39:THR:O	7:G:43:GLY:HA2	2.15	0.45
14:P:2:C:O2'	14:P:3:G:H5'	2.16	0.45
1:A:71:GLN:HG3	1:A:72:GLU:N	2.31	0.45
1:A:500:GLU:OE2	2:B:1145:SER:N	2.49	0.45
1:A:526:ASP:OD1	2:B:1013:ASN:ND2	2.48	0.45
1:A:711:ARG:HA	9:I:97:MET:HE2	1.99	0.45
1:A:730:GLY:O	1:A:733:ALA:N	2.49	0.45
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.16	0.45
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	1.98	0.45
1:A:1381:LEU:HD23	1:A:1381:LEU:HA	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:758:PHE:HZ	2:B:1031:LEU:HD22	1.82	0.45
2:B:1177:HIS:C	2:B:1179:GLN:H	2.25	0.45
3:C:236:GLY:C	3:C:238:ILE:N	2.73	0.45
5:E:35:VAL:C	5:E:37:LEU:N	2.75	0.45
5:E:191:LYS:O	5:E:192:ARG:C	2.58	0.45
1:A:26:GLU:O	1:A:27:VAL:C	2.59	0.45
1:A:361:LEU:HA	1:A:471:ASN:ND2	2.31	0.45
1:A:667:GLY:HA3	3:C:192:TRP:CH2	2.51	0.45
1:A:915:SER:O	1:A:919:ILE:HG13	2.16	0.45
1:A:963:ILE:HD13	1:A:1049:ILE:CG1	2.47	0.45
1:A:1021:LEU:O	1:A:1024:SER:HB3	2.16	0.45
1:A:1171:GLN:HA	1:A:1174:PHE:HD1	1.80	0.45
1:A:1394:THR:O	1:A:1395:GLY:O	2.34	0.45
1:A:1444:MET:HE3	1:A:1444:MET:HB2	1.78	0.45
2:B:29:ASP:O	2:B:30:SER:C	2.60	0.45
2:B:96:TYR:HE1	2:B:131:ASP:OD2	1.99	0.45
2:B:364:ILE:CG1	2:B:585:VAL:HG13	2.38	0.45
2:B:570:VAL:HG23	2:B:573:GLN:HB3	1.97	0.45
2:B:640:VAL:O	2:B:640:VAL:HG12	2.16	0.45
2:B:825:VAL:HG21	2:B:1092:TYR:HE1	1.80	0.45
2:B:1065:GLN:HB2	3:C:201:TRP:CZ3	2.51	0.45
3:C:184:ASN:HD21	3:C:187:LYS:HA	1.80	0.45
9:I:29:CYS:SG	9:I:31:THR:N	2.86	0.45
10:J:45:CYS:O	10:J:48:ARG:HG3	2.17	0.45
13:N:6:DC:H1'	13:N:7:DT:H5'	1.97	0.45
1:A:396:PRO:HG3	1:A:416:ARG:HB3	1.97	0.45
1:A:885:THR:O	1:A:885:THR:HG22	2.16	0.45
1:A:1111:MET:CE	1:A:1330:ASN:OD1	2.64	0.45
1:A:1364:ASN:HD22	1:A:1364:ASN:C	2.24	0.45
2:B:833:TYR:CZ	11:K:66:PRO:HG3	2.51	0.45
2:B:1182:CYS:O	2:B:1183:LYS:O	2.35	0.45
3:C:113:VAL:CG2	3:C:147:LEU:HD21	2.47	0.45
4:D:29:LEU:HB3	7:G:82:PHE:CE2	2.52	0.45
4:D:52:LEU:C	4:D:54:GLU:N	2.69	0.45
5:E:156:LEU:HD12	5:E:195:VAL:CB	2.47	0.45
8:H:40:LEU:HB2	8:H:123:MET:HG3	1.99	0.45
8:H:82:PRO:C	8:H:84:ALA:N	2.73	0.45
10:J:13:VAL:C	10:J:14:VAL:HG23	2.40	0.45
11:K:11:LEU:HD22	11:K:11:LEU:N	2.32	0.45
11:K:65:HIS:CG	11:K:66:PRO:HD2	2.51	0.45
12:L:27:LEU:HD23	12:L:27:LEU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HB2	2:B:1193:GLN:OE1	2.16	0.45
1:A:32:VAL:HG21	1:A:68:GLN:NE2	2.32	0.45
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.52	0.45
1:A:381:THR:HG23	1:A:382:PRO:CD	2.47	0.45
1:A:408:ASP:C	1:A:410:GLY:H	2.24	0.45
1:A:481:ASP:OD1	1:A:483:ASP:CG	2.60	0.45
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.50	0.45
1:A:1134:ILE:O	1:A:1135:ARG:C	2.59	0.45
2:B:337:ARG:C	2:B:338:GLY:CA	2.90	0.45
2:B:502:ILE:CD1	2:B:502:ILE:N	2.78	0.45
2:B:854:LEU:HB3	2:B:856:PHE:HE1	1.80	0.45
2:B:895:ASP:C	2:B:897:GLY:N	2.74	0.45
3:C:20:PHE:HE1	3:C:22:LEU:CD1	2.30	0.45
3:C:123:ASN:ND2	3:C:125:MET:CG	2.79	0.45
3:C:176:ILE:CG2	3:C:177:GLU:N	2.79	0.45
3:C:191:TYR:HD2	3:C:201:TRP:CD1	2.34	0.45
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.84	0.45
8:H:99:GLY:HA3	8:H:117:SER:O	2.17	0.45
10:J:43:ARG:O	10:J:47:ARG:HB2	2.17	0.45
1:A:19:PHE:HE1	1:A:1396:ALA:HB3	1.82	0.45
1:A:23:SER:O	1:A:26:GLU:N	2.49	0.45
1:A:1064:VAL:O	1:A:1064:VAL:HG12	2.16	0.45
2:B:58:THR:O	2:B:62:ILE:HG13	2.17	0.45
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.99	0.45
2:B:294:ASP:C	2:B:296:GLU:H	2.24	0.45
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.97	0.45
8:H:4:THR:HG22	8:H:5:LEU:H	1.81	0.45
8:H:91:ASP:C	8:H:93:TYR:N	2.74	0.45
9:I:69:PRO:HG2	9:I:85:PHE:CD2	2.52	0.45
11:K:15:GLY:O	11:K:16:GLU:HG3	2.17	0.45
1:A:166:GLY:O	1:A:167:CYS:SG	2.74	0.45
1:A:244:PRO:CG	1:A:245:PRO:HD3	2.47	0.45
1:A:414:ASP:OD1	1:A:414:ASP:C	2.60	0.45
1:A:723:ASN:C	1:A:725:ALA:N	2.72	0.45
1:A:939:ASP:O	1:A:940:ARG:C	2.59	0.45
2:B:223:VAL:HG21	2:B:380:TYR:CE2	2.51	0.45
2:B:497:ARG:NH2	2:B:775:LYS:HZ3	2.13	0.45
2:B:704:ALA:HB2	2:B:738:PHE:CD2	2.52	0.45
2:B:765:PRO:O	2:B:766:ARG:C	2.59	0.45
2:B:1006:ILE:HD13	10:J:44:TYR:CZ	2.51	0.45
2:B:1031:LEU:HD11	2:B:1042:GLY:HA3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:ASP:O	3:C:17:ASN:CG	2.59	0.45
3:C:99:LEU:HD23	3:C:99:LEU:N	2.32	0.45
5:E:124:VAL:HB	5:E:125:PRO:CD	2.47	0.45
1:A:120:GLU:HA	1:A:123:ARG:HG3	1.99	0.45
1:A:185:TRP:CZ3	1:A:200:ARG:HG2	2.52	0.45
1:A:482:PHE:O	1:A:484:GLY:N	2.49	0.45
1:A:508:PRO:O	1:A:511:ILE:HG13	2.16	0.45
1:A:549:MET:SD	1:A:577:ILE:CD1	3.04	0.45
1:A:666:ILE:CD1	1:A:667:GLY:N	2.80	0.45
1:A:674:PRO:C	1:A:676:MET:N	2.72	0.45
1:A:1146:VAL:HG11	1:A:1207:LEU:HD12	1.99	0.45
2:B:244:LEU:HD11	2:B:366:GLN:HE22	1.81	0.45
2:B:360:PHE:CD2	2:B:361:LEU:HB2	2.51	0.45
2:B:582:VAL:HG12	2:B:587:HIS:NE2	2.32	0.45
2:B:802:PRO:HB3	2:B:1091:TYR:CD2	2.51	0.45
2:B:911:ILE:O	2:B:911:ILE:HG22	2.17	0.45
2:B:954:VAL:HA	2:B:964:VAL:HG22	1.98	0.45
3:C:168:ALA:C	3:C:170:TRP:H	2.24	0.45
3:C:249:ASP:O	3:C:250:THR:C	2.60	0.45
5:E:60:PHE:CE2	5:E:80:VAL:HB	2.51	0.45
9:I:34:TYR:O	9:I:35:VAL:HG23	2.17	0.45
9:I:70:ARG:HH11	9:I:84:VAL:HB	1.81	0.45
11:K:82:ASP:O	11:K:85:ASP:HB2	2.17	0.45
12:L:28:LYS:HB2	12:L:39:SER:HB2	1.99	0.45
1:A:41:MET:O	1:A:42:ASP:C	2.59	0.45
1:A:65:LEU:O	1:A:66:LYS:C	2.59	0.45
1:A:313:GLN:O	1:A:314:ALA:HB3	2.17	0.45
1:A:349:ALA:C	2:B:1128:LEU:HD11	2.42	0.45
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.52	0.45
1:A:545:GLN:C	1:A:547:LEU:N	2.73	0.45
1:A:567:LYS:HD2	1:A:568:PRO:CD	2.38	0.45
1:A:710:LEU:HD13	9:I:94:ASP:O	2.16	0.45
1:A:779:PHE:O	1:A:780:VAL:C	2.60	0.45
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.17	0.45
1:A:1333:ILE:HG22	1:A:1334:ASP:N	2.32	0.45
2:B:405:ARG:HA	2:B:631:GLY:O	2.16	0.45
2:B:814:PHE:C	2:B:816:GLU:H	2.24	0.45
2:B:1164:GLY:HA3	2:B:1190:ASP:OD2	2.16	0.45
3:C:27:LEU:HD13	3:C:228:PHE:HE2	1.81	0.45
3:C:215:GLU:O	3:C:217:ASP:N	2.50	0.45
5:E:24:LYS:CG	5:E:25:ASP:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:20:PRO:CG	7:G:21:ARG:N	2.80	0.45
8:H:10:PHE:CE1	8:H:57:VAL:HB	2.52	0.45
11:K:31:VAL:O	11:K:74:ARG:HA	2.17	0.45
1:A:1206:ASP:O	1:A:1274:ARG:NH1	2.51	0.44
1:A:1334:ASP:C	1:A:1336:MET:N	2.73	0.44
2:B:27:ALA:C	2:B:29:ASP:N	2.74	0.44
2:B:96:TYR:HB2	2:B:129:PHE:HB2	1.99	0.44
2:B:118:ARG:CG	2:B:204:ILE:HD13	2.47	0.44
2:B:280:ILE:CD1	2:B:334:ILE:HG12	2.44	0.44
2:B:295:GLY:O	2:B:299:GLU:HG3	2.18	0.44
2:B:364:ILE:HG12	2:B:585:VAL:CG1	2.38	0.44
3:C:35:ARG:HH11	11:K:41:THR:HA	1.81	0.44
4:D:33:PHE:CZ	7:G:80:LYS:HE3	2.53	0.44
4:D:153:ARG:C	4:D:154:PHE:CG	2.95	0.44
5:E:112:TYR:CZ	5:E:136:ASN:HB2	2.52	0.44
5:E:163:GLU:O	5:E:166:LYS:N	2.50	0.44
6:F:109:VAL:HG12	6:F:110:ASP:N	2.31	0.44
7:G:7:LEU:O	7:G:73:LYS:HD2	2.17	0.44
7:G:9:LEU:HD23	7:G:30:LEU:HD12	2.00	0.44
7:G:87:VAL:HG23	7:G:103:VAL:HG21	1.99	0.44
10:J:56:LEU:O	10:J:59:LYS:N	2.44	0.44
11:K:35:PHE:CD1	11:K:71:PHE:CE1	3.05	0.44
11:K:110:ASN:C	11:K:111:LEU:CG	2.89	0.44
15:T:16:DT:H1'	15:T:17:DT:H5'	1.98	0.44
1:A:34:LYS:CB	1:A:36:ARG:HE	2.28	0.44
1:A:67:CYS:O	1:A:68:GLN:CB	2.65	0.44
1:A:75:ASN:O	1:A:76:GLU:HB2	2.17	0.44
1:A:285:PRO:O	1:A:287:HIS:N	2.50	0.44
1:A:334:GLY:O	1:A:335:ARG:C	2.59	0.44
1:A:337:ARG:HH12	15:T:18:DT:P	2.39	0.44
1:A:469:ARG:NH2	2:B:991:GLY:O	2.50	0.44
1:A:567:LYS:HE3	8:H:46:LEU:CB	2.42	0.44
1:A:572:TRP:HA	1:A:576:GLN:OE1	2.17	0.44
1:A:849:MET:HE3	1:A:1061:GLY:O	2.17	0.44
1:A:1074:GLU:C	1:A:1076:ALA:H	2.25	0.44
1:A:1265:ASN:O	1:A:1268:LEU:N	2.47	0.44
1:A:1277:GLU:C	1:A:1279:ILE:H	2.24	0.44
2:B:209:GLU:CD	2:B:788:ARG:HH22	2.25	0.44
2:B:283:VAL:O	2:B:286:PHE:N	2.50	0.44
2:B:776:GLN:NE2	14:P:8:G:H5'	2.30	0.44
5:E:30:ILE:HG22	5:E:31:THR:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:90:ARG:CG	6:F:91:ALA:N	2.81	0.44
7:G:1:MET:HG2	7:G:85:GLU:CD	2.43	0.44
8:H:91:ASP:O	8:H:93:TYR:N	2.50	0.44
8:H:143:LEU:N	8:H:143:LEU:CD1	2.79	0.44
9:I:4:PHE:CD1	9:I:4:PHE:C	2.95	0.44
11:K:6:ARG:O	11:K:8:GLU:N	2.50	0.44
1:A:418:SER:C	1:A:420:ARG:N	2.76	0.44
1:A:524:VAL:HG12	1:A:525:GLN:HE21	1.81	0.44
2:B:744:HIS:CG	2:B:745:PRO:HD2	2.52	0.44
2:B:848:ARG:HD2	10:J:7:CYS:O	2.18	0.44
3:C:45:ALA:HA	3:C:72:LEU:CD1	2.47	0.44
5:E:18:THR:O	5:E:19:VAL:C	2.59	0.44
5:E:147:HIS:CD2	5:E:149:LEU:H	2.35	0.44
5:E:180:ARG:HB2	5:E:215:MET:OXT	2.17	0.44
7:G:1:MET:SD	7:G:79:PHE:HD1	2.40	0.44
7:G:106:MET:HG2	7:G:107:LYS:N	2.31	0.44
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.52	0.44
9:I:55:THR:HG22	9:I:55:THR:O	2.18	0.44
9:I:78:CYS:HB3	9:I:106:CYS:SG	2.58	0.44
10:J:57:ILE:HA	10:J:60:PHE:HB2	1.98	0.44
15:T:15:DT:H6	15:T:15:DT:H2'	1.61	0.44
1:A:606:LEU:HB3	1:A:614:PHE:CD2	2.52	0.44
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.99	0.44
1:A:1334:ASP:O	1:A:1337:GLU:N	2.50	0.44
2:B:240:ILE:HG23	2:B:240:ILE:O	2.17	0.44
2:B:377:PHE:O	2:B:378:LEU:C	2.60	0.44
2:B:597:MET:C	2:B:599:THR:N	2.73	0.44
2:B:1027:ILE:O	2:B:1028:GLU:C	2.59	0.44
2:B:1223:ASP:HB3	2:B:1224:PHE:H	1.58	0.44
3:C:3:GLU:O	3:C:4:GLU:HG3	2.18	0.44
4:D:7:THR:O	4:D:7:THR:HG23	2.17	0.44
4:D:13:ARG:C	4:D:17:LYS:NZ	2.75	0.44
6:F:140:ASP:C	6:F:140:ASP:OD1	2.61	0.44
7:G:91:VAL:HG12	7:G:92:VAL:N	2.32	0.44
8:H:84:ALA:C	8:H:86:ASP:N	2.74	0.44
9:I:50:THR:HG22	9:I:51:ASN:N	2.32	0.44
9:I:75:CYS:SG	9:I:78:CYS:C	3.01	0.44
1:A:401:GLY:O	1:A:435:HIS:CD2	2.71	0.44
1:A:404:TYR:CE2	1:A:414:ASP:HA	2.53	0.44
1:A:415:LEU:HA	1:A:415:LEU:HD23	1.69	0.44
1:A:452:LYS:HE2	1:A:452:LYS:HB3	1.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ALA:O	1:A:509:LEU:HB2	2.17	0.44
1:A:806:ARG:NH1	2:B:729:ILE:HG13	2.32	0.44
1:A:929:LEU:CD2	1:A:983:ILE:HG21	2.48	0.44
1:A:968:GLN:C	1:A:970:THR:H	2.26	0.44
1:A:979:SER:HG	1:A:981:LEU:HG	1.80	0.44
1:A:1332:PHE:O	1:A:1333:ILE:C	2.59	0.44
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.17	0.44
2:B:43:LEU:HD11	2:B:811:TYR:O	2.17	0.44
2:B:210:LYS:HA	2:B:481:GLN:O	2.18	0.44
2:B:487:THR:CG2	2:B:488:TYR:N	2.81	0.44
2:B:560:GLU:O	2:B:561:TRP:CD1	2.71	0.44
3:C:18:VAL:O	3:C:20:PHE:CD2	2.70	0.44
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.53	0.44
4:D:27:LEU:HG	4:D:197:SER:HB2	1.98	0.44
4:D:146:GLN:O	4:D:149:THR:HG22	2.17	0.44
5:E:23:VAL:HG13	5:E:78:LEU:HD13	2.00	0.44
7:G:73:LYS:HE2	7:G:74:TYR:O	2.18	0.44
11:K:82:ASP:OD1	11:K:84:LYS:N	2.46	0.44
1:A:35:ILE:HD13	1:A:241:VAL:HG11	1.99	0.44
1:A:55:ASP:C	1:A:57:ARG:N	2.74	0.44
1:A:56:PRO:O	1:A:57:ARG:HG3	2.18	0.44
1:A:172:PRO:HD3	1:A:185:TRP:NE1	2.33	0.44
1:A:299:HIS:C	1:A:301:ALA:N	2.74	0.44
1:A:368:LYS:O	1:A:369:SER:C	2.61	0.44
1:A:664:THR:CG2	1:A:665:GLY:N	2.80	0.44
1:A:816:HIS:CD2	2:B:764:SER:H	2.36	0.44
1:A:986:ILE:HD12	1:A:1032:LEU:HD11	1.98	0.44
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.32	0.44
1:A:1102:LYS:HG2	1:A:1106:ASN:HD21	1.82	0.44
2:B:223:VAL:CG1	2:B:381:MET:HG2	2.48	0.44
2:B:314:LEU:O	2:B:317:CYS:HB3	2.17	0.44
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.89	0.44
2:B:782:LEU:CD1	2:B:788:ARG:HH11	2.29	0.44
3:C:44:LEU:HD21	3:C:159:ALA:HB1	1.99	0.44
7:G:48:VAL:HA	7:G:76:ALA:HB2	1.99	0.44
7:G:166:ASP:O	7:G:167:TYR:C	2.61	0.44
11:K:18:LYS:NZ	11:K:37:LYS:O	2.51	0.44
1:A:262:LEU:C	1:A:264:PHE:H	2.24	0.44
1:A:418:SER:C	1:A:420:ARG:H	2.25	0.44
1:A:673:GLY:O	1:A:676:MET:HB2	2.17	0.44
1:A:709:THR:CG2	1:A:710:LEU:N	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:GLU:OE2	6:F:88:TYR:OH	2.35	0.44
2:B:293:PRO:HG2	2:B:296:GLU:HB3	2.00	0.44
2:B:682:SER:O	2:B:685:LEU:HB3	2.17	0.44
2:B:806:THR:HG22	2:B:808:ALA:HB3	1.99	0.44
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.81	0.44
3:C:238:ILE:HD11	3:C:246:ARG:NH1	2.33	0.44
3:C:259:LEU:CD1	11:K:91:CYS:HB2	2.47	0.44
5:E:90:VAL:O	5:E:90:VAL:HG22	2.17	0.44
6:F:89:GLU:HB3	6:F:134:ILE:HD13	2.00	0.44
9:I:15:TYR:N	9:I:15:TYR:HD1	2.14	0.44
9:I:32:CYS:SG	9:I:33:SER:N	2.90	0.44
9:I:34:TYR:CD2	9:I:34:TYR:C	2.95	0.44
9:I:70:ARG:NH1	9:I:84:VAL:HB	2.33	0.44
11:K:65:HIS:CD2	11:K:65:HIS:C	2.95	0.44
14:P:4:A:C2'	14:P:5:C:H5'	2.47	0.44
15:T:18:DT:C3'	15:T:19:TT:C5'	2.96	0.44
1:A:113:LEU:HG	1:A:218:ASP:OD1	2.17	0.44
1:A:548:ASN:OD1	11:K:60:ALA:HB1	2.18	0.44
1:A:719:VAL:O	1:A:721:PHE:N	2.51	0.44
1:A:760:GLN:HG2	1:A:765:VAL:O	2.17	0.44
1:A:1006:ILE:CD1	5:E:163:GLU:HG3	2.45	0.44
1:A:1094:VAL:CG1	1:A:1095:THR:N	2.63	0.44
2:B:113:TYR:HB3	2:B:114:PRO:HD2	1.99	0.44
2:B:259:TYR:HD1	2:B:259:TYR:N	2.16	0.44
2:B:386:LEU:C	2:B:388:CYS:N	2.74	0.44
2:B:1087:PHE:CD2	2:B:1088:GLY:N	2.76	0.44
4:D:51:ASN:O	4:D:52:LEU:C	2.58	0.44
5:E:197:LYS:HE2	5:E:199:ILE:HD11	2.00	0.44
7:G:125:SER:OG	7:G:128:PRO:HA	2.18	0.44
9:I:110:PHE:H	9:I:110:PHE:HD2	1.66	0.44
13:N:3:DG:H2''	13:N:4:DT:OP2	2.18	0.44
1:A:34:LYS:H	1:A:57:ARG:HH21	1.66	0.44
1:A:34:LYS:HZ1	1:A:57:ARG:NH1	2.15	0.44
1:A:82:GLY:O	1:A:241:VAL:N	2.37	0.44
1:A:388:LEU:HD22	1:A:432:VAL:HG21	2.00	0.44
1:A:523:ILE:HG22	1:A:528:LEU:HB2	2.00	0.44
1:A:543:LEU:O	1:A:544:ASP:C	2.60	0.44
1:A:773:LYS:H	1:A:773:LYS:HG3	1.49	0.44
1:A:1315:GLU:C	1:A:1317:MET:N	2.72	0.44
2:B:212:LEU:HD21	2:B:466:TRP:CH2	2.53	0.44
2:B:311:LEU:O	2:B:312:GLU:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:ILE:HG21	2:B:348:ARG:CA	2.47	0.44
2:B:770:GLN:OE1	2:B:983:ARG:CA	2.58	0.44
2:B:806:THR:CG2	2:B:808:ALA:HB3	2.48	0.44
2:B:1183:LYS:O	2:B:1183:LYS:HE3	2.17	0.44
3:C:36:VAL:HG21	3:C:251:LEU:HD22	2.00	0.44
3:C:70:ILE:O	3:C:70:ILE:HG22	2.17	0.44
3:C:255:VAL:O	3:C:255:VAL:HG12	2.18	0.44
4:D:24:ALA:C	4:D:26:THR:N	2.75	0.44
5:E:168:TYR:C	5:E:169:ARG:HG3	2.43	0.44
6:F:128:LYS:HD3	6:F:149:GLU:O	2.18	0.44
7:G:31:LEU:CD2	7:G:48:VAL:HG21	2.48	0.44
7:G:39:THR:CG2	7:G:40:GLY:N	2.76	0.44
7:G:131:GLN:HG2	7:G:136:VAL:HG22	1.99	0.44
8:H:40:LEU:HG	8:H:41:ASP:O	2.18	0.44
14:P:5:C:C2'	14:P:6:C:O4'	2.55	0.44
1:A:37:PHE:HD1	1:A:37:PHE:H	1.65	0.43
1:A:230:ARG:N	1:A:233:TRP:CE3	2.65	0.43
1:A:242:PRO:HA	1:A:243:PRO:HD2	1.75	0.43
1:A:265:LYS:CE	1:A:322:VAL:HG13	2.47	0.43
1:A:337:ARG:HD3	2:B:1132:GLU:CD	2.43	0.43
1:A:483:ASP:OD2	1:A:483:ASP:C	2.61	0.43
1:A:783:THR:CG2	1:A:815:PHE:CE2	3.00	0.43
1:A:1280:GLU:O	1:A:1281:ARG:C	2.60	0.43
2:B:615:MET:HE3	2:B:615:MET:HB2	1.75	0.43
2:B:640:VAL:HB	2:B:738:PHE:O	2.19	0.43
2:B:798:TYR:HE2	3:C:62:PHE:HZ	1.63	0.43
2:B:798:TYR:CE2	3:C:62:PHE:CE2	3.06	0.43
2:B:1034:VAL:C	2:B:1036:ALA:N	2.75	0.43
2:B:1068:GLY:O	2:B:1069:PHE:C	2.61	0.43
2:B:1183:LYS:N	2:B:1183:LYS:HE3	2.33	0.43
4:D:18:VAL:O	4:D:19:GLU:HB3	2.18	0.43
6:F:75:PRO:HG2	6:F:78:GLN:HB2	2.00	0.43
7:G:18:PHE:HZ	7:G:68:ALA:HB2	1.83	0.43
7:G:80:LYS:O	7:G:82:PHE:CE1	2.71	0.43
1:A:218:ASP:O	1:A:219:PHE:C	2.59	0.43
1:A:442:VAL:O	1:A:457:ALA:HA	2.17	0.43
1:A:474:VAL:HG22	1:A:474:VAL:O	2.19	0.43
1:A:547:LEU:HB3	11:K:58:PHE:CE1	2.52	0.43
1:A:577:ILE:O	1:A:580:VAL:HG23	2.18	0.43
1:A:907:THR:HG22	1:A:908:LEU:N	2.33	0.43
1:A:935:GLN:O	1:A:938:LYS:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1350:LYS:O	1:A:1354:ASN:ND2	2.47	0.43
2:B:181:LEU:HD22	2:B:189:LEU:CD2	2.48	0.43
2:B:331:LEU:HD12	2:B:331:LEU:N	2.33	0.43
2:B:449:ASN:O	2:B:451:LYS:N	2.51	0.43
2:B:530:GLY:O	2:B:531:GLN:C	2.61	0.43
2:B:570:VAL:HA	2:B:571:PRO:HD2	1.74	0.43
2:B:642:ASP:HB3	2:B:649:LYS:HG3	2.00	0.43
3:C:249:ASP:O	3:C:252:GLN:HB3	2.18	0.43
3:C:256:ALA:C	3:C:258:ILE:H	2.24	0.43
4:D:122:GLU:HA	4:D:125:SER:OG	2.18	0.43
4:D:141:LEU:HD12	4:D:141:LEU:HA	1.80	0.43
5:E:117:THR:C	5:E:119:SER:H	2.26	0.43
9:I:7:CYS:HB2	9:I:34:TYR:CD1	2.53	0.43
12:L:70:ARG:HG2	12:L:70:ARG:NH1	2.32	0.43
15:T:24:DG:C2'	15:T:25:DT:O5'	2.63	0.43
1:A:248:PRO:O	1:A:260:ASP:HB2	2.18	0.43
1:A:699:ALA:HB2	9:I:114:GLN:NE2	2.32	0.43
1:A:780:VAL:O	1:A:782:ARG:HG2	2.18	0.43
1:A:1208:THR:O	1:A:1209:MET:C	2.60	0.43
1:A:1243:VAL:HG12	1:A:1244:ARG:N	2.32	0.43
1:A:1290:LYS:O	1:A:1291:VAL:HG23	2.19	0.43
1:A:1341:ILE:O	1:A:1344:GLY:N	2.51	0.43
1:A:1450:LEU:HD11	6:F:108:PHE:HZ	1.79	0.43
2:B:234:ILE:HD12	2:B:234:ILE:N	2.33	0.43
2:B:616:ILE:N	2:B:616:ILE:CD1	2.81	0.43
2:B:707:PRO:O	2:B:711:GLU:HG3	2.18	0.43
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.84	0.43
3:C:8:VAL:HG12	3:C:9:LYS:H	1.83	0.43
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.42	0.43
4:D:209:ARG:O	4:D:212:LYS:HB2	2.19	0.43
9:I:33:SER:O	9:I:34:TYR:C	2.61	0.43
9:I:85:PHE:CD1	9:I:99:LEU:HD13	2.54	0.43
11:K:45:LEU:C	11:K:47:ARG:H	2.25	0.43
11:K:88:LYS:O	11:K:89:ASN:C	2.61	0.43
1:A:347:PHE:CE2	1:A:493:GLN:OE1	2.72	0.43
1:A:353:ILE:CG2	1:A:487:MET:HG3	2.45	0.43
1:A:388:LEU:HD22	1:A:432:VAL:HB	1.99	0.43
1:A:526:ASP:O	1:A:527:THR:C	2.59	0.43
1:A:546:VAL:O	1:A:546:VAL:HG12	2.18	0.43
1:A:639:PRO:HG2	1:A:640:GLN:N	2.33	0.43
1:A:699:ALA:HB1	9:I:114:GLN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:802:ASN:ND2	1:A:812:GLU:OE1	2.42	0.43
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.99	0.43
1:A:1213:GLY:O	1:A:1216:ILE:N	2.52	0.43
1:A:1305:VAL:CG1	1:A:1306:LEU:N	2.81	0.43
2:B:114:PRO:HG2	2:B:115:GLN:N	2.28	0.43
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.34	0.43
2:B:309:GLN:HG3	9:I:52:ILE:CD1	2.48	0.43
2:B:526:GLU:CD	2:B:752:ALA:HB2	2.43	0.43
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.48	0.43
2:B:681:TRP:O	2:B:684:LEU:N	2.51	0.43
2:B:957:ASN:O	2:B:960:GLY:N	2.47	0.43
2:B:1123:SER:HB3	15:T:24:DG:P	2.58	0.43
2:B:1156:ASP:O	2:B:1157:ALA:O	2.37	0.43
2:B:1181:GLU:O	2:B:1182:CYS:HB2	2.17	0.43
4:D:13:ARG:C	4:D:17:LYS:HZ3	2.26	0.43
4:D:55:ALA:HB3	4:D:148:LEU:HD21	1.99	0.43
5:E:88:VAL:HG12	5:E:89:GLY:N	2.33	0.43
7:G:26:LEU:HD23	7:G:26:LEU:HA	1.85	0.43
8:H:23:VAL:HG22	8:H:43:ASN:HA	2.00	0.43
8:H:95:TYR:HB3	8:H:144:ILE:HB	1.99	0.43
15:T:10:DA:H1'	15:T:11:DG:C8	2.54	0.43
1:A:239:LEU:HA	1:A:240:PRO:HD2	1.89	0.43
1:A:472:LEU:CD1	2:B:835:GLN:CD	2.92	0.43
1:A:567:LYS:HZ2	8:H:47:PHE:CB	2.31	0.43
1:A:608:ILE:HG13	1:A:613:ILE:HD12	2.01	0.43
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.52	0.43
1:A:958:VAL:HG12	1:A:960:ILE:HG13	2.01	0.43
1:A:1209:MET:CE	1:A:1236:LEU:HB3	2.48	0.43
1:A:1226:VAL:HG22	1:A:1240:CYS:HB3	2.00	0.43
1:A:1316:VAL:O	1:A:1316:VAL:HG12	2.19	0.43
1:A:1404:GLU:O	1:A:1407:GLU:HB2	2.18	0.43
2:B:352:ALA:O	2:B:353:LYS:C	2.62	0.43
2:B:496:ARG:HB3	2:B:496:ARG:NH1	2.33	0.43
2:B:765:PRO:O	2:B:768:THR:N	2.51	0.43
2:B:1040:ASN:O	2:B:1041:GLU:C	2.60	0.43
2:B:1072:MET:HE3	2:B:1085:ILE:HD13	2.01	0.43
2:B:1074:ASN:HB2	2:B:1081:LEU:HD21	2.00	0.43
3:C:86:CYS:O	3:C:88:CYS:N	2.52	0.43
3:C:213:PRO:O	3:C:214:ASN:CB	2.60	0.43
5:E:20:LYS:O	5:E:21:GLU:C	2.61	0.43
5:E:46:TYR:CE2	5:E:58:MET:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:153:HIS:O	5:E:154:ILE:CG1	2.67	0.43
6:F:118:LEU:O	6:F:118:LEU:HG	2.18	0.43
7:G:9:LEU:HD12	7:G:10:ASN:N	2.34	0.43
10:J:36:LEU:O	10:J:37:SER:C	2.61	0.43
10:J:53:HIS:NE2	10:J:55:ASP:HA	2.34	0.43
13:N:0:DT:O4	15:T:18:DT:O2	2.35	0.43
1:A:47:ARG:O	1:A:48:ALA:HB2	2.18	0.43
1:A:335:ARG:N	1:A:339:ASN:HD22	2.17	0.43
1:A:455:MET:HE3	2:B:1134:GLU:HG3	2.01	0.43
1:A:618:GLU:OE2	1:A:620:LYS:HB2	2.19	0.43
2:B:193:LYS:NZ	12:L:32:ALA:HB1	2.32	0.43
2:B:247:GLY:O	2:B:249:ARG:N	2.51	0.43
2:B:371:GLU:CD	2:B:371:GLU:N	2.77	0.43
2:B:681:TRP:O	2:B:682:SER:C	2.61	0.43
2:B:825:VAL:HG12	2:B:826:ALA:N	2.33	0.43
2:B:857:ARG:HH21	2:B:942:ARG:NH1	2.16	0.43
2:B:1115:THR:HG22	2:B:1117:GLN:HG3	2.00	0.43
3:C:189:THR:CG2	3:C:190:ASP:N	2.81	0.43
4:D:13:ARG:HB2	4:D:17:LYS:NZ	2.34	0.43
4:D:47:LEU:CD1	4:D:48:ILE:N	2.81	0.43
5:E:124:VAL:CG1	5:E:132:ILE:HB	2.46	0.43
5:E:136:ASN:OD1	5:E:138:ALA:N	2.52	0.43
7:G:99:PHE:CZ	7:G:143:ILE:HD13	2.54	0.43
9:I:33:SER:O	9:I:35:VAL:HG23	2.18	0.43
1:A:265:LYS:HE2	1:A:322:VAL:HG13	1.98	0.43
1:A:482:PHE:C	1:A:484:GLY:N	2.71	0.43
1:A:525:GLN:O	1:A:526:ASP:C	2.61	0.43
1:A:696:GLU:O	1:A:696:GLU:HG2	2.18	0.43
1:A:842:VAL:C	1:A:844:ALA:N	2.76	0.43
1:A:857:ARG:NH2	6:F:139:PRO:HG3	2.33	0.43
1:A:877:HIS:O	1:A:878:ILE:HG12	2.19	0.43
1:A:1116:LEU:C	1:A:1116:LEU:HD12	2.43	0.43
1:A:1313:LEU:HD23	1:A:1338:VAL:HB	2.01	0.43
1:A:1362:TYR:HD1	1:A:1363:VAL:H	1.65	0.43
2:B:29:ASP:HB3	2:B:658:ILE:HD11	1.99	0.43
2:B:39:ARG:HH21	2:B:665:GLU:CG	2.31	0.43
2:B:258:LEU:HG	2:B:258:LEU:O	2.18	0.43
2:B:410:GLY:O	2:B:412:LEU:N	2.52	0.43
3:C:69:LEU:HB3	10:J:6:ARG:HD3	1.99	0.43
3:C:262:LEU:HD23	3:C:262:LEU:HA	1.84	0.43
4:D:71:LYS:HA	4:D:74:GLN:CB	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:112:LYS:NZ	7:G:120:THR:HA	2.33	0.43
9:I:33:SER:C	9:I:34:TYR:O	2.62	0.43
11:K:44:ASN:N	11:K:61:TYR:CE1	2.87	0.43
1:A:35:ILE:HB	1:A:83:HIS:O	2.18	0.43
1:A:236:LEU:HD11	1:A:304:MET:HE1	2.00	0.43
1:A:503:GLN:C	1:A:504:LEU:HD12	2.43	0.43
1:A:653:VAL:O	1:A:654:ASN:C	2.62	0.43
1:A:839:ARG:O	1:A:840:ARG:C	2.62	0.43
1:A:971:PHE:O	1:A:972:HIS:C	2.62	0.43
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	2.01	0.43
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.99	0.43
2:B:515:HIS:O	2:B:518:HIS:HB2	2.19	0.43
2:B:583:ASN:OD1	2:B:628:THR:N	2.50	0.43
2:B:685:LEU:C	2:B:687:GLU:H	2.26	0.43
7:G:51:TYR:CD2	7:G:51:TYR:O	2.71	0.43
8:H:62:SER:C	8:H:64:ASN:N	2.74	0.43
12:L:43:THR:HG22	12:L:43:THR:O	2.19	0.43
1:A:76:GLU:O	1:A:78:PRO:HD3	2.19	0.43
1:A:204:THR:O	1:A:205:GLU:C	2.61	0.43
1:A:370:ILE:O	1:A:373:THR:N	2.43	0.43
1:A:481:ASP:OD1	1:A:483:ASP:OD2	2.37	0.43
1:A:570:PRO:O	1:A:571:LEU:HD12	2.18	0.43
1:A:719:VAL:C	1:A:721:PHE:H	2.26	0.43
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.44	0.43
2:B:27:ALA:C	2:B:29:ASP:H	2.27	0.43
2:B:47:GLN:O	2:B:173:MET:HE1	2.19	0.43
2:B:376:PHE:HE2	2:B:569:TYR:HD2	1.65	0.43
2:B:566:LEU:O	2:B:567:GLU:C	2.61	0.43
2:B:614:SER:C	2:B:615:MET:HG3	2.43	0.43
2:B:642:ASP:CA	2:B:649:LYS:HA	2.40	0.43
2:B:763:GLN:O	2:B:764:SER:C	2.61	0.43
2:B:797:TYR:HB2	2:B:852:ARG:O	2.19	0.43
2:B:860:MET:CG	2:B:861:ASP:N	2.80	0.43
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.63	0.43
2:B:1064:TYR:O	2:B:1065:GLN:O	2.37	0.43
2:B:1065:GLN:NE2	2:B:1067:ARG:HG2	2.33	0.43
2:B:1099:VAL:C	2:B:1101:ASP:N	2.77	0.43
2:B:1135:ARG:C	2:B:1137:CYS:N	2.76	0.43
2:B:1147:LEU:CD2	2:B:1151:LEU:HD22	2.48	0.43
3:C:176:ILE:HG22	3:C:177:GLU:O	2.19	0.43
5:E:153:HIS:C	5:E:154:ILE:HG13	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:195:VAL:HG22	5:E:213:ILE:HG13	2.01	0.43
8:H:30:SER:CB	8:H:36:CYS:HB3	2.48	0.43
8:H:39:THR:HB	8:H:124:ARG:HB3	2.00	0.43
10:J:2:ILE:HG22	10:J:3:VAL:O	2.18	0.43
11:K:57:LEU:HB2	11:K:76:GLN:HG2	2.01	0.43
1:A:49:LYS:CE	1:A:61:ILE:HD12	2.42	0.43
1:A:78:PRO:HB2	2:B:1201:LYS:HE3	2.01	0.43
1:A:399:HIS:O	1:A:400:PRO:C	2.60	0.43
1:A:601:LYS:HB2	1:A:603:ASN:HD21	1.84	0.43
1:A:1130:GLN:O	1:A:1134:ILE:HG13	2.19	0.43
2:B:60:GLN:OE1	2:B:95:ILE:HG22	2.19	0.43
2:B:343:ILE:HB	2:B:348:ARG:HE	1.84	0.43
2:B:361:LEU:N	2:B:362:PRO:CD	2.81	0.43
2:B:595:ARG:O	2:B:596:LEU:C	2.62	0.43
2:B:806:THR:C	2:B:808:ALA:N	2.71	0.43
2:B:890:TYR:O	2:B:892:LYS:N	2.51	0.43
3:C:3:GLU:O	3:C:4:GLU:CG	2.67	0.43
3:C:27:LEU:HD13	3:C:228:PHE:CE2	2.54	0.43
3:C:38:ILE:HA	3:C:173:ALA:HB2	2.00	0.43
3:C:120:ILE:HD11	3:C:130:GLY:O	2.19	0.43
4:D:51:ASN:ND2	4:D:54:GLU:OE2	2.52	0.43
4:D:60:LYS:O	4:D:64:VAL:HG23	2.19	0.43
5:E:55:ARG:HD2	5:E:83:CYS:O	2.19	0.43
7:G:34:VAL:HG11	7:G:74:TYR:HE1	1.84	0.43
8:H:59:ILE:O	8:H:60:ALA:HB3	2.18	0.43
11:K:57:LEU:N	11:K:76:GLN:O	2.52	0.43
1:A:203:SER:OG	1:A:206:GLU:HB2	2.19	0.42
1:A:350:ARG:HG3	1:A:350:ARG:NH1	2.33	0.42
1:A:356:ASP:C	1:A:358:ASN:H	2.27	0.42
1:A:925:LEU:O	1:A:927:VAL:N	2.52	0.42
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.19	0.42
1:A:1025:ARG:O	1:A:1026:LEU:HD23	2.19	0.42
2:B:382:ILE:O	2:B:386:LEU:HG	2.19	0.42
2:B:764:SER:HB3	2:B:765:PRO:CD	2.49	0.42
3:C:47:ASP:HA	3:C:169:LYS:HZ2	1.84	0.42
3:C:61:GLU:HA	3:C:64:ALA:HB3	2.00	0.42
4:D:145:MET:O	4:D:149:THR:HB	2.19	0.42
6:F:101:ILE:HD11	6:F:124:GLU:OE1	2.18	0.42
7:G:79:PHE:CE2	7:G:105:PRO:HG2	2.54	0.42
1:A:92:HIS:HD2	1:A:304:MET:CE	2.32	0.42
1:A:412:ARG:NH2	2:B:1108:ARG:HH12	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:TYR:O	1:A:418:SER:C	2.61	0.42
1:A:600:PRO:C	1:A:602:ASP:N	2.75	0.42
1:A:1057:VAL:CG1	1:A:1058:VAL:N	2.82	0.42
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	2.01	0.42
2:B:60:GLN:CD	2:B:95:ILE:HG22	2.44	0.42
2:B:693:ILE:HG22	2:B:694:ASP:O	2.20	0.42
2:B:971:THR:HG1	3:C:61:GLU:HG3	1.83	0.42
2:B:1197:PRO:O	2:B:1200:ALA:N	2.51	0.42
3:C:41:ILE:HD11	3:C:247:GLY:HA2	2.00	0.42
5:E:157:SER:O	5:E:159:ASP:N	2.51	0.42
5:E:160:GLU:O	5:E:163:GLU:HB3	2.19	0.42
7:G:15:PRO:HG3	7:G:66:GLY:C	2.44	0.42
8:H:56:THR:HG21	8:H:145:ARG:HE	1.84	0.42
9:I:101:PHE:HB2	9:I:110:PHE:CE2	2.55	0.42
12:L:43:THR:C	12:L:45:ALA:H	2.28	0.42
1:A:49:LYS:HZ2	1:A:60:SER:HA	1.84	0.42
1:A:372:LYS:HA	1:A:435:HIS:HD1	1.81	0.42
1:A:870:GLU:HG2	5:E:208:TYR:CD1	2.54	0.42
1:A:894:GLU:C	1:A:896:ARG:H	2.27	0.42
1:A:907:THR:HG23	1:A:908:LEU:N	2.33	0.42
1:A:1400:CYS:O	1:A:1405:THR:HG23	2.20	0.42
1:A:1430:LEU:HB2	1:A:1432:GLN:HG3	2.00	0.42
1:A:1437:GLY:C	1:A:1439:GLY:N	2.77	0.42
2:B:37:PHE:CE2	2:B:542:MET:HA	2.55	0.42
2:B:185:THR:O	2:B:186:GLU:C	2.62	0.42
2:B:857:ARG:NH2	2:B:942:ARG:NH1	2.68	0.42
2:B:1162:ILE:O	2:B:1171:VAL:HG21	2.19	0.42
4:D:118:THR:HG22	4:D:118:THR:O	2.19	0.42
5:E:61:GLN:HG2	5:E:62:ALA:H	1.83	0.42
5:E:179:GLN:HB2	5:E:182:ASP:HB2	2.01	0.42
7:G:13:LEU:HD21	7:G:17:PHE:CB	2.28	0.42
8:H:89:LEU:C	8:H:91:ASP:N	2.78	0.42
1:A:207:ILE:O	1:A:208:LEU:C	2.62	0.42
1:A:353:ILE:HG21	1:A:487:MET:CE	2.49	0.42
1:A:774:ARG:CZ	1:A:797:LYS:HG3	2.48	0.42
1:A:815:PHE:O	1:A:816:HIS:C	2.60	0.42
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.83	0.42
1:A:1386:ARG:HE	1:A:1386:ARG:HB3	1.68	0.42
1:A:1387:HIS:CE1	13:N:4:DT:C4'	3.00	0.42
2:B:221:ASN:OD1	2:B:242:SER:HA	2.18	0.42
2:B:283:VAL:O	2:B:284:ILE:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:ILE:HG22	2:B:365:THR:N	2.33	0.42
2:B:467:GLY:CA	2:B:475:SER:HB3	2.49	0.42
2:B:519:TRP:CD1	2:B:519:TRP:C	2.98	0.42
2:B:1060:ARG:C	2:B:1062:HIS:N	2.77	0.42
3:C:45:ALA:O	3:C:159:ALA:HA	2.20	0.42
7:G:27:LYS:O	7:G:28:THR:C	2.60	0.42
8:H:95:TYR:CE2	8:H:97:MET:CG	3.02	0.42
9:I:53:GLY:O	9:I:89:GLN:HB2	2.18	0.42
11:K:61:TYR:CD2	11:K:61:TYR:O	2.72	0.42
1:A:208:LEU:O	1:A:208:LEU:HD23	2.20	0.42
1:A:332:LYS:C	1:A:334:GLY:N	2.75	0.42
1:A:852:TYR:CE1	6:F:136:ARG:HG2	2.54	0.42
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.83	0.42
1:A:907:THR:HG23	1:A:908:LEU:H	1.85	0.42
1:A:1198:ASP:HB3	1:A:1201:ALA:HB3	2.01	0.42
1:A:1370:LEU:O	1:A:1373:ASP:HB2	2.20	0.42
1:A:1398:MET:HB2	1:A:1426:GLU:OE2	2.19	0.42
2:B:37:PHE:CD1	2:B:37:PHE:C	2.97	0.42
2:B:45:SER:OG	2:B:46:GLN:N	2.49	0.42
2:B:129:PHE:HE2	2:B:166:PHE:CD1	2.37	0.42
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.35	0.42
2:B:405:ARG:NE	2:B:632:ARG:HG2	2.34	0.42
2:B:708:GLU:O	2:B:709:ASP:C	2.62	0.42
2:B:758:PHE:N	2:B:759:PRO:HD2	2.34	0.42
2:B:806:THR:HG22	2:B:808:ALA:CB	2.49	0.42
2:B:1222:ARG:O	2:B:1222:ARG:HG2	2.19	0.42
3:C:94:LYS:HE3	3:C:94:LYS:HB2	1.87	0.42
3:C:239:PRO:O	3:C:241:ASP:N	2.53	0.42
7:G:115:MET:CB	7:G:116:PRO:CD	2.98	0.42
8:H:10:PHE:HA	8:H:29:ALA:O	2.18	0.42
10:J:1:MET:H3	10:J:56:LEU:H	1.67	0.42
1:A:144:THR:O	1:A:146:MET:HE2	2.20	0.42
1:A:477:PRO:HG3	1:A:521:MET:HG2	2.02	0.42
1:A:543:LEU:HD12	1:A:547:LEU:HG	2.01	0.42
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.54	0.42
1:A:842:VAL:O	1:A:844:ALA:N	2.52	0.42
2:B:618:ASP:O	2:B:619:ILE:C	2.62	0.42
2:B:641:GLU:OE1	2:B:641:GLU:HA	2.20	0.42
2:B:995:ARG:O	2:B:996:ARG:C	2.62	0.42
2:B:1208:MET:O	2:B:1211:ASN:N	2.51	0.42
3:C:47:ASP:CA	12:L:69:ALA:CB	2.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:7:THR:HB	7:G:42:PHE:CZ	2.55	0.42
4:D:40:HIS:C	4:D:42:GLY:H	2.28	0.42
5:E:58:MET:O	5:E:59:SER:C	2.62	0.42
5:E:180:ARG:NH2	5:E:192:ARG:HD2	2.34	0.42
8:H:95:TYR:HE2	8:H:97:MET:CG	2.32	0.42
9:I:100:PHE:N	9:I:100:PHE:CD1	2.88	0.42
12:L:29:TYR:N	12:L:29:TYR:CD2	2.84	0.42
12:L:60:ARG:HG2	12:L:61:THR:N	2.35	0.42
1:A:453:MET:C	1:A:455:MET:H	2.28	0.42
1:A:507:VAL:N	1:A:508:PRO:CD	2.82	0.42
1:A:746:MET:CE	2:B:1018:PRO:HG2	2.50	0.42
1:A:846:GLU:HB2	1:A:847:ASP:H	1.68	0.42
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.35	0.42
1:A:1118:VAL:O	1:A:1305:VAL:HG13	2.20	0.42
1:A:1121:GLU:O	1:A:1122:PRO:C	2.63	0.42
1:A:1131:ALA:O	1:A:1132:LYS:C	2.62	0.42
1:A:1226:VAL:HG22	1:A:1240:CYS:CB	2.50	0.42
1:A:1349:TYR:O	1:A:1350:LYS:C	2.62	0.42
2:B:205:ILE:O	2:B:206:ASN:C	2.63	0.42
2:B:519:TRP:HE1	2:B:635:ARG:NH2	2.18	0.42
2:B:559:SER:HA	2:B:563:MET:HB3	2.02	0.42
2:B:604:ARG:C	2:B:606:LYS:N	2.78	0.42
2:B:693:ILE:HD11	2:B:740:HIS:CD2	2.54	0.42
2:B:781:PHE:O	2:B:782:LEU:HD23	2.19	0.42
3:C:204:SER:C	3:C:206:ASN:N	2.76	0.42
5:E:96:PHE:O	5:E:97:VAL:C	2.63	0.42
6:F:87:LYS:HG3	6:F:88:TYR:CE1	2.54	0.42
12:L:28:LYS:HB2	12:L:39:SER:HA	2.02	0.42
1:A:381:THR:O	1:A:384:ASN:N	2.50	0.42
1:A:393:ARG:O	1:A:394:ASN:C	2.60	0.42
1:A:841:LEU:O	1:A:845:LEU:HG	2.20	0.42
1:A:1447:GLU:OE2	7:G:23:LYS:HB2	2.19	0.42
2:B:102:VAL:HG23	2:B:112:LEU:HB2	2.02	0.42
2:B:865:LYS:C	2:B:866:TYR:CD1	2.98	0.42
3:C:124:LEU:HD22	3:C:129:ILE:HG22	2.01	0.42
4:D:170:THR:CG2	4:D:172:LEU:HG	2.50	0.42
6:F:81:THR:HB	6:F:136:ARG:HH11	1.85	0.42
7:G:1:MET:O	7:G:1:MET:HE2	2.20	0.42
7:G:56:ILE:O	7:G:57:GLN:HB2	2.20	0.42
15:T:12:DT:H2"	15:T:13:DA:OP2	2.18	0.42
1:A:115:LEU:O	1:A:122:MET:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:VAL:HG12	1:A:163:SER:N	2.34	0.42
1:A:785:PRO:HG2	1:A:786:HIS:CD2	2.52	0.42
1:A:1437:GLY:HA3	6:F:88:TYR:CD2	2.55	0.42
1:A:1438:THR:HB	2:B:1144:ALA:CB	2.46	0.42
1:A:1441:PHE:CE2	6:F:89:GLU:HG2	2.55	0.42
2:B:235:SER:HA	2:B:261:ARG:NH1	2.34	0.42
2:B:251:ILE:O	2:B:251:ILE:HG22	2.19	0.42
2:B:314:LEU:C	2:B:316:PRO:HD2	2.44	0.42
2:B:597:MET:O	2:B:599:THR:N	2.53	0.42
2:B:616:ILE:HG12	2:B:697:GLU:HA	2.01	0.42
2:B:765:PRO:C	2:B:767:ASN:N	2.75	0.42
2:B:798:TYR:HE2	3:C:62:PHE:CE2	2.36	0.42
2:B:914:LYS:HD3	2:B:937:ALA:CB	2.50	0.42
2:B:1085:ILE:N	2:B:1085:ILE:CD1	2.79	0.42
3:C:23:SER:O	3:C:24:ASN:HB3	2.19	0.42
3:C:166:GLU:O	3:C:167:HIS:HB2	2.20	0.42
3:C:213:PRO:HG2	3:C:214:ASN:H	1.84	0.42
4:D:146:GLN:O	4:D:147:TYR:C	2.63	0.42
5:E:73:PRO:O	5:E:75:MET:N	2.48	0.42
5:E:98:ILE:C	5:E:100:ILE:N	2.77	0.42
5:E:161:LYS:C	5:E:163:GLU:H	2.27	0.42
9:I:4:PHE:HE1	9:I:6:PHE:CE2	2.38	0.42
9:I:58:VAL:O	9:I:59:VAL:C	2.63	0.42
11:K:101:LEU:HD23	11:K:101:LEU:C	2.45	0.42
1:A:7:SER:OG	2:B:1193:GLN:NE2	2.53	0.42
1:A:382:PRO:CB	1:A:428:TYR:CE2	2.97	0.42
1:A:472:LEU:O	1:A:475:THR:CB	2.60	0.42
1:A:856:THR:CB	1:A:865:GLN:HB2	2.47	0.42
1:A:975:HIS:HA	1:A:1036:ARG:HG3	2.02	0.42
1:A:1013:ASP:C	1:A:1015:VAL:H	2.27	0.42
1:A:1215:ARG:HA	1:A:1215:ARG:HD2	1.72	0.42
1:A:1279:ILE:HG23	1:A:1308:THR:OG1	2.20	0.42
2:B:28:GLU:O	2:B:28:GLU:HG3	2.20	0.42
2:B:763:GLN:O	2:B:765:PRO:N	2.53	0.42
2:B:882:THR:HG21	2:B:884:ARG:HB2	2.02	0.42
2:B:977:GLY:HA3	2:B:1099:VAL:CG2	2.49	0.42
2:B:1006:ILE:HD13	10:J:44:TYR:HE2	1.81	0.42
5:E:144:ILE:HD13	5:E:183:PRO:HB3	2.01	0.42
7:G:25:TYR:O	7:G:26:LEU:C	2.63	0.42
7:G:38:CYS:HB3	7:G:155:SER:HA	2.02	0.42
7:G:144:ARG:O	7:G:168:LEU:HD22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:10:PHE:HE1	8:H:57:VAL:HB	1.85	0.42
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.50	0.42
11:K:103:THR:C	11:K:105:PHE:H	2.27	0.42
12:L:52:GLY:O	12:L:53:HIS:C	2.62	0.42
14:P:1:U:O2'	14:P:2:C:C5'	2.67	0.42
1:A:61:ILE:HG22	1:A:62:ASP:N	2.32	0.41
1:A:130:ASP:HB3	1:A:133:LYS:HB2	2.02	0.41
1:A:146:MET:HA	1:A:171:GLN:HB2	2.01	0.41
1:A:755:PHE:O	1:A:756:ILE:C	2.62	0.41
1:A:786:HIS:O	1:A:787:PHE:HD2	2.03	0.41
1:A:920:LEU:C	1:A:920:LEU:CD2	2.92	0.41
2:B:753:ALA:O	2:B:755:ILE:N	2.53	0.41
2:B:769:TYR:O	2:B:772:ALA:N	2.53	0.41
2:B:953:LEU:HD23	2:B:965:LYS:H	1.85	0.41
2:B:1138:MET:HA	2:B:1138:MET:CE	2.38	0.41
3:C:26:ASP:O	3:C:27:LEU:C	2.61	0.41
3:C:187:LYS:C	3:C:189:THR:H	2.26	0.41
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.83	0.41
7:G:22:MET:O	7:G:25:TYR:N	2.53	0.41
7:G:91:VAL:HA	7:G:101:VAL:HA	2.02	0.41
8:H:139:ASN:O	8:H:140:ALA:HB2	2.19	0.41
11:K:42:LEU:HD21	11:K:46:ILE:CD1	2.50	0.41
1:A:16:GLU:CD	2:B:1220:ARG:HA	2.45	0.41
1:A:98:LYS:O	1:A:101:LYS:N	2.54	0.41
1:A:108:MET:O	1:A:109:HIS:HB2	2.19	0.41
1:A:469:ARG:HH11	1:A:469:ARG:HB3	1.85	0.41
1:A:497:THR:O	1:A:498:ARG:C	2.62	0.41
1:A:646:PHE:O	1:A:647:GLY:C	2.63	0.41
1:A:809:THR:O	1:A:810:PRO:C	2.63	0.41
1:A:1209:MET:HE1	1:A:1236:LEU:HB3	2.01	0.41
1:A:1394:THR:HG22	1:A:1395:GLY:N	2.35	0.41
2:B:53:GLN:NE2	2:B:57:TYR:HB2	2.35	0.41
2:B:236:HIS:C	2:B:237:VAL:HG23	2.46	0.41
2:B:523:CYS:SG	2:B:524:PRO:HD2	2.60	0.41
2:B:620:ARG:NH2	9:I:89:GLN:NE2	2.68	0.41
2:B:661:LEU:C	2:B:663:ALA:H	2.28	0.41
2:B:862:GLN:CG	2:B:963:PHE:HD1	2.33	0.41
3:C:51:VAL:HG22	3:C:155:LEU:HD22	2.01	0.41
3:C:53:THR:O	3:C:153:LEU:HA	2.20	0.41
4:D:180:LEU:HD23	4:D:180:LEU:HA	1.88	0.41
5:E:9:ILE:C	5:E:11:ARG:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:92:THR:HG22	5:E:92:THR:O	2.20	0.41
5:E:157:SER:OG	5:E:159:ASP:HB2	2.21	0.41
5:E:177:ARG:HD3	5:E:215:MET:HG2	2.02	0.41
8:H:20:TYR:O	8:H:22:LYS:N	2.52	0.41
8:H:76:THR:O	8:H:76:THR:HG22	2.19	0.41
9:I:54:GLU:HB3	9:I:100:PHE:CE2	2.55	0.41
1:A:68:GLN:C	1:A:70:CYS:N	2.66	0.41
1:A:73:GLY:O	1:A:74:MET:C	2.64	0.41
1:A:90:VAL:HG12	1:A:91:PHE:N	2.34	0.41
1:A:688:LYS:C	1:A:690:VAL:N	2.78	0.41
1:A:722:LEU:HD21	1:A:794:PRO:HB3	2.03	0.41
1:A:1329:THR:CG2	1:A:1331:SER:HB3	2.51	0.41
2:B:95:ILE:HB	2:B:130:VAL:HG22	2.01	0.41
2:B:169:ARG:N	2:B:454:THR:OG1	2.54	0.41
2:B:224:GLN:HA	2:B:396:ASP:OD2	2.19	0.41
2:B:235:SER:C	2:B:236:HIS:HD2	2.28	0.41
2:B:429:PHE:HA	2:B:432:MET:CE	2.50	0.41
2:B:1176:ASN:C	2:B:1178:ASN:N	2.75	0.41
8:H:83:GLN:O	8:H:85:GLY:N	2.53	0.41
11:K:91:CYS:O	11:K:94:ILE:HB	2.21	0.41
1:A:11:LEU:O	1:A:11:LEU:HG	2.16	0.41
1:A:453:MET:C	1:A:455:MET:N	2.77	0.41
1:A:825:ILE:O	1:A:828:ALA:N	2.48	0.41
1:A:1044:TRP:O	1:A:1045:VAL:C	2.64	0.41
1:A:1444:MET:HG2	7:G:59:GLY:O	2.20	0.41
1:A:1451:VAL:C	1:A:1453:TYR:N	2.77	0.41
2:B:48:LEU:O	2:B:51:PHE:N	2.51	0.41
2:B:51:PHE:CD2	2:B:173:MET:HB3	2.56	0.41
2:B:97:VAL:HG12	2:B:178:ASN:HD21	1.85	0.41
2:B:179:CYS:O	2:B:180:TYR:C	2.63	0.41
2:B:273:LEU:HD12	2:B:280:ILE:HD12	2.01	0.41
2:B:336:ARG:NH2	2:B:345:LYS:CE	2.77	0.41
2:B:581:PHE:HA	2:B:585:VAL:O	2.20	0.41
2:B:778:MET:HE2	2:B:1094:ARG:CD	2.51	0.41
2:B:1085:ILE:CG2	2:B:1086:PHE:N	2.82	0.41
2:B:1115:THR:CG2	2:B:1117:GLN:CG	2.98	0.41
4:D:33:PHE:CE2	7:G:80:LYS:NZ	2.82	0.41
4:D:68:ARG:C	4:D:70:PHE:H	2.28	0.41
10:J:2:ILE:HG12	10:J:57:ILE:HD12	2.02	0.41
10:J:22:LEU:O	10:J:25:LEU:HB2	2.20	0.41
1:A:265:LYS:NZ	1:A:322:VAL:HG13	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:HB3	1:A:336:ILE:H	1.68	0.41
1:A:562:THR:HA	1:A:563:PRO:HD3	1.87	0.41
1:A:605:MET:HE2	1:A:607:ILE:HG13	2.01	0.41
1:A:818:MET:HG2	2:B:514:LEU:HG	2.03	0.41
1:A:886:ILE:HG22	1:A:887:GLY:H	1.78	0.41
1:A:909:ASP:C	1:A:911:SER:H	2.29	0.41
1:A:1018:PHE:O	1:A:1021:LEU:HB3	2.20	0.41
1:A:1027:ALA:O	1:A:1028:THR:C	2.62	0.41
1:A:1445:ILE:H	1:A:1445:ILE:CD1	1.98	0.41
2:B:446:LEU:N	2:B:446:LEU:HD23	2.36	0.41
2:B:807:ARG:O	2:B:811:TYR:HE1	2.03	0.41
2:B:980:PHE:HE2	2:B:1094:ARG:CB	2.33	0.41
2:B:1002:THR:O	2:B:1003:ALA:C	2.62	0.41
2:B:1142:GLY:O	2:B:1144:ALA:N	2.53	0.41
3:C:70:ILE:HA	3:C:71:PRO:HD2	1.89	0.41
3:C:116:LYS:HD3	3:C:140:ASN:HA	2.02	0.41
4:D:55:ALA:O	4:D:56:ARG:C	2.63	0.41
10:J:32:GLU:O	10:J:35:ALA:N	2.53	0.41
10:J:53:HIS:CD2	10:J:54:VAL:N	2.88	0.41
12:L:53:HIS:C	12:L:55:ILE:H	2.29	0.41
1:A:47:ARG:HH12	1:A:254:GLU:CG	2.33	0.41
1:A:62:ASP:HB3	1:A:64:ASN:HD21	1.83	0.41
1:A:860:LEU:HD11	1:A:1393:ASN:HB2	2.02	0.41
1:A:1067:LEU:C	1:A:1067:LEU:CD1	2.94	0.41
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.50	0.41
1:A:1317:MET:HE1	1:A:1338:VAL:HG11	2.03	0.41
2:B:384:ARG:O	2:B:385:LEU:C	2.64	0.41
2:B:400:HIS:O	2:B:402:GLY:N	2.53	0.41
2:B:458:LYS:O	2:B:462:ALA:N	2.54	0.41
2:B:651:LEU:HD11	2:B:707:PRO:CB	2.51	0.41
2:B:863:GLU:OE1	2:B:962:LYS:HB2	2.20	0.41
2:B:948:ILE:C	2:B:949:VAL:O	2.61	0.41
2:B:1002:THR:CG2	2:B:1006:ILE:HG13	2.49	0.41
2:B:1074:ASN:O	2:B:1078:GLY:N	2.51	0.41
2:B:1110:PRO:HB2	2:B:1119:VAL:CG2	2.51	0.41
3:C:76:ASP:O	3:C:79:GLN:HG2	2.21	0.41
3:C:168:ALA:O	3:C:169:LYS:C	2.62	0.41
5:E:134:THR:C	5:E:135:PHE:HD1	2.27	0.41
6:F:99:LEU:C	6:F:99:LEU:CD1	2.92	0.41
6:F:147:SER:OG	6:F:150:GLU:HG3	2.20	0.41
7:G:62:LEU:HD23	7:G:62:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:165:GLU:HB2	7:G:168:LEU:HD12	2.02	0.41
12:L:40:LEU:HD22	12:L:44:ASP:CB	2.51	0.41
14:P:6:C:H2'	14:P:7:A:O4'	2.20	0.41
1:A:42:ASP:OD1	1:A:45:GLN:O	2.39	0.41
1:A:89:PRO:HB3	1:A:208:LEU:HD12	2.03	0.41
1:A:392:VAL:O	1:A:393:ARG:C	2.64	0.41
1:A:629:LEU:O	1:A:633:VAL:HG23	2.21	0.41
1:A:688:LYS:C	1:A:690:VAL:H	2.27	0.41
1:A:849:MET:HE1	1:A:1440:ALA:HB2	2.01	0.41
1:A:1364:ASN:C	1:A:1364:ASN:ND2	2.79	0.41
2:B:449:ASN:C	2:B:451:LYS:N	2.78	0.41
2:B:469:GLN:HB2	2:B:470:LYS:H	1.52	0.41
2:B:642:ASP:CA	2:B:649:LYS:HG3	2.50	0.41
3:C:75:MET:HB2	3:C:75:MET:HE3	1.99	0.41
3:C:183:TRP:O	3:C:184:ASN:C	2.63	0.41
5:E:114:ASN:O	5:E:115:ASN:CB	2.63	0.41
6:F:97:ARG:NH2	6:F:106:PRO:O	2.54	0.41
7:G:25:TYR:CD2	7:G:25:TYR:C	2.98	0.41
10:J:57:ILE:HG23	10:J:58:GLU:N	2.35	0.41
15:T:16:DT:C4	15:T:17:DT:C4	3.09	0.41
1:A:42:ASP:O	1:A:44:THR:N	2.38	0.41
1:A:56:PRO:O	1:A:57:ARG:NE	2.47	0.41
1:A:98:LYS:O	1:A:100:LYS:N	2.53	0.41
1:A:98:LYS:C	1:A:100:LYS:N	2.77	0.41
1:A:135:PHE:HB2	1:A:223:GLY:H	1.85	0.41
1:A:322:VAL:O	1:A:322:VAL:HG12	2.19	0.41
1:A:1170:ILE:H	1:A:1170:ILE:HG13	1.55	0.41
1:A:1214:GLU:OE1	1:A:1214:GLU:HA	2.21	0.41
2:B:762:ASN:OD1	2:B:1024:ALA:HB3	2.21	0.41
2:B:1034:VAL:O	2:B:1036:ALA:N	2.54	0.41
2:B:1177:HIS:C	2:B:1179:GLN:N	2.78	0.41
2:B:1197:PRO:O	2:B:1198:TYR:C	2.63	0.41
3:C:66:ARG:CZ	10:J:2:ILE:CG2	2.98	0.41
3:C:143:LEU:HD21	3:C:146:LYS:HE2	2.03	0.41
3:C:256:ALA:O	3:C:258:ILE:N	2.54	0.41
4:D:187:THR:HG22	4:D:188:ALA:H	1.84	0.41
4:D:192:LYS:HB3	4:D:192:LYS:NZ	2.34	0.41
6:F:89:GLU:O	6:F:93:ILE:HG13	2.20	0.41
7:G:1:MET:HE1	7:G:80:LYS:C	2.46	0.41
7:G:87:VAL:CG2	7:G:103:VAL:HG21	2.51	0.41
9:I:101:PHE:CE1	9:I:112:SER:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:60:ARG:HH21	12:L:65:VAL:HG21	1.86	0.41
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.56	0.41
1:A:24:PRO:HD2	1:A:233:TRP:CD1	2.55	0.41
1:A:41:MET:O	1:A:50:ILE:HG13	2.21	0.41
1:A:63:ARG:HA	1:A:74:MET:HE2	2.01	0.41
1:A:68:GLN:HE22	1:A:80:HIS:CG	2.39	0.41
1:A:265:LYS:O	1:A:269:ILE:HG13	2.21	0.41
1:A:266:LEU:O	1:A:267:ALA:C	2.63	0.41
1:A:269:ILE:HG12	1:A:299:HIS:HB3	2.03	0.41
1:A:335:ARG:CA	1:A:339:ASN:HD22	2.28	0.41
1:A:337:ARG:CZ	1:A:839:ARG:NH1	2.84	0.41
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.86	0.41
1:A:536:LEU:O	1:A:537:ARG:C	2.63	0.41
1:A:573:SER:OG	1:A:576:GLN:HB2	2.21	0.41
1:A:608:ILE:O	1:A:610:GLY:N	2.54	0.41
1:A:722:LEU:HD22	1:A:799:PHE:CG	2.56	0.41
1:A:976:THR:HG23	8:H:136:LYS:NZ	2.36	0.41
1:A:1161:THR:HG22	1:A:1162:VAL:N	2.35	0.41
1:A:1334:ASP:C	1:A:1336:MET:H	2.29	0.41
2:B:24:PRO:O	2:B:655:LYS:HB2	2.21	0.41
2:B:189:LEU:O	2:B:192:LEU:HB2	2.21	0.41
2:B:205:ILE:N	2:B:205:ILE:CD1	2.83	0.41
2:B:490:SER:O	2:B:491:THR:C	2.63	0.41
2:B:583:ASN:HD21	2:B:628:THR:HB	1.86	0.41
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.51	0.41
2:B:603:LEU:HD22	2:B:603:LEU:HA	1.95	0.41
2:B:751:VAL:HG13	2:B:812:LEU:CD2	2.47	0.41
2:B:1001:PHE:CD1	2:B:1001:PHE:C	2.99	0.41
2:B:1010:LEU:HD12	2:B:1010:LEU:HA	1.81	0.41
2:B:1107:ALA:O	2:B:1108:ARG:O	2.39	0.41
4:D:56:ARG:NH2	4:D:57:LEU:HD21	2.35	0.41
4:D:164:ILE:O	4:D:165:GLN:C	2.62	0.41
4:D:176:GLU:HG2	4:D:197:SER:OG	2.21	0.41
5:E:56:LYS:HE3	5:E:84:ASP:HB2	2.02	0.41
5:E:58:MET:O	5:E:59:SER:O	2.38	0.41
5:E:60:PHE:CD2	5:E:60:PHE:C	2.99	0.41
5:E:153:HIS:O	5:E:154:ILE:HG13	2.20	0.41
6:F:95:GLY:O	6:F:96:THR:C	2.63	0.41
7:G:27:LYS:O	7:G:30:LEU:N	2.54	0.41
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.56	0.41
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:18:DT:O3'	15:T:19:TT:C4'	2.63	0.41
1:A:106:VAL:HA	1:A:114:LEU:HD21	2.04	0.41
1:A:188:ASP:OD1	1:A:189:ARG:N	2.53	0.41
1:A:354:SER:HA	1:A:482:PHE:CD2	2.56	0.41
1:A:532:ARG:O	1:A:535:THR:HB	2.21	0.41
1:A:604:GLY:O	1:A:605:MET:HB2	2.21	0.41
1:A:1001:ARG:O	1:A:1002:GLY:C	2.64	0.41
1:A:1332:PHE:HE1	1:A:1348:LEU:HD13	1.85	0.41
2:B:743:ILE:H	2:B:743:ILE:HG12	1.64	0.41
2:B:953:LEU:HD22	2:B:965:LYS:HB2	1.98	0.41
3:C:97:VAL:HG12	3:C:99:LEU:HD21	2.03	0.41
3:C:174:ALA:O	3:C:175:ALA:CB	2.67	0.41
7:G:21:ARG:HD3	7:G:21:ARG:HA	1.81	0.41
7:G:34:VAL:HG11	7:G:74:TYR:CE1	2.56	0.41
8:H:145:ARG:O	8:H:146:ARG:HB2	2.21	0.41
9:I:77:LYS:O	9:I:79:HIS:N	2.54	0.41
10:J:57:ILE:O	10:J:60:PHE:HB2	2.21	0.41
11:K:42:LEU:O	11:K:42:LEU:HG	2.22	0.41
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.56	0.41
1:A:31:SER:HA	1:A:81:PHE:O	2.22	0.40
1:A:70:CYS:O	1:A:71:GLN:C	2.64	0.40
1:A:219:PHE:O	1:A:222:LEU:O	2.38	0.40
1:A:230:ARG:O	1:A:231:PRO:C	2.64	0.40
1:A:391:LEU:O	1:A:394:ASN:HB2	2.21	0.40
1:A:547:LEU:HD13	11:K:58:PHE:CD1	2.56	0.40
1:A:606:LEU:CB	1:A:614:PHE:CE2	3.03	0.40
1:A:823:GLY:O	1:A:824:LEU:C	2.64	0.40
1:A:1142:THR:O	1:A:1143:LEU:C	2.64	0.40
2:B:95:ILE:CB	2:B:130:VAL:HG22	2.51	0.40
2:B:638:PHE:HB3	2:B:651:LEU:HD22	2.03	0.40
2:B:710:LEU:C	2:B:711:GLU:HG2	2.46	0.40
2:B:710:LEU:O	2:B:711:GLU:OE2	2.38	0.40
2:B:744:HIS:CD2	2:B:746:SER:HB3	2.56	0.40
2:B:834:ASN:CA	2:B:838:SER:O	2.69	0.40
2:B:999:MET:HG2	2:B:1007:VAL:HG22	2.02	0.40
3:C:172:PRO:O	3:C:235:VAL:HG23	2.20	0.40
4:D:195:ILE:N	4:D:196:PRO:CD	2.85	0.40
8:H:39:THR:O	8:H:124:ARG:N	2.52	0.40
9:I:34:TYR:O	9:I:35:VAL:CG2	2.69	0.40
1:A:308:ILE:HG22	1:A:309:ALA:N	2.25	0.40
1:A:376:TYR:HA	1:A:377:PRO:HD2	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:GLN:HG3	2:B:836:GLU:HG2	2.02	0.40
1:A:567:LYS:NZ	8:H:47:PHE:HB3	2.36	0.40
1:A:824:LEU:HD23	1:A:824:LEU:HA	1.85	0.40
1:A:879:GLU:OE1	1:A:962:ARG:NH2	2.53	0.40
1:A:964:ILE:O	1:A:966:ASN:N	2.54	0.40
1:A:1111:MET:HE2	1:A:1114:PRO:HA	2.03	0.40
1:A:1405:THR:HB	1:A:1406:VAL:H	1.55	0.40
1:A:1409:LEU:O	1:A:1412:ALA:HB3	2.21	0.40
2:B:175:ARG:NH1	2:B:175:ARG:CG	2.84	0.40
2:B:298:LEU:N	2:B:298:LEU:HD22	2.36	0.40
2:B:448:ILE:O	2:B:450:ALA:N	2.55	0.40
2:B:558:LEU:C	2:B:560:GLU:N	2.79	0.40
2:B:773:MET:HB3	2:B:1095:LEU:HD23	2.02	0.40
3:C:131:HIS:O	3:C:132:PRO:C	2.64	0.40
3:C:181:ASP:N	3:C:182:PRO:CD	2.84	0.40
4:D:192:LYS:HG2	4:D:207:LEU:CD2	2.51	0.40
5:E:72:PHE:CE2	5:E:155:ARG:NH2	2.89	0.40
5:E:129:PRO:O	5:E:130:ALA:C	2.65	0.40
8:H:59:ILE:CG2	8:H:60:ALA:N	2.65	0.40
9:I:103:CYS:CB	9:I:106:CYS:SG	3.09	0.40
11:K:46:ILE:O	11:K:50:LEU:HB2	2.21	0.40
11:K:50:LEU:HD11	11:K:75:ILE:HD13	2.04	0.40
12:L:46:VAL:HG12	12:L:46:VAL:O	2.22	0.40
12:L:49:LYS:O	12:L:50:ASP:HB3	2.22	0.40
1:A:34:LYS:H	1:A:57:ARG:HH22	1.68	0.40
1:A:58:LEU:HG	1:A:59:GLY:H	1.82	0.40
1:A:220:THR:O	1:A:221:SER:C	2.62	0.40
1:A:225:ASN:HD22	1:A:228:PHE:N	1.88	0.40
1:A:230:ARG:N	1:A:233:TRP:HE3	2.11	0.40
1:A:356:ASP:HB2	1:A:469:ARG:HH12	1.81	0.40
1:A:834:THR:HG22	1:A:835:GLY:N	2.35	0.40
1:A:869:GLY:O	1:A:870:GLU:HB2	2.21	0.40
1:A:1031:VAL:O	1:A:1031:VAL:HG12	2.22	0.40
1:A:1053:PHE:O	1:A:1056:SER:N	2.51	0.40
1:A:1450:LEU:CD1	6:F:108:PHE:CZ	3.04	0.40
2:B:309:GLN:CG	9:I:52:ILE:HD11	2.51	0.40
2:B:315:LYS:N	2:B:316:PRO:CD	2.83	0.40
2:B:658:ILE:O	2:B:661:LEU:N	2.42	0.40
2:B:774:GLY:HA2	2:B:1093:GLN:HE22	1.85	0.40
2:B:824:ILE:CG2	2:B:1087:PHE:CE2	2.95	0.40
2:B:911:ILE:C	2:B:912:ILE:HG13	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:147:SER:C	6:F:149:GLU:N	2.77	0.40
7:G:17:PHE:N	7:G:17:PHE:HD2	2.17	0.40
7:G:27:LYS:O	7:G:30:LEU:HB3	2.20	0.40
7:G:109:PHE:O	7:G:160:ILE:HA	2.22	0.40
8:H:84:ALA:C	8:H:87:ARG:H	2.29	0.40
9:I:8:ARG:O	9:I:10:CYS:N	2.54	0.40
9:I:56:ALA:O	9:I:57:GLY:O	2.39	0.40
11:K:89:ASN:O	11:K:90:ALA:C	2.64	0.40
1:A:263:THR:O	1:A:263:THR:HG22	2.22	0.40
1:A:332:LYS:O	1:A:334:GLY:N	2.55	0.40
1:A:388:LEU:HD22	1:A:432:VAL:CB	2.51	0.40
1:A:466:SER:HB3	2:B:1103:ILE:HG12	2.02	0.40
1:A:711:ARG:O	1:A:714:PHE:HB3	2.21	0.40
1:A:823:GLY:O	1:A:825:ILE:N	2.55	0.40
1:A:852:TYR:CD1	6:F:136:ARG:HB3	2.56	0.40
2:B:22:SER:HA	2:B:654:ARG:HG3	2.03	0.40
2:B:288:ALA:HA	2:B:331:LEU:CD1	2.49	0.40
2:B:460:ALA:HB1	2:B:466:TRP:CZ3	2.57	0.40
2:B:732:SER:HB2	2:B:734:HIS:CD2	2.57	0.40
2:B:782:LEU:HB3	2:B:784:ASN:OD1	2.21	0.40
2:B:1030:LEU:HD12	2:B:1030:LEU:HA	1.96	0.40
3:C:10:ILE:HG22	3:C:11:ARG:O	2.21	0.40
3:C:58:LEU:CD2	3:C:58:LEU:N	2.84	0.40
3:C:58:LEU:N	3:C:58:LEU:HD22	2.37	0.40
3:C:187:LYS:HG3	3:C:219:PHE:CE1	2.56	0.40
4:D:29:LEU:O	4:D:30:GLY:C	2.65	0.40
5:E:117:THR:C	5:E:119:SER:N	2.80	0.40
7:G:14:HIS:ND1	7:G:15:PRO:CD	2.78	0.40
8:H:38:LEU:HD13	8:H:125:LEU:CD1	2.51	0.40
1:A:34:LYS:N	1:A:57:ARG:NH2	2.65	0.40
1:A:56:PRO:O	1:A:57:ARG:CG	2.70	0.40
1:A:351:THR:CG2	2:B:1103:ILE:HG13	2.51	0.40
1:A:682:THR:O	1:A:682:THR:HG22	2.22	0.40
1:A:685:GLU:HG3	1:A:686:ALA:N	2.36	0.40
1:A:1019:CYS:O	1:A:1022:LEU:N	2.54	0.40
1:A:1036:ARG:NH1	1:A:1036:ARG:CG	2.80	0.40
1:A:1168:GLU:O	1:A:1172:LEU:HG	2.21	0.40
1:A:1260:LEU:O	1:A:1260:LEU:CG	2.70	0.40
2:B:223:VAL:HG11	2:B:381:MET:HG2	2.03	0.40
2:B:225:VAL:O	2:B:226:PHE:CD2	2.74	0.40
2:B:766:ARG:HD3	2:B:766:ARG:HA	1.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:785:TYR:CD1	2:B:786:ASN:N	2.89	0.40
2:B:1198:TYR:C	2:B:1198:TYR:CD2	3.00	0.40
3:C:137:LYS:HB3	3:C:138:GLU:OE1	2.21	0.40
3:C:241:ASP:CG	3:C:242:GLN:N	2.80	0.40
4:D:207:LEU:O	4:D:211:LEU:HG	2.22	0.40
5:E:11:ARG:HH21	5:E:141:VAL:HG21	1.87	0.40
5:E:114:ASN:HD22	5:E:114:ASN:HA	1.68	0.40
6:F:111:LEU:O	6:F:113:GLY:N	2.52	0.40
10:J:53:HIS:CD2	10:J:53:HIS:C	2.99	0.40
11:K:58:PHE:HB3	11:K:76:GLN:HB3	2.03	0.40
11:K:62:LYS:O	11:K:71:PHE:HB2	2.21	0.40
11:K:83:PRO:O	11:K:84:LYS:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1410/1733 (81%)	962 (68%)	299 (21%)	149 (11%)	0	6
2	B	1096/1224 (90%)	767 (70%)	219 (20%)	110 (10%)	0	7
3	C	264/318 (83%)	171 (65%)	62 (24%)	31 (12%)	0	4
4	D	173/221 (78%)	125 (72%)	29 (17%)	19 (11%)	0	5
5	E	212/215 (99%)	157 (74%)	44 (21%)	11 (5%)	1	17
6	F	84/155 (54%)	67 (80%)	15 (18%)	2 (2%)	4	29
7	G	169/171 (99%)	125 (74%)	34 (20%)	10 (6%)	1	15
8	H	131/146 (90%)	84 (64%)	30 (23%)	17 (13%)	0	3
9	I	114/122 (93%)	80 (70%)	21 (18%)	13 (11%)	0	5
10	J	63/70 (90%)	35 (56%)	13 (21%)	15 (24%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	112/120 (93%)	86 (77%)	16 (14%)	10 (9%)	0	9
12	L	44/70 (63%)	17 (39%)	17 (39%)	10 (23%)	0	0
All	All	3872/4565 (85%)	2676 (69%)	799 (21%)	397 (10%)	0	6

All (397) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	48	ALA
1	A	57	ARG
1	A	62	ASP
1	A	65	LEU
1	A	74	MET
1	A	93	VAL
1	A	167	CYS
1	A	219	PHE
1	A	223	GLY
1	A	255	SER
1	A	286	HIS
1	A	311	GLN
1	A	312	PRO
1	A	318	SER
1	A	322	VAL
1	A	335	ARG
1	A	385	ILE
1	A	423	ASP
1	A	465	TYR
1	A	536	LEU
1	A	543	LEU
1	A	567	LYS
1	A	597	LEU
1	A	626	ASN
1	A	666	ILE
1	A	753	GLY
1	A	789	LYS
1	A	847	ASP
1	A	875	ALA
1	A	968	GLN
1	A	969	GLN
1	A	986	ILE
1	A	1002	GLY

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Mol	Chain	Res	Type
1	A	1036	ARG
1	A	1096	SER
1	A	1114	PRO
1	A	1115	SER
1	A	1122	PRO
1	A	1212	VAL
1	A	1223	ASP
1	A	1281	ARG
1	A	1314	SER
1	A	1341	ILE
1	A	1365	TYR
1	A	1378	GLN
1	A	1405	THR
1	A	1438	THR
2	B	45	SER
2	B	46	GLN
2	B	108	VAL
2	B	115	GLN
2	B	186	GLU
2	B	258	LEU
2	B	345	LYS
2	B	367	LEU
2	B	467	GLY
2	B	474	SER
2	B	643	ASP
2	B	709	ASP
2	B	727	LYS
2	B	731	VAL
2	B	764	SER
2	B	831	SER
2	B	943	SER
2	B	958	GLN
2	B	1046	PRO
2	B	1069	PHE
2	B	1097	HIS
2	B	1108	ARG
2	B	1156	ASP
2	B	1157	ALA
2	B	1167	GLY
2	B	1175	LEU
2	B	1178	ASN
2	B	1181	GLU

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Mol	Chain	Res	Type
2	B	1182	CYS
2	B	1188	LYS
3	C	4	GLU
3	C	6	PRO
3	C	78	GLU
3	C	87	PHE
3	C	141	GLY
3	C	149	LYS
3	C	156	THR
3	C	161	LYS
3	C	184	ASN
3	C	209	TYR
3	C	214	ASN
3	C	215	GLU
4	D	5	THR
4	D	8	PHE
4	D	19	GLU
4	D	20	GLU
4	D	52	LEU
4	D	131	GLU
4	D	177	VAL
4	D	199	ASN
5	E	3	GLN
5	E	36	GLU
5	E	59	SER
5	E	73	PRO
5	E	74	ASP
5	E	106	GLN
5	E	130	ALA
5	E	206	GLY
7	G	63	PRO
7	G	139	ILE
8	H	17	PRO
8	H	62	SER
8	H	81	PRO
8	H	82	PRO
8	H	108	SER
8	H	128	ASN
9	I	3	THR
9	I	9	ASP
9	I	79	HIS
10	J	2	ILE

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Mol	Chain	Res	Type
10	J	6	ARG
10	J	32	GLU
10	J	64	ASN
11	K	110	ASN
12	L	35	SER
12	L	50	ASP
12	L	59	ALA
12	L	60	ARG
1	A	42	ASP
1	A	54	ASN
1	A	59	GLY
1	A	61	ILE
1	A	66	LYS
1	A	70	CYS
1	A	76	GLU
1	A	84	ILE
1	A	148	CYS
1	A	154	SER
1	A	250	ILE
1	A	253	ASN
1	A	283	GLY
1	A	386	ASP
1	A	394	ASN
1	A	399	HIS
1	A	439	ASN
1	A	517	ASN
1	A	619	LYS
1	A	661	GLY
1	A	731	ARG
1	A	780	VAL
1	A	979	SER
1	A	1054	LEU
1	A	1116	LEU
1	A	1120	LEU
1	A	1124	HIS
1	A	1127	ASP
1	A	1233	ASP
1	A	1280	GLU
1	A	1377	THR
1	A	1386	ARG
1	A	1395	GLY
1	A	1402	PHE

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Mol	Chain	Res	Type
2	B	28	GLU
2	B	48	LEU
2	B	65	GLU
2	B	260	GLY
2	B	264	SER
2	B	266	ALA
2	B	282	ILE
2	B	387	LEU
2	B	401	PHE
2	B	450	ALA
2	B	466	TRP
2	B	605	ARG
2	B	613	VAL
2	B	619	ILE
2	B	641	GLU
2	B	655	LYS
2	B	708	GLU
2	B	746	SER
2	B	751	VAL
2	B	792	MET
2	B	869	SER
2	B	881	ASN
2	B	891	ASP
2	B	907	GLY
2	B	945	GLU
2	B	1065	GLN
2	B	1100	ASP
2	B	1155	SER
2	B	1171	VAL
2	B	1183	LYS
2	B	1186	ASP
3	C	81	GLU
3	C	110	THR
3	C	175	ALA
3	C	213	PRO
3	C	216	GLY
3	C	240	VAL
4	D	12	ARG
4	D	21	GLU
4	D	65	GLU
4	D	192	LYS
5	E	45	LYS

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Mol	Chain	Res	Type
7	G	19	GLY
8	H	21	ASN
8	H	32	THR
8	H	59	ILE
8	H	77	ARG
8	H	84	ALA
8	H	140	ALA
9	I	11	ASN
9	I	34	TYR
9	I	57	GLY
9	I	78	CYS
9	I	106	CYS
10	J	14	VAL
10	J	17	LYS
10	J	27	GLU
10	J	28	ASP
10	J	29	GLU
11	K	7	PHE
11	K	15	GLY
12	L	26	THR
12	L	53	HIS
12	L	55	ILE
1	A	263	THR
1	A	336	ILE
1	A	409	SER
1	A	418	SER
1	A	424	ILE
1	A	525	GLN
1	A	526	ASP
1	A	544	ASP
1	A	592	ASP
1	A	648	ASN
1	A	649	ILE
1	A	673	GLY
1	A	759	ALA
1	A	846	GLU
1	A	871	ASP
1	A	1014	ALA
1	A	1165	GLU
1	A	1221	LYS
1	A	1335	ILE
1	A	1392	SER

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Mol	Chain	Res	Type
2	B	94	LYS
2	B	114	PRO
2	B	124	TYR
2	B	259	TYR
2	B	591	ARG
2	B	629	ASP
2	B	711	GLU
2	B	754	SER
2	B	772	ALA
2	B	818	PRO
2	B	951	GLN
2	B	1041	GLU
3	C	51	VAL
3	C	56	THR
3	C	60	ASP
3	C	148	ARG
3	C	264	GLN
4	D	6	SER
4	D	9	GLN
4	D	30	GLY
4	D	53	SER
5	E	115	ASN
5	E	192	ARG
6	F	81	THR
7	G	140	LYS
8	H	92	ASP
9	I	47	GLU
9	I	62	ILE
10	J	24	LEU
10	J	33	GLY
10	J	55	ASP
11	K	29	ASN
11	K	53	ASP
11	K	88	LYS
11	K	104	ASN
1	A	113	LEU
1	A	169	ASN
1	A	245	PRO
1	A	317	LYS
1	A	332	LYS
1	A	483	ASP
1	A	516	SER

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Mol	Chain	Res	Type
1	A	591	PHE
1	A	605	MET
1	A	636	GLU
1	A	975	HIS
1	A	1277	GLU
1	A	1366	ARG
1	A	1454	MET
2	B	56	ASP
2	B	58	THR
2	B	229	ALA
2	B	257	LYS
2	B	283	VAL
2	B	322	PHE
2	B	389	ALA
2	B	894	ASP
2	B	1003	ALA
2	B	1017	ILE
2	B	1035	ALA
3	C	117	ASP
3	C	167	HIS
6	F	154	ASP
7	G	17	PHE
7	G	20	PRO
7	G	62	LEU
7	G	154	VAL
8	H	52	GLN
8	H	90	ALA
9	I	107	SER
9	I	113	ASP
10	J	8	PHE
10	J	63	TYR
11	K	90	ALA
1	A	69	THR
1	A	86	LEU
1	A	226	GLU
1	A	244	PRO
1	A	290	GLU
1	A	400	PRO
1	A	604	GLY
1	A	720	ARG
1	A	824	LEU
1	A	895	LYS

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Mol	Chain	Res	Type
1	A	926	GLN
1	A	958	VAL
1	A	1389	PHE
2	B	61	ASP
2	B	231	PRO
2	B	245	GLU
2	B	248	SER
2	B	365	THR
2	B	369	GLY
2	B	571	PRO
2	B	728	ARG
2	B	770	GLN
2	B	848	ARG
2	B	880	THR
2	B	1103	ILE
3	C	142	VAL
3	C	208	GLU
4	D	119	ARG
4	D	218	GLU
7	G	115	MET
8	H	43	ASN
8	H	44	VAL
9	I	59	VAL
10	J	18	TRP
11	K	112	GLN
12	L	39	SER
12	L	57	LEU
1	A	43	GLU
1	A	71	GLN
1	A	96	ILE
1	A	111	GLY
1	A	135	PHE
1	A	825	ILE
2	B	100	PRO
2	B	341	LEU
2	B	530	GLY
2	B	752	ALA
2	B	824	ILE
3	C	126	GLY
4	D	196	PRO
11	K	41	THR
12	L	54	ARG

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Mol	Chain	Res	Type
1	A	196	GLU
2	B	1018	PRO
2	B	1214	PRO
1	A	55	ASP
1	A	1158	PRO
1	A	1164	PRO
2	B	364	ILE
2	B	611	PRO
2	B	729	ILE
2	B	901	PRO
7	G	34	VAL
1	A	357	PRO
1	A	364	VAL
1	A	410	GLY
1	A	492	PRO
1	A	718	VAL
3	C	212	PRO
3	C	255	VAL
1	A	35	ILE
1	A	99	ILE
1	A	842	VAL
2	B	758	PHE
2	B	867	GLY
3	C	139	GLY
1	A	652	VAL
1	A	653	VAL
2	B	636	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1244/1520 (82%)	1118 (90%)	126 (10%)	7	27
2	B	967/1061 (91%)	889 (92%)	78 (8%)	11	35
3	C	235/274 (86%)	211 (90%)	24 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	159/200 (80%)	133 (84%)	26 (16%)	2	14
5	E	196/197 (100%)	190 (97%)	6 (3%)	35	57
6	F	77/137 (56%)	70 (91%)	7 (9%)	9	32
7	G	152/152 (100%)	139 (91%)	13 (9%)	10	33
8	H	119/128 (93%)	113 (95%)	6 (5%)	22	47
9	I	110/116 (95%)	97 (88%)	13 (12%)	5	22
10	J	60/65 (92%)	56 (93%)	4 (7%)	15	41
11	K	99/102 (97%)	89 (90%)	10 (10%)	7	27
12	L	40/57 (70%)	37 (92%)	3 (8%)	12	38
All	All	3458/4009 (86%)	3142 (91%)	316 (9%)	9	32

All (316) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	5	GLN
1	A	11	LEU
1	A	32	VAL
1	A	34	LYS
1	A	37	PHE
1	A	38	PRO
1	A	62	ASP
1	A	67	CYS
1	A	93	VAL
1	A	108	MET
1	A	130	ASP
1	A	142	CYS
1	A	198	GLU
1	A	200	ARG
1	A	215	SER
1	A	245	PRO
1	A	270	LEU
1	A	302	THR
1	A	312	PRO
1	A	320	ARG
1	A	321	PRO
1	A	326	ARG
1	A	335	ARG
1	A	344	ARG

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Mol	Chain	Res	Type
1	A	345	VAL
1	A	350	ARG
1	A	379	VAL
1	A	381	THR
1	A	385	ILE
1	A	388	LEU
1	A	404	TYR
1	A	406	ILE
1	A	407	ARG
1	A	408	ASP
1	A	412	ARG
1	A	418	SER
1	A	425	GLN
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	460	VAL
1	A	461	LYS
1	A	462	VAL
1	A	466	SER
1	A	469	ARG
1	A	475	THR
1	A	493	GLN
1	A	497	THR
1	A	512	VAL
1	A	515	GLN
1	A	524	VAL
1	A	527	THR
1	A	528	LEU
1	A	535	THR
1	A	560	ILE
1	A	562	THR
1	A	577	ILE
1	A	590	ARG
1	A	618	GLU
1	A	629	LEU
1	A	657	LEU
1	A	666	ILE
1	A	670	ILE
1	A	711	ARG
1	A	715	GLU

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Mol	Chain	Res	Type
1	A	741	ASN
1	A	768	GLN
1	A	774	ARG
1	A	821	ARG
1	A	827	THR
1	A	831	THR
1	A	834	THR
1	A	845	LEU
1	A	854	ASN
1	A	858	ASN
1	A	859	SER
1	A	886	ILE
1	A	890	ASP
1	A	902	LEU
1	A	907	THR
1	A	929	LEU
1	A	937	VAL
1	A	940	ARG
1	A	941	LYS
1	A	969	GLN
1	A	983	ILE
1	A	992	ASP
1	A	1006	ILE
1	A	1029	ARG
1	A	1030	ARG
1	A	1035	TYR
1	A	1052	GLN
1	A	1067	LEU
1	A	1110	ASN
1	A	1116	LEU
1	A	1122	PRO
1	A	1127	ASP
1	A	1152	ILE
1	A	1170	ILE
1	A	1187	GLN
1	A	1206	ASP
1	A	1264	GLU
1	A	1271	ILE
1	A	1276	VAL
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU

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Mol	Chain	Res	Type
1	A	1325	THR
1	A	1329	THR
1	A	1332	PHE
1	A	1333	ILE
1	A	1359	ASP
1	A	1371	LEU
1	A	1372	VAL
1	A	1376	THR
1	A	1378	GLN
1	A	1385	THR
1	A	1386	ARG
1	A	1405	THR
1	A	1432	GLN
1	A	1442	ASP
1	A	1443	VAL
1	A	1444	MET
1	A	1445	ILE
2	B	30	SER
2	B	57	TYR
2	B	104	GLU
2	B	106	ASP
2	B	128	LEU
2	B	175	ARG
2	B	180	TYR
2	B	188	ASP
2	B	194	GLU
2	B	223	VAL
2	B	258	LEU
2	B	268	THR
2	B	298	LEU
2	B	323	VAL
2	B	365	THR
2	B	371	GLU
2	B	393	LYS
2	B	396	ASP
2	B	399	ASP
2	B	427	ASP
2	B	463	THR
2	B	465	ASN
2	B	466	TRP
2	B	487	THR
2	B	498	THR

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Mol	Chain	Res	Type
2	B	502	ILE
2	B	513	GLN
2	B	516	ASN
2	B	557	PHE
2	B	582	VAL
2	B	593	PRO
2	B	603	LEU
2	B	615	MET
2	B	628	THR
2	B	635	ARG
2	B	644	GLU
2	B	649	LYS
2	B	682	SER
2	B	684	LEU
2	B	724	ASP
2	B	737	THR
2	B	742	GLU
2	B	748	ILE
2	B	790	ASP
2	B	811	TYR
2	B	835	GLN
2	B	837	ASP
2	B	839	MET
2	B	857	ARG
2	B	878	GLN
2	B	901	PRO
2	B	909	ASP
2	B	935	ARG
2	B	939	THR
2	B	953	LEU
2	B	999	MET
2	B	1002	THR
2	B	1006	ILE
2	B	1010	LEU
2	B	1022	THR
2	B	1034	VAL
2	B	1047	PHE
2	B	1069	PHE
2	B	1084	GLN
2	B	1095	LEU
2	B	1099	VAL
2	B	1103	ILE

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Mol	Chain	Res	Type
2	B	1133	MET
2	B	1159	ARG
2	B	1160	VAL
2	B	1165	ILE
2	B	1169	MET
2	B	1170	THR
2	B	1176	ASN
2	B	1183	LYS
2	B	1202	LEU
2	B	1212	ILE
2	B	1216	LEU
3	C	8	VAL
3	C	22	LEU
3	C	48	SER
3	C	56	THR
3	C	57	VAL
3	C	58	LEU
3	C	77	ILE
3	C	93	ASP
3	C	99	LEU
3	C	108	GLU
3	C	129	ILE
3	C	140	ASN
3	C	145	CYS
3	C	147	LEU
3	C	163	ILE
3	C	166	GLU
3	C	193	TYR
3	C	214	ASN
3	C	233	GLU
3	C	238	ILE
3	C	240	VAL
3	C	245	VAL
3	C	259	LEU
3	C	266	ASP
4	D	8	PHE
4	D	13	ARG
4	D	16	LYS
4	D	17	LYS
4	D	19	GLU
4	D	22	GLU
4	D	32	GLU

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Mol	Chain	Res	Type
4	D	47	LEU
4	D	63	LEU
4	D	70	PHE
4	D	126	ILE
4	D	137	ASN
4	D	139	LYS
4	D	148	LEU
4	D	149	THR
4	D	156	ASP
4	D	159	THR
4	D	170	THR
4	D	174	PRO
4	D	182	SER
4	D	187	THR
4	D	192	LYS
4	D	193	THR
4	D	206	GLU
4	D	208	GLU
4	D	221	TYR
5	E	40	GLU
5	E	60	PHE
5	E	74	ASP
5	E	78	LEU
5	E	114	ASN
5	E	183	PRO
6	F	79	ARG
6	F	90	ARG
6	F	99	LEU
6	F	111	LEU
6	F	119	ARG
6	F	148	VAL
6	F	153	VAL
7	G	1	MET
7	G	13	LEU
7	G	17	PHE
7	G	45	ILE
7	G	74	TYR
7	G	78	VAL
7	G	80	LYS
7	G	88	ASP
7	G	96	GLN
7	G	115	MET

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Mol	Chain	Res	Type
7	G	118	ASP
7	G	126	ASN
7	G	171	ILE
8	H	42	ILE
8	H	86	ASP
8	H	93	TYR
8	H	102	TYR
8	H	130	ARG
8	H	143	LEU
9	I	8	ARG
9	I	9	ASP
9	I	15	TYR
9	I	40	SER
9	I	59	VAL
9	I	75	CYS
9	I	78	CYS
9	I	85	PHE
9	I	86	PHE
9	I	94	ASP
9	I	98	VAL
9	I	99	LEU
9	I	101	PHE
10	J	9	SER
10	J	10	CYS
10	J	44	TYR
10	J	46	CYS
11	K	10	PHE
11	K	25	THR
11	K	47	ARG
11	K	50	LEU
11	K	61	TYR
11	K	68	PHE
11	K	78	THR
11	K	111	LEU
11	K	112	GLN
11	K	113	THR
12	L	51	CYS
12	L	55	ILE
12	L	65	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	54	ASN
1	A	64	ASN
1	A	68	GLN
1	A	71	GLN
1	A	83	HIS
1	A	160	GLN
1	A	225	ASN
1	A	339	ASN
1	A	358	ASN
1	A	399	HIS
1	A	435	HIS
1	A	479	ASN
1	A	631	HIS
1	A	654	ASN
1	A	660	ASN
1	A	698	GLN
1	A	736	ASN
1	A	741	ASN
1	A	742	ASN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	935	GLN
1	A	965	GLN
1	A	1009	ASN
1	A	1040	GLN
1	A	1140	HIS
1	A	1171	GLN
1	A	1218	GLN
1	A	1387	HIS
1	A	1432	GLN
2	B	47	GLN
2	B	53	GLN
2	B	178	ASN
2	B	236	HIS
2	B	366	GLN
2	B	449	ASN
2	B	465	ASN
2	B	515	HIS

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Mol	Chain	Res	Type
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	734	HIS
2	B	744	HIS
2	B	776	GLN
2	B	794	ASN
2	B	821	GLN
2	B	834	ASN
2	B	842	ASN
2	B	975	GLN
2	B	1015	HIS
2	B	1025	HIS
2	B	1065	GLN
2	B	1076	HIS
2	B	1084	GLN
2	B	1097	HIS
2	B	1117	GLN
2	B	1141	HIS
2	B	1179	GLN
2	B	1193	GLN
3	C	73	GLN
3	C	112	ASN
3	C	123	ASN
3	C	140	ASN
3	C	151	GLN
3	C	167	HIS
3	C	203	GLN
3	C	231	ASN
4	D	28	GLN
4	D	39	ASN
4	D	40	HIS
4	D	132	GLN
4	D	137	ASN
5	E	8	ASN
5	E	101	GLN
5	E	104	ASN
5	E	114	ASN
5	E	146	HIS
5	E	147	HIS
5	E	179	GLN
6	F	104	ASN

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Mol	Chain	Res	Type
7	G	53	ASN
7	G	97	HIS
7	G	102	GLN
7	G	122	ASN
7	G	126	ASN
7	G	158	HIS
8	H	139	ASN
9	I	12	ASN
9	I	51	ASN
9	I	89	GLN
9	I	90	GLN
10	J	53	HIS
10	J	64	ASN
11	K	29	ASN
11	K	44	ASN
11	K	65	HIS
11	K	76	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	9/11 (81%)	3 (33%)	1 (11%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	7	A
14	P	8	G
14	P	9	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	7	A

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	BRU	T	22	14,15	18,21,22	0.46	0	25,30,33	1.00	1 (4%)
15	TT	T	19	15	40,43,44	5.14	11 (27%)	58,69,72	2.48	19 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BRU	T	22	14,15	-	0/7/21/22	0/2/2/2
15	TT	T	19	15	-	11/18/105/106	0/5/6/6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	19	TT	C5-C6	-22.15	1.31	1.55
15	T	19	TT	C5T-C6T	-21.11	1.32	1.55
15	T	19	TT	C6-N1	-5.42	1.38	1.46
15	T	19	TT	C1'-N1	4.00	1.50	1.45
15	T	19	TT	C6T-N1T	-3.76	1.40	1.46
15	T	19	TT	C2-N1	2.76	1.41	1.36
15	T	19	TT	O3'-C3'	2.74	1.48	1.43
15	T	19	TT	C6T-C6	2.71	1.64	1.56
15	T	19	TT	C1R-N1T	2.53	1.49	1.45
15	T	19	TT	O4-C4	2.26	1.26	1.22
15	T	19	TT	C4-N3	2.09	1.40	1.37

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	19	TT	C5-C6-N1	8.88	127.43	115.65
15	T	19	TT	C5T-C6T-N1T	6.46	124.22	115.65
15	T	19	TT	C5T-C5-C6	6.41	95.86	88.36
15	T	19	TT	C5-C6-C6T	-6.09	79.91	89.26
15	T	19	TT	C5-C5T-C6T	-5.79	81.59	88.36
15	T	19	TT	O4-C4-C5	3.28	125.77	122.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	19	TT	N3T-C2T-N1T	-3.00	113.64	116.78
15	T	19	TT	C5'-C4'-C3'	2.95	121.57	114.57
15	T	19	TT	O4R-C4R-C5R	2.91	118.67	109.33
15	T	19	TT	N3-C2-N1	-2.62	114.04	116.78
15	T	22	BRU	C6-C5-C4	-2.62	118.02	120.67
15	T	19	TT	C6-C6T-N1T	2.55	128.06	118.51
15	T	19	TT	C5A-C5-C6	-2.46	107.08	114.44
15	T	19	TT	C5T-C6T-C6	2.42	92.99	89.26
15	T	19	TT	C2R-C1R-N1T	-2.31	112.47	115.59
15	T	19	TT	C5-C4-N3	-2.24	114.20	116.09
15	T	19	TT	C5-C5T-C4T	2.11	119.69	112.84
15	T	19	TT	C5A-C5-C4	-2.08	104.77	108.19
15	T	19	TT	O3R-C3R-C4R	-2.07	102.21	110.07
15	T	19	TT	O4T-C4T-C5T	2.01	124.58	122.71

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	19	TT	C4'-C5'-O5'-P
15	T	19	TT	O3'-C7-O5R-C5R
15	T	19	TT	C2R-C1R-N1T-C6T
15	T	19	TT	C2'-C1'-N1-C6
15	T	19	TT	C2'-C1'-N1-C2
15	T	19	TT	O4'-C1'-N1-C2
15	T	19	TT	O4'-C1'-N1-C6
15	T	19	TT	O4R-C1R-N1T-C6T
15	T	19	TT	O5R-C7-O3'-C3'
15	T	19	TT	C4R-C5R-O5R-C7
15	T	19	TT	C2'-C3'-O3'-C7

There are no ring outliers.

2 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	T	22	BRU	5	0
15	T	19	TT	26	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2
3	C	1
6	F	1
1	A	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	4.15
1	B	18:PHE	C	19:GLU	N	3.85
1	F	69:LEU	C	70:LYS	N	3.50
1	A	1175:SER	C	1176:LEU	N	3.39
1	B	337:ARG	C	338:GLY	N	2.64

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1421/1733 (81%)	0.02	38 (2%) 56 38	17, 78, 152, 199	0
2	B	1115/1224 (91%)	0.22	56 (5%) 34 25	20, 91, 167, 200	0
3	C	267/318 (83%)	-0.11	2 (0%) 84 65	39, 77, 139, 165	0
4	D	177/221 (80%)	0.33	9 (5%) 33 25	61, 111, 160, 175	0
5	E	214/215 (99%)	0.29	4 (1%) 66 45	50, 133, 184, 188	0
6	F	87/155 (56%)	-0.24	4 (4%) 37 27	27, 56, 100, 138	0
7	G	171/171 (100%)	0.21	7 (4%) 41 30	57, 80, 126, 137	0
8	H	135/146 (92%)	0.92	15 (11%) 10 13	95, 138, 173, 183	0
9	I	116/122 (95%)	0.48	7 (6%) 27 22	75, 134, 166, 186	0
10	J	65/70 (92%)	-0.08	2 (3%) 51 35	42, 73, 117, 125	0
11	K	114/120 (95%)	-0.06	2 (1%) 67 46	38, 83, 112, 167	0
12	L	46/70 (65%)	0.88	8 (17%) 4 6	78, 156, 175, 181	0
13	N	8/14 (57%)	1.19	1 (12%) 8 12	129, 140, 153, 155	0
14	P	10/11 (90%)	1.10	3 (30%) 1 2	115, 126, 152, 158	0
15	T	17/25 (68%)	1.08	3 (17%) 4 6	125, 138, 151, 153	0
All	All	3963/4615 (85%)	0.16	161 (4%) 41 30	17, 89, 165, 200	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1081	LEU	8.1
2	B	882	THR	7.4
8	H	65	LEU	6.1
4	D	25	ALA	6.0
1	A	1257	ASP	5.7
2	B	879	ARG	5.6
2	B	471	LYS	5.3

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Mol	Chain	Res	Type	RSRZ
6	F	69	LEU	5.2
2	B	883	LEU	4.9
1	A	1176	LEU	4.7
8	H	90	ALA	4.7
4	D	24	ALA	4.4
1	A	3	GLY	4.3
14	P	8	G	4.3
1	A	1173	HIS	4.2
1	A	1245	PRO	4.2
8	H	76	THR	4.1
8	H	139	ASN	4.1
1	A	252	PHE	4.0
2	B	884	ARG	3.9
8	H	136	LYS	3.8
1	A	1254	ALA	3.8
2	B	963	PHE	3.8
1	A	171	GLN	3.7
4	D	4	SER	3.7
8	H	135	LEU	3.6
1	A	69	THR	3.6
14	P	0	U	3.6
3	C	2	SER	3.6
2	B	730	ARG	3.5
2	B	881	ASN	3.4
2	B	731	VAL	3.4
8	H	137	GLN	3.3
7	G	85	GLU	3.2
7	G	21	ARG	3.2
1	A	56	PRO	3.2
11	K	114	LEU	3.2
11	K	113	THR	3.2
12	L	25	ALA	3.2
8	H	119	GLY	3.2
6	F	155	LEU	3.2
1	A	25	GLU	3.1
1	A	251	SER	3.1
1	A	333	GLU	3.1
2	B	472	ALA	3.1
2	B	732	SER	3.1
14	P	9	A	3.0
2	B	70	ILE	3.0
1	A	667	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
4	D	155	ARG	2.9
1	A	51	GLY	2.9
2	B	880	THR	2.9
4	D	8	PHE	2.9
9	I	2	THR	2.9
8	H	140	ALA	2.9
12	L	27	LEU	2.8
8	H	86	ASP	2.8
2	B	860	MET	2.8
2	B	641	GLU	2.8
8	H	120	GLY	2.8
9	I	93	LYS	2.8
1	A	1125	ALA	2.8
1	A	147	VAL	2.7
4	D	13	ARG	2.7
2	B	885	MET	2.6
2	B	804	GLY	2.6
9	I	44	TYR	2.6
1	A	1175	SER	2.6
2	B	964	VAL	2.6
8	H	112	ILE	2.6
2	B	571	PRO	2.6
2	B	487	THR	2.6
2	B	1224	PHE	2.6
1	A	1158	PRO	2.6
2	B	246	LYS	2.6
4	D	18	VAL	2.6
2	B	230	ALA	2.6
8	H	81	PRO	2.6
2	B	446	LEU	2.5
5	E	110	PHE	2.5
1	A	1097	GLY	2.5
2	B	110	HIS	2.5
6	F	70	LYS	2.5
13	N	0	DT	2.5
2	B	710	LEU	2.5
1	A	316	GLN	2.5
4	D	14	ARG	2.5
9	I	117	LYS	2.4
1	A	587	HIS	2.4
1	A	1280	GLU	2.4
2	B	734	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	510	LYS	2.4
2	B	934	LYS	2.4
6	F	72	LYS	2.4
8	H	129	TYR	2.4
15	T	10	DA	2.4
2	B	310	MET	2.4
1	A	1191	TRP	2.3
12	L	35	SER	2.3
2	B	728	ARG	2.3
12	L	28	LYS	2.3
12	L	43	THR	2.3
5	E	192	ARG	2.3
1	A	292	ALA	2.3
1	A	149	GLU	2.3
1	A	253	ASN	2.3
2	B	461	LEU	2.3
10	J	65	PRO	2.3
1	A	2	VAL	2.3
7	G	124	GLY	2.3
2	B	101	MET	2.3
7	G	113	HIS	2.3
8	H	46	LEU	2.3
2	B	113	TYR	2.3
1	A	79	GLY	2.3
2	B	694	ASP	2.3
2	B	935	ARG	2.3
1	A	1217	LYS	2.2
7	G	164	LYS	2.2
1	A	1256	GLU	2.2
3	C	130	GLY	2.2
1	A	1080	THR	2.2
2	B	887	HIS	2.2
1	A	128	ILE	2.2
2	B	243	ALA	2.2
9	I	64	SER	2.2
1	A	1110	ASN	2.2
2	B	468	GLU	2.2
12	L	32	ALA	2.2
2	B	709	ASP	2.2
1	A	68	GLN	2.2
12	L	64	LEU	2.2
2	B	282	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	18	PHE	2.2
2	B	262	GLU	2.2
7	G	128	PRO	2.2
9	I	55	THR	2.2
2	B	371	GLU	2.1
2	B	473	MET	2.1
2	B	305	VAL	2.1
2	B	486	TYR	2.1
2	B	245	GLU	2.1
1	A	265	LYS	2.1
15	T	14	DC	2.1
15	T	23	DG	2.1
7	G	148	GLU	2.1
12	L	26	THR	2.1
2	B	775	LYS	2.1
2	B	469	GLN	2.1
4	D	20	GLU	2.1
9	I	63	GLY	2.0
2	B	241	ARG	2.0
2	B	435	THR	2.0
1	A	830	LYS	2.0
2	B	250	PHE	2.0
10	J	30	LEU	2.0
5	E	88	VAL	2.0
5	E	5	ASN	2.0
2	B	876	LYS	2.0
2	B	254	LEU	2.0
2	B	933	SER	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	BRU	T	22	20/21	0.78	0.15	112,118,124,128	0
15	TT	T	19	38/39	0.83	0.18	130,144,163,166	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	ZN	A	2461	1/1	0.98	0.05	200,200,200,200	0
17	ZN	A	2464	1/1	0.98	0.04	87,87,87,87	0
17	ZN	A	2458	1/1	0.99	0.05	57,57,57,57	0
17	ZN	A	2459	1/1	0.99	0.04	125,125,125,125	0
16	MG	A	2457	1/1	1.00	0.01	35,35,35,35	0
17	ZN	A	2462	1/1	1.00	0.01	39,39,39,39	0
17	ZN	A	2463	1/1	1.00	0.01	47,47,47,47	0
17	ZN	A	2460	1/1	1.00	0.05	88,88,88,88	0
17	ZN	A	2465	1/1	1.00	0.05	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.