



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:50 PM UTC

PDB ID : 8KAK / pdb_00008kak
Title : Crystal structure of SpyCas9 in complex with sgRNA and 18nt target DNA
Authors : Chen, Y.; Chen, J.; Liu, L.
Deposited on : 2023-08-03
Resolution : 3.60 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

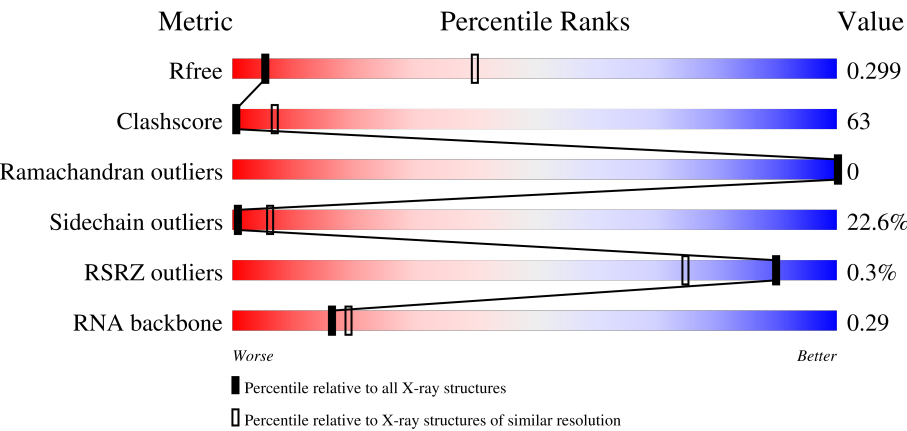
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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.



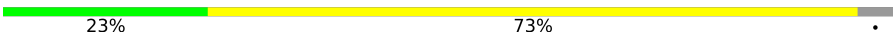
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

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

Mol	Chain	Length	Quality of chain
1	A	98	16% 55% 24% .
1	E	98	16% 54% 26% .
2	B	1368	28% 50% 18% ..
2	F	1368	% 29% 49% 18% ..

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Mol	Chain	Length	Quality of chain
3	C	26	 23% 73% .
3	G	26	 23% 73% .
4	D	11	 27% 73%
4	H	11	 27% 73%

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
5	SO4	B	1401	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27148 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called RNA (98-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	P	0	0	0
			2009	899	362	654	94			
1	E	94	Total	C	N	O	P	0	0	0
			2009	899	362	654	94			

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1326	Total	C	N	O	S	0	0	0
			10827	6897	1879	2029	22			
2	F	1326	Total	C	N	O	S	0	0	0
			10827	6897	1879	2029	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	ALA	ASP	engineered mutation	UNP Q99ZW2
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2
F	10	ALA	ASP	engineered mutation	UNP Q99ZW2
F	840	ALA	HIS	engineered mutation	UNP Q99ZW2

- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	25	Total	C	N	O	P	0	0	0
			505	243	93	145	24			
3	G	25	Total	C	N	O	P	0	0	0
			505	243	93	145	24			

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total	C	N	O	P	0	0	0
			225	110	37	68	10			
4	H	11	Total	C	N	O	P	0	0	0
			225	110	37	68	10			

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		

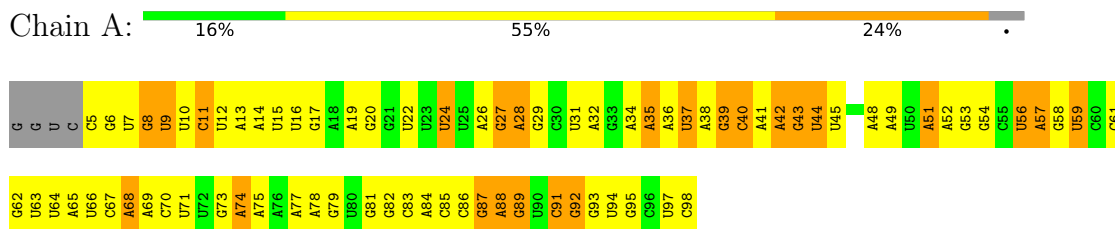
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	B	1	Total	O	0	0
			1	1		
6	F	4	Total	O	0	0
			4	4		

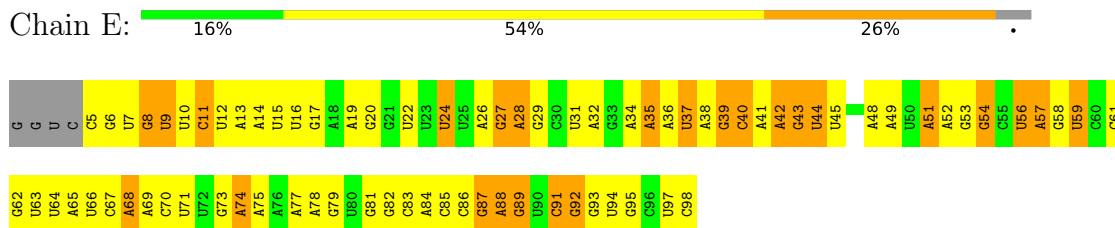
3 Residue-property plots

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.

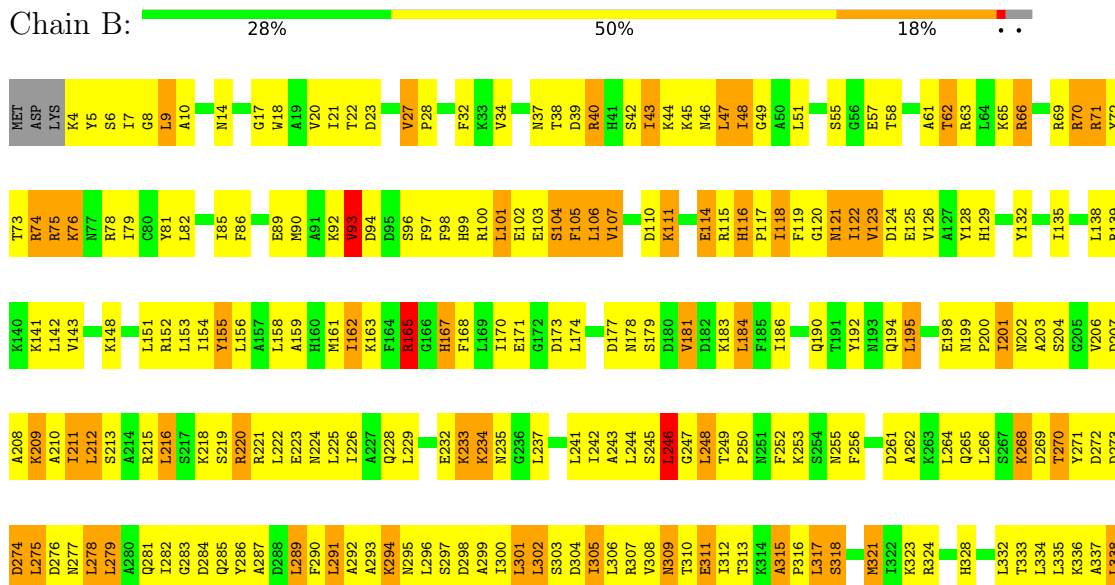
- Molecule 1: RNA (98-MER)



- Molecule 1: RNA (98-MER)



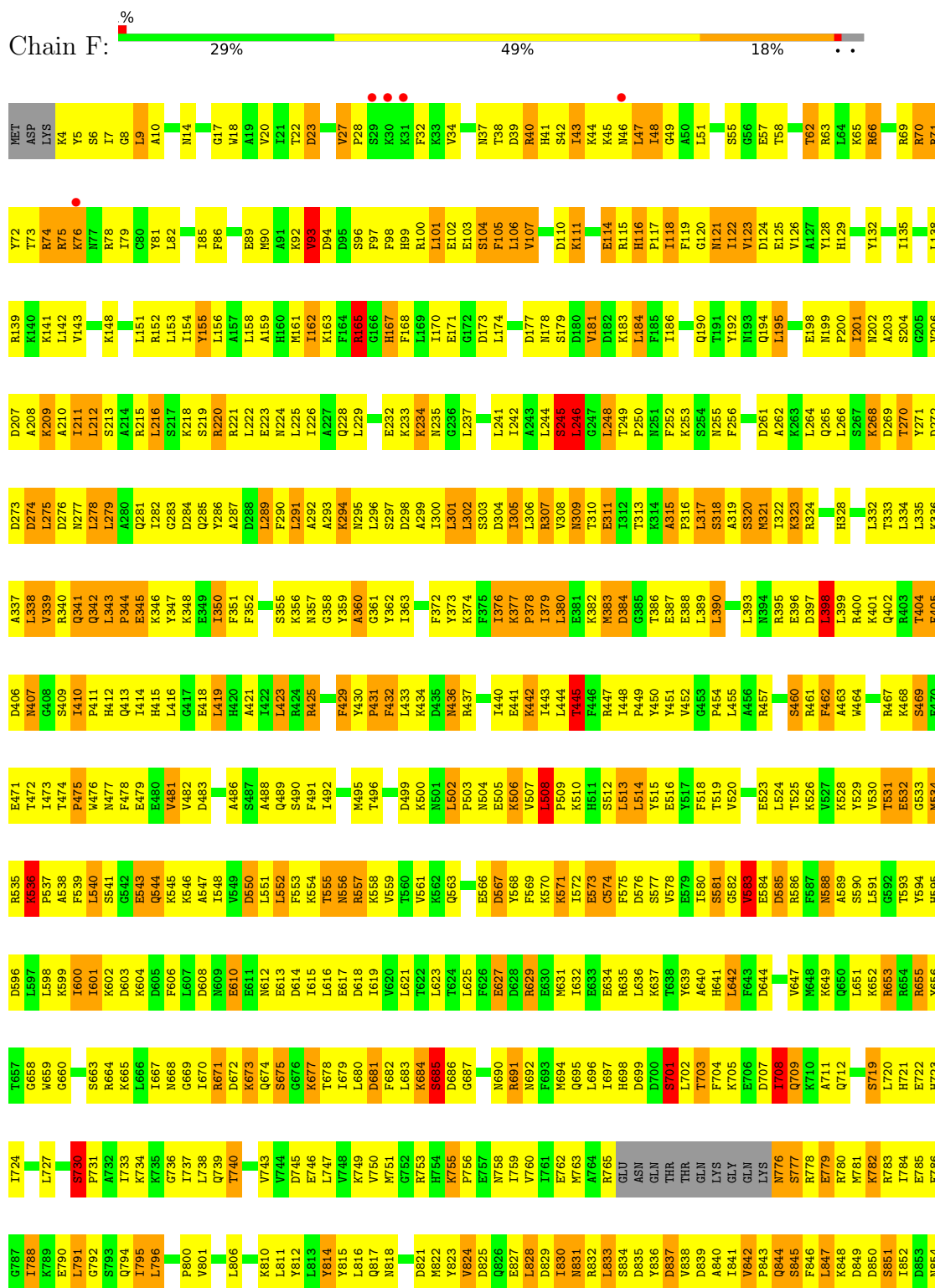
- Molecule 2: CRISPR-associated endonuclease Cas9/Csn1

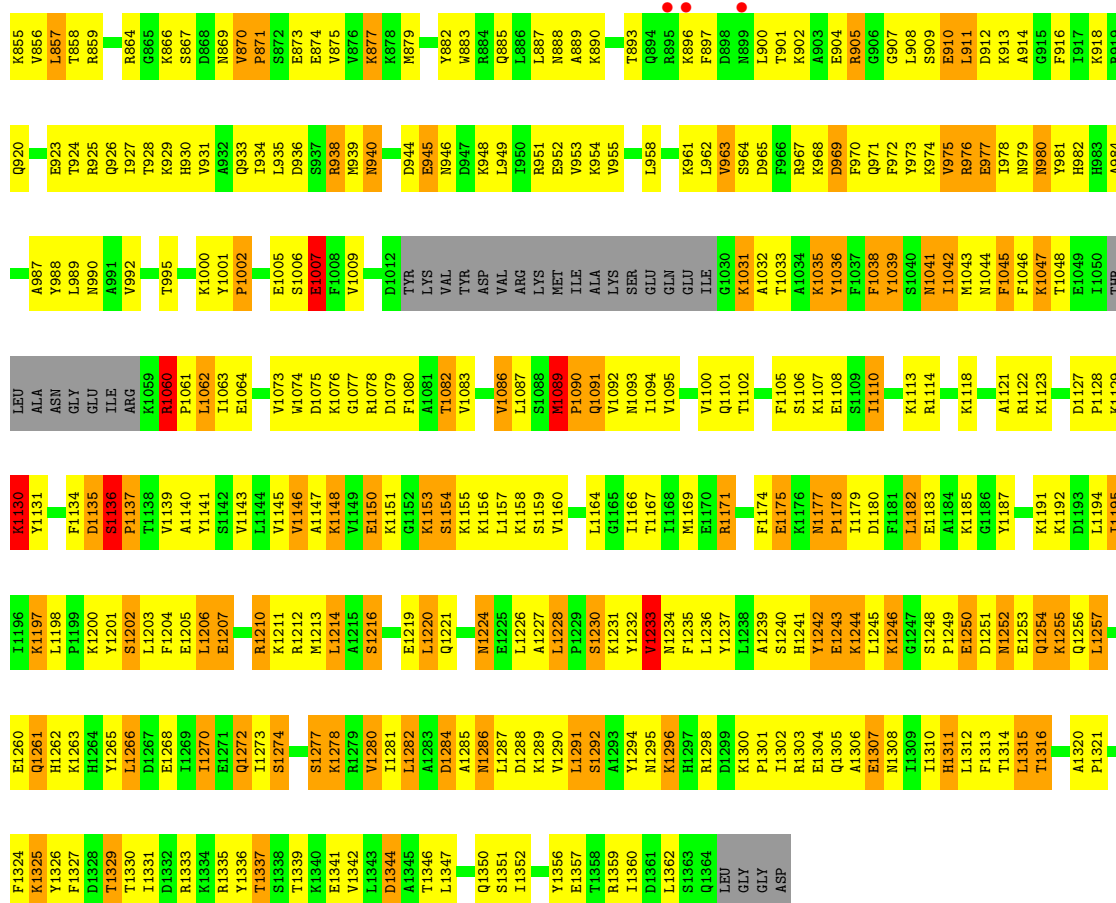






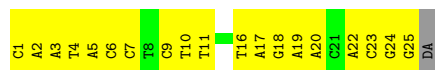
● Molecule 2: CRISPR-associated endonuclease Cas9/Csn1





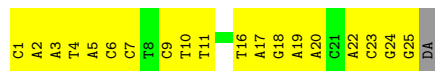
• Molecule 3: DNA (26-MER)

Chain C: 23% 73%



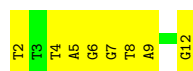
• Molecule 3: DNA (26-MER)

Chain G: 23% 73%

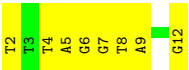
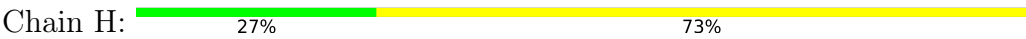


• Molecule 4: DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP*G)-3')

Chain D: 27% 73%



• Molecule 4: DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.74Å 104.97Å 184.31Å 75.82° 78.67° 72.63°	Depositor
Resolution (Å)	24.97 – 3.60 24.97 – 3.60	Depositor EDS
% Data completeness (in resolution range)	73.7 (24.97-3.60) 73.9 (24.97-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.265 , 0.297 0.264 , 0.299	Depositor DCC
R_{free} test set	2067 reflections (3.66%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.942	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 19.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.107 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	27148	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.47	0/2249	0.69	0/3503
1	E	0.47	0/2249	0.69	0/3503
2	B	0.81	30/11019 (0.3%)	1.08	93/14807 (0.6%)
2	F	0.81	31/11019 (0.3%)	1.10	102/14807 (0.7%)
3	C	0.63	0/566	0.77	0/870
3	G	0.63	0/566	0.77	0/870
4	D	0.63	0/251	0.74	0/387
4	H	0.63	0/251	0.74	0/387
All	All	0.76	61/28170 (0.2%)	1.01	195/39134 (0.5%)

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	27	VAL	CA-C	13.90	1.67	1.52
2	B	27	VAL	CA-C	13.84	1.67	1.52
2	B	755	LYS	C-N	6.24	1.40	1.33
2	F	755	LYS	C-N	6.23	1.40	1.33
2	B	508	LEU	C-N	6.09	1.40	1.33
2	F	508	LEU	C-N	6.04	1.40	1.33
2	F	1300	LYS	C-N	5.97	1.40	1.33
2	B	1198	LEU	C-N	5.91	1.40	1.33
2	B	1300	LYS	C-N	5.90	1.40	1.33
2	F	1198	LEU	C-N	5.90	1.40	1.33
2	F	410	ILE	C-N	5.84	1.40	1.33
2	B	410	ILE	C-N	5.83	1.40	1.33
2	B	1060	ARG	C-N	5.75	1.41	1.33
2	F	1228	LEU	C-N	5.74	1.41	1.33
2	B	1001	TYR	C-N	5.73	1.40	1.33
2	F	1001	TYR	C-N	5.71	1.40	1.33
2	B	536	LYS	C-N	5.69	1.41	1.33
2	F	1060	ARG	C-N	5.67	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	536	LYS	C-N	5.66	1.41	1.33
2	F	870	VAL	C-N	5.64	1.41	1.33
2	F	1089	MET	C-N	5.64	1.40	1.34
2	B	1089	MET	C-N	5.63	1.40	1.34
2	B	1177	ASN	C-N	5.62	1.40	1.34
2	B	1228	LEU	C-N	5.62	1.41	1.33
2	F	1177	ASN	C-N	5.58	1.40	1.34
2	B	870	VAL	C-N	5.58	1.40	1.33
2	F	343	LEU	C-N	5.58	1.40	1.33
2	B	343	LEU	C-N	5.55	1.40	1.33
2	B	1136	SER	C-N	5.42	1.40	1.33
2	F	1002	PRO	N-CD	5.41	1.55	1.47
2	F	1136	SER	C-N	5.40	1.40	1.33
2	B	431	PRO	N-CD	5.39	1.55	1.47
2	F	344	PRO	N-CD	5.37	1.55	1.47
2	F	431	PRO	N-CD	5.36	1.55	1.47
2	B	1002	PRO	N-CD	5.35	1.55	1.47
2	F	842	VAL	C-N	5.28	1.40	1.33
2	B	344	PRO	N-CD	5.27	1.55	1.47
2	B	842	VAL	C-N	5.26	1.40	1.33
2	B	1301	PRO	N-CD	5.25	1.55	1.47
2	F	475	PRO	N-CD	5.25	1.55	1.47
2	B	475	PRO	N-CD	5.19	1.55	1.47
2	F	1301	PRO	N-CD	5.18	1.55	1.47
2	B	316	PRO	N-CD	5.17	1.54	1.47
2	F	1137	PRO	N-CD	5.17	1.54	1.47
2	F	1061	PRO	N-CD	5.17	1.54	1.47
2	B	1061	PRO	N-CD	5.15	1.54	1.47
2	F	316	PRO	N-CD	5.14	1.54	1.47
2	F	377	LYS	C-N	5.13	1.41	1.34
2	B	377	LYS	C-N	5.12	1.41	1.34
2	B	1137	PRO	N-CD	5.11	1.54	1.47
2	F	1178	PRO	N-CD	5.11	1.54	1.47
2	B	871	PRO	N-CD	5.11	1.54	1.47
2	B	1178	PRO	N-CD	5.09	1.54	1.47
2	B	1229	PRO	N-CD	5.07	1.54	1.47
2	F	871	PRO	N-CD	5.07	1.54	1.47
2	F	1090	PRO	N-CD	5.06	1.54	1.47
2	B	1249	PRO	N-CD	5.05	1.54	1.47
2	B	731	PRO	N-CD	5.03	1.54	1.47
2	F	378	PRO	N-CD	5.02	1.54	1.47
2	F	1249	PRO	N-CD	5.02	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	800	PRO	N-CD	5.01	1.54	1.47

All (195) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	685	SER	N-CA-C	24.49	144.85	111.54
2	F	684	LYS	N-CA-C	-14.18	86.15	109.96
2	B	684	LYS	N-CA-C	-14.17	86.15	109.96
2	F	200	PRO	CB-CA-C	10.22	128.42	111.56
2	B	246	LEU	N-CA-C	-9.85	96.61	110.50
2	B	200	PRO	CB-CA-C	9.61	127.41	111.56
2	F	687	GLY	N-CA-C	9.51	123.53	112.50
2	F	462	PHE	N-CA-C	8.97	121.14	111.36
2	B	462	PHE	N-CA-C	8.96	121.13	111.36
2	F	201	ILE	N-CA-C	-8.63	94.80	108.86
2	B	600	ILE	N-CA-C	8.54	119.34	110.72
2	F	600	ILE	N-CA-C	8.48	119.29	110.72
2	B	398	LEU	N-CA-C	8.39	120.04	111.07
2	F	398	LEU	N-CA-C	8.38	120.04	111.07
2	B	685	SER	N-CA-C	8.22	122.84	111.74
2	B	201	ILE	N-CA-C	-8.11	95.65	108.86
2	B	66	ARG	N-CA-C	-7.65	102.89	111.07
2	F	66	ARG	N-CA-C	-7.61	102.93	111.07
2	B	582	GLY	N-CA-C	7.40	121.61	112.73
2	F	582	GLY	N-CA-C	7.38	121.59	112.73
2	B	1198	LEU	CA-C-N	-7.23	113.22	120.31
2	B	1198	LEU	C-N-CA	-7.23	113.22	120.31
2	F	27	VAL	O-C-N	7.23	129.34	121.10
2	F	1198	LEU	CA-C-N	-7.21	113.24	120.31
2	F	1198	LEU	C-N-CA	-7.21	113.24	120.31
2	B	27	VAL	O-C-N	7.17	129.28	121.10
2	B	755	LYS	CA-C-N	-6.94	113.51	120.31
2	B	755	LYS	C-N-CA	-6.94	113.51	120.31
2	F	755	LYS	CA-C-N	-6.89	113.56	120.31
2	F	755	LYS	C-N-CA	-6.89	113.56	120.31
2	B	1007	GLU	N-CA-C	6.87	118.84	111.36
2	F	1007	GLU	N-CA-C	6.82	118.79	111.36
2	B	536	LYS	CA-C-N	-6.81	112.75	119.76
2	B	536	LYS	C-N-CA	-6.81	112.75	119.76
2	F	536	LYS	CA-C-N	-6.80	112.75	119.76
2	F	536	LYS	C-N-CA	-6.80	112.75	119.76
2	F	1130	LYS	N-CA-C	6.80	118.77	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	824	VAL	N-CA-C	6.79	120.18	113.53
2	B	504	ASN	N-CA-C	6.78	118.75	111.36
2	F	824	VAL	N-CA-C	6.78	120.17	113.53
2	F	504	ASN	N-CA-C	6.76	118.73	111.36
2	F	410	ILE	CA-C-N	-6.71	113.39	120.03
2	F	410	ILE	C-N-CA	-6.71	113.39	120.03
2	F	1280	VAL	N-CA-C	6.68	116.90	111.62
2	B	410	ILE	CA-C-N	-6.63	113.46	120.03
2	B	410	ILE	C-N-CA	-6.63	113.46	120.03
2	F	118	ILE	N-CA-C	6.63	117.42	110.72
2	B	1280	VAL	N-CA-C	6.60	116.84	111.62
2	B	118	ILE	N-CA-C	6.59	117.38	110.72
2	F	685	SER	N-CA-CB	-6.56	102.07	111.84
2	B	445	THR	N-CA-C	6.55	118.50	111.36
2	F	445	THR	N-CA-C	6.53	118.48	111.36
2	B	123	VAL	N-CA-C	6.49	116.65	110.42
2	F	1228	LEU	CA-C-N	-6.46	113.11	119.76
2	F	1228	LEU	C-N-CA	-6.46	113.11	119.76
2	F	70	ARG	N-CA-C	-6.44	104.27	111.28
2	F	123	VAL	N-CA-C	6.43	116.59	110.42
2	B	684	LYS	CB-CA-C	-6.42	98.93	109.53
2	F	1300	LYS	CA-C-N	-6.42	113.68	120.03
2	F	1300	LYS	C-N-CA	-6.42	113.68	120.03
2	B	70	ARG	N-CA-C	-6.41	104.29	111.28
2	B	1228	LEU	CA-C-N	-6.41	113.16	119.76
2	B	1228	LEU	C-N-CA	-6.41	113.16	119.76
2	F	508	LEU	CA-C-N	-6.41	113.69	120.03
2	F	508	LEU	C-N-CA	-6.41	113.69	120.03
2	F	684	LYS	CB-CA-C	-6.41	98.96	109.53
2	F	870	VAL	CA-C-N	-6.41	113.16	119.76
2	F	870	VAL	C-N-CA	-6.41	113.16	119.76
2	B	1300	LYS	CA-C-N	-6.39	113.70	120.03
2	B	1300	LYS	C-N-CA	-6.39	113.70	120.03
2	F	23	ASP	N-CA-C	6.38	119.92	111.75
2	F	1216	SER	N-CA-C	-6.38	99.29	108.60
2	B	533	GLY	N-CA-C	6.37	120.38	112.73
2	B	1216	SER	N-CA-C	-6.37	99.31	108.60
2	B	1136	SER	CA-C-N	-6.36	113.40	119.76
2	B	1136	SER	C-N-CA	-6.36	113.40	119.76
2	F	533	GLY	N-CA-C	6.36	120.36	112.73
2	B	870	VAL	CA-C-N	-6.35	113.22	119.76
2	B	870	VAL	C-N-CA	-6.35	113.22	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1136	SER	CA-C-N	-6.34	113.42	119.76
2	F	1136	SER	C-N-CA	-6.34	113.42	119.76
2	B	508	LEU	CA-C-N	-6.33	113.76	120.03
2	B	508	LEU	C-N-CA	-6.33	113.76	120.03
2	F	842	VAL	CA-C-N	-6.32	113.27	119.78
2	F	842	VAL	C-N-CA	-6.32	113.27	119.78
2	B	842	VAL	CA-C-N	-6.31	113.28	119.78
2	B	842	VAL	C-N-CA	-6.31	113.28	119.78
2	F	583	VAL	N-CA-C	6.29	119.32	108.95
2	B	583	VAL	N-CA-C	6.27	119.30	108.95
2	B	1060	ARG	CA-C-N	-6.21	113.57	119.85
2	B	1060	ARG	C-N-CA	-6.21	113.57	119.85
2	F	1060	ARG	CA-C-N	-6.21	113.58	119.85
2	F	1060	ARG	C-N-CA	-6.21	113.58	119.85
2	B	343	LEU	CA-C-N	-6.20	113.23	119.56
2	B	343	LEU	C-N-CA	-6.20	113.23	119.56
2	F	343	LEU	CA-C-N	-6.16	113.28	119.56
2	F	343	LEU	C-N-CA	-6.16	113.28	119.56
2	F	71	ARG	N-CA-C	6.12	117.62	111.07
2	B	71	ARG	N-CA-C	6.09	117.59	111.07
2	F	552	LEU	N-CA-C	6.04	117.66	111.14
2	B	1001	TYR	CA-C-N	-6.02	113.42	119.56
2	B	1001	TYR	C-N-CA	-6.02	113.42	119.56
2	B	552	LEU	N-CA-C	6.01	117.63	111.14
2	F	1001	TYR	CA-C-N	-5.99	113.45	119.56
2	F	1001	TYR	C-N-CA	-5.99	113.45	119.56
2	B	116	HIS	CA-C-N	-5.99	112.35	119.84
2	B	116	HIS	C-N-CA	-5.99	112.35	119.84
2	B	1077	GLY	N-CA-C	5.98	119.72	112.49
2	F	116	HIS	CA-C-N	-5.97	112.38	119.84
2	F	116	HIS	C-N-CA	-5.97	112.38	119.84
2	F	1077	GLY	N-CA-C	5.94	119.68	112.49
2	B	831	ASN	N-CA-C	5.87	117.47	111.14
2	F	831	ASN	N-CA-C	5.82	117.43	111.14
2	B	681	ASP	N-CA-C	-5.78	104.98	111.28
2	F	681	ASP	N-CA-C	-5.77	104.99	111.28
2	B	1130	LYS	N-CA-C	5.76	117.36	111.14
2	F	246	LEU	N-CA-C	-5.72	102.43	110.50
2	B	1039	TYR	N-CA-C	5.72	117.59	111.36
2	F	155	TYR	N-CA-C	-5.70	105.07	111.28
2	B	155	TYR	N-CA-C	-5.67	105.10	111.28
2	F	1039	TYR	N-CA-C	5.66	117.53	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	409	SER	N-CA-C	-5.61	105.64	112.88
2	B	409	SER	N-CA-C	-5.59	105.66	112.88
2	F	245	SER	N-CA-C	-5.59	105.19	111.28
2	B	1210	ARG	N-CA-C	-5.59	102.13	110.23
2	F	1210	ARG	N-CA-C	-5.57	102.16	110.23
2	B	200	PRO	CA-N-CD	-5.54	104.24	112.00
2	B	478	PHE	N-CA-C	5.54	116.99	111.07
2	F	200	PRO	CA-N-CD	-5.50	104.30	112.00
2	F	478	PHE	N-CA-C	5.50	116.95	111.07
2	F	708	ILE	N-CA-C	-5.47	105.04	110.62
2	B	708	ILE	N-CA-C	-5.46	105.05	110.62
2	B	1233	VAL	CB-CA-C	-5.46	104.97	111.97
2	F	360	ALA	N-CA-C	-5.46	105.33	111.28
2	F	377	LYS	CA-C-N	-5.45	113.00	119.05
2	F	377	LYS	C-N-CA	-5.45	113.00	119.05
2	F	1286	ASN	N-CA-C	5.45	117.30	111.36
2	B	1316	THR	N-CA-C	5.45	117.22	111.28
2	B	1286	ASN	N-CA-C	5.44	117.29	111.36
2	F	1233	VAL	CB-CA-C	-5.44	105.01	111.97
2	F	1316	THR	N-CA-C	5.40	117.17	111.28
2	F	481	VAL	N-CA-C	5.40	116.17	110.72
2	F	567	ASP	N-CA-C	5.40	117.24	111.36
2	B	377	LYS	CA-C-N	-5.39	113.06	119.05
2	B	377	LYS	C-N-CA	-5.39	113.06	119.05
2	B	534	MET	N-CA-C	5.39	118.26	110.28
2	B	567	ASP	N-CA-C	5.39	117.24	111.36
2	F	534	MET	N-CA-C	5.39	118.26	110.28
2	B	481	VAL	N-CA-C	5.38	116.16	110.72
2	F	581	SER	N-CA-C	5.37	117.22	111.36
2	B	1177	ASN	CA-C-N	-5.35	113.02	118.85
2	B	1177	ASN	C-N-CA	-5.35	113.02	118.85
2	B	701	SER	N-CA-C	-5.34	105.45	111.28
2	B	581	SER	N-CA-C	5.33	117.17	111.36
2	F	1177	ASN	CA-C-N	-5.32	113.05	118.85
2	F	1177	ASN	C-N-CA	-5.32	113.05	118.85
2	F	701	SER	N-CA-C	-5.31	105.49	111.28
2	F	1337	THR	N-CA-C	5.31	119.74	113.16
2	B	406	ASP	N-CA-C	5.30	117.06	111.28
2	B	1337	THR	N-CA-C	5.29	119.73	113.16
2	F	406	ASP	N-CA-C	5.28	117.03	111.28
2	B	869	ASN	N-CA-C	5.26	116.79	108.96
2	F	22	THR	CB-CA-C	-5.24	99.56	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	105	PHE	N-CA-C	5.23	116.98	111.28
2	B	1129	LYS	N-CA-C	-5.21	105.49	111.07
2	F	105	PHE	N-CA-C	5.20	116.95	111.28
2	F	93	VAL	N-CA-C	5.20	115.42	110.53
2	B	93	VAL	N-CA-C	5.19	115.41	110.53
2	F	869	ASN	N-CA-C	5.19	116.69	108.96
2	F	1129	LYS	N-CA-C	-5.19	105.52	111.07
2	F	588	ASN	N-CA-C	5.17	116.73	111.14
2	B	588	ASN	N-CA-C	5.15	116.70	111.14
2	F	800	PRO	CA-N-CD	-5.11	104.84	112.00
2	F	199	ASN	CA-C-N	-5.11	113.46	119.84
2	F	199	ASN	C-N-CA	-5.11	113.46	119.84
2	B	800	PRO	CA-N-CD	-5.10	104.86	112.00
2	F	1089	MET	CA-C-N	-5.09	113.30	118.85
2	F	1089	MET	C-N-CA	-5.09	113.30	118.85
2	B	350	ILE	N-CA-C	5.09	115.86	110.72
2	B	199	ASN	CA-C-N	-5.08	113.49	119.84
2	B	199	ASN	C-N-CA	-5.08	113.49	119.84
2	B	1261	GLN	N-CA-C	-5.07	105.76	111.28
2	F	1261	GLN	N-CA-C	-5.07	105.76	111.28
2	B	1089	MET	CA-C-N	-5.07	113.33	118.85
2	B	1089	MET	C-N-CA	-5.07	113.33	118.85
2	B	165	ARG	N-CA-C	5.05	120.82	114.31
2	F	350	ILE	N-CA-C	5.05	115.82	110.72
2	F	1036	TYR	N-CA-C	-5.05	105.78	111.28
2	F	165	ARG	N-CA-C	5.02	120.79	114.31
2	B	315	ALA	CA-C-N	-5.01	113.48	119.05
2	B	315	ALA	C-N-CA	-5.01	113.48	119.05
2	F	730	SER	CA-C-N	-5.01	113.49	119.05
2	F	730	SER	C-N-CA	-5.01	113.49	119.05
2	F	315	ALA	CA-C-N	-5.01	113.49	119.05
2	F	315	ALA	C-N-CA	-5.01	113.49	119.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2009	0	1009	111	0
1	E	2009	0	1009	112	0
2	B	10827	0	10973	1538	0
2	F	10827	0	10972	1594	0
3	C	505	0	283	31	0
3	G	505	0	283	31	0
4	D	225	0	129	18	0
4	H	225	0	129	19	0
5	B	5	0	0	3	0
5	F	5	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	F	4	0	0	0	0
All	All	27148	0	24787	3258	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 63.

All (3258) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:181:VAL:HG11	2:F:300:ILE:CD1	1.14	1.57
2:B:181:VAL:HG11	2:B:300:ILE:CD1	1.14	1.57
2:F:342:GLN:HG3	2:F:383:MET:CE	1.09	1.54
2:F:1270:ILE:HD12	2:F:1294:TYR:CE2	1.37	1.54
2:B:181:VAL:CG1	2:B:300:ILE:CD1	1.83	1.53
2:F:181:VAL:CG1	2:F:300:ILE:CD1	1.83	1.53
2:B:1270:ILE:HD12	2:B:1294:TYR:CE2	1.37	1.53
2:B:1270:ILE:CD1	2:B:1294:TYR:CE2	1.91	1.52
2:F:1270:ILE:CD1	2:F:1294:TYR:CE2	1.91	1.51
2:F:1294:TYR:HE1	2:F:1305:GLN:NE2	1.14	1.44
2:B:1294:TYR:HE1	2:B:1305:GLN:NE2	1.14	1.43
2:F:179:SER:CB	2:F:310:THR:CB	1.93	1.43
2:B:179:SER:CB	2:B:310:THR:CB	1.93	1.42
2:F:181:VAL:CG1	2:F:300:ILE:HD11	1.40	1.42
2:B:181:VAL:CG1	2:B:300:ILE:HD11	1.40	1.42
2:B:981:TYR:CZ	2:B:1092:VAL:HG12	1.54	1.41
2:F:981:TYR:CZ	2:F:1092:VAL:HG12	1.54	1.41
2:B:1000:LYS:NZ	2:B:1045:PHE:HD2	1.18	1.41
2:F:1000:LYS:NZ	2:F:1045:PHE:HD2	1.19	1.40
2:F:297:SER:OG	2:F:301:LEU:CD1	1.68	1.39
2:B:297:SER:OG	2:B:301:LEU:CD1	1.68	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1270:ILE:CD1	2:B:1294:TYR:CD2	2.04	1.39
2:F:1270:ILE:CD1	2:F:1294:TYR:CD2	2.04	1.38
2:B:665:LYS:CA	2:B:669:GLY:HA3	1.53	1.37
2:F:665:LYS:CA	2:F:669:GLY:HA3	1.52	1.37
2:B:1000:LYS:HE3	2:B:1073:VAL:CG2	1.53	1.36
2:F:342:GLN:CG	2:F:383:MET:CE	2.01	1.36
2:F:1000:LYS:HE3	2:F:1073:VAL:CG2	1.53	1.36
2:F:324:ARG:HD3	2:F:400:ARG:CG	1.55	1.34
2:F:1000:LYS:CE	2:F:1073:VAL:CG2	2.07	1.33
2:B:1000:LYS:CE	2:B:1073:VAL:CG2	2.07	1.33
2:F:1000:LYS:CE	2:F:1073:VAL:HG21	1.56	1.33
2:F:324:ARG:NH2	2:F:400:ARG:NH1	1.77	1.32
2:F:530:VAL:CG2	2:F:537:PRO:HB3	1.57	1.32
2:B:1000:LYS:CE	2:B:1073:VAL:HG21	1.56	1.32
2:F:179:SER:HB2	2:F:310:THR:CB	1.51	1.32
2:B:179:SER:HB2	2:B:310:THR:CB	1.51	1.32
2:B:530:VAL:CG2	2:B:537:PRO:HB3	1.57	1.31
2:F:1000:LYS:NZ	2:F:1045:PHE:CD2	1.96	1.31
2:B:1000:LYS:NZ	2:B:1045:PHE:CD2	1.95	1.30
2:B:178:ASN:O	2:B:299:ALA:CB	1.80	1.28
2:F:178:ASN:O	2:F:299:ALA:CB	1.80	1.28
2:F:1294:TYR:CE1	2:F:1305:GLN:NE2	2.00	1.28
2:B:557:ARG:HH22	2:B:599:LYS:NZ	1.28	1.28
2:F:324:ARG:CZ	2:F:400:ARG:HH11	1.45	1.28
2:B:1060:ARG:NH1	2:B:1064:GLU:OE2	1.66	1.27
2:B:1294:TYR:CE1	2:B:1305:GLN:NE2	2.00	1.27
2:F:324:ARG:CD	2:F:400:ARG:HG2	1.64	1.27
2:F:557:ARG:HH22	2:F:599:LYS:NZ	1.28	1.27
2:F:1060:ARG:NH1	2:F:1064:GLU:OE2	1.66	1.26
2:F:178:ASN:O	2:F:299:ALA:HB1	1.14	1.26
2:B:178:ASN:O	2:B:299:ALA:HB1	1.14	1.26
2:B:178:ASN:HB3	2:B:299:ALA:CB	1.65	1.26
2:F:181:VAL:CG2	2:F:209:LYS:CG	2.12	1.25
2:B:181:VAL:CG2	2:B:209:LYS:CG	2.12	1.25
2:F:178:ASN:HB3	2:F:299:ALA:CB	1.65	1.25
2:F:195:LEU:HD21	2:F:286:TYR:CD2	1.72	1.24
2:B:195:LEU:HD21	2:B:286:TYR:CD2	1.71	1.24
2:B:178:ASN:CB	2:B:299:ALA:HB2	1.69	1.22
2:F:178:ASN:CB	2:F:299:ALA:HB2	1.69	1.22
2:F:207:ASP:HB3	2:F:210:ALA:CB	1.69	1.22
2:B:780:ARG:NH1	2:B:812:TYR:CD2	2.08	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:ASP:HB3	2:B:210:ALA:CB	1.69	1.22
2:F:780:ARG:NH1	2:F:812:TYR:CD2	2.08	1.22
2:F:324:ARG:NH2	2:F:400:ARG:HH11	1.30	1.21
2:F:665:LYS:HA	2:F:669:GLY:CA	1.70	1.21
2:B:665:LYS:HA	2:B:669:GLY:CA	1.70	1.21
2:F:979:ASN:ND2	2:F:981:TYR:CD1	2.09	1.20
2:F:672:ASP:OD1	2:F:703:THR:HG22	1.02	1.19
2:F:1251:ASP:HA	2:F:1254:GLN:NE2	1.57	1.19
2:B:672:ASP:OD1	2:B:703:THR:HG22	1.02	1.18
2:B:1251:ASP:HA	2:B:1254:GLN:NE2	1.57	1.18
2:B:1146:VAL:HG11	2:B:1194:LEU:CD1	1.73	1.18
2:B:870:VAL:HG23	2:B:908:LEU:HG	1.26	1.18
2:F:297:SER:OG	2:F:301:LEU:HD11	1.43	1.18
2:F:870:VAL:HG23	2:F:908:LEU:HG	1.26	1.18
2:F:1146:VAL:HG11	2:F:1194:LEU:CD1	1.73	1.18
2:B:297:SER:OG	2:B:301:LEU:HD11	1.43	1.17
2:B:1251:ASP:HA	2:B:1254:GLN:CD	1.69	1.17
2:F:1251:ASP:HA	2:F:1254:GLN:CD	1.69	1.17
2:F:926:GLN:HA	2:F:929:LYS:HG3	1.22	1.16
2:F:755:LYS:NZ	2:F:939:MET:O	1.78	1.16
2:B:755:LYS:NZ	2:B:939:MET:O	1.78	1.16
2:B:926:GLN:HA	2:B:929:LYS:HG3	1.21	1.16
2:B:195:LEU:CD2	2:B:286:TYR:CD2	2.27	1.16
2:F:195:LEU:CD2	2:F:286:TYR:CD2	2.27	1.16
2:F:905:ARG:NH1	3:G:24:DG:OP1	1.78	1.16
2:B:905:ARG:NH1	3:C:24:DG:OP1	1.78	1.15
2:F:207:ASP:CB	2:F:210:ALA:HB3	1.74	1.15
2:B:207:ASP:CB	2:B:210:ALA:HB3	1.74	1.14
2:B:981:TYR:CE2	2:B:1092:VAL:CG1	2.30	1.14
2:F:362:TYR:HD1	2:F:372:PHE:CD2	1.65	1.14
2:F:981:TYR:CE2	2:F:1092:VAL:CG1	2.30	1.14
2:F:342:GLN:HG3	2:F:383:MET:HE1	1.15	1.14
2:F:178:ASN:ND2	2:F:298:ASP:HB2	1.62	1.14
2:F:297:SER:OG	2:F:301:LEU:HD12	1.42	1.13
2:B:178:ASN:ND2	2:B:298:ASP:HB2	1.62	1.13
2:B:297:SER:OG	2:B:301:LEU:HD12	1.42	1.12
2:F:362:TYR:CD1	2:F:372:PHE:CD2	2.38	1.12
2:F:178:ASN:ND2	2:F:298:ASP:CB	2.12	1.12
2:F:1270:ILE:HD12	2:F:1294:TYR:CD2	1.78	1.12
2:B:178:ASN:ND2	2:B:298:ASP:CB	2.12	1.12
2:B:278:LEU:HD11	2:B:282:ILE:HD11	1.28	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1062:LEU:O	2:F:1076:LYS:HG3	1.45	1.12
2:B:1270:ILE:HD12	2:B:1294:TYR:CD2	1.78	1.11
2:B:672:ASP:OD1	2:B:703:THR:CG2	1.97	1.11
2:F:181:VAL:CG2	2:F:209:LYS:HG3	1.79	1.11
2:B:181:VAL:CG2	2:B:209:LYS:HG3	1.79	1.11
2:F:278:LEU:HD11	2:F:282:ILE:HD11	1.28	1.11
2:F:672:ASP:OD1	2:F:703:THR:CG2	1.97	1.11
2:B:1062:LEU:O	2:B:1076:LYS:HG3	1.46	1.11
2:F:181:VAL:CG1	2:F:300:ILE:HD13	1.60	1.11
2:F:179:SER:HB3	2:F:310:THR:CB	1.71	1.10
2:F:1205:GLU:O	2:F:1346:THR:OG1	1.69	1.10
2:B:1205:GLU:O	2:B:1346:THR:OG1	1.69	1.10
2:F:324:ARG:CD	2:F:400:ARG:CG	2.24	1.10
2:B:974:LYS:NZ	2:B:976:ARG:HH12	1.49	1.10
2:F:810:LYS:O	2:F:833:LEU:CD1	1.99	1.10
2:B:58:THR:HG22	2:B:731:PRO:HG3	1.30	1.10
2:B:181:VAL:CG1	2:B:300:ILE:HD13	1.60	1.10
2:F:58:THR:HG22	2:F:731:PRO:HG3	1.30	1.10
2:B:378:PRO:HG2	2:B:379:ILE:HD12	1.15	1.09
2:B:121:ASN:HD21	2:B:124:ASP:HB2	1.15	1.09
2:B:179:SER:HB3	2:B:310:THR:CB	1.71	1.09
2:B:810:LYS:O	2:B:833:LEU:CD1	1.99	1.09
2:F:107:VAL:HG22	2:F:1131:TYR:OH	1.51	1.09
2:F:195:LEU:CD2	2:F:286:TYR:CE2	2.36	1.09
2:F:324:ARG:HD3	2:F:400:ARG:HG3	1.11	1.09
2:F:378:PRO:HG2	2:F:379:ILE:HD12	1.15	1.09
2:B:195:LEU:CD2	2:B:286:TYR:CE2	2.36	1.09
2:B:107:VAL:HG22	2:B:1131:TYR:OH	1.51	1.08
2:B:530:VAL:HG22	2:B:537:PRO:HB3	1.23	1.08
2:F:121:ASN:HD21	2:F:124:ASP:HB2	1.15	1.08
2:B:557:ARG:NH2	2:B:599:LYS:NZ	2.00	1.08
2:F:704:PHE:O	2:F:708:ILE:HG12	1.51	1.08
2:F:914:ALA:HB1	2:F:1035:LYS:HD3	1.29	1.08
2:F:1146:VAL:CG1	2:F:1194:LEU:HD12	1.84	1.08
1:A:63:U:O2'	2:B:62:THR:HG23	1.54	1.08
2:B:704:PHE:O	2:B:708:ILE:HG12	1.51	1.08
2:B:981:TYR:CZ	2:B:1092:VAL:CG1	2.36	1.08
2:B:1146:VAL:CG1	2:B:1194:LEU:HD12	1.84	1.08
2:F:557:ARG:NH2	2:F:599:LYS:NZ	2.00	1.08
2:F:981:TYR:CZ	2:F:1092:VAL:CG1	2.36	1.08
1:E:63:U:O2'	2:F:62:THR:HG23	1.54	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:335:LEU:O	2:F:339:VAL:HG23	1.53	1.08
2:F:530:VAL:HG22	2:F:537:PRO:HB3	1.23	1.08
2:F:1062:LEU:HA	2:F:1076:LYS:HD2	1.36	1.08
2:B:914:ALA:HB1	2:B:1035:LYS:HD3	1.29	1.07
2:B:1062:LEU:HA	2:B:1076:LYS:HD2	1.36	1.07
2:B:1326:TYR:CE2	2:B:1327:PHE:CE2	2.41	1.07
2:F:665:LYS:C	2:F:669:GLY:HA3	1.77	1.07
2:F:1270:ILE:HD13	2:F:1294:TYR:CD2	1.80	1.07
2:F:1326:TYR:CE2	2:F:1327:PHE:CE2	2.41	1.07
2:B:335:LEU:O	2:B:339:VAL:HG23	1.53	1.07
2:B:665:LYS:C	2:B:669:GLY:HA3	1.77	1.07
2:B:551:LEU:O	2:B:555:THR:OG1	1.71	1.07
2:B:832:ARG:NH1	2:B:835:ASP:OD2	1.88	1.07
2:F:832:ARG:NH1	2:F:835:ASP:OD2	1.88	1.07
2:F:551:LEU:O	2:F:555:THR:OG1	1.71	1.07
2:B:1270:ILE:HD13	2:B:1294:TYR:CD2	1.80	1.06
2:B:14:ASN:OD1	2:B:55:SER:OG	1.71	1.06
2:B:1270:ILE:HD11	2:B:1294:TYR:CE2	1.87	1.06
2:F:668:ASN:OD1	2:F:678:THR:OG1	1.74	1.06
2:B:278:LEU:CD1	2:B:282:ILE:HD11	1.86	1.06
2:B:668:ASN:OD1	2:B:678:THR:OG1	1.74	1.06
2:F:1000:LYS:HE3	2:F:1073:VAL:HG23	1.38	1.06
2:B:215:ARG:NE	2:B:215:ARG:O	1.88	1.05
2:F:278:LEU:CD1	2:F:282:ILE:HD11	1.86	1.05
2:F:14:ASN:OD1	2:F:55:SER:OG	1.71	1.05
2:F:215:ARG:O	2:F:215:ARG:NE	1.88	1.05
2:F:665:LYS:O	2:F:669:GLY:CA	2.04	1.05
1:A:19:A:H4'	2:B:407:ASN:O	1.57	1.05
2:B:665:LYS:O	2:B:669:GLY:CA	2.04	1.05
2:F:273:ASP:O	2:F:277:ASN:N	1.88	1.05
2:F:324:ARG:NE	2:F:400:ARG:HG2	1.70	1.05
2:F:806:LEU:HD22	2:F:811:LEU:HD12	1.32	1.05
2:B:273:ASP:O	2:B:277:ASN:N	1.88	1.05
2:B:1292:SER:OG	2:B:1296:LYS:NZ	1.88	1.05
1:E:19:A:H4'	2:F:407:ASN:O	1.57	1.05
2:B:1000:LYS:HE3	2:B:1073:VAL:HG23	1.38	1.05
2:F:1270:ILE:HD11	2:F:1294:TYR:CE2	1.87	1.05
2:B:530:VAL:HG22	2:B:537:PRO:CB	1.86	1.04
2:B:596:ASP:OD2	2:B:656:TYR:OH	1.75	1.04
2:B:806:LEU:HD22	2:B:811:LEU:HD12	1.32	1.04
2:F:596:ASP:OD2	2:F:656:TYR:OH	1.75	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:981:TYR:CE2	2:B:1092:VAL:HG12	1.92	1.04
2:F:530:VAL:HG22	2:F:537:PRO:CB	1.86	1.04
2:F:1292:SER:OG	2:F:1296:LYS:NZ	1.88	1.04
2:B:665:LYS:HA	2:B:669:GLY:HA3	1.09	1.04
2:F:393:LEU:HD12	2:F:398:LEU:HD12	1.08	1.04
2:B:704:PHE:O	2:B:708:ILE:CG1	2.05	1.04
2:F:704:PHE:O	2:F:708:ILE:CG1	2.05	1.04
2:B:275:LEU:HD12	2:B:279:LEU:HB2	1.40	1.03
2:F:665:LYS:HA	2:F:669:GLY:HA3	1.08	1.03
2:B:393:LEU:HD12	2:B:398:LEU:HD12	1.08	1.03
2:B:846:PHE:O	2:B:916:PHE:HB3	1.57	1.03
2:F:275:LEU:HD12	2:F:279:LEU:HB2	1.40	1.03
2:B:181:VAL:HG11	2:B:300:ILE:HD13	1.20	1.02
2:B:672:ASP:HA	2:B:703:THR:CG2	1.89	1.02
2:F:846:PHE:O	2:F:916:PHE:HB3	1.57	1.02
2:B:1326:TYR:CE2	2:B:1327:PHE:HE2	1.76	1.02
2:F:672:ASP:HA	2:F:703:THR:CG2	1.89	1.02
2:F:978:ILE:HG12	2:F:1313:PHE:CE2	1.93	1.02
2:B:1210:ARG:HH22	2:B:1341:GLU:CD	1.66	1.02
2:F:70:ARG:NH2	2:F:462:PHE:HD2	1.56	1.02
2:F:1326:TYR:CE2	2:F:1327:PHE:HE2	1.76	1.02
2:B:1143:VAL:CG1	2:B:1195:ILE:CG2	2.38	1.02
2:F:1143:VAL:CG1	2:F:1195:ILE:CG2	2.38	1.02
2:B:70:ARG:NH2	2:B:462:PHE:HD2	1.56	1.01
2:F:1000:LYS:HE2	2:F:1073:VAL:CG2	1.87	1.01
2:B:1000:LYS:HE2	2:B:1073:VAL:CG2	1.87	1.01
2:B:1224:ASN:CG	2:B:1280:VAL:HG11	1.85	1.01
2:F:641:HIS:CD2	2:F:642:LEU:HG	1.95	1.01
2:F:1210:ARG:HH22	2:F:1341:GLU:CD	1.66	1.01
2:F:1224:ASN:CG	2:F:1280:VAL:HG11	1.85	1.01
1:A:59:U:OP1	2:B:467:ARG:NH2	1.93	1.01
2:B:525:THR:HG23	2:B:690:ASN:HD22	1.22	1.01
2:B:641:HIS:CD2	2:B:642:LEU:HG	1.95	1.01
2:F:342:GLN:HG3	2:F:383:MET:HE2	1.42	1.01
1:E:59:U:OP1	2:F:467:ARG:NH2	1.93	1.01
2:F:181:VAL:HG11	2:F:300:ILE:HD13	1.20	1.01
2:F:378:PRO:HG2	2:F:379:ILE:CD1	1.91	1.01
2:B:378:PRO:HG2	2:B:379:ILE:CD1	1.91	1.00
2:B:1239:ALA:HB1	2:B:1306:ALA:HB1	1.40	1.00
2:F:1239:ALA:HB1	2:F:1306:ALA:HB1	1.40	1.00
2:B:376:ILE:HD12	2:B:376:ILE:H	1.27	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:195:LEU:HD23	2:F:286:TYR:CE2	1.97	1.00
2:F:376:ILE:H	2:F:376:ILE:HD12	1.27	1.00
2:B:114:GLU:OE2	2:B:120:GLY:O	1.77	1.00
2:B:195:LEU:HD23	2:B:286:TYR:CE2	1.97	1.00
2:B:979:ASN:ND2	2:B:981:TYR:CD1	2.26	1.00
2:F:114:GLU:OE2	2:F:120:GLY:O	1.77	1.00
2:F:780:ARG:NH1	2:F:812:TYR:HD2	1.53	1.00
2:F:530:VAL:HG21	2:F:537:PRO:HB3	1.42	0.99
2:B:178:ASN:HB3	2:B:299:ALA:HB2	1.03	0.99
2:B:1305:GLN:HA	2:B:1327:PHE:CZ	1.97	0.99
2:F:178:ASN:HB3	2:F:299:ALA:HB2	1.03	0.99
2:F:528:LYS:HB2	2:F:581:SER:OG	1.63	0.99
2:F:1305:GLN:HA	2:F:1327:PHE:CZ	1.97	0.99
2:B:530:VAL:HG21	2:B:537:PRO:HB3	1.42	0.99
2:B:393:LEU:CD1	2:B:398:LEU:HD12	1.91	0.99
2:F:393:LEU:CD1	2:F:398:LEU:HD12	1.91	0.99
2:F:696:LEU:CD1	2:F:702:LEU:CD1	2.40	0.99
2:B:393:LEU:HD12	2:B:398:LEU:CD1	1.93	0.99
2:B:528:LYS:HB2	2:B:581:SER:OG	1.63	0.99
2:B:696:LEU:CD1	2:B:702:LEU:CD1	2.40	0.99
2:F:340:ARG:O	2:F:344:PRO:HG3	1.61	0.99
2:F:1305:GLN:HA	2:F:1327:PHE:HZ	1.26	0.99
2:B:340:ARG:O	2:B:344:PRO:HG3	1.61	0.99
2:F:1230:SER:HA	2:F:1233:VAL:HG23	1.45	0.99
2:B:249:THR:HG22	2:B:265:GLN:NE2	1.78	0.99
2:F:359:TYR:HE1	2:F:399:LEU:HD23	1.26	0.99
2:F:393:LEU:HD12	2:F:398:LEU:CD1	1.93	0.99
2:F:70:ARG:NH2	2:F:462:PHE:CD2	2.31	0.98
2:B:1230:SER:HA	2:B:1233:VAL:HG23	1.45	0.98
2:B:1305:GLN:HA	2:B:1327:PHE:HZ	1.26	0.98
2:B:70:ARG:NH2	2:B:462:PHE:CD2	2.31	0.98
2:F:945:GLU:OE1	2:F:945:GLU:N	1.94	0.98
2:B:945:GLU:N	2:B:945:GLU:OE1	1.94	0.98
2:B:849:ASP:HB3	2:B:854:ASN:HD22	1.29	0.98
2:F:342:GLN:HG3	2:F:383:MET:HE3	1.02	0.98
2:F:981:TYR:CE2	2:F:1092:VAL:HG12	1.92	0.98
2:F:849:ASP:HB3	2:F:854:ASN:HD22	1.29	0.98
2:B:277:ASN:HD22	2:B:653:ARG:HD3	1.27	0.98
2:B:780:ARG:NH1	2:B:812:TYR:HD2	1.53	0.98
2:F:704:PHE:O	2:F:708:ILE:CD1	2.12	0.98
2:B:704:PHE:O	2:B:708:ILE:CD1	2.12	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:342:GLN:CG	2:F:383:MET:HE3	1.74	0.98
2:F:181:VAL:HG21	2:F:209:LYS:CG	1.93	0.97
2:F:525:THR:HG22	2:F:690:ASN:HB3	1.43	0.97
2:F:1062:LEU:CD2	2:F:1063:ILE:HG13	1.93	0.97
2:B:1146:VAL:HG11	2:B:1194:LEU:HD12	0.98	0.97
2:F:195:LEU:HD21	2:F:286:TYR:CE2	1.99	0.97
2:B:311:GLU:OE1	2:B:311:GLU:N	1.97	0.97
2:F:311:GLU:OE1	2:F:311:GLU:N	1.97	0.97
2:F:1146:VAL:HG11	2:F:1194:LEU:HD12	0.98	0.97
2:B:195:LEU:HD21	2:B:286:TYR:CE2	1.99	0.97
2:B:207:ASP:HB3	2:B:210:ALA:HB3	0.98	0.97
2:F:207:ASP:HB3	2:F:210:ALA:HB3	0.98	0.97
2:F:277:ASN:HD22	2:F:653:ARG:HD3	1.26	0.97
2:F:1270:ILE:HD12	2:F:1294:TYR:HE2	1.25	0.97
2:B:181:VAL:HG21	2:B:209:LYS:CG	1.93	0.97
2:B:1000:LYS:HE3	2:B:1073:VAL:HG21	1.19	0.97
2:B:1062:LEU:CD2	2:B:1063:ILE:HG13	1.93	0.97
2:B:181:VAL:HG21	2:B:209:LYS:HG2	1.44	0.97
2:B:372:PHE:O	2:B:376:ILE:HD11	1.65	0.97
2:F:372:PHE:O	2:F:376:ILE:HD11	1.65	0.97
2:F:343:LEU:HD21	2:F:346:LYS:HB2	1.44	0.97
2:B:343:LEU:HD21	2:B:346:LYS:HB2	1.44	0.97
2:B:1143:VAL:HG11	2:B:1195:ILE:CG2	1.95	0.97
2:B:1270:ILE:HD12	2:B:1294:TYR:HE2	1.25	0.97
2:F:1143:VAL:HG11	2:F:1195:ILE:CG2	1.95	0.97
2:B:178:ASN:HB3	2:B:299:ALA:CA	1.95	0.96
2:B:279:LEU:HD11	2:B:287:ALA:HA	1.47	0.96
2:F:279:LEU:HD11	2:F:287:ALA:HA	1.47	0.96
2:B:686:ASP:OD2	2:B:691:ARG:N	1.96	0.96
2:F:178:ASN:HB3	2:F:299:ALA:CA	1.95	0.96
2:F:181:VAL:CG2	2:F:209:LYS:HG2	1.95	0.96
2:F:279:LEU:HD11	2:F:287:ALA:CA	1.95	0.96
2:F:181:VAL:HG21	2:F:209:LYS:HG2	1.43	0.96
2:F:181:VAL:HG12	2:F:300:ILE:CD1	1.94	0.96
2:F:279:LEU:HD11	2:F:287:ALA:CB	1.95	0.96
2:F:979:ASN:HD21	2:F:981:TYR:HD1	1.10	0.96
3:C:24:DG:H2''	3:C:25:DG:H5'	1.47	0.96
2:F:1326:TYR:HE2	2:F:1327:PHE:CE2	1.80	0.96
2:B:279:LEU:HD11	2:B:287:ALA:CA	1.95	0.96
2:F:340:ARG:O	2:F:344:PRO:CG	2.14	0.96
2:B:279:LEU:HD11	2:B:287:ALA:CB	1.95	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:340:ARG:O	2:B:344:PRO:CG	2.14	0.96
2:B:432:PHE:O	2:B:436:ASN:ND2	1.99	0.96
2:B:181:VAL:CG2	2:B:209:LYS:HG2	1.95	0.95
2:B:1326:TYR:HE2	2:B:1327:PHE:CE2	1.80	0.95
2:F:432:PHE:O	2:F:436:ASN:ND2	1.99	0.95
3:G:24:DG:H2''	3:G:25:DG:H5'	1.46	0.95
2:B:681:ASP:O	2:B:684:LYS:O	1.83	0.95
2:F:184:LEU:HD12	2:F:296:LEU:HA	1.47	0.95
2:F:359:TYR:CE1	2:F:399:LEU:HD23	2.01	0.95
2:F:681:ASP:O	2:F:684:LYS:O	1.83	0.95
2:F:1000:LYS:HE3	2:F:1073:VAL:HG21	1.18	0.95
2:B:181:VAL:HG12	2:B:300:ILE:CD1	1.93	0.95
2:B:278:LEU:HD11	2:B:282:ILE:CD1	1.96	0.95
2:B:1210:ARG:NH2	2:B:1341:GLU:CD	2.24	0.95
2:F:318:SER:OG	2:F:418:GLU:OE2	1.82	0.95
2:F:1210:ARG:NH2	2:F:1341:GLU:CD	2.24	0.95
2:B:184:LEU:HD12	2:B:296:LEU:HA	1.47	0.95
2:F:278:LEU:HD11	2:F:282:ILE:CD1	1.96	0.95
2:B:70:ARG:HH22	2:B:462:PHE:HB2	1.32	0.95
2:B:244:LEU:HG	2:B:266:LEU:CD1	1.96	0.95
2:B:870:VAL:CG2	2:B:908:LEU:HG	1.96	0.95
2:F:70:ARG:HH22	2:F:462:PHE:HB2	1.32	0.95
2:F:244:LEU:HG	2:F:266:LEU:CD1	1.96	0.95
3:G:23:DC:H2''	3:G:24:DG:H5'	1.44	0.95
2:F:870:VAL:CG2	2:F:908:LEU:HG	1.96	0.95
2:B:1148:LYS:HB3	2:B:1158:LYS:O	1.65	0.95
2:F:1148:LYS:HB3	2:F:1158:LYS:O	1.65	0.94
2:F:1313:PHE:O	2:F:1316:THR:OG1	1.85	0.94
2:B:1313:PHE:O	2:B:1316:THR:OG1	1.85	0.94
3:C:23:DC:H2''	3:C:24:DG:H5'	1.44	0.94
2:B:342:GLN:OE1	2:B:384:ASP:O	1.86	0.94
2:F:844:GLN:HE21	2:F:848:LYS:HG2	1.32	0.94
2:F:248:LEU:HD13	2:F:249:THR:H	1.29	0.94
2:F:784:ILE:HG22	2:F:788:ILE:HD11	1.50	0.94
2:B:1204:PHE:CE2	2:B:1214:LEU:HD12	2.03	0.94
2:F:696:LEU:HD13	2:F:702:LEU:CD1	1.97	0.94
2:F:1135:ASP:OD1	2:F:1136:SER:OG	1.85	0.94
1:A:89:G:N1	2:B:1272:GLN:OE1	2.01	0.94
2:B:784:ILE:HG22	2:B:788:ILE:HD11	1.50	0.94
2:B:844:GLN:HE21	2:B:848:LYS:HG2	1.32	0.94
2:B:1171:ARG:HG2	2:B:1171:ARG:HH11	1.33	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:G:N1	2:F:1272:GLN:OE1	2.01	0.94
2:F:318:SER:OG	2:F:418:GLU:CD	2.09	0.94
2:F:1204:PHE:CE2	2:F:1214:LEU:HD12	2.03	0.94
2:B:181:VAL:HG22	2:B:209:LYS:HG3	1.47	0.94
2:B:696:LEU:HD13	2:B:702:LEU:CD1	1.97	0.94
2:B:1135:ASP:OD1	2:B:1136:SER:OG	1.85	0.94
2:B:525:THR:HG22	2:B:690:ASN:HB3	1.49	0.94
2:F:275:LEU:O	2:F:279:LEU:N	2.01	0.94
2:F:1171:ARG:HG2	2:F:1171:ARG:HH11	1.33	0.94
2:B:275:LEU:O	2:B:279:LEU:N	2.01	0.93
2:F:703:THR:OG1	2:F:707:ASP:OD2	1.85	0.93
2:B:359:TYR:HE1	2:B:399:LEU:HD23	1.30	0.93
2:F:181:VAL:HG22	2:F:209:LYS:HG3	1.47	0.93
1:A:32:A:N6	1:A:37:U:O4	2.01	0.93
2:B:703:THR:OG1	2:B:707:ASP:OD2	1.85	0.93
2:F:1314:THR:HG21	2:F:1324:PHE:CB	1.98	0.93
2:B:1273:ILE:O	2:B:1277:SER:OG	1.85	0.93
1:E:32:A:N6	1:E:37:U:O4	2.01	0.93
2:B:1224:ASN:OD1	2:B:1280:VAL:HG11	1.68	0.93
2:B:1314:THR:HG21	2:B:1324:PHE:CB	1.98	0.93
2:F:806:LEU:CD2	2:F:811:LEU:HD12	1.97	0.93
1:A:57:A:H5'	2:B:457:ARG:NH2	1.83	0.93
2:B:806:LEU:CD2	2:B:811:LEU:HD12	1.97	0.93
2:F:1273:ILE:O	2:F:1277:SER:OG	1.85	0.93
1:E:57:A:H5'	2:F:457:ARG:NH2	1.83	0.93
2:F:1224:ASN:OD1	2:F:1280:VAL:HG11	1.69	0.93
2:B:1105:PHE:CD2	2:B:1169:MET:HG3	2.04	0.93
2:F:1105:PHE:CD2	2:F:1169:MET:HG3	2.04	0.93
2:F:1326:TYR:HE2	2:F:1327:PHE:HE2	0.98	0.92
1:A:63:U:H2'	2:B:62:THR:CG2	1.99	0.92
1:E:63:U:H2'	2:F:62:THR:CG2	1.99	0.92
1:A:24:U:O2	2:B:105:PHE:CD1	2.23	0.92
2:F:248:LEU:HD13	2:F:249:THR:N	1.84	0.92
2:B:1045:PHE:CZ	2:B:1046:PHE:CE2	2.57	0.92
2:F:1045:PHE:CZ	2:F:1046:PHE:CE2	2.57	0.92
2:B:299:ALA:O	2:B:302:LEU:CD2	2.18	0.92
2:B:181:VAL:HG21	2:B:209:LYS:HA	1.52	0.92
2:B:691:ARG:NH1	2:B:699:ASP:OD2	2.03	0.92
2:F:691:ARG:NH1	2:F:699:ASP:OD2	2.03	0.92
1:E:24:U:O2	2:F:105:PHE:CD1	2.23	0.91
2:F:181:VAL:HG21	2:F:209:LYS:HA	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:299:ALA:O	2:F:302:LEU:CD2	2.18	0.91
2:F:305:ILE:HD13	2:F:306:LEU:N	1.84	0.91
2:B:285:GLN:OE1	2:B:285:GLN:N	2.03	0.91
2:F:181:VAL:HG12	2:F:300:ILE:HD11	1.52	0.91
2:F:1260:GLU:HA	2:F:1263:LYS:HB2	1.51	0.91
2:F:195:LEU:HD23	2:F:286:TYR:HE2	1.29	0.91
2:F:285:GLN:OE1	2:F:285:GLN:N	2.03	0.91
2:B:195:LEU:CD2	2:B:286:TYR:HD2	1.81	0.91
2:B:195:LEU:HD23	2:B:286:TYR:HE2	1.29	0.91
2:B:305:ILE:HD13	2:B:306:LEU:N	1.84	0.91
2:F:209:LYS:O	2:F:213:SER:CB	2.19	0.91
2:F:970:PHE:HE1	2:F:1080:PHE:HZ	1.18	0.91
2:B:178:ASN:CA	2:B:299:ALA:HB2	2.01	0.91
2:B:1000:LYS:NZ	2:B:1064:GLU:HG3	1.85	0.91
2:B:1260:GLU:HA	2:B:1263:LYS:HB2	1.51	0.91
2:F:178:ASN:CA	2:F:299:ALA:HB2	2.01	0.91
2:B:209:LYS:O	2:B:213:SER:CB	2.19	0.91
2:B:1294:TYR:HE1	2:B:1305:GLN:HE22	1.14	0.91
2:B:181:VAL:HG12	2:B:300:ILE:HD11	1.52	0.91
2:B:569:PHE:O	2:B:574:CYS:N	2.04	0.91
2:B:665:LYS:O	2:B:669:GLY:HA3	1.68	0.91
2:B:1270:ILE:HD11	2:B:1294:TYR:CZ	2.06	0.91
3:G:23:DC:C2'	3:G:24:DG:H5'	2.01	0.91
2:B:849:ASP:OD1	2:B:851:SER:OG	1.88	0.90
1:E:63:U:C2'	2:F:62:THR:CG2	2.49	0.90
2:F:665:LYS:O	2:F:669:GLY:HA3	1.68	0.90
2:F:849:ASP:OD1	2:F:851:SER:OG	1.88	0.90
2:F:1000:LYS:NZ	2:F:1064:GLU:HG3	1.85	0.90
2:F:1230:SER:HA	2:F:1233:VAL:CG2	2.01	0.90
2:B:926:GLN:CA	2:B:929:LYS:HG3	2.02	0.90
2:B:970:PHE:HE1	2:B:1080:PHE:HZ	1.18	0.90
3:C:23:DC:C2'	3:C:24:DG:H5'	2.01	0.90
2:F:569:PHE:O	2:F:574:CYS:N	2.04	0.90
2:F:1270:ILE:HD11	2:F:1294:TYR:CZ	2.06	0.90
1:A:63:U:C2'	2:B:62:THR:CG2	2.49	0.90
2:F:305:ILE:HD13	2:F:306:LEU:H	1.36	0.90
2:B:557:ARG:HH11	2:B:557:ARG:HG3	1.34	0.90
2:F:342:GLN:HE22	2:F:384:ASP:HB2	1.37	0.90
2:B:1230:SER:HA	2:B:1233:VAL:CG2	2.01	0.90
2:F:926:GLN:CA	2:F:929:LYS:HG3	2.02	0.90
2:B:1000:LYS:CG	2:B:1073:VAL:HG21	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1294:TYR:HE1	2:F:1305:GLN:HE22	1.13	0.90
2:B:755:LYS:HD3	2:B:939:MET:CE	2.02	0.90
2:F:1000:LYS:CG	2:F:1073:VAL:HG21	2.02	0.90
2:F:1091:GLN:O	2:F:1091:GLN:NE2	2.05	0.90
2:B:305:ILE:HD13	2:B:306:LEU:H	1.35	0.89
2:B:1091:GLN:NE2	2:B:1091:GLN:O	2.05	0.89
2:B:1243:GLU:O	2:B:1244:LYS:NZ	2.05	0.89
1:E:63:U:C2'	2:F:62:THR:HG23	2.02	0.89
2:F:178:ASN:HD22	2:F:298:ASP:CB	1.86	0.89
2:F:195:LEU:CD2	2:F:286:TYR:HD2	1.81	0.89
2:F:755:LYS:HD3	2:F:939:MET:CE	2.02	0.89
2:F:1243:GLU:O	2:F:1244:LYS:NZ	2.05	0.89
2:B:1114:ARG:NH1	4:D:9:DA:OP1	2.04	0.89
2:B:1221:GLN:NE2	4:D:6:DG:OP2	2.05	0.89
2:B:1326:TYR:HE2	2:B:1327:PHE:HE2	0.98	0.89
2:B:178:ASN:HD22	2:B:298:ASP:CB	1.86	0.89
2:F:178:ASN:ND2	2:F:298:ASP:HB3	1.87	0.89
1:A:63:U:C2'	2:B:62:THR:HG23	2.02	0.89
2:B:143:VAL:HG11	2:B:315:ALA:HB2	1.55	0.89
2:F:557:ARG:HH11	2:F:557:ARG:HG3	1.34	0.89
2:F:914:ALA:HB1	2:F:1035:LYS:CD	2.02	0.89
2:F:1114:ARG:NH1	4:H:9:DA:OP1	2.04	0.89
2:F:143:VAL:HG11	2:F:315:ALA:HB2	1.55	0.89
2:F:249:THR:CG2	2:F:265:GLN:NE2	2.34	0.89
2:F:1221:GLN:NE2	4:H:6:DG:OP2	2.05	0.89
2:B:634:GLU:HA	2:B:637:LYS:HE2	1.55	0.89
2:B:914:ALA:HB1	2:B:1035:LYS:CD	2.03	0.89
2:F:634:GLU:HA	2:F:637:LYS:HE2	1.55	0.89
2:B:178:ASN:ND2	2:B:298:ASP:HB3	1.87	0.88
2:B:531:THR:HG22	2:B:534:MET:SD	2.13	0.88
2:F:531:THR:HG22	2:F:534:MET:SD	2.13	0.88
2:B:905:ARG:HG2	2:B:905:ARG:HH11	1.39	0.88
2:F:905:ARG:HG2	2:F:905:ARG:HH11	1.39	0.88
2:B:600:ILE:O	2:B:647:VAL:HG13	1.74	0.88
2:B:981:TYR:CE2	2:B:1092:VAL:HB	2.08	0.88
2:F:981:TYR:CE2	2:F:1092:VAL:HB	2.08	0.88
2:F:600:ILE:O	2:F:647:VAL:HG13	1.74	0.88
2:F:107:VAL:HG22	2:F:1131:TYR:CZ	2.08	0.88
2:B:244:LEU:HD12	2:B:250:PRO:CD	2.04	0.88
2:B:369:GLN:OE1	2:B:400:ARG:NH1	2.07	0.88
2:F:244:LEU:HD12	2:F:250:PRO:CD	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:ARG:NH1	2:B:162:ILE:O	2.06	0.87
2:B:107:VAL:HG22	2:B:1131:TYR:CZ	2.08	0.87
2:B:641:HIS:HD2	2:B:642:LEU:HG	1.30	0.87
1:E:24:U:O2	2:F:105:PHE:HD1	1.57	0.87
2:F:78:ARG:NH1	2:F:162:ILE:O	2.06	0.87
2:F:1000:LYS:HZ3	2:F:1045:PHE:HD2	0.90	0.87
2:B:1326:TYR:CD2	2:B:1327:PHE:CD2	2.63	0.87
2:F:1326:TYR:CD2	2:F:1327:PHE:CD2	2.63	0.87
2:B:665:LYS:CA	2:B:669:GLY:CA	2.41	0.87
2:B:974:LYS:NZ	2:B:976:ARG:NH1	2.23	0.87
2:F:324:ARG:CZ	2:F:400:ARG:NH1	2.27	0.87
2:B:1062:LEU:HD23	2:B:1063:ILE:H	1.36	0.87
1:A:24:U:C2	2:B:105:PHE:CE1	2.63	0.87
2:B:226:ILE:HD11	2:F:574:CYS:SG	2.15	0.87
2:B:557:ARG:NH2	2:B:599:LYS:HZ2	1.67	0.87
1:E:24:U:C2	2:F:105:PHE:CE1	2.63	0.87
2:F:641:HIS:HD2	2:F:642:LEU:HG	1.30	0.87
1:A:24:U:O2	2:B:105:PHE:HD1	1.56	0.87
2:B:544:GLN:O	2:B:548:ILE:HG13	1.74	0.87
2:F:665:LYS:CA	2:F:669:GLY:CA	2.40	0.87
2:B:372:PHE:O	2:B:376:ILE:CD1	2.22	0.86
2:F:220:ARG:HG3	2:F:220:ARG:HH11	1.40	0.86
2:B:220:ARG:HH11	2:B:220:ARG:HG3	1.40	0.86
2:F:372:PHE:O	2:F:376:ILE:CD1	2.22	0.86
2:F:699:ASP:OD1	2:F:701:SER:OG	1.93	0.86
2:B:699:ASP:OD1	2:B:701:SER:OG	1.93	0.86
2:B:974:LYS:HZ2	2:B:976:ARG:HH12	0.92	0.86
2:F:544:GLN:O	2:F:548:ILE:HG13	1.74	0.86
2:F:1062:LEU:HD23	2:F:1063:ILE:H	1.36	0.86
2:B:195:LEU:HD22	2:B:289:LEU:CD1	2.05	0.86
2:B:1357:GLU:OE1	2:B:1359:ARG:NH1	2.09	0.86
2:F:342:GLN:CD	2:F:383:MET:HE2	2.01	0.86
2:B:181:VAL:CG2	2:B:209:LYS:CB	2.53	0.86
2:B:1204:PHE:HE2	2:B:1214:LEU:HD12	1.37	0.86
2:F:1357:GLU:OE1	2:F:1359:ARG:NH1	2.09	0.86
2:B:525:THR:CG2	2:B:690:ASN:HD22	1.87	0.86
2:F:181:VAL:CG2	2:F:209:LYS:CB	2.53	0.86
2:F:195:LEU:HD22	2:F:289:LEU:CD1	2.05	0.86
2:F:679:ILE:HD11	2:F:704:PHE:CD1	2.11	0.86
2:F:1204:PHE:HE2	2:F:1214:LEU:HD12	1.37	0.86
2:B:70:ARG:O	2:B:74:ARG:HD2	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:679:ILE:HD11	2:B:704:PHE:CD1	2.11	0.86
2:B:909:SER:N	2:B:912:ASP:OD2	2.08	0.86
2:B:1314:THR:HG21	2:B:1324:PHE:HB3	1.58	0.86
2:F:1314:THR:HG21	2:F:1324:PHE:HB3	1.58	0.86
2:F:931:VAL:O	2:F:935:LEU:HD13	1.75	0.85
2:F:70:ARG:O	2:F:74:ARG:HD2	1.75	0.85
2:F:557:ARG:NH2	2:F:599:LYS:HZ2	1.67	0.85
2:F:909:SER:N	2:F:912:ASP:OD2	2.08	0.85
2:B:557:ARG:NH2	2:B:599:LYS:HZ3	1.64	0.85
2:B:981:TYR:CE2	2:B:1092:VAL:CB	2.59	0.85
2:F:981:TYR:CE2	2:F:1092:VAL:CB	2.59	0.85
2:B:1062:LEU:HD23	2:B:1063:ILE:N	1.90	0.85
2:F:121:ASN:HD21	2:F:124:ASP:CB	1.89	0.85
2:F:178:ASN:CB	2:F:299:ALA:CA	2.54	0.85
2:B:931:VAL:O	2:B:935:LEU:HD13	1.75	0.85
2:F:1062:LEU:HD23	2:F:1063:ILE:N	1.90	0.85
2:B:279:LEU:CD1	2:B:287:ALA:HB2	2.06	0.85
2:F:342:GLN:CG	2:F:383:MET:HE2	1.99	0.85
2:F:1290:VAL:HG22	2:F:1331:ILE:HD13	1.57	0.85
2:F:557:ARG:NH2	2:F:599:LYS:HZ3	1.64	0.85
2:B:121:ASN:HD21	2:B:124:ASP:CB	1.89	0.85
2:B:178:ASN:CB	2:B:299:ALA:CA	2.54	0.85
2:B:317:LEU:HD12	2:B:317:LEU:O	1.76	0.85
2:F:279:LEU:CD1	2:F:287:ALA:HB2	2.06	0.85
2:F:977:GLU:HG3	2:F:1310:ILE:CG2	2.06	0.85
2:B:671:ARG:HG3	2:B:678:THR:HG22	1.58	0.85
2:F:27:VAL:CG1	2:F:1086:VAL:HG13	2.06	0.85
2:F:318:SER:HG	2:F:418:GLU:CD	1.82	0.85
2:F:671:ARG:HG3	2:F:678:THR:HG22	1.58	0.85
2:F:806:LEU:HD22	2:F:811:LEU:CD1	2.07	0.85
2:B:1105:PHE:CG	2:B:1169:MET:HG3	2.11	0.84
2:B:1290:VAL:HG22	2:B:1331:ILE:HD13	1.57	0.84
2:F:317:LEU:HD12	2:F:317:LEU:O	1.76	0.84
2:F:1105:PHE:CG	2:F:1169:MET:HG3	2.11	0.84
2:B:181:VAL:HG23	2:B:209:LYS:CB	2.06	0.84
2:F:563:GLN:O	2:F:567:ASP:HB2	1.77	0.84
2:B:27:VAL:CG1	2:B:1086:VAL:HG13	2.06	0.84
2:B:806:LEU:HD22	2:B:811:LEU:CD1	2.07	0.84
1:E:17:G:OP2	2:F:74:ARG:NH1	2.10	0.84
2:F:297:SER:C	2:F:301:LEU:HD12	2.01	0.84
2:F:362:TYR:CE2	2:F:401:LYS:HE3	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:297:SER:C	2:B:301:LEU:HD12	2.01	0.84
2:B:563:GLN:O	2:B:567:ASP:HB2	1.77	0.84
2:B:672:ASP:HA	2:B:703:THR:HG21	1.59	0.84
2:F:1305:GLN:CA	2:F:1327:PHE:HZ	1.89	0.84
1:A:17:G:OP2	2:B:74:ARG:NH1	2.10	0.84
2:F:181:VAL:HG23	2:F:209:LYS:CB	2.06	0.84
2:F:181:VAL:HG23	2:F:209:LYS:CG	2.07	0.84
2:B:530:VAL:CG2	2:B:537:PRO:CB	2.46	0.84
2:B:1305:GLN:CA	2:B:1327:PHE:HZ	1.89	0.84
2:F:691:ARG:HB3	2:F:696:LEU:HD22	1.60	0.84
2:B:961:LYS:NZ	2:B:965:ASP:OD2	2.10	0.84
2:F:961:LYS:NZ	2:F:965:ASP:OD2	2.10	0.84
2:B:569:PHE:HD1	2:B:575:PHE:CD2	1.96	0.84
2:B:691:ARG:HB3	2:B:696:LEU:HD22	1.60	0.84
2:F:569:PHE:HD1	2:F:575:PHE:CD2	1.96	0.84
2:F:672:ASP:HA	2:F:703:THR:HG21	1.59	0.84
2:B:557:ARG:HH22	2:B:599:LYS:HZ3	0.86	0.83
2:B:810:LYS:O	2:B:833:LEU:HD13	1.76	0.83
2:B:181:VAL:HG23	2:B:209:LYS:CG	2.07	0.83
2:B:229:LEU:HD13	2:B:232:GLU:H	1.42	0.83
2:B:696:LEU:HD12	2:B:702:LEU:HD13	1.60	0.83
2:F:436:ASN:O	2:F:440:ILE:HD12	1.78	0.83
2:B:436:ASN:O	2:B:440:ILE:HD12	1.78	0.83
3:C:19:DA:H8	3:C:19:DA:H5"	1.42	0.83
2:F:1000:LYS:CD	2:F:1073:VAL:HG21	2.08	0.83
2:B:1302:ILE:O	2:B:1306:ALA:CB	2.27	0.83
2:F:557:ARG:HH22	2:F:599:LYS:HZ3	0.86	0.83
2:F:696:LEU:HD12	2:F:702:LEU:HD13	1.60	0.83
2:B:704:PHE:O	2:B:708:ILE:HD11	1.77	0.83
2:F:530:VAL:CG2	2:F:537:PRO:CB	2.46	0.83
2:F:810:LYS:O	2:F:833:LEU:HD13	1.76	0.83
2:B:1232:TYR:OH	2:B:1268:GLU:HG2	1.77	0.83
2:F:229:LEU:HD13	2:F:232:GLU:H	1.42	0.83
2:F:1302:ILE:O	2:F:1306:ALA:CB	2.27	0.83
2:B:359:TYR:CE1	2:B:399:LEU:HD23	2.12	0.83
2:B:1244:LYS:N	2:B:1244:LYS:HD3	1.94	0.83
2:F:297:SER:HG	2:F:301:LEU:HD11	1.39	0.83
2:F:979:ASN:ND2	2:F:981:TYR:HD1	1.69	0.83
2:F:1000:LYS:HE2	2:F:1073:VAL:HG22	1.59	0.83
2:B:870:VAL:HG12	2:B:871:PRO:CD	2.08	0.83
2:B:1000:LYS:CD	2:B:1073:VAL:HG21	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1203:LEU:CD1	2:F:1213:MET:HG3	2.08	0.83
2:F:1244:LYS:HD3	2:F:1244:LYS:N	1.94	0.83
3:G:19:DA:H5"	3:G:19:DA:H8	1.42	0.83
2:F:1000:LYS:HZ3	2:F:1064:GLU:HG3	1.42	0.83
2:B:1000:LYS:HE2	2:B:1073:VAL:HG22	1.59	0.83
2:B:1203:LEU:CD1	2:B:1213:MET:HG3	2.08	0.83
2:F:704:PHE:O	2:F:708:ILE:HD11	1.77	0.83
2:F:870:VAL:HG12	2:F:871:PRO:CD	2.08	0.82
2:B:395:ARG:O	2:B:396:GLU:HB2	1.79	0.82
2:F:209:LYS:O	2:F:213:SER:HB2	1.78	0.82
2:F:1230:SER:CA	2:F:1233:VAL:HG23	2.09	0.82
2:B:209:LYS:O	2:B:213:SER:HB2	1.78	0.82
2:B:1143:VAL:CG1	2:B:1195:ILE:HG23	2.09	0.82
2:F:121:ASN:ND2	2:F:124:ASP:HB2	1.93	0.82
2:F:1143:VAL:CG1	2:F:1195:ILE:HG23	2.09	0.82
2:B:1230:SER:CA	2:B:1233:VAL:HG23	2.09	0.82
2:F:324:ARG:HH21	2:F:400:ARG:NH1	1.72	0.82
2:F:395:ARG:O	2:F:396:GLU:HB2	1.79	0.82
2:B:121:ASN:ND2	2:B:124:ASP:HB2	1.93	0.82
2:B:569:PHE:HD1	2:B:575:PHE:HD2	1.26	0.82
2:F:70:ARG:HH21	2:F:462:PHE:HD2	1.26	0.82
2:F:672:ASP:CG	2:F:703:THR:HG22	2.02	0.82
2:B:733:ILE:O	2:B:737:ILE:HG13	1.80	0.82
2:B:1062:LEU:HD21	2:B:1063:ILE:HG13	1.61	0.82
2:F:569:PHE:HD1	2:F:575:PHE:HD2	1.26	0.82
2:F:733:ILE:O	2:F:737:ILE:HG13	1.80	0.82
2:B:672:ASP:CG	2:B:703:THR:HG22	2.02	0.82
2:B:181:VAL:HG13	2:B:300:ILE:HD13	1.61	0.82
2:F:1062:LEU:HD21	2:F:1063:ILE:HG13	1.61	0.82
2:B:181:VAL:HG11	2:B:300:ILE:HD11	0.83	0.82
2:B:279:LEU:HD11	2:B:287:ALA:HB2	1.62	0.82
2:F:279:LEU:HD11	2:F:287:ALA:HB2	1.62	0.82
2:B:679:ILE:HG12	2:B:704:PHE:CE1	2.14	0.81
2:F:181:VAL:HG11	2:F:300:ILE:HD11	0.83	0.81
2:F:679:ILE:HG12	2:F:704:PHE:CE1	2.14	0.81
2:B:70:ARG:HH21	2:B:462:PHE:HD2	1.26	0.81
2:B:241:LEU:HD21	2:B:290:PHE:HE2	1.45	0.81
2:B:244:LEU:HG	2:B:266:LEU:HD12	1.62	0.81
2:B:398:LEU:O	2:B:399:LEU:HD12	1.80	0.81
2:B:508:LEU:HD12	2:B:663:SER:C	2.04	0.81
2:B:1107:LYS:NZ	3:C:7:DC:O2	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1243:GLU:C	2:B:1244:LYS:HD3	2.04	0.81
2:B:1314:THR:CG2	2:B:1324:PHE:CG	2.62	0.81
2:F:241:LEU:HD21	2:F:290:PHE:HE2	1.45	0.81
2:F:1314:THR:CG2	2:F:1324:PHE:CG	2.62	0.81
2:F:181:VAL:HG13	2:F:300:ILE:HD13	1.61	0.81
2:F:244:LEU:HG	2:F:266:LEU:HD12	1.62	0.81
2:B:101:LEU:O	2:B:104:SER:OG	1.97	0.81
2:B:926:GLN:HA	2:B:929:LYS:CG	2.06	0.81
2:B:1127:ASP:HB3	2:B:1130:LYS:HB2	1.62	0.81
2:F:398:LEU:O	2:F:399:LEU:HD12	1.80	0.81
2:F:508:LEU:HD12	2:F:663:SER:C	2.04	0.81
2:F:1107:LYS:NZ	3:G:7:DC:O2	2.13	0.81
2:F:101:LEU:O	2:F:104:SER:OG	1.97	0.81
2:F:1243:GLU:C	2:F:1244:LYS:HD3	2.04	0.81
1:A:62:G:C8	2:B:69:ARG:NH1	2.49	0.81
2:B:277:ASN:ND2	2:B:653:ARG:HD3	1.94	0.81
2:F:99:HIS:O	2:F:103:GLU:HG2	1.80	0.81
2:F:277:ASN:ND2	2:F:653:ARG:HD3	1.94	0.81
4:H:6:DG:H2''	4:H:7:DG:H5'	1.61	0.81
2:B:955:VAL:O	2:B:1009:VAL:HG13	1.81	0.81
2:F:926:GLN:HA	2:F:929:LYS:CG	2.06	0.81
2:B:513:LEU:HD11	2:B:616:LEU:CB	2.10	0.81
2:B:852:ILE:HG13	5:B:1401:SO4:O1	1.81	0.81
4:D:6:DG:H2''	4:D:7:DG:H5'	1.61	0.81
1:E:62:G:C8	2:F:69:ARG:NH1	2.49	0.81
2:F:324:ARG:NH2	2:F:400:ARG:HH12	1.77	0.81
2:F:955:VAL:O	2:F:1009:VAL:HG13	1.81	0.81
2:B:99:HIS:O	2:B:103:GLU:HG2	1.80	0.80
2:B:745:ASP:OD2	2:B:938:ARG:NH2	2.14	0.80
2:F:107:VAL:CG2	2:F:1131:TYR:OH	2.28	0.80
2:F:745:ASP:OD2	2:F:938:ARG:NH2	2.14	0.80
2:B:1251:ASP:HA	2:B:1254:GLN:OE1	1.81	0.80
2:F:513:LEU:HD11	2:F:616:LEU:CB	2.10	0.80
2:B:249:THR:CG2	2:B:265:GLN:NE2	2.44	0.80
2:B:974:LYS:HZ2	2:B:976:ARG:NH1	1.77	0.80
2:F:342:GLN:OE1	2:F:383:MET:HE2	1.79	0.80
2:B:107:VAL:CG2	2:B:1131:TYR:OH	2.28	0.80
2:F:1045:PHE:CZ	2:F:1046:PHE:HE2	1.95	0.80
2:B:207:ASP:O	2:B:211:ILE:N	2.14	0.80
2:B:665:LYS:O	2:B:669:GLY:N	2.13	0.80
2:B:842:VAL:HG12	2:B:854:ASN:OD1	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1312:LEU:HD11	2:B:1326:TYR:CD1	2.16	0.80
2:B:970:PHE:HE1	2:B:1080:PHE:CZ	2.00	0.80
2:B:1302:ILE:O	2:B:1306:ALA:N	2.15	0.80
2:F:528:LYS:HB2	2:F:581:SER:HG	1.47	0.80
2:F:665:LYS:O	2:F:669:GLY:N	2.13	0.80
2:F:842:VAL:HG12	2:F:854:ASN:OD1	1.82	0.80
2:F:1251:ASP:HA	2:F:1254:GLN:OE1	1.81	0.80
2:B:1045:PHE:CZ	2:B:1046:PHE:HE2	1.95	0.80
2:B:1207:GLU:OE2	2:B:1210:ARG:HD3	1.82	0.80
2:F:637:LYS:HA	2:F:640:ALA:HB2	1.63	0.80
2:F:970:PHE:HE1	2:F:1080:PHE:CZ	2.00	0.80
2:F:1207:GLU:OE2	2:F:1210:ARG:HD3	1.82	0.80
2:F:979:ASN:OD1	2:F:980:ASN:N	2.15	0.80
2:F:1206:LEU:C	2:F:1207:GLU:HG3	2.07	0.80
2:F:1302:ILE:O	2:F:1306:ALA:N	2.15	0.80
2:B:1206:LEU:C	2:B:1207:GLU:HG3	2.06	0.80
2:F:207:ASP:O	2:F:211:ILE:N	2.14	0.80
2:F:518:PHE:CD1	2:F:667:ILE:HG23	2.17	0.80
2:F:1312:LEU:HD11	2:F:1326:TYR:CD1	2.16	0.80
2:B:637:LYS:HA	2:B:640:ALA:HB2	1.63	0.80
2:F:1236:LEU:HD22	2:F:1310:ILE:HG13	1.64	0.80
1:A:59:U:OP2	2:B:472:THR:HG23	1.81	0.79
2:B:518:PHE:CD1	2:B:667:ILE:HG23	2.17	0.79
2:B:788:ILE:O	2:B:792:GLY:N	2.15	0.79
2:B:1179:ILE:O	2:B:1183:GLU:HG3	1.82	0.79
2:B:1236:LEU:HD22	2:B:1310:ILE:HG13	1.64	0.79
2:F:1179:ILE:O	2:F:1183:GLU:HG3	1.82	0.79
2:B:1062:LEU:O	2:B:1076:LYS:CG	2.27	0.79
2:B:1224:ASN:CG	2:B:1280:VAL:CG1	2.55	0.79
2:F:89:GLU:O	2:F:93:VAL:HG23	1.81	0.79
2:F:343:LEU:CD2	2:F:346:LYS:HB2	2.12	0.79
2:F:788:ILE:O	2:F:792:GLY:N	2.15	0.79
2:B:343:LEU:CD2	2:B:346:LYS:HB2	2.12	0.79
1:E:59:U:OP2	2:F:472:THR:HG23	1.81	0.79
1:A:56:U:O2	1:A:58:G:N2	2.15	0.79
2:B:89:GLU:O	2:B:93:VAL:HG23	1.81	0.79
2:B:100:ARG:NE	2:B:117:PRO:O	2.16	0.79
2:F:539:PHE:CE1	2:F:690:ASN:HB2	2.17	0.79
2:F:874:GLU:O	2:F:877:LYS:HG3	1.82	0.79
2:F:1062:LEU:O	2:F:1076:LYS:CG	2.27	0.79
1:E:56:U:O2	1:E:58:G:N2	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1224:ASN:CG	2:F:1280:VAL:CG1	2.55	0.79
1:E:19:A:O2'	2:F:405:PHE:O	2.00	0.79
2:F:100:ARG:NE	2:F:117:PRO:O	2.16	0.79
1:A:19:A:O2'	2:B:405:PHE:O	2.00	0.79
2:B:874:GLU:O	2:B:877:LYS:HG3	1.82	0.79
2:B:1303:ARG:O	2:B:1307:GLU:HG3	1.82	0.79
1:E:52:A:H1'	2:F:1169:MET:HE3	1.65	0.78
2:B:1086:VAL:O	2:B:1089:MET:HE2	1.82	0.78
2:B:1242:TYR:HD1	2:B:1242:TYR:H	1.32	0.78
2:F:340:ARG:C	2:F:344:PRO:HG3	2.08	0.78
2:F:1251:ASP:CA	2:F:1254:GLN:NE2	2.39	0.78
2:B:665:LYS:C	2:B:669:GLY:CA	2.52	0.78
2:B:1045:PHE:CE1	2:B:1046:PHE:CE2	2.71	0.78
2:F:321:MET:HA	2:F:321:MET:HE3	1.65	0.78
1:A:52:A:H1'	2:B:1169:MET:HE3	1.65	0.78
2:B:340:ARG:C	2:B:344:PRO:HG3	2.08	0.78
2:B:512:SER:OG	2:B:617:GLU:OE1	2.02	0.78
2:B:1000:LYS:HZ1	2:B:1064:GLU:HG3	1.49	0.78
2:F:1045:PHE:CE1	2:F:1046:PHE:CE2	2.71	0.78
2:F:1242:TYR:HD1	2:F:1242:TYR:H	1.32	0.78
2:F:1303:ARG:O	2:F:1307:GLU:HG3	1.82	0.78
1:A:41:A:H2'	1:A:42:A:H5''	1.65	0.78
2:B:45:LYS:HE3	2:B:1093:ASN:OD1	1.83	0.78
2:B:1326:TYR:HD2	2:B:1327:PHE:HD2	1.31	0.78
2:F:512:SER:OG	2:F:617:GLU:OE1	2.02	0.78
1:E:41:A:H2'	1:E:42:A:H5''	1.65	0.78
2:F:8:GLY:O	2:F:987:ALA:HB1	1.83	0.78
2:F:114:GLU:HG2	2:F:120:GLY:HA2	1.63	0.78
2:F:249:THR:HG22	2:F:265:GLN:HB2	1.66	0.78
2:F:1143:VAL:HG13	2:F:1195:ILE:HG22	1.65	0.78
2:B:870:VAL:HG12	2:B:871:PRO:HD2	1.66	0.78
2:F:1326:TYR:HD2	2:F:1327:PHE:HD2	1.31	0.78
1:A:24:U:H1'	2:B:105:PHE:CE1	2.18	0.78
2:B:219:SER:O	2:B:222:LEU:HG	1.84	0.78
2:B:1041:ASN:HB3	2:B:1044:ASN:OD1	1.82	0.78
2:B:1143:VAL:HG13	2:B:1195:ILE:HG22	1.65	0.78
1:E:24:U:H1'	2:F:105:PHE:CE1	2.18	0.78
2:F:219:SER:O	2:F:222:LEU:HG	1.84	0.78
2:F:1086:VAL:O	2:F:1089:MET:HE2	1.82	0.78
2:B:8:GLY:O	2:B:987:ALA:HB1	1.83	0.78
2:B:212:LEU:HD21	2:B:225:LEU:HD12	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:45:LYS:HE3	2:F:1093:ASN:OD1	1.83	0.78
2:F:362:TYR:CE1	2:F:372:PHE:CD2	2.72	0.78
2:B:278:LEU:CD1	2:B:282:ILE:CD1	2.59	0.78
2:F:870:VAL:HG12	2:F:871:PRO:HD2	1.66	0.78
2:F:1041:ASN:HB3	2:F:1044:ASN:OD1	1.82	0.78
2:F:777:SER:HG	4:H:2:DT:HO5'	1.25	0.77
2:B:114:GLU:HG2	2:B:120:GLY:HA2	1.63	0.77
2:B:1256:GLN:NE2	2:B:1260:GLU:OE2	2.17	0.77
2:B:914:ALA:CB	2:B:1035:LYS:HD3	2.13	0.77
2:B:1000:LYS:HE2	2:B:1064:GLU:HB3	1.64	0.77
2:F:212:LEU:HD21	2:F:225:LEU:HD12	1.65	0.77
2:F:1000:LYS:HE2	2:F:1064:GLU:HB3	1.65	0.77
2:F:278:LEU:CD1	2:F:282:ILE:CD1	2.59	0.77
2:F:1256:GLN:NE2	2:F:1260:GLU:OE2	2.17	0.77
2:F:362:TYR:HD1	2:F:372:PHE:CG	2.03	0.77
2:F:914:ALA:CB	2:F:1035:LYS:HD3	2.13	0.77
2:B:847:LEU:HD21	2:B:849:ASP:HB2	1.66	0.77
2:F:78:ARG:NE	2:F:165:ARG:HH11	1.83	0.77
2:F:321:MET:HA	2:F:321:MET:CE	2.15	0.77
2:F:842:VAL:HG12	2:F:854:ASN:CG	2.10	0.77
2:F:847:LEU:HD21	2:F:849:ASP:HB2	1.66	0.77
2:F:1143:VAL:CG1	2:F:1195:ILE:HG22	2.13	0.77
2:B:279:LEU:CD1	2:B:287:ALA:CB	2.61	0.77
2:B:1287:LEU:HD12	2:B:1287:LEU:O	1.84	0.77
2:F:165:ARG:HH21	2:F:168:PHE:HZ	1.29	0.77
2:F:178:ASN:CB	2:F:299:ALA:CB	2.41	0.77
2:F:812:TYR:CE1	2:F:816:LEU:HD21	2.19	0.77
2:B:78:ARG:NE	2:B:165:ARG:HH11	1.83	0.77
2:B:842:VAL:HG12	2:B:854:ASN:CG	2.10	0.77
2:B:977:GLU:HG3	2:B:1310:ILE:CG2	2.14	0.77
2:B:1272:GLN:C	2:B:1272:GLN:HE21	1.93	0.77
2:F:1272:GLN:HE21	2:F:1272:GLN:C	1.93	0.77
2:B:114:GLU:HG2	2:B:120:GLY:CA	2.15	0.77
2:F:1287:LEU:HD12	2:F:1287:LEU:O	1.84	0.77
2:B:45:LYS:CE	2:B:1093:ASN:OD1	2.33	0.77
2:B:545:LYS:HZ2	2:B:690:ASN:ND2	1.83	0.77
2:F:114:GLU:HG2	2:F:120:GLY:CA	2.15	0.77
2:B:812:TYR:CE1	2:B:816:LEU:HD21	2.19	0.76
2:F:279:LEU:CD1	2:F:287:ALA:CB	2.61	0.76
2:F:45:LYS:CE	2:F:1093:ASN:OD1	2.33	0.76
2:F:98:PHE:O	2:F:102:GLU:HG3	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1303:ARG:O	2:F:1307:GLU:CG	2.34	0.76
2:B:1206:LEU:O	2:B:1207:GLU:HG3	1.84	0.76
2:B:1303:ARG:O	2:B:1307:GLU:CG	2.34	0.76
2:F:621:LEU:O	2:F:625:LEU:HB2	1.85	0.76
2:F:1206:LEU:O	2:F:1207:GLU:HG3	1.84	0.76
2:F:1290:VAL:HG22	2:F:1331:ILE:CD1	2.15	0.76
2:B:178:ASN:CB	2:B:299:ALA:CB	2.41	0.76
2:B:483:ASP:OD1	2:B:486:ALA:HB3	1.86	0.76
2:B:842:VAL:CG1	2:B:854:ASN:HD21	1.99	0.76
2:B:1143:VAL:CG1	2:B:1195:ILE:HG22	2.13	0.76
2:B:1290:VAL:HG22	2:B:1331:ILE:CD1	2.15	0.76
2:F:483:ASP:OD1	2:F:486:ALA:HB3	1.86	0.76
2:F:842:VAL:CG1	2:F:854:ASN:HD21	1.99	0.76
2:B:106:LEU:O	2:B:111:LYS:HE3	1.84	0.76
2:F:106:LEU:O	2:F:111:LYS:HE3	1.84	0.76
2:B:98:PHE:O	2:B:102:GLU:HG3	1.85	0.76
2:B:275:LEU:CD1	2:B:279:LEU:HB2	2.16	0.76
2:B:621:LEU:O	2:B:625:LEU:HB2	1.85	0.76
2:F:275:LEU:CD1	2:F:279:LEU:HB2	2.16	0.76
2:B:165:ARG:HH21	2:B:168:PHE:HZ	1.29	0.76
2:F:386:THR:O	2:F:389:LEU:HB2	1.86	0.76
2:B:839:ASP:OD1	2:B:864:ARG:NH1	2.18	0.76
2:B:970:PHE:CE1	2:B:1080:PHE:CZ	2.73	0.76
2:F:970:PHE:CE1	2:F:1080:PHE:CZ	2.73	0.76
2:B:181:VAL:HG23	2:B:209:LYS:HB2	1.68	0.76
1:E:15:U:H2'	1:E:16:U:H6	1.50	0.76
2:F:839:ASP:OD1	2:F:864:ARG:NH1	2.18	0.76
2:F:181:VAL:HG23	2:F:209:LYS:HB2	1.67	0.75
2:F:784:ILE:CG2	2:F:788:ILE:HD11	2.16	0.75
2:F:818:ASN:O	2:F:818:ASN:ND2	2.19	0.75
2:F:1082:THR:O	2:F:1086:VAL:HG23	1.85	0.75
2:B:818:ASN:ND2	2:B:818:ASN:O	2.19	0.75
2:B:970:PHE:CE1	2:B:1080:PHE:HZ	2.04	0.75
2:B:1274:SER:O	2:B:1278:LYS:HG3	1.84	0.75
1:E:24:U:C2	2:F:105:PHE:HE1	2.01	0.75
2:F:307:ARG:NH1	2:F:323:LYS:NZ	2.34	0.75
2:F:518:PHE:HD1	2:F:667:ILE:HG23	1.51	0.75
2:F:1274:SER:O	2:F:1278:LYS:HG3	1.84	0.75
1:A:15:U:H2'	1:A:16:U:H6	1.50	0.75
1:A:24:U:C2	2:B:105:PHE:CD1	2.75	0.75
2:B:518:PHE:HD1	2:B:667:ILE:HG23	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:784:ILE:CG2	2:B:788:ILE:HD11	2.16	0.75
2:B:1082:THR:O	2:B:1086:VAL:HG23	1.85	0.75
1:E:24:U:C2	2:F:105:PHE:CD1	2.75	0.75
2:F:234:LYS:HD3	2:F:235:ASN:ND2	2.02	0.75
2:F:341:GLN:HG3	2:F:342:GLN:HG2	1.69	0.75
2:F:970:PHE:CE1	2:F:1080:PHE:HZ	2.04	0.75
2:F:1246:LYS:HZ2	2:F:1246:LYS:HB2	1.52	0.75
2:B:178:ASN:HD22	2:B:298:ASP:HB3	1.46	0.75
2:B:234:LYS:HD3	2:B:235:ASN:ND2	2.02	0.75
2:B:341:GLN:HG3	2:B:342:GLN:HG2	1.69	0.75
2:F:398:LEU:HD22	2:F:399:LEU:HD13	1.67	0.75
2:B:1314:THR:HG21	2:B:1324:PHE:CG	2.22	0.74
2:F:1105:PHE:CD2	2:F:1169:MET:CG	2.70	0.74
2:F:1314:THR:HG21	2:F:1324:PHE:CG	2.22	0.74
1:A:24:U:C2	2:B:105:PHE:HE1	2.01	0.74
2:B:299:ALA:O	2:B:302:LEU:HD22	1.84	0.74
2:B:398:LEU:HD22	2:B:399:LEU:HD13	1.67	0.74
2:B:679:ILE:HD11	2:B:704:PHE:CE1	2.22	0.74
2:B:810:LYS:C	2:B:833:LEU:HD12	2.11	0.74
2:F:178:ASN:HD22	2:F:298:ASP:HB3	1.46	0.74
2:F:299:ALA:O	2:F:302:LEU:HD22	1.84	0.74
2:F:981:TYR:CD2	2:F:1092:VAL:HG11	2.22	0.74
2:B:114:GLU:CG	2:B:120:GLY:HA2	2.17	0.74
2:B:981:TYR:CD2	2:B:1092:VAL:HG11	2.22	0.74
2:F:100:ARG:NH2	2:F:117:PRO:O	2.19	0.74
2:B:1105:PHE:CD2	2:B:1169:MET:CG	2.70	0.74
2:F:810:LYS:C	2:F:833:LEU:HD12	2.11	0.74
2:F:679:ILE:HD11	2:F:704:PHE:CE1	2.22	0.74
2:B:100:ARG:NH2	2:B:117:PRO:O	2.19	0.74
2:F:78:ARG:NE	2:F:165:ARG:NH1	2.35	0.74
2:B:234:LYS:HB2	2:F:572:ILE:O	1.87	0.74
2:B:297:SER:HG	2:B:301:LEU:CD1	1.97	0.74
2:B:939:MET:HE2	2:B:953:VAL:HG21	1.70	0.74
2:B:967:ARG:NH1	2:B:974:LYS:HB2	2.01	0.74
2:F:963:VAL:HG21	2:F:990:ASN:ND2	2.02	0.74
2:B:78:ARG:NE	2:B:165:ARG:NH1	2.35	0.74
2:B:940:ASN:OD1	2:B:951:ARG:HA	1.88	0.74
2:F:114:GLU:CG	2:F:120:GLY:HA2	2.17	0.74
2:F:940:ASN:OD1	2:F:951:ARG:HA	1.88	0.74
2:F:967:ARG:NH1	2:F:974:LYS:HB2	2.01	0.74
2:B:244:LEU:CD1	2:B:250:PRO:CD	2.66	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:19:DA:H5''	3:C:19:DA:C8	2.22	0.74
2:F:696:LEU:HD12	2:F:702:LEU:CD1	2.15	0.74
2:F:874:GLU:HA	2:F:877:LYS:HD2	1.68	0.74
2:F:939:MET:HE2	2:F:953:VAL:HG21	1.70	0.74
2:B:963:VAL:HG21	2:B:990:ASN:ND2	2.02	0.73
2:F:244:LEU:CD1	2:F:250:PRO:CD	2.66	0.73
2:B:618:ASP:OD2	2:B:639:TYR:OH	2.03	0.73
2:B:979:ASN:OD1	2:B:981:TYR:HD1	1.72	0.73
2:F:842:VAL:HG12	2:F:854:ASN:ND2	2.03	0.73
2:B:285:GLN:H	2:B:285:GLN:CD	1.97	0.73
2:B:830:ILE:N	2:B:830:ILE:HD12	2.04	0.73
2:B:842:VAL:HG12	2:B:854:ASN:ND2	2.03	0.73
2:F:278:LEU:HD12	2:F:278:LEU:O	1.88	0.73
2:F:285:GLN:H	2:F:285:GLN:CD	1.97	0.73
2:F:830:ILE:HD12	2:F:830:ILE:N	2.03	0.73
3:G:19:DA:H5''	3:G:19:DA:C8	2.22	0.73
2:B:340:ARG:NH2	2:B:347:TYR:CE1	2.57	0.73
2:F:618:ASP:OD2	2:F:639:TYR:OH	2.03	0.73
2:F:1304:GLU:HB3	2:F:1327:PHE:HE1	1.52	0.73
2:B:278:LEU:HD12	2:B:278:LEU:O	1.88	0.73
2:B:545:LYS:NZ	2:B:690:ASN:HD21	1.86	0.73
2:B:961:LYS:HG2	2:B:965:ASP:OD2	1.88	0.73
2:B:1221:GLN:NE2	2:B:1320:ALA:HB2	2.03	0.73
2:F:340:ARG:NH2	2:F:347:TYR:CE1	2.57	0.73
2:F:755:LYS:HD3	2:F:939:MET:HE1	1.71	0.73
2:F:1221:GLN:NE2	2:F:1320:ALA:HB2	2.03	0.73
2:B:27:VAL:HG12	2:B:1086:VAL:HG13	1.70	0.73
2:B:696:LEU:HD12	2:B:702:LEU:CD1	2.15	0.73
2:B:780:ARG:HD2	2:B:812:TYR:CE2	2.23	0.73
2:B:874:GLU:HA	2:B:877:LYS:HD2	1.68	0.73
1:E:45:U:H5'	2:F:402:GLN:HG2	1.68	0.73
2:F:27:VAL:HG12	2:F:1086:VAL:HG13	1.70	0.73
2:F:244:LEU:HG	2:F:266:LEU:HD11	1.70	0.73
2:B:244:LEU:HG	2:B:266:LEU:HD11	1.70	0.73
2:B:545:LYS:NZ	2:B:690:ASN:ND2	2.36	0.73
2:B:686:ASP:OD2	2:B:691:ARG:HB2	1.88	0.73
2:B:755:LYS:HD3	2:B:939:MET:HE1	1.71	0.73
2:F:178:ASN:HB3	2:F:299:ALA:N	2.04	0.73
2:F:362:TYR:CE1	2:F:372:PHE:HD2	2.07	0.73
2:F:780:ARG:HD2	2:F:812:TYR:CE2	2.23	0.73
2:B:178:ASN:HB3	2:B:299:ALA:N	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:ASN:C	2:B:299:ALA:CB	2.61	0.73
2:B:870:VAL:CG2	2:B:908:LEU:CG	2.67	0.73
2:F:979:ASN:OD1	2:F:981:TYR:N	2.20	0.73
1:A:45:U:H5'	2:B:402:GLN:HG2	1.68	0.73
2:F:870:VAL:CG2	2:F:908:LEU:CG	2.67	0.73
2:B:34:VAL:HG21	2:B:43:ILE:HG13	1.71	0.73
2:B:27:VAL:HG11	2:B:1086:VAL:HG13	1.70	0.72
2:B:1304:GLU:HB3	2:B:1327:PHE:HE1	1.52	0.72
1:E:63:U:H2'	2:F:62:THR:HG22	1.69	0.72
2:F:178:ASN:C	2:F:299:ALA:CB	2.61	0.72
2:F:284:ASP:N	2:F:285:GLN:OE1	2.22	0.72
2:F:302:LEU:HD23	2:F:303:SER:N	2.03	0.72
2:F:961:LYS:HG2	2:F:965:ASP:OD2	1.88	0.72
2:B:284:ASP:N	2:B:285:GLN:OE1	2.22	0.72
2:F:34:VAL:HG21	2:F:43:ILE:HG13	1.71	0.72
2:F:1246:LYS:HB2	2:F:1246:LYS:NZ	2.04	0.72
2:B:22:THR:HG22	2:B:23:ASP:H	1.54	0.72
2:B:241:LEU:HD21	2:B:290:PHE:CE2	2.24	0.72
2:B:1246:LYS:HB2	2:B:1246:LYS:NZ	2.04	0.72
2:F:841:ILE:HD13	2:F:900:LEU:HD23	1.71	0.72
2:F:963:VAL:HG21	2:F:990:ASN:CG	2.15	0.72
2:F:1243:GLU:C	2:F:1244:LYS:HZ2	1.94	0.72
1:A:63:U:H2'	2:B:62:THR:HG22	1.69	0.72
2:B:106:LEU:HD23	2:B:110:ASP:CG	2.14	0.72
2:B:302:LEU:HD23	2:B:303:SER:N	2.03	0.72
2:B:963:VAL:HG21	2:B:990:ASN:CG	2.15	0.72
2:B:841:ILE:HD13	2:B:900:LEU:HD23	1.71	0.72
2:B:1135:ASP:OD1	2:B:1136:SER:N	2.22	0.72
2:B:1171:ARG:HG2	2:B:1171:ARG:NH1	2.01	0.72
2:B:1203:LEU:HD12	2:B:1213:MET:HG3	1.71	0.72
2:F:241:LEU:HD21	2:F:290:PHE:CE2	2.24	0.72
2:F:273:ASP:OD1	2:F:274:ASP:N	2.22	0.72
2:F:635:ARG:HG3	2:F:635:ARG:NH1	2.04	0.72
2:B:273:ASP:OD1	2:B:274:ASP:N	2.22	0.72
2:B:449:PRO:HD2	2:B:452:VAL:HG21	1.71	0.72
2:B:1243:GLU:C	2:B:1244:LYS:HZ2	1.94	0.72
2:F:755:LYS:HD3	2:F:939:MET:HE3	1.69	0.72
2:F:1135:ASP:OD1	2:F:1136:SER:N	2.22	0.72
2:B:244:LEU:HD12	2:B:250:PRO:HD3	1.71	0.72
2:B:297:SER:O	2:B:301:LEU:HD12	1.88	0.72
2:B:324:ARG:HD3	2:B:400:ARG:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:70:ARG:NH1	2:F:454:PRO:HG3	2.04	0.72
2:F:249:THR:HG23	2:F:265:GLN:NE2	2.04	0.72
2:F:1203:LEU:HD12	2:F:1213:MET:HG3	1.71	0.72
2:B:70:ARG:NH1	2:B:454:PRO:HG3	2.04	0.72
2:B:178:ASN:HD21	2:B:298:ASP:HB2	1.51	0.72
2:B:216:LEU:HD23	2:B:216:LEU:N	2.03	0.72
2:B:275:LEU:HD12	2:B:275:LEU:C	2.15	0.72
2:B:635:ARG:HG3	2:B:635:ARG:NH1	2.04	0.72
2:B:1224:ASN:OD1	2:B:1280:VAL:CG1	2.37	0.72
2:F:27:VAL:HG11	2:F:1086:VAL:HG13	1.70	0.72
2:F:275:LEU:HD12	2:F:275:LEU:C	2.15	0.72
2:F:297:SER:O	2:F:301:LEU:HD12	1.88	0.72
2:F:449:PRO:HD2	2:F:452:VAL:HG21	1.71	0.72
2:F:1171:ARG:HG2	2:F:1171:ARG:NH1	2.01	0.72
2:F:216:LEU:N	2:F:216:LEU:HD23	2.03	0.72
2:F:844:GLN:NE2	2:F:848:LYS:HG2	2.04	0.72
2:B:746:GLU:O	2:B:750:VAL:HG23	1.90	0.72
2:B:1000:LYS:HZ3	2:B:1045:PHE:HD2	0.74	0.72
2:F:178:ASN:HB2	2:F:299:ALA:HA	1.72	0.72
2:F:178:ASN:HD21	2:F:298:ASP:HB2	1.51	0.72
2:F:746:GLU:O	2:F:750:VAL:HG23	1.90	0.72
2:B:178:ASN:HD21	2:B:298:ASP:CB	2.00	0.71
2:B:178:ASN:HB2	2:B:299:ALA:HA	1.72	0.71
2:B:379:ILE:HD12	2:B:379:ILE:H	1.55	0.71
2:B:844:GLN:NE2	2:B:848:LYS:HG2	2.04	0.71
2:B:1060:ARG:HH12	2:B:1064:GLU:CD	1.98	0.71
2:F:1060:ARG:HH12	2:F:1064:GLU:CD	1.98	0.71
2:F:1224:ASN:OD1	2:F:1280:VAL:CG1	2.37	0.71
2:B:181:VAL:HG21	2:B:209:LYS:CA	2.20	0.71
2:B:393:LEU:HD23	2:B:393:LEU:C	2.14	0.71
2:B:755:LYS:HD3	2:B:939:MET:HE3	1.69	0.71
2:B:1127:ASP:O	2:B:1131:TYR:N	2.22	0.71
2:F:181:VAL:HG21	2:F:209:LYS:CA	2.20	0.71
2:F:283:GLY:C	2:F:285:GLN:OE1	2.33	0.71
2:F:373:TYR:HA	2:F:376:ILE:HD11	1.71	0.71
2:F:393:LEU:C	2:F:393:LEU:HD23	2.14	0.71
2:B:278:LEU:HD12	2:B:278:LEU:C	2.16	0.71
2:B:283:GLY:C	2:B:285:GLN:OE1	2.33	0.71
2:B:317:LEU:HD12	2:B:317:LEU:C	2.16	0.71
2:F:244:LEU:HD12	2:F:250:PRO:HD3	1.71	0.71
2:F:317:LEU:HD12	2:F:317:LEU:C	2.16	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:513:LEU:HD11	2:F:616:LEU:HB3	1.71	0.71
2:F:557:ARG:HH12	2:F:599:LYS:NZ	1.88	0.71
2:B:373:TYR:HA	2:B:376:ILE:HD11	1.71	0.71
2:B:981:TYR:CE1	2:B:1092:VAL:HG12	2.24	0.71
2:B:70:ARG:HH22	2:B:462:PHE:CB	2.04	0.71
2:B:557:ARG:HH12	2:B:599:LYS:NZ	1.89	0.71
2:B:974:LYS:HD3	2:B:976:ARG:NH1	2.05	0.71
2:F:70:ARG:HH22	2:F:462:PHE:CB	2.04	0.71
2:F:379:ILE:HD12	2:F:379:ILE:H	1.54	0.71
2:F:407:ASN:H	2:F:407:ASN:ND2	1.86	0.71
2:B:513:LEU:HD11	2:B:616:LEU:HB3	1.71	0.71
1:E:45:U:H5"	2:F:402:GLN:HB2	1.72	0.71
2:F:278:LEU:HD12	2:F:278:LEU:C	2.16	0.71
2:B:841:ILE:HD13	2:B:900:LEU:CD2	2.20	0.71
2:B:1308:ASN:O	2:B:1311:HIS:HB2	1.89	0.71
2:F:340:ARG:O	2:F:344:PRO:HG2	1.91	0.71
2:F:981:TYR:CE1	2:F:1092:VAL:HG12	2.24	0.71
1:A:24:U:N1	2:B:105:PHE:HE1	1.88	0.71
1:A:45:U:H5"	2:B:402:GLN:HB2	1.72	0.71
2:B:407:ASN:ND2	2:B:407:ASN:H	1.86	0.71
2:B:780:ARG:HD3	5:B:1401:SO4:O3	1.90	0.71
1:E:24:U:N1	2:F:105:PHE:HE1	1.88	0.71
2:F:178:ASN:HD21	2:F:298:ASP:CB	2.00	0.71
2:F:1031:LYS:H	2:F:1031:LYS:HD2	1.56	0.71
2:F:1127:ASP:O	2:F:1131:TYR:N	2.22	0.71
2:F:1308:ASN:O	2:F:1311:HIS:HB2	1.89	0.71
2:F:1326:TYR:CD2	2:F:1327:PHE:HD2	2.06	0.71
2:B:209:LYS:O	2:B:213:SER:HB3	1.89	0.71
2:B:340:ARG:O	2:B:344:PRO:HG2	1.91	0.71
2:B:967:ARG:HA	2:B:972:PHE:HB2	1.73	0.71
2:B:978:ILE:HG12	2:B:1313:PHE:CE2	2.25	0.71
2:B:1246:LYS:HB2	2:B:1246:LYS:HZ2	1.56	0.71
2:F:981:TYR:CE2	2:F:1092:VAL:HG11	2.24	0.71
2:B:379:ILE:HD12	2:B:379:ILE:N	2.05	0.71
2:B:489:GLN:HG3	2:B:625:LEU:HD21	1.73	0.71
2:F:870:VAL:HG21	2:F:908:LEU:CD2	2.21	0.70
2:F:967:ARG:HA	2:F:972:PHE:HB2	1.73	0.70
2:B:870:VAL:HG21	2:B:908:LEU:CD2	2.21	0.70
2:F:209:LYS:O	2:F:213:SER:HB3	1.89	0.70
2:F:1252:ASN:N	2:F:1252:ASN:HD22	1.89	0.70
2:B:1000:LYS:HZ1	2:B:1064:GLU:CB	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1252:ASN:HD22	2:B:1252:ASN:N	1.89	0.70
1:E:61:C:OP1	2:F:70:ARG:NH2	2.24	0.70
2:F:181:VAL:HG23	2:F:209:LYS:HG3	1.67	0.70
2:F:379:ILE:HD12	2:F:379:ILE:N	2.05	0.70
2:F:489:GLN:HG3	2:F:625:LEU:HD21	1.73	0.70
2:F:841:ILE:HD13	2:F:900:LEU:CD2	2.20	0.70
2:B:195:LEU:HD22	2:B:289:LEU:HD13	1.73	0.70
2:F:178:ASN:O	2:F:299:ALA:HB2	1.87	0.70
2:F:302:LEU:HD23	2:F:302:LEU:C	2.16	0.70
2:F:350:ILE:HG22	2:F:351:PHE:CD2	2.26	0.70
2:F:810:LYS:C	2:F:833:LEU:CD1	2.63	0.70
2:F:1060:ARG:NH1	2:F:1064:GLU:CD	2.48	0.70
1:A:61:C:OP1	2:B:70:ARG:NH2	2.24	0.70
2:B:181:VAL:HG23	2:B:209:LYS:HG3	1.67	0.70
2:B:296:LEU:HD23	2:B:296:LEU:C	2.15	0.70
2:B:350:ILE:HG22	2:B:351:PHE:CD2	2.26	0.70
2:B:1000:LYS:HZ3	2:B:1064:GLU:HG3	1.56	0.70
2:F:249:THR:CG2	2:F:265:GLN:HE21	2.04	0.70
2:F:265:GLN:HB3	2:F:268:LYS:HB2	1.73	0.70
2:F:342:GLN:CB	2:F:383:MET:HE3	2.21	0.70
2:B:302:LEU:HD23	2:B:302:LEU:C	2.16	0.70
2:F:1143:VAL:HG13	2:F:1195:ILE:CG2	2.17	0.70
2:F:195:LEU:HD22	2:F:289:LEU:HD13	1.73	0.70
2:F:1344:ASP:OD2	2:F:1344:ASP:N	2.24	0.70
2:B:265:GLN:HB3	2:B:268:LYS:HB2	1.73	0.70
2:B:794:GLN:H	2:B:794:GLN:CD	2.00	0.70
2:B:842:VAL:CG1	2:B:854:ASN:ND2	2.54	0.70
2:B:1000:LYS:HZ1	2:B:1064:GLU:CG	2.05	0.70
2:F:296:LEU:HD23	2:F:296:LEU:C	2.15	0.70
2:F:780:ARG:HH12	2:F:812:TYR:HD2	1.37	0.70
2:F:842:VAL:CG1	2:F:854:ASN:ND2	2.54	0.70
2:B:178:ASN:O	2:B:299:ALA:HB2	1.87	0.70
2:B:1243:GLU:HA	2:B:1243:GLU:OE1	1.92	0.70
2:B:1326:TYR:CD2	2:B:1327:PHE:HD2	2.06	0.70
2:B:1344:ASP:OD2	2:B:1344:ASP:N	2.25	0.70
2:F:1230:SER:C	2:F:1233:VAL:HG23	2.17	0.70
2:F:1243:GLU:OE1	2:F:1243:GLU:HA	1.92	0.70
2:B:679:ILE:CG1	2:B:704:PHE:CE1	2.75	0.70
2:B:810:LYS:C	2:B:833:LEU:CD1	2.64	0.70
2:B:1060:ARG:NH1	2:B:1064:GLU:CD	2.48	0.70
2:B:1230:SER:C	2:B:1233:VAL:HG23	2.17	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1256:GLN:NE2	2:B:1260:GLU:CD	2.49	0.70
2:B:1315:LEU:HD12	2:B:1315:LEU:O	1.92	0.70
2:F:794:GLN:CD	2:F:794:GLN:H	2.00	0.70
2:B:679:ILE:CD1	2:B:704:PHE:CE1	2.75	0.69
2:B:1232:TYR:OH	2:B:1268:GLU:CG	2.40	0.69
2:F:317:LEU:HB2	2:F:414:ILE:HD12	1.73	0.69
2:F:679:ILE:CD1	2:F:704:PHE:CE1	2.75	0.69
2:F:1302:ILE:O	2:F:1306:ALA:HB3	1.91	0.69
2:F:1315:LEU:HD12	2:F:1315:LEU:O	1.92	0.69
2:B:317:LEU:HB2	2:B:414:ILE:HD12	1.73	0.69
2:B:780:ARG:HH12	2:B:812:TYR:HD2	1.37	0.69
2:F:167:HIS:ND1	2:F:411:PRO:HA	2.07	0.69
2:B:148:LYS:HE3	2:B:429:PHE:HB3	1.72	0.69
2:B:181:VAL:HG22	2:B:209:LYS:CG	2.05	0.69
2:B:275:LEU:HD12	2:B:275:LEU:O	1.92	0.69
2:B:1302:ILE:O	2:B:1306:ALA:HB3	1.91	0.69
2:F:557:ARG:CZ	2:F:599:LYS:NZ	2.55	0.69
2:F:679:ILE:CG1	2:F:704:PHE:CE1	2.75	0.69
2:F:979:ASN:ND2	2:F:981:TYR:CG	2.60	0.69
2:B:167:HIS:ND1	2:B:411:PRO:HA	2.07	0.69
2:B:444:LEU:O	2:B:444:LEU:HD23	1.92	0.69
2:B:557:ARG:CZ	2:B:599:LYS:NZ	2.55	0.69
2:B:1219:GLU:HG3	2:B:1336:TYR:O	1.91	0.69
2:F:1256:GLN:NE2	2:F:1260:GLU:CD	2.49	0.69
2:B:539:PHE:CD1	2:B:690:ASN:HB2	2.28	0.69
2:B:696:LEU:HD13	2:B:702:LEU:HD12	1.74	0.69
2:F:275:LEU:HD12	2:F:275:LEU:O	1.92	0.69
2:F:784:ILE:O	2:F:788:ILE:HG12	1.93	0.69
2:B:343:LEU:O	2:B:343:LEU:HD23	1.93	0.69
2:B:696:LEU:HD13	2:B:702:LEU:HD11	1.75	0.69
2:B:1143:VAL:HG13	2:B:1195:ILE:CG2	2.17	0.69
2:F:343:LEU:HD23	2:F:343:LEU:O	1.93	0.69
1:A:35:A:H2'	1:A:36:A:C8	2.28	0.69
2:B:208:ALA:O	2:B:212:LEU:HB2	1.92	0.69
2:B:784:ILE:O	2:B:788:ILE:HG12	1.93	0.69
2:B:940:ASN:HD22	2:B:940:ASN:N	1.90	0.69
2:B:1204:PHE:CE1	2:B:1347:LEU:HG	2.28	0.69
1:E:35:A:H2'	1:E:36:A:C8	2.28	0.69
2:F:148:LYS:HE3	2:F:429:PHE:HB3	1.72	0.69
2:F:208:ALA:O	2:F:212:LEU:HB2	1.92	0.69
2:F:359:TYR:CE1	2:F:399:LEU:CD2	2.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:444:LEU:HD23	2:F:444:LEU:O	1.92	0.69
2:F:696:LEU:HD13	2:F:702:LEU:HD11	1.75	0.69
2:F:696:LEU:HD13	2:F:702:LEU:HD12	1.74	0.69
2:F:730:SER:O	2:F:733:ILE:HG22	1.93	0.69
2:F:1219:GLU:HG3	2:F:1336:TYR:O	1.91	0.69
2:B:507:VAL:HG11	2:B:660:GLY:O	1.93	0.69
2:B:117:PRO:HD2	2:B:125:GLU:OE2	1.93	0.69
2:B:373:TYR:CE1	2:B:398:LEU:HB3	2.28	0.69
2:B:730:SER:O	2:B:733:ILE:HG22	1.93	0.69
2:F:117:PRO:HD2	2:F:125:GLU:OE2	1.93	0.69
2:B:223:GLU:OE1	2:F:574:CYS:HB3	1.92	0.68
2:F:373:TYR:CE1	2:F:398:LEU:HB3	2.28	0.68
2:F:507:VAL:HG11	2:F:660:GLY:O	1.93	0.68
2:F:940:ASN:N	2:F:940:ASN:HD22	1.91	0.68
2:F:1204:PHE:CE1	2:F:1347:LEU:HG	2.28	0.68
2:B:500:LYS:O	2:B:712:GLN:NE2	2.27	0.68
2:F:324:ARG:NH1	2:F:400:ARG:HD2	2.08	0.68
2:F:806:LEU:CD2	2:F:811:LEU:CD1	2.69	0.68
2:B:51:LEU:HD13	2:B:1352:ILE:HG13	1.75	0.68
2:B:806:LEU:CD2	2:B:811:LEU:CD1	2.69	0.68
2:F:51:LEU:HD13	2:F:1352:ILE:HG13	1.75	0.68
2:F:500:LYS:O	2:F:712:GLN:NE2	2.27	0.68
2:F:106:LEU:HD23	2:F:110:ASP:HB3	1.75	0.68
2:F:107:VAL:HG23	2:F:110:ASP:HB2	1.75	0.68
2:B:1257:LEU:H	2:B:1257:LEU:HD12	1.58	0.68
2:F:699:ASP:HB3	2:F:702:LEU:HB2	1.75	0.68
2:B:376:ILE:HD12	2:B:376:ILE:N	2.03	0.68
2:B:1272:GLN:O	2:B:1272:GLN:NE2	2.26	0.68
2:F:1257:LEU:H	2:F:1257:LEU:HD12	1.59	0.68
2:B:699:ASP:HB3	2:B:702:LEU:HB2	1.75	0.68
2:F:433:LEU:O	2:F:437:ARG:N	2.27	0.68
2:F:1272:GLN:NE2	2:F:1272:GLN:O	2.26	0.68
2:B:433:LEU:O	2:B:437:ARG:N	2.27	0.68
2:B:483:ASP:OD1	2:B:486:ALA:CB	2.42	0.68
2:B:1326:TYR:CE2	2:B:1327:PHE:CD2	2.81	0.68
2:F:1236:LEU:HD22	2:F:1310:ILE:CG1	2.23	0.68
2:F:1326:TYR:CE2	2:F:1327:PHE:CD2	2.81	0.68
2:B:687:GLY:HA3	2:B:688:PHE:C	2.17	0.68
2:F:181:VAL:HG22	2:F:209:LYS:CG	2.05	0.68
2:B:513:LEU:HD11	2:B:616:LEU:HB2	1.75	0.67
2:B:1260:GLU:HA	2:B:1263:LYS:CB	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:376:ILE:HD12	2:F:376:ILE:N	2.03	0.67
2:F:483:ASP:OD1	2:F:486:ALA:CB	2.41	0.67
2:F:817:GLN:OE1	2:F:856:VAL:HG13	1.94	0.67
2:F:1260:GLU:HA	2:F:1263:LYS:CB	2.24	0.67
2:B:845:SER:O	2:B:920:GLN:NE2	2.27	0.67
2:B:1236:LEU:HD22	2:B:1310:ILE:CG1	2.23	0.67
2:F:569:PHE:CD1	2:F:575:PHE:CD2	2.81	0.67
2:B:1045:PHE:H	2:B:1045:PHE:HD1	1.41	0.67
2:F:1062:LEU:CG	2:F:1063:ILE:HG13	2.23	0.67
2:B:817:GLN:OE1	2:B:856:VAL:HG13	1.94	0.67
2:B:901:THR:O	2:B:904:GLU:HG2	1.95	0.67
2:B:1062:LEU:CG	2:B:1063:ILE:HG13	2.24	0.67
2:F:362:TYR:HE2	2:F:401:LYS:HE3	1.58	0.67
2:F:901:THR:O	2:F:904:GLU:HG2	1.95	0.67
2:F:979:ASN:CG	2:F:981:TYR:H	2.01	0.67
2:F:1045:PHE:HD1	2:F:1045:PHE:H	1.41	0.67
2:B:143:VAL:HG22	2:B:421:ALA:HB3	1.77	0.67
2:B:569:PHE:CD1	2:B:575:PHE:CD2	2.81	0.67
2:F:513:LEU:HD11	2:F:616:LEU:HB2	1.75	0.67
2:F:845:SER:O	2:F:920:GLN:NE2	2.27	0.67
2:B:212:LEU:HD12	2:B:246:LEU:HD11	1.75	0.67
2:B:530:VAL:HG22	2:B:537:PRO:CA	2.25	0.67
2:F:442:LYS:HE2	2:F:476:TRP:HA	1.75	0.67
2:B:1000:LYS:NZ	2:B:1045:PHE:CE2	2.51	0.67
2:F:143:VAL:HG22	2:F:421:ALA:HB3	1.77	0.67
2:F:530:VAL:HG22	2:F:537:PRO:CA	2.25	0.67
2:B:247:GLY:O	2:B:248:LEU:HD22	1.95	0.67
2:B:350:ILE:HG22	2:B:351:PHE:CE2	2.30	0.67
2:B:442:LYS:HE2	2:B:476:TRP:HA	1.75	0.67
2:F:279:LEU:HD13	2:F:287:ALA:HB2	1.76	0.67
2:F:350:ILE:HG22	2:F:351:PHE:CE2	2.30	0.67
2:B:93:VAL:HG21	2:B:151:LEU:HD23	1.76	0.67
2:B:918:LYS:HG3	2:B:1039:TYR:CE2	2.30	0.67
2:B:279:LEU:HD13	2:B:287:ALA:HB2	1.76	0.66
2:F:495:MET:O	3:G:17:DA:H2"	1.94	0.66
2:F:552:LEU:O	2:F:556:ASN:ND2	2.28	0.66
2:F:1063:ILE:HG23	2:F:1074:TRP:O	1.94	0.66
2:B:141:LYS:HG2	2:B:142:LEU:HD23	1.77	0.66
2:B:539:PHE:CE1	2:B:690:ASN:HB2	2.31	0.66
2:B:552:LEU:O	2:B:556:ASN:ND2	2.28	0.66
2:F:141:LYS:HG2	2:F:142:LEU:HD23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:635:ARG:HG3	2:F:635:ARG:HH11	1.60	0.66
2:F:665:LYS:C	2:F:669:GLY:CA	2.52	0.66
2:F:918:LYS:HG3	2:F:1039:TYR:CE2	2.30	0.66
2:B:58:THR:HG22	2:B:731:PRO:CG	2.17	0.66
2:B:256:PHE:CD2	2:B:282:ILE:HD13	2.30	0.66
2:B:495:MET:O	3:C:17:DA:H2''	1.94	0.66
2:B:557:ARG:NH1	2:B:599:LYS:NZ	2.43	0.66
2:B:1045:PHE:CE1	2:B:1046:PHE:HE2	2.12	0.66
2:B:1063:ILE:HG23	2:B:1074:TRP:O	1.94	0.66
2:B:1312:LEU:HD11	2:B:1326:TYR:CE1	2.31	0.66
2:F:256:PHE:CD2	2:F:282:ILE:HD13	2.31	0.66
2:F:1000:LYS:HG3	2:F:1073:VAL:HG21	1.77	0.66
2:F:1325:LYS:HB2	2:F:1329:THR:O	1.95	0.66
2:B:178:ASN:C	2:B:299:ALA:HB2	2.20	0.66
2:B:1062:LEU:CA	2:B:1076:LYS:HD2	2.22	0.66
2:B:1281:ILE:HG21	2:B:1315:LEU:HD11	1.77	0.66
2:F:317:LEU:HD23	2:F:414:ILE:HG13	1.77	0.66
2:F:318:SER:OG	2:F:418:GLU:OE1	2.14	0.66
2:F:362:TYR:CD2	2:F:401:LYS:HE3	2.31	0.66
2:F:407:ASN:H	2:F:407:ASN:HD22	1.44	0.66
2:F:557:ARG:NH1	2:F:599:LYS:NZ	2.43	0.66
2:F:1062:LEU:CA	2:F:1076:LYS:HD2	2.22	0.66
2:F:1281:ILE:HG21	2:F:1315:LEU:HD11	1.77	0.66
2:B:635:ARG:HG3	2:B:635:ARG:HH11	1.61	0.66
2:B:1325:LYS:HB2	2:B:1329:THR:O	1.95	0.66
2:F:93:VAL:HG21	2:F:151:LEU:HD23	1.76	0.66
2:F:307:ARG:HH11	2:F:323:LYS:NZ	1.93	0.66
2:F:692:ASN:HB3	2:F:695:GLN:HG3	1.76	0.66
2:F:1045:PHE:CE1	2:F:1046:PHE:HE2	2.12	0.66
2:B:407:ASN:H	2:B:407:ASN:HD22	1.44	0.66
2:B:1044:ASN:O	2:B:1047:LYS:HG3	1.95	0.66
2:F:178:ASN:C	2:F:299:ALA:HB2	2.20	0.66
2:F:830:ILE:CD1	2:F:831:ASN:H	2.09	0.66
2:B:229:LEU:CD1	2:B:232:GLU:H	2.09	0.66
2:B:317:LEU:HD23	2:B:414:ILE:HG13	1.77	0.66
2:B:386:THR:O	2:B:389:LEU:HB2	1.95	0.66
2:F:229:LEU:CD1	2:F:232:GLU:H	2.09	0.66
2:F:844:GLN:HE21	2:F:848:LYS:CG	2.08	0.66
2:F:873:GLU:HG2	2:F:874:GLU:N	2.09	0.66
2:F:1122:ARG:HD3	2:F:1134:PHE:CE2	2.31	0.66
2:F:1239:ALA:HB1	2:F:1306:ALA:CB	2.21	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1248:SER:O	2:F:1252:ASN:ND2	2.29	0.66
2:F:1307:GLU:O	2:F:1310:ILE:HB	1.95	0.66
2:B:830:ILE:CD1	2:B:831:ASN:H	2.09	0.66
2:B:1000:LYS:NZ	2:B:1064:GLU:CG	2.58	0.66
2:B:1122:ARG:HD3	2:B:1134:PHE:CE2	2.31	0.66
2:B:1248:SER:O	2:B:1252:ASN:ND2	2.29	0.66
2:B:1307:GLU:O	2:B:1310:ILE:HB	1.95	0.66
2:F:1000:LYS:NZ	2:F:1064:GLU:CG	2.58	0.66
2:F:1312:LEU:HD11	2:F:1326:TYR:CE1	2.31	0.66
2:B:902:LYS:O	2:B:905:ARG:N	2.27	0.66
2:F:58:THR:HG22	2:F:731:PRO:CG	2.17	0.66
2:F:291:LEU:HD23	2:F:291:LEU:C	2.21	0.66
2:F:944:ASP:OD1	2:F:946:ASN:O	2.13	0.66
2:F:945:GLU:CD	2:F:946:ASN:H	2.04	0.66
2:F:981:TYR:CD2	2:F:1092:VAL:CG1	2.78	0.66
2:F:1044:ASN:O	2:F:1047:LYS:HG3	1.95	0.66
1:A:78:A:H2'	1:A:79:G:H8	1.60	0.66
2:B:692:ASN:HB3	2:B:695:GLN:HG3	1.76	0.66
2:B:873:GLU:HG2	2:B:874:GLU:N	2.09	0.66
2:B:981:TYR:CD2	2:B:1092:VAL:CG1	2.78	0.66
2:B:107:VAL:HG22	2:B:1131:TYR:CE1	2.31	0.65
2:B:844:GLN:HE21	2:B:848:LYS:CG	2.08	0.65
2:B:944:ASP:OD1	2:B:946:ASN:O	2.13	0.65
2:B:945:GLU:CD	2:B:946:ASN:H	2.04	0.65
2:B:979:ASN:CG	2:B:981:TYR:HD1	2.04	0.65
2:F:107:VAL:HG22	2:F:1131:TYR:CE1	2.31	0.65
2:F:821:ASP:OD1	2:F:858:THR:OG1	2.13	0.65
2:B:291:LEU:HD23	2:B:291:LEU:C	2.21	0.65
2:F:252:PHE:CZ	2:F:264:LEU:HD13	2.31	0.65
2:F:275:LEU:HD11	2:F:279:LEU:CG	2.26	0.65
2:F:307:ARG:HH11	2:F:323:LYS:HZ3	1.43	0.65
2:F:1230:SER:O	2:F:1233:VAL:HG23	1.96	0.65
1:A:59:U:OP1	2:B:473:ILE:HG13	1.96	0.65
2:B:1230:SER:O	2:B:1233:VAL:HG23	1.96	0.65
2:B:1239:ALA:HB1	2:B:1306:ALA:CB	2.21	0.65
2:F:665:LYS:HA	2:F:669:GLY:HA2	1.76	0.65
2:F:902:LYS:O	2:F:905:ARG:N	2.27	0.65
1:A:57:A:H5'	2:B:457:ARG:HH21	1.60	0.65
2:B:275:LEU:HD11	2:B:279:LEU:CG	2.26	0.65
2:B:870:VAL:HG21	2:B:908:LEU:HD21	1.78	0.65
2:B:958:LEU:HD22	2:B:962:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1257:LEU:HD12	2:B:1257:LEU:N	2.11	0.65
1:E:78:A:H2'	1:E:79:G:H8	1.60	0.65
2:F:275:LEU:O	2:F:279:LEU:HB2	1.96	0.65
2:B:821:ASP:OD1	2:B:858:THR:OG1	2.13	0.65
1:E:15:U:H2'	1:E:16:U:C6	2.31	0.65
2:F:958:LEU:HD22	2:F:962:LEU:HD12	1.78	0.65
2:F:1257:LEU:H	2:F:1257:LEU:CD1	2.10	0.65
1:A:15:U:H2'	1:A:16:U:C6	2.31	0.65
2:B:100:ARG:CZ	2:B:117:PRO:O	2.45	0.65
2:B:252:PHE:CZ	2:B:264:LEU:HD13	2.32	0.65
2:B:1257:LEU:H	2:B:1257:LEU:CD1	2.10	0.65
1:E:59:U:OP1	2:F:473:ILE:HG13	1.97	0.65
2:F:870:VAL:HG21	2:F:908:LEU:HD21	1.78	0.65
2:B:970:PHE:HD1	2:B:1080:PHE:CE1	2.15	0.65
3:C:24:DG:H2''	3:C:25:DG:C5'	2.26	0.65
1:E:57:A:H5'	2:F:457:ARG:HH21	1.60	0.65
2:B:665:LYS:HA	2:B:669:GLY:HA2	1.76	0.65
2:B:1256:GLN:HE22	2:B:1260:GLU:CD	2.05	0.65
2:F:100:ARG:CZ	2:F:117:PRO:O	2.45	0.65
2:F:569:PHE:CD1	2:F:575:PHE:HD2	2.13	0.65
2:F:970:PHE:HD1	2:F:1080:PHE:CE1	2.15	0.65
2:F:970:PHE:CD1	2:F:1080:PHE:CE1	2.84	0.65
2:F:1062:LEU:HA	2:F:1076:LYS:CD	2.21	0.65
2:B:275:LEU:O	2:B:279:LEU:HB2	1.96	0.65
2:B:569:PHE:CD1	2:B:575:PHE:HD2	2.13	0.65
2:B:1220:LEU:HD11	2:B:1339:THR:HA	1.79	0.65
2:B:1251:ASP:CA	2:B:1254:GLN:NE2	2.39	0.65
2:F:1257:LEU:HD12	2:F:1257:LEU:N	2.11	0.65
3:G:19:DA:H2''	3:G:20:DA:O4'	1.97	0.65
3:G:24:DG:H2''	3:G:25:DG:C5'	2.26	0.65
2:B:970:PHE:CD1	2:B:1080:PHE:CE1	2.84	0.65
2:F:615:ILE:O	2:F:619:ILE:N	2.28	0.65
2:F:1220:LEU:HD11	2:F:1339:THR:HA	1.79	0.65
2:F:1256:GLN:HE22	2:F:1260:GLU:CD	2.05	0.65
2:B:615:ILE:O	2:B:619:ILE:N	2.28	0.64
2:B:672:ASP:OD2	2:B:675:SER:OG	2.13	0.64
2:B:1062:LEU:HA	2:B:1076:LYS:CD	2.21	0.64
2:B:1143:VAL:HG11	2:B:1195:ILE:HG21	1.79	0.64
3:C:19:DA:H2''	3:C:20:DA:O4'	1.97	0.64
2:F:121:ASN:OD1	2:F:124:ASP:N	2.25	0.64
2:F:696:LEU:CD1	2:F:702:LEU:HD11	2.24	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:737:ILE:HG23	2:F:931:VAL:HG13	1.79	0.64
2:F:1143:VAL:HG11	2:F:1195:ILE:HG21	1.79	0.64
2:B:264:LEU:HD11	2:B:278:LEU:HD23	1.79	0.64
2:B:627:GLU:OE1	2:B:627:GLU:N	2.30	0.64
2:B:737:ILE:HG23	2:B:931:VAL:HG13	1.79	0.64
2:B:1045:PHE:CE1	2:B:1046:PHE:CD2	2.85	0.64
2:F:398:LEU:HD22	2:F:399:LEU:CD1	2.27	0.64
2:F:539:PHE:CD1	2:F:690:ASN:HB2	2.32	0.64
2:F:672:ASP:OD2	2:F:675:SER:OG	2.13	0.64
2:F:1045:PHE:CE1	2:F:1046:PHE:CD2	2.84	0.64
2:B:696:LEU:CD1	2:B:702:LEU:HD11	2.24	0.64
2:B:972:PHE:CE1	2:B:1083:VAL:HG12	2.33	0.64
2:F:46:ASN:ND2	2:F:1089:MET:SD	2.71	0.64
2:F:192:TYR:HE1	2:F:237:LEU:HD23	1.62	0.64
2:F:264:LEU:HD11	2:F:278:LEU:HD23	1.80	0.64
2:B:398:LEU:HD22	2:B:399:LEU:CD1	2.27	0.64
2:F:627:GLU:N	2:F:627:GLU:OE1	2.30	0.64
2:F:930:HIS:O	2:F:934:ILE:HG13	1.98	0.64
2:F:972:PHE:CE1	2:F:1083:VAL:HG12	2.33	0.64
2:F:1108:GLU:N	3:G:9:DC:OP1	2.30	0.64
2:B:46:ASN:ND2	2:B:1089:MET:SD	2.71	0.64
2:B:106:LEU:CD2	2:B:110:ASP:CG	2.71	0.64
2:B:192:TYR:HE1	2:B:237:LEU:HD23	1.62	0.64
2:B:930:HIS:O	2:B:934:ILE:HG13	1.97	0.64
2:B:1108:GLU:N	3:C:9:DC:OP1	2.30	0.64
2:B:1326:TYR:HD2	2:B:1327:PHE:CD2	2.08	0.64
2:F:317:LEU:HD22	2:F:414:ILE:HD11	1.80	0.64
2:F:1305:GLN:CA	2:F:1327:PHE:CZ	2.73	0.64
2:B:317:LEU:HD22	2:B:414:ILE:HD11	1.80	0.64
2:B:557:ARG:HH12	2:B:599:LYS:HZ1	1.46	0.64
2:B:873:GLU:O	2:B:877:LYS:HG2	1.98	0.64
2:F:841:ILE:CD1	2:F:900:LEU:CD2	2.76	0.64
1:A:28:A:OP2	2:B:126:VAL:HG13	1.97	0.64
2:B:121:ASN:OD1	2:B:124:ASP:N	2.25	0.64
2:B:841:ILE:CD1	2:B:900:LEU:CD2	2.76	0.64
2:F:557:ARG:HH12	2:F:599:LYS:HZ1	1.45	0.64
2:B:763:MET:HE2	2:B:928:THR:HG22	1.79	0.64
2:F:554:LYS:HD3	2:F:594:TYR:CZ	2.33	0.64
2:F:873:GLU:O	2:F:877:LYS:HG2	1.98	0.64
2:B:252:PHE:CE1	2:B:264:LEU:HD13	2.34	0.63
2:B:554:LYS:HD3	2:B:594:TYR:CZ	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:979:ASN:CG	2:B:981:TYR:CD1	2.76	0.63
2:F:559:VAL:HA	2:F:563:GLN:OE1	1.98	0.63
2:F:763:MET:HE2	2:F:928:THR:HG22	1.79	0.63
2:F:1000:LYS:HZ1	2:F:1064:GLU:HG3	1.63	0.63
2:F:1216:SER:HB2	4:H:6:DG:H3'	1.80	0.63
1:A:26:A:OP1	2:B:115:ARG:NH1	2.31	0.63
2:B:341:GLN:HE21	2:B:342:GLN:HG2	1.63	0.63
2:B:356:LYS:O	2:B:357:ASN:HB2	1.98	0.63
2:B:1216:SER:HB2	4:D:6:DG:H3'	1.80	0.63
2:B:1305:GLN:CA	2:B:1327:PHE:CZ	2.73	0.63
2:F:342:GLN:OE1	2:F:384:ASP:O	2.15	0.63
2:F:379:ILE:O	2:F:383:MET:HB2	1.98	0.63
2:B:97:PHE:CE1	2:B:152:ARG:HB3	2.33	0.63
2:B:184:LEU:CD1	2:B:296:LEU:HA	2.26	0.63
2:B:244:LEU:CG	2:B:266:LEU:HD11	2.28	0.63
2:B:559:VAL:HA	2:B:563:GLN:OE1	1.99	0.63
1:E:28:A:OP2	2:F:126:VAL:HG13	1.97	0.63
2:F:252:PHE:CE1	2:F:264:LEU:HD13	2.34	0.63
2:F:341:GLN:HE21	2:F:342:GLN:HG2	1.63	0.63
2:F:1326:TYR:HD2	2:F:1327:PHE:CD2	2.08	0.63
2:B:429:PHE:HB2	2:B:430:TYR:CD1	2.34	0.63
2:B:441:GLU:O	2:B:445:THR:OG1	2.16	0.63
2:B:614:ASP:OD1	2:B:664:ARG:NH2	2.31	0.63
2:F:429:PHE:HB2	2:F:430:TYR:CD1	2.34	0.63
2:F:441:GLU:O	2:F:445:THR:OG1	2.16	0.63
2:B:234:LYS:HE2	2:B:234:LYS:O	1.97	0.63
2:B:525:THR:HG23	2:B:690:ASN:ND2	2.05	0.63
2:B:596:ASP:CG	2:B:656:TYR:HH	1.95	0.63
1:E:26:A:OP1	2:F:115:ARG:NH1	2.31	0.63
2:F:97:PHE:CE1	2:F:152:ARG:HB3	2.33	0.63
2:F:184:LEU:CD1	2:F:296:LEU:HA	2.26	0.63
2:F:244:LEU:CG	2:F:266:LEU:HD11	2.28	0.63
2:F:614:ASP:OD1	2:F:664:ARG:NH2	2.31	0.63
2:F:1039:TYR:O	2:F:1042:ILE:HG22	1.98	0.63
2:B:1079:ASP:HA	2:B:1082:THR:OG1	1.99	0.63
2:F:830:ILE:HD12	2:F:830:ILE:H	1.63	0.63
2:F:1079:ASP:HA	2:F:1082:THR:OG1	1.99	0.63
2:B:1039:TYR:O	2:B:1042:ILE:HG22	1.99	0.63
2:F:338:LEU:O	2:F:383:MET:HE1	1.99	0.63
2:F:1200:LYS:NZ	4:H:6:DG:OP1	2.31	0.63
3:G:10:DT:H2'	3:G:11:DT:C6	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:557:ARG:CZ	2:B:599:LYS:HZ2	2.12	0.63
2:B:680:LEU:O	2:B:684:LYS:HG3	1.97	0.63
2:B:1007:GLU:N	2:B:1007:GLU:OE2	2.31	0.63
2:B:1200:LYS:NZ	4:D:6:DG:OP1	2.31	0.63
3:C:24:DG:C2'	3:C:25:DG:H5'	2.25	0.63
3:C:10:DT:H2'	3:C:11:DT:C6	2.34	0.63
2:F:234:LYS:HE2	2:F:234:LYS:O	1.97	0.63
2:F:1000:LYS:HD2	2:F:1045:PHE:CE2	2.34	0.63
2:F:1127:ASP:HB3	2:F:1130:LYS:HB2	1.81	0.63
2:B:334:LEU:O	2:B:338:LEU:HB2	1.98	0.62
2:B:830:ILE:HD12	2:B:830:ILE:H	1.64	0.62
2:B:1000:LYS:HD2	2:B:1045:PHE:CE2	2.34	0.62
2:F:680:LEU:O	2:F:684:LYS:HG3	1.97	0.62
2:F:1145:VAL:HG11	2:F:1182:LEU:HD13	1.81	0.62
3:G:24:DG:C2'	3:G:25:DG:H5'	2.25	0.62
2:B:341:GLN:NE2	2:B:342:GLN:HG2	2.13	0.62
2:F:334:LEU:O	2:F:338:LEU:HB2	1.98	0.62
2:B:171:GLU:OE1	2:B:269:ASP:HB3	1.98	0.62
2:B:1145:VAL:HG11	2:B:1182:LEU:HD13	1.81	0.62
2:B:1150:GLU:HG2	2:B:1157:LEU:HD21	1.81	0.62
2:F:195:LEU:HD22	2:F:286:TYR:HD2	1.63	0.62
2:F:1007:GLU:N	2:F:1007:GLU:OE2	2.31	0.62
2:B:889:ALA:O	2:B:890:LYS:HB2	1.98	0.62
2:B:1000:LYS:HG3	2:B:1073:VAL:HG21	1.77	0.62
2:F:275:LEU:HD11	2:F:279:LEU:HG	1.80	0.62
2:F:828:LEU:HD13	2:F:836:TYR:CE2	2.34	0.62
2:F:1062:LEU:HG	2:F:1063:ILE:HG13	1.80	0.62
2:F:1150:GLU:HG2	2:F:1157:LEU:HD21	1.81	0.62
1:A:17:G:O2'	2:B:168:PHE:CD1	2.53	0.62
2:B:275:LEU:HD11	2:B:279:LEU:HG	1.80	0.62
2:B:828:LEU:HD13	2:B:836:TYR:CE2	2.34	0.62
2:F:171:GLU:OE1	2:F:269:ASP:HB3	1.98	0.62
2:F:1315:LEU:HB2	2:F:1324:PHE:CZ	2.34	0.62
2:B:158:LEU:O	2:B:162:ILE:HG13	1.99	0.62
2:B:1325:LYS:CB	2:B:1330:THR:HA	2.29	0.62
1:E:17:G:O2'	2:F:168:PHE:CD1	2.53	0.62
2:F:341:GLN:NE2	2:F:342:GLN:HG2	2.13	0.62
2:B:378:PRO:O	2:B:382:LYS:HG2	2.00	0.62
2:B:1270:ILE:HD13	2:B:1294:TYR:CG	2.35	0.62
2:B:1315:LEU:HB2	2:B:1324:PHE:CZ	2.34	0.62
2:F:70:ARG:NH1	2:F:454:PRO:CG	2.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:423:LEU:N	2:F:423:LEU:HD23	2.13	0.62
2:F:889:ALA:O	2:F:890:LYS:HB2	1.98	0.62
2:F:977:GLU:HG3	2:F:1310:ILE:HG21	1.79	0.62
2:F:1325:LYS:CB	2:F:1330:THR:HA	2.29	0.62
2:B:61:ALA:O	2:B:65:LYS:HG2	1.99	0.62
2:B:244:LEU:CD2	2:B:266:LEU:HD11	2.30	0.62
2:B:545:LYS:HZ3	2:B:690:ASN:HD21	1.47	0.62
2:F:158:LEU:O	2:F:162:ILE:HG13	1.99	0.62
2:F:1292:SER:O	2:F:1296:LYS:HE3	2.00	0.62
2:B:195:LEU:HD22	2:B:286:TYR:HD2	1.63	0.62
2:B:665:LYS:O	2:B:670:ILE:N	2.33	0.62
2:B:1062:LEU:HG	2:B:1063:ILE:HG13	1.80	0.62
2:F:244:LEU:CD2	2:F:266:LEU:HD11	2.30	0.62
2:F:244:LEU:O	2:F:266:LEU:HD13	1.99	0.62
2:F:842:VAL:HG13	2:F:854:ASN:HD21	1.64	0.62
2:B:70:ARG:NH1	2:B:454:PRO:CG	2.63	0.62
2:B:1292:SER:O	2:B:1296:LYS:HE3	2.00	0.62
2:F:979:ASN:CG	2:F:981:TYR:HD1	2.07	0.62
2:B:842:VAL:HG13	2:B:854:ASN:HD21	1.64	0.61
2:F:324:ARG:CG	2:F:400:ARG:HG2	2.29	0.61
2:F:665:LYS:O	2:F:670:ILE:N	2.33	0.61
2:F:1270:ILE:HD13	2:F:1294:TYR:CG	2.35	0.61
2:B:318:SER:OG	2:B:418:GLU:OE2	2.16	0.61
2:B:423:LEU:N	2:B:423:LEU:HD23	2.13	0.61
2:B:1164:LEU:HD22	2:B:1187:TYR:HE2	1.65	0.61
2:F:972:PHE:CE1	2:F:1083:VAL:CG1	2.83	0.61
2:F:1164:LEU:HD22	2:F:1187:TYR:HE2	1.65	0.61
2:B:229:LEU:HD22	2:B:232:GLU:HB2	1.82	0.61
2:B:244:LEU:O	2:B:266:LEU:HD13	1.99	0.61
2:B:981:TYR:OH	2:B:1092:VAL:HG12	2.00	0.61
2:B:1302:ILE:CG2	2:B:1306:ALA:HB2	2.30	0.61
2:F:1079:ASP:O	2:F:1082:THR:OG1	2.15	0.61
2:F:1292:SER:O	2:F:1296:LYS:HD2	2.00	0.61
2:B:972:PHE:CE1	2:B:1083:VAL:CG1	2.83	0.61
2:B:1079:ASP:O	2:B:1082:THR:OG1	2.16	0.61
2:F:167:HIS:CE1	2:F:411:PRO:HA	2.35	0.61
2:F:229:LEU:HD22	2:F:232:GLU:HB2	1.82	0.61
2:F:1302:ILE:CG2	2:F:1306:ALA:HB2	2.30	0.61
1:A:8:G:H2'	1:A:9:U:C6	2.36	0.61
2:B:167:HIS:CE1	2:B:411:PRO:HA	2.35	0.61
2:B:870:VAL:CG2	2:B:908:LEU:CD2	2.78	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1292:SER:O	2:B:1296:LYS:HD2	2.00	0.61
1:E:8:G:H2'	1:E:9:U:C6	2.36	0.61
2:F:342:GLN:NE2	2:F:384:ASP:HB2	2.13	0.61
2:B:655:ARG:HH11	2:B:655:ARG:CG	2.13	0.61
2:F:460:SER:OG	2:F:463:ALA:N	2.32	0.61
2:F:870:VAL:CG2	2:F:908:LEU:CD2	2.78	0.61
2:F:935:LEU:O	2:F:939:MET:HG2	2.00	0.61
2:F:1239:ALA:CB	2:F:1306:ALA:HB1	2.25	0.61
2:F:1282:LEU:O	2:F:1282:LEU:HD22	2.00	0.61
2:B:269:ASP:N	2:B:269:ASP:OD1	2.33	0.61
2:B:979:ASN:OD1	2:B:980:ASN:N	2.34	0.61
2:B:1042:ILE:O	2:B:1042:ILE:HD12	2.01	0.61
2:B:1245:LEU:HD12	2:B:1245:LEU:O	2.01	0.61
2:F:269:ASP:OD1	2:F:269:ASP:N	2.33	0.61
2:B:106:LEU:O	2:B:111:LYS:CE	2.49	0.60
2:B:244:LEU:CD1	2:B:250:PRO:HD2	2.29	0.60
2:F:244:LEU:CD1	2:F:250:PRO:HD2	2.29	0.60
2:F:1042:ILE:HD12	2:F:1042:ILE:O	2.01	0.60
2:F:324:ARG:HH21	2:F:400:ARG:HH12	1.39	0.60
2:F:655:ARG:CG	2:F:655:ARG:HH11	2.13	0.60
2:F:791:LEU:HD13	2:F:889:ALA:HB2	1.83	0.60
2:B:460:SER:OG	2:B:463:ALA:N	2.32	0.60
2:B:721:HIS:ND1	2:B:738:LEU:HD11	2.16	0.60
2:B:935:LEU:O	2:B:939:MET:HG2	2.00	0.60
2:B:1147:ALA:O	2:B:1160:VAL:HG22	2.01	0.60
2:B:1239:ALA:CB	2:B:1306:ALA:HB1	2.25	0.60
2:B:1282:LEU:O	2:B:1282:LEU:HD22	2.00	0.60
2:B:1304:GLU:HB3	2:B:1327:PHE:CE1	2.35	0.60
2:F:10:ALA:N	2:F:17:GLY:O	2.28	0.60
2:F:324:ARG:HG2	2:F:400:ARG:HB3	1.83	0.60
1:E:70:C:H2'	1:E:71:U:C6	2.36	0.60
2:F:106:LEU:O	2:F:111:LYS:CE	2.49	0.60
2:F:307:ARG:NH1	2:F:323:LYS:HZ1	1.97	0.60
2:F:340:ARG:NH2	2:F:347:TYR:CZ	2.63	0.60
2:F:379:ILE:CD1	2:F:379:ILE:H	2.15	0.60
2:F:720:LEU:O	2:F:724:ILE:HG13	2.01	0.60
2:F:1147:ALA:O	2:F:1160:VAL:HG22	2.01	0.60
2:B:340:ARG:NH2	2:B:347:TYR:CZ	2.63	0.60
2:B:526:LYS:NZ	2:B:695:GLN:OE1	2.28	0.60
2:B:791:LEU:HD13	2:B:889:ALA:HB2	1.83	0.60
2:F:663:SER:OG	2:F:664:ARG:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:721:HIS:ND1	2:F:738:LEU:HD11	2.16	0.60
2:F:1245:LEU:O	2:F:1245:LEU:HD12	2.01	0.60
2:F:1284:ASP:O	2:F:1285:ALA:C	2.43	0.60
2:F:1304:GLU:HB3	2:F:1327:PHE:CE1	2.34	0.60
2:B:720:LEU:O	2:B:724:ILE:HG13	2.01	0.60
2:B:1075:ASP:OD1	2:B:1078:ARG:N	2.27	0.60
2:B:1166:ILE:HG13	2:B:1174:PHE:CE2	2.37	0.60
2:B:1284:ASP:O	2:B:1285:ALA:C	2.43	0.60
2:F:526:LYS:NZ	2:F:695:GLN:OE1	2.28	0.60
2:F:1166:ILE:HG13	2:F:1174:PHE:CE2	2.37	0.60
1:A:70:C:H2'	1:A:71:U:C6	2.36	0.60
2:B:10:ALA:N	2:B:17:GLY:O	2.28	0.60
2:B:379:ILE:CD1	2:B:379:ILE:H	2.15	0.60
2:B:275:LEU:CD1	2:B:279:LEU:HG	2.32	0.60
2:B:379:ILE:O	2:B:383:MET:CG	2.49	0.60
2:B:557:ARG:O	2:B:590:SER:HB2	2.01	0.60
2:B:663:SER:OG	2:B:664:ARG:N	2.35	0.60
2:F:170:ILE:O	2:F:413:GLN:NE2	2.35	0.60
2:F:812:TYR:HE1	2:F:816:LEU:HD21	1.64	0.60
2:F:923:GLU:OE2	2:F:925:ARG:NE	2.32	0.60
2:F:1150:GLU:HG2	2:F:1157:LEU:CD2	2.32	0.60
2:B:170:ILE:O	2:B:413:GLN:NE2	2.35	0.60
2:B:491:PHE:CZ	3:C:16:DT:H1'	2.37	0.60
2:B:830:ILE:HD12	2:B:831:ASN:H	1.67	0.60
2:B:830:ILE:HD13	2:B:831:ASN:OD1	2.01	0.60
2:B:1150:GLU:HG2	2:B:1157:LEU:CD2	2.32	0.60
2:B:1312:LEU:HD11	2:B:1326:TYR:HD1	1.65	0.60
2:F:275:LEU:CD1	2:F:279:LEU:HG	2.32	0.60
2:F:557:ARG:O	2:F:590:SER:HB2	2.01	0.60
2:F:830:ILE:HD13	2:F:831:ASN:OD1	2.01	0.60
2:F:557:ARG:CZ	2:F:599:LYS:HZ2	2.12	0.60
2:F:1075:ASP:OD1	2:F:1078:ARG:N	2.27	0.60
2:B:508:LEU:HD11	2:B:664:ARG:HB2	1.84	0.59
2:B:727:LEU:O	2:B:734:LYS:HE2	2.01	0.59
2:B:812:TYR:HE1	2:B:816:LEU:HD21	1.64	0.59
2:B:1254:GLN:HB2	2:B:1255:LYS:HE3	1.84	0.59
2:F:491:PHE:CZ	3:G:16:DT:H1'	2.37	0.59
2:F:830:ILE:HD12	2:F:831:ASN:H	1.67	0.59
2:B:118:ILE:CG2	2:B:119:PHE:CE2	2.86	0.59
2:B:1266:LEU:O	2:B:1270:ILE:HG13	2.01	0.59
2:F:516:GLU:HA	2:F:519:THR:HG22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:665:LYS:CB	2:F:669:GLY:HA3	2.30	0.59
2:F:727:LEU:O	2:F:734:LYS:HE2	2.01	0.59
2:B:115:ARG:HG3	2:B:116:HIS:ND1	2.16	0.59
1:E:5:C:H42	3:G:24:DG:H1	1.49	0.59
1:E:24:U:C1'	2:F:105:PHE:CE1	2.85	0.59
2:F:115:ARG:HG3	2:F:116:HIS:ND1	2.16	0.59
2:F:118:ILE:CG2	2:F:119:PHE:CE2	2.86	0.59
2:F:252:PHE:HZ	2:F:264:LEU:HD22	1.66	0.59
2:F:297:SER:CB	2:F:301:LEU:HD12	2.30	0.59
2:F:508:LEU:HD11	2:F:664:ARG:HB2	1.84	0.59
2:F:1203:LEU:CD1	2:F:1213:MET:CG	2.80	0.59
2:B:252:PHE:HZ	2:B:264:LEU:HD22	1.66	0.59
2:B:516:GLU:HA	2:B:519:THR:HG22	1.85	0.59
2:B:923:GLU:OE2	2:B:925:ARG:NE	2.32	0.59
2:F:1254:GLN:HB2	2:F:1255:LYS:HE3	1.84	0.59
2:F:1266:LEU:O	2:F:1270:ILE:HG13	2.02	0.59
1:A:5:C:H42	3:C:24:DG:H1	1.49	0.59
2:B:665:LYS:CB	2:B:669:GLY:HA3	2.30	0.59
2:B:675:SER:O	2:B:677:LYS:HG3	2.03	0.59
2:B:981:TYR:CE2	2:B:1092:VAL:HG11	2.24	0.59
2:B:256:PHE:HD2	2:B:282:ILE:HD13	1.66	0.59
2:B:524:LEU:CD2	2:B:540:LEU:HD23	2.32	0.59
2:B:672:ASP:CA	2:B:703:THR:CG2	2.74	0.59
1:E:83:C:H2'	1:E:84:A:H8	1.68	0.59
2:F:524:LEU:CD2	2:F:540:LEU:HD23	2.32	0.59
2:F:675:SER:O	2:F:677:LYS:HG3	2.03	0.59
2:F:1177:ASN:ND2	2:F:1180:ASP:OD2	2.33	0.59
2:F:1312:LEU:HD11	2:F:1326:TYR:HD1	1.65	0.59
2:B:143:VAL:CG1	2:B:315:ALA:HB2	2.31	0.59
2:B:297:SER:CB	2:B:301:LEU:HD12	2.30	0.59
2:B:936:ASP:OD2	2:B:951:ARG:NE	2.36	0.59
2:B:1177:ASN:ND2	2:B:1180:ASP:OD2	2.33	0.59
2:B:1241:HIS:CD2	2:B:1303:ARG:NH1	2.71	0.59
2:F:454:PRO:HB2	2:F:463:ALA:HB2	1.84	0.59
2:F:936:ASP:OD2	2:F:951:ARG:NE	2.36	0.59
2:F:1086:VAL:HG13	2:F:1089:MET:HE1	1.84	0.59
1:A:83:C:H2'	1:A:84:A:H8	1.68	0.59
2:B:841:ILE:O	2:B:864:ARG:NH2	2.34	0.59
2:B:1086:VAL:HG13	2:B:1089:MET:HE1	1.84	0.59
2:F:270:THR:OG1	2:F:274:ASP:OD1	2.21	0.59
2:F:297:SER:O	2:F:301:LEU:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1241:HIS:CD2	2:F:1303:ARG:NH1	2.71	0.59
2:B:297:SER:O	2:B:301:LEU:HB2	2.03	0.59
2:B:454:PRO:HB2	2:B:463:ALA:HB2	1.84	0.59
2:F:143:VAL:CG1	2:F:315:ALA:HB2	2.31	0.59
2:F:841:ILE:O	2:F:864:ARG:NH2	2.34	0.59
2:B:606:PHE:HE2	2:B:612:ASN:CG	2.10	0.59
2:F:324:ARG:NE	2:F:400:ARG:CG	2.55	0.59
2:F:981:TYR:HE2	2:F:1092:VAL:HB	1.64	0.59
2:B:93:VAL:HG21	2:B:151:LEU:CD2	2.33	0.58
2:B:114:GLU:OE1	2:B:115:ARG:N	2.35	0.58
2:B:270:THR:OG1	2:B:274:ASP:OD1	2.21	0.58
2:B:810:LYS:O	2:B:833:LEU:HD11	1.97	0.58
2:F:359:TYR:CZ	2:F:363:ILE:HD11	2.38	0.58
2:F:596:ASP:CG	2:F:656:TYR:HH	1.98	0.58
2:F:606:PHE:HE2	2:F:612:ASN:CG	2.10	0.58
2:F:1000:LYS:NZ	2:F:1045:PHE:CE2	2.51	0.58
2:F:1064:GLU:HB2	2:F:1074:TRP:HB3	1.85	0.58
2:F:93:VAL:HG21	2:F:151:LEU:CD2	2.33	0.58
2:F:979:ASN:CG	2:F:981:TYR:HB2	2.27	0.58
1:A:89:G:C6	2:B:1272:GLN:OE1	2.55	0.58
2:B:178:ASN:CB	2:B:299:ALA:N	2.64	0.58
2:B:328:HIS:CD2	2:B:399:LEU:HG	2.38	0.58
2:B:1064:GLU:HB2	2:B:1074:TRP:HB3	1.85	0.58
1:E:85:C:H2'	1:E:86:C:H6	1.68	0.58
2:F:114:GLU:OE1	2:F:115:ARG:N	2.35	0.58
2:F:978:ILE:HG21	2:F:1228:LEU:HD23	1.85	0.58
2:F:1000:LYS:NZ	2:F:1064:GLU:CB	2.66	0.58
1:A:24:U:C1'	2:B:105:PHE:CE1	2.85	0.58
1:A:85:C:H2'	1:A:86:C:H6	1.68	0.58
2:B:1000:LYS:NZ	2:B:1064:GLU:CB	2.66	0.58
2:B:1095:VAL:HG22	2:B:1350:GLN:OE1	2.03	0.58
2:B:1255:LYS:HE2	2:B:1255:LYS:CA	2.33	0.58
1:E:89:G:C6	2:F:1272:GLN:OE1	2.55	0.58
2:F:319:ALA:HA	2:F:322:ILE:HD12	1.85	0.58
2:F:1095:VAL:HG22	2:F:1350:GLN:OE1	2.03	0.58
2:B:167:HIS:HD1	2:B:411:PRO:HA	1.69	0.58
2:B:508:LEU:CD1	2:B:663:SER:C	2.75	0.58
2:B:1344:ASP:HA	2:B:1362:LEU:O	2.04	0.58
1:E:5:C:N4	3:G:24:DG:H1	2.01	0.58
2:F:499:ASP:O	2:F:502:LEU:O	2.22	0.58
2:F:672:ASP:CA	2:F:703:THR:CG2	2.74	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1255:LYS:HE2	2:F:1255:LYS:CA	2.33	0.58
1:A:88:A:C2	2:B:1090:PRO:HD2	2.38	0.58
2:B:78:ARG:CD	2:B:165:ARG:NH1	2.67	0.58
2:B:457:ARG:HB2	2:B:467:ARG:HH12	1.68	0.58
2:B:846:PHE:HB3	2:B:916:PHE:CD2	2.39	0.58
1:E:88:A:C2	2:F:1090:PRO:HD2	2.38	0.58
2:F:167:HIS:HD1	2:F:411:PRO:HA	1.69	0.58
2:F:256:PHE:HD2	2:F:282:ILE:HD13	1.66	0.58
2:F:328:HIS:CD2	2:F:399:LEU:HG	2.39	0.58
2:F:674:GLN:OE1	2:F:674:GLN:HA	2.02	0.58
2:F:1344:ASP:HA	2:F:1362:LEU:O	2.04	0.58
1:A:5:C:N4	3:C:24:DG:H1	2.01	0.58
1:A:19:A:H4'	2:B:407:ASN:C	2.27	0.58
2:B:499:ASP:O	2:B:502:LEU:O	2.22	0.58
2:B:674:GLN:OE1	2:B:674:GLN:HA	2.02	0.58
2:F:78:ARG:CD	2:F:165:ARG:NH1	2.67	0.58
2:F:846:PHE:HB3	2:F:916:PHE:CD2	2.39	0.58
2:B:359:TYR:CE1	2:B:399:LEU:CD2	2.85	0.58
2:F:178:ASN:CB	2:F:299:ALA:N	2.64	0.58
2:F:356:LYS:O	2:F:357:ASN:HB2	2.02	0.58
2:F:1216:SER:HB2	4:H:6:DG:C3'	2.34	0.58
2:B:48:ILE:HG12	2:B:49:GLY:N	2.17	0.58
2:B:233:LYS:HD2	2:F:543:GLU:CD	2.28	0.58
2:B:286:TYR:O	2:B:289:LEU:N	2.37	0.58
2:B:1135:ASP:OD2	4:D:8:DT:C5'	2.52	0.58
2:B:1232:TYR:CZ	2:B:1268:GLU:HB3	2.39	0.58
2:F:457:ARG:HB2	2:F:467:ARG:HH12	1.68	0.58
2:F:1135:ASP:OD2	4:H:8:DT:C5'	2.52	0.58
2:B:277:ASN:HB3	2:B:653:ARG:CZ	2.34	0.58
2:B:672:ASP:HA	2:B:703:THR:HG23	1.82	0.58
2:B:1203:LEU:HD12	2:B:1213:MET:CG	2.33	0.58
1:E:14:A:H5''	2:F:66:ARG:HH12	1.68	0.58
1:E:22:U:O2	2:F:1110:ILE:HD12	2.04	0.58
2:F:277:ASN:HB3	2:F:653:ARG:CZ	2.34	0.58
2:F:508:LEU:CD1	2:F:663:SER:C	2.75	0.58
2:F:810:LYS:O	2:F:833:LEU:HD11	1.97	0.58
2:F:1000:LYS:CE	2:F:1064:GLU:HB3	2.34	0.58
1:A:14:A:H5''	2:B:66:ARG:HH12	1.68	0.57
2:B:981:TYR:HE2	2:B:1092:VAL:HB	1.64	0.57
2:B:1000:LYS:CE	2:B:1064:GLU:HB3	2.34	0.57
2:B:1216:SER:HB2	4:D:6:DG:C3'	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:48:ILE:HG12	2:F:49:GLY:N	2.17	0.57
2:F:181:VAL:HG21	2:F:209:LYS:CB	2.26	0.57
2:F:286:TYR:O	2:F:289:LEU:N	2.37	0.57
1:A:22:U:O2	2:B:1110:ILE:HD12	2.04	0.57
2:B:66:ARG:NH2	2:B:462:PHE:CE2	2.61	0.57
2:B:336:LYS:HD3	2:B:347:TYR:OH	2.03	0.57
2:B:350:ILE:CG2	2:B:351:PHE:CE2	2.88	0.57
2:B:843:PRO:HD2	2:B:846:PHE:HD2	1.69	0.57
1:E:19:A:H4'	2:F:407:ASN:C	2.27	0.57
2:F:673:LYS:H	2:F:703:THR:HG21	1.69	0.57
2:F:843:PRO:HD2	2:F:846:PHE:HD2	1.69	0.57
2:F:1148:LYS:HE2	2:F:1159:SER:OG	2.03	0.57
1:A:85:C:H2'	1:A:86:C:C6	2.38	0.57
2:B:503:PRO:HD3	2:B:711:ALA:HB1	1.86	0.57
2:B:524:LEU:HD23	2:B:540:LEU:HD23	1.85	0.57
1:E:85:C:H2'	1:E:86:C:C6	2.38	0.57
2:F:503:PRO:HD3	2:F:711:ALA:HB1	1.86	0.57
2:F:777:SER:OG	4:H:2:DT:O5'	2.01	0.57
2:F:1203:LEU:HD12	2:F:1213:MET:CG	2.33	0.57
2:B:244:LEU:HD13	2:B:250:PRO:HG2	1.87	0.57
2:B:601:ILE:CD1	2:B:603:ASP:HB3	2.33	0.57
2:B:673:LYS:H	2:B:703:THR:HG21	1.69	0.57
2:B:1148:LYS:HE2	2:B:1159:SER:OG	2.03	0.57
2:F:341:GLN:HE21	2:F:342:GLN:CG	2.16	0.57
2:F:350:ILE:CG2	2:F:351:PHE:CE2	2.88	0.57
2:F:601:ILE:CD1	2:F:603:ASP:HB3	2.33	0.57
2:F:244:LEU:HD13	2:F:250:PRO:HG2	1.87	0.57
2:F:273:ASP:HA	2:F:276:ASP:HB3	1.86	0.57
2:F:430:TYR:CD1	2:F:430:TYR:N	2.73	0.57
2:F:601:ILE:HD11	2:F:603:ASP:HB3	1.87	0.57
2:F:694:MET:O	2:F:697:ILE:HG22	2.04	0.57
2:F:852:ILE:HG13	5:F:1401:SO4:O4	2.05	0.57
2:F:978:ILE:HG12	2:F:1313:PHE:CZ	2.38	0.57
2:F:1315:LEU:HD12	2:F:1315:LEU:C	2.29	0.57
2:B:339:VAL:O	2:B:342:GLN:O	2.22	0.57
2:B:430:TYR:CD1	2:B:430:TYR:N	2.73	0.57
2:B:694:MET:O	2:B:697:ILE:HG22	2.04	0.57
2:B:905:ARG:NH1	2:B:905:ARG:HG2	2.13	0.57
2:F:336:LYS:HD3	2:F:347:TYR:OH	2.03	0.57
2:F:339:VAL:O	2:F:342:GLN:O	2.22	0.57
2:F:524:LEU:HD23	2:F:540:LEU:HD23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:790:GLU:OE2	2:F:888:ASN:O	2.23	0.57
2:F:829:ASP:OD1	2:F:832:ARG:N	2.32	0.57
2:F:905:ARG:NH1	2:F:905:ARG:HG2	2.13	0.57
2:F:973:TYR:HD2	2:F:1234:ASN:OD1	1.88	0.57
2:B:273:ASP:HA	2:B:276:ASP:HB3	1.86	0.57
2:B:341:GLN:HE21	2:B:342:GLN:CG	2.16	0.57
2:B:601:ILE:HD11	2:B:603:ASP:HB3	1.87	0.57
2:F:672:ASP:HA	2:F:703:THR:HG23	1.82	0.57
2:F:738:LEU:C	2:F:738:LEU:HD23	2.30	0.57
2:B:790:GLU:OE2	2:B:888:ASN:O	2.23	0.57
2:B:1212:ARG:CZ	2:B:1336:TYR:HE2	2.18	0.57
2:F:979:ASN:ND2	2:F:981:TYR:HB2	2.19	0.57
2:B:973:TYR:HD2	2:B:1234:ASN:OD1	1.88	0.57
1:E:6:G:H2'	1:E:7:U:O4'	2.05	0.57
2:F:1045:PHE:N	2:F:1045:PHE:CD1	2.73	0.57
1:A:6:G:H2'	1:A:7:U:O4'	2.05	0.57
2:B:181:VAL:HG21	2:B:209:LYS:CB	2.26	0.57
2:B:738:LEU:HD23	2:B:738:LEU:C	2.30	0.57
2:B:1315:LEU:HD12	2:B:1315:LEU:C	2.29	0.57
2:F:249:THR:HG22	2:F:265:GLN:NE2	2.18	0.57
2:F:1212:ARG:CZ	2:F:1336:TYR:HE2	2.18	0.57
2:F:1230:SER:HA	2:F:1233:VAL:HG21	1.86	0.56
1:A:89:G:N2	2:B:1227:ALA:O	2.39	0.56
2:B:275:LEU:HD11	2:B:279:LEU:HD12	1.88	0.56
2:B:811:LEU:HD13	2:B:811:LEU:C	2.29	0.56
2:B:822:MET:HG3	2:B:883:TRP:HE1	1.69	0.56
2:B:824:VAL:O	2:B:824:VAL:HG12	2.05	0.56
2:B:829:ASP:OD1	2:B:832:ARG:N	2.32	0.56
2:B:1086:VAL:CG1	2:B:1089:MET:HE1	2.36	0.56
2:B:1230:SER:HA	2:B:1233:VAL:HG21	1.86	0.56
1:E:89:G:N2	2:F:1227:ALA:O	2.39	0.56
2:F:128:TYR:HD1	2:F:132:TYR:HD2	1.53	0.56
2:F:275:LEU:HD11	2:F:279:LEU:HD12	1.88	0.56
2:F:811:LEU:C	2:F:811:LEU:HD13	2.29	0.56
2:F:1086:VAL:CG1	2:F:1089:MET:HE1	2.36	0.56
2:B:318:SER:OG	2:B:418:GLU:CD	2.48	0.56
2:B:1202:SER:O	2:B:1213:MET:HA	2.05	0.56
2:F:979:ASN:CG	2:F:981:TYR:CD1	2.81	0.56
2:F:1204:PHE:CZ	2:F:1214:LEU:HD12	2.40	0.56
2:F:1000:LYS:HZ1	2:F:1064:GLU:CB	2.18	0.56
2:F:1202:SER:O	2:F:1213:MET:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:TYR:HD1	2:B:132:TYR:HD2	1.53	0.56
2:B:350:ILE:O	2:B:359:TYR:N	2.39	0.56
2:B:557:ARG:HG3	2:B:557:ARG:NH1	2.09	0.56
2:B:1204:PHE:CZ	2:B:1214:LEU:HD12	2.40	0.56
2:F:207:ASP:HB3	2:F:210:ALA:HB2	1.79	0.56
2:F:824:VAL:O	2:F:824:VAL:HG12	2.05	0.56
2:F:972:PHE:CZ	2:F:1083:VAL:HG11	2.41	0.56
1:A:27:G:H5'	1:A:28:A:H5''	1.87	0.56
2:B:186:ILE:HD11	2:B:203:ALA:HB1	1.88	0.56
2:B:341:GLN:HE21	2:B:342:GLN:CB	2.18	0.56
2:B:566:GLU:O	2:B:571:LYS:HD2	2.06	0.56
2:B:837:ASP:OD2	2:B:859:ARG:O	2.23	0.56
2:B:972:PHE:CZ	2:B:1083:VAL:HG11	2.41	0.56
2:B:1303:ARG:O	2:B:1307:GLU:HG2	2.06	0.56
1:E:8:G:H2'	1:E:9:U:H6	1.70	0.56
1:E:17:G:O2'	2:F:168:PHE:HD1	1.89	0.56
1:E:27:G:H5'	1:E:28:A:H5''	1.88	0.56
2:F:822:MET:HG3	2:F:883:TRP:HE1	1.69	0.56
2:F:1237:TYR:O	2:F:1242:TYR:HE1	1.88	0.56
2:B:297:SER:HG	2:B:301:LEU:HD11	1.61	0.56
2:F:362:TYR:CD1	2:F:372:PHE:CG	2.87	0.56
2:F:691:ARG:HB3	2:F:696:LEU:CD2	2.35	0.56
1:A:17:G:O2'	2:B:168:PHE:HD1	1.89	0.56
2:B:9:LEU:HA	2:B:17:GLY:O	2.06	0.56
2:B:18:TRP:CZ3	2:B:747:LEU:HD21	2.41	0.56
2:B:691:ARG:HB3	2:B:696:LEU:CD2	2.35	0.56
2:B:1101:GLN:HB2	2:B:1140:ALA:HA	1.88	0.56
2:B:1203:LEU:CD1	2:B:1213:MET:CG	2.80	0.56
2:F:186:ILE:HD11	2:F:203:ALA:HB1	1.88	0.56
2:F:837:ASP:OD2	2:F:859:ARG:O	2.23	0.56
2:F:1101:GLN:HB2	2:F:1140:ALA:HA	1.88	0.56
2:F:1303:ARG:O	2:F:1307:GLU:HG2	2.06	0.56
1:A:8:G:H2'	1:A:9:U:H6	1.70	0.56
2:B:207:ASP:HB3	2:B:210:ALA:HB2	1.80	0.56
2:B:244:LEU:HD23	2:B:266:LEU:HD11	1.86	0.56
2:B:393:LEU:HB2	2:B:398:LEU:HD12	1.88	0.56
2:B:1241:HIS:CD2	2:B:1303:ARG:HH11	2.22	0.56
2:F:9:LEU:HA	2:F:17:GLY:O	2.06	0.56
2:F:18:TRP:CZ3	2:F:747:LEU:HD21	2.41	0.56
2:F:244:LEU:HD23	2:F:266:LEU:HD11	1.86	0.56
2:F:324:ARG:CZ	2:F:400:ARG:HD2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:341:GLN:HE21	2:F:342:GLN:CB	2.18	0.56
2:F:393:LEU:HB2	2:F:398:LEU:HD12	1.88	0.56
2:F:566:GLU:O	2:F:571:LYS:HD2	2.06	0.56
2:F:655:ARG:HG3	2:F:655:ARG:NH1	2.21	0.56
2:F:679:ILE:O	2:F:683:LEU:N	2.34	0.56
2:B:79:ILE:HD12	2:B:159:ALA:HB1	1.87	0.55
2:B:489:GLN:HG3	2:B:625:LEU:CD2	2.36	0.55
2:B:1210:ARG:NH2	2:B:1341:GLU:OE2	2.39	0.55
2:B:1237:TYR:O	2:B:1242:TYR:HE1	1.88	0.55
2:B:1302:ILE:HG23	2:B:1306:ALA:HB2	1.88	0.55
2:F:489:GLN:HG3	2:F:625:LEU:CD2	2.36	0.55
2:F:686:ASP:OD2	2:F:691:ARG:HB2	2.05	0.55
2:F:1241:HIS:CD2	2:F:1303:ARG:HH11	2.22	0.55
2:F:1302:ILE:HG23	2:F:1306:ALA:HB2	1.88	0.55
2:B:148:LYS:CD	2:B:429:PHE:CD1	2.72	0.55
2:B:309:ASN:OD1	2:B:309:ASN:N	2.36	0.55
2:B:679:ILE:O	2:B:683:LEU:N	2.34	0.55
2:F:758:ASN:HD22	2:F:995:THR:HG22	1.71	0.55
2:F:1294:TYR:CD1	2:F:1305:GLN:NE2	2.68	0.55
2:B:655:ARG:HG3	2:B:655:ARG:NH1	2.21	0.55
2:B:758:ASN:HD22	2:B:995:THR:HG22	1.71	0.55
2:F:79:ILE:HD12	2:F:159:ALA:HB1	1.87	0.55
2:F:229:LEU:HD13	2:F:232:GLU:N	2.18	0.55
2:F:694:MET:SD	2:F:698:HIS:CD2	2.99	0.55
2:B:694:MET:SD	2:B:698:HIS:CD2	3.00	0.55
2:B:823:TYR:CD1	2:B:875:VAL:HG11	2.42	0.55
2:B:940:ASN:OD1	2:B:952:GLU:N	2.40	0.55
2:B:1325:LYS:HB2	2:B:1330:THR:HA	1.87	0.55
3:C:23:DC:C2'	3:C:24:DG:C5'	2.82	0.55
2:F:161:MET:SD	2:F:419:LEU:HD12	2.46	0.55
2:F:557:ARG:HG3	2:F:557:ARG:NH1	2.09	0.55
2:F:1210:ARG:NH2	2:F:1341:GLU:OE2	2.39	0.55
2:B:161:MET:SD	2:B:419:LEU:HD12	2.46	0.55
2:B:229:LEU:HD13	2:B:232:GLU:N	2.18	0.55
2:B:1272:GLN:HE21	2:B:1272:GLN:CA	2.18	0.55
2:F:342:GLN:CG	2:F:383:MET:HE1	2.02	0.55
2:F:457:ARG:O	2:F:457:ARG:HG2	2.07	0.55
2:F:823:TYR:CD1	2:F:875:VAL:HG11	2.42	0.55
2:F:940:ASN:OD1	2:F:952:GLU:N	2.40	0.55
1:A:19:A:C4'	2:B:407:ASN:O	2.45	0.55
2:B:38:THR:HG22	2:B:39:ASP:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:ILE:HA	2:B:379:ILE:HD13	1.87	0.55
2:B:457:ARG:HG2	2:B:457:ARG:O	2.07	0.55
2:F:842:VAL:HG12	2:F:854:ASN:HD21	1.66	0.55
3:G:23:DC:C2'	3:G:24:DG:C5'	2.82	0.55
2:B:51:LEU:CD1	2:B:1352:ILE:HG13	2.35	0.55
2:B:207:ASP:O	2:B:210:ALA:N	2.40	0.55
2:B:380:LEU:O	2:B:386:THR:HG21	2.07	0.55
2:F:309:ASN:OD1	2:F:309:ASN:N	2.36	0.55
2:F:681:ASP:HA	2:F:684:LYS:HE2	1.89	0.55
2:F:969:ASP:C	2:F:970:PHE:CD2	2.85	0.55
2:F:1272:GLN:HE21	2:F:1272:GLN:CA	2.18	0.55
2:B:681:ASP:HA	2:B:684:LYS:HE2	1.89	0.55
2:B:1294:TYR:CD1	2:B:1305:GLN:NE2	2.68	0.55
2:F:38:THR:HG22	2:F:39:ASP:N	2.20	0.55
2:F:988:TYR:CZ	2:F:1086:VAL:HG21	2.42	0.55
2:F:1325:LYS:HB2	2:F:1330:THR:HA	1.88	0.55
2:B:567:ASP:O	2:B:571:LYS:HB2	2.06	0.55
2:B:606:PHE:CE2	2:B:612:ASN:CG	2.85	0.55
2:B:969:ASP:C	2:B:970:PHE:CD2	2.85	0.55
2:F:207:ASP:O	2:F:210:ALA:N	2.40	0.55
2:F:376:ILE:HA	2:F:379:ILE:HD13	1.88	0.55
2:F:523:GLU:OE2	2:F:588:ASN:N	2.35	0.55
2:F:843:PRO:HD2	2:F:846:PHE:CD2	2.42	0.55
2:F:1230:SER:O	2:F:1233:VAL:N	2.40	0.55
2:F:1304:GLU:CB	2:F:1327:PHE:HE1	2.17	0.55
2:B:842:VAL:HG12	2:B:854:ASN:HD21	1.66	0.55
2:B:843:PRO:HD2	2:B:846:PHE:CD2	2.42	0.55
2:B:1230:SER:O	2:B:1233:VAL:N	2.40	0.55
2:F:606:PHE:CE2	2:F:612:ASN:CG	2.85	0.55
2:F:830:ILE:HD13	2:F:831:ASN:CG	2.32	0.55
2:B:988:TYR:CZ	2:B:1086:VAL:HG21	2.42	0.54
2:B:1270:ILE:CD1	2:B:1294:TYR:CG	2.84	0.54
2:F:51:LEU:CD1	2:F:1352:ILE:HG13	2.35	0.54
2:F:342:GLN:CD	2:F:383:MET:CE	2.63	0.54
2:B:233:LYS:CG	2:F:543:GLU:OE1	2.56	0.54
2:B:1277:SER:HB2	2:B:1287:LEU:HD22	1.88	0.54
2:F:212:LEU:HD12	2:F:246:LEU:HD11	1.87	0.54
2:F:567:ASP:O	2:F:571:LYS:HB2	2.06	0.54
2:F:905:ARG:HH11	2:F:905:ARG:CG	2.14	0.54
2:B:167:HIS:HE1	2:B:411:PRO:HG3	1.72	0.54
2:B:244:LEU:CD1	2:B:250:PRO:CG	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:790:GLU:OE2	2:B:888:ASN:C	2.50	0.54
2:B:1038:PHE:CD1	2:B:1038:PHE:C	2.85	0.54
2:F:148:LYS:CD	2:F:429:PHE:CD1	2.72	0.54
2:F:814:TYR:CD1	2:F:814:TYR:C	2.85	0.54
2:F:1277:SER:HB2	2:F:1287:LEU:HD22	1.88	0.54
2:B:195:LEU:HD22	2:B:289:LEU:HD12	1.87	0.54
2:B:261:ASP:OD1	2:B:261:ASP:N	2.38	0.54
2:B:1146:VAL:O	2:B:1146:VAL:HG13	2.07	0.54
2:B:1304:GLU:CB	2:B:1327:PHE:HE1	2.17	0.54
2:F:114:GLU:HG2	2:F:120:GLY:O	2.08	0.54
2:F:307:ARG:NH1	2:F:323:LYS:HZ3	2.02	0.54
2:F:495:MET:HB3	3:G:17:DA:H1'	1.89	0.54
2:B:114:GLU:HG2	2:B:120:GLY:O	2.08	0.54
2:B:495:MET:HB3	3:C:17:DA:H1'	1.89	0.54
2:B:814:TYR:C	2:B:814:TYR:CD1	2.85	0.54
2:B:830:ILE:HD13	2:B:831:ASN:CG	2.32	0.54
1:E:91:C:H2'	2:F:44:LYS:O	2.07	0.54
2:F:167:HIS:HE1	2:F:411:PRO:HG3	1.71	0.54
2:F:832:ARG:HH11	2:F:835:ASP:CG	2.10	0.54
2:F:1038:PHE:CD1	2:F:1038:PHE:C	2.85	0.54
2:F:1314:THR:HG23	2:F:1324:PHE:CG	2.43	0.54
1:A:91:C:H2'	2:B:44:LYS:O	2.07	0.54
2:B:1220:LEU:HD21	2:B:1342:VAL:HG21	1.89	0.54
2:B:1241:HIS:CE1	2:B:1244:LYS:C	2.85	0.54
1:E:19:A:C4'	2:F:407:ASN:O	2.45	0.54
1:E:81:G:N1	2:F:1356:TYR:HB3	2.23	0.54
2:F:790:GLU:OE2	2:F:888:ASN:C	2.50	0.54
2:F:1146:VAL:HG13	2:F:1146:VAL:O	2.07	0.54
2:B:181:VAL:CG2	2:B:209:LYS:CA	2.84	0.54
2:B:317:LEU:HD22	2:B:414:ILE:CD1	2.38	0.54
2:B:864:ARG:HA	2:B:875:VAL:HG21	1.88	0.54
2:B:905:ARG:HH11	2:B:905:ARG:CG	2.14	0.54
2:B:1314:THR:HG23	2:B:1324:PHE:CG	2.43	0.54
2:F:195:LEU:HD22	2:F:289:LEU:HD12	1.87	0.54
2:F:1220:LEU:HD21	2:F:1342:VAL:HG21	1.89	0.54
1:A:81:G:N1	2:B:1356:TYR:HB3	2.23	0.54
2:F:244:LEU:CD1	2:F:250:PRO:CG	2.85	0.54
2:F:277:ASN:HB3	2:F:653:ARG:NE	2.23	0.54
2:F:317:LEU:HD22	2:F:414:ILE:CD1	2.38	0.54
2:F:1235:PHE:C	2:F:1235:PHE:CD2	2.86	0.54
2:B:1200:LYS:O	2:B:1201:TYR:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:A:O2'	1:E:43:G:OP1	2.23	0.54
2:F:220:ARG:HG3	2:F:220:ARG:NH1	2.14	0.54
2:F:1270:ILE:CD1	2:F:1294:TYR:CG	2.84	0.54
2:B:823:TYR:OH	2:B:839:ASP:OD2	2.19	0.54
2:F:261:ASP:N	2:F:261:ASP:OD1	2.38	0.54
2:F:1241:HIS:CE1	2:F:1244:LYS:C	2.86	0.54
1:A:24:U:N1	2:B:105:PHE:CE1	2.74	0.53
2:B:1235:PHE:C	2:B:1235:PHE:CD2	2.86	0.53
2:B:1237:TYR:C	2:B:1237:TYR:CD1	2.85	0.53
2:F:696:LEU:CD1	2:F:702:LEU:HD13	2.20	0.53
2:F:864:ARG:HA	2:F:875:VAL:HG21	1.88	0.53
2:F:1048:THR:HA	2:F:1076:LYS:HZ2	1.73	0.53
2:F:1200:LYS:O	2:F:1201:TYR:HB2	2.08	0.53
3:G:17:DA:H2'	3:G:18:DG:C8	2.43	0.53
2:B:69:ARG:O	2:B:73:THR:HG23	2.09	0.53
2:B:114:GLU:CD	2:B:120:GLY:O	2.50	0.53
2:B:277:ASN:HB3	2:B:653:ARG:NE	2.23	0.53
2:B:360:ALA:O	2:B:364:ASP:HB2	2.08	0.53
2:B:432:PHE:CD1	2:B:433:LEU:N	2.77	0.53
2:B:437:ARG:O	2:B:441:GLU:HG3	2.08	0.53
2:B:927:ILE:O	2:B:931:VAL:HG23	2.08	0.53
2:B:1000:LYS:HE2	2:B:1073:VAL:HG21	1.62	0.53
3:C:17:DA:H2'	3:C:18:DG:C8	2.43	0.53
2:F:69:ARG:O	2:F:73:THR:HG23	2.09	0.53
2:F:181:VAL:CG2	2:F:209:LYS:CA	2.84	0.53
2:F:437:ARG:O	2:F:441:GLU:HG3	2.08	0.53
2:F:1237:TYR:CD1	2:F:1237:TYR:C	2.86	0.53
2:B:275:LEU:HD11	2:B:279:LEU:CD1	2.38	0.53
2:B:665:LYS:O	2:B:669:GLY:C	2.51	0.53
2:B:870:VAL:CG1	2:B:871:PRO:CD	2.85	0.53
2:B:963:VAL:HG21	2:B:990:ASN:OD1	2.08	0.53
2:B:1325:LYS:HG3	2:B:1326:TYR:O	2.08	0.53
2:B:736:GLY:O	2:B:740:THR:HG22	2.09	0.53
2:B:832:ARG:HH11	2:B:835:ASP:CG	2.10	0.53
2:F:432:PHE:CD1	2:F:433:LEU:N	2.77	0.53
2:F:530:VAL:HG22	2:F:537:PRO:HA	1.90	0.53
2:F:736:GLY:O	2:F:740:THR:HG22	2.09	0.53
2:F:927:ILE:O	2:F:931:VAL:HG23	2.08	0.53
1:E:24:U:N1	2:F:105:PHE:CE1	2.74	0.53
2:F:762:GLU:OE1	2:F:990:ASN:ND2	2.41	0.53
2:B:1038:PHE:HD1	2:B:1038:PHE:O	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:207:ASP:HB2	2:F:210:ALA:HB3	1.84	0.53
2:F:270:THR:OG1	2:F:629:ARG:NH1	2.41	0.53
2:F:1038:PHE:O	2:F:1038:PHE:HD1	1.92	0.53
2:F:1135:ASP:OD2	4:H:8:DT:H5''	2.09	0.53
2:F:1325:LYS:HG3	2:F:1326:TYR:O	2.08	0.53
2:B:7:ILE:O	2:B:759:ILE:HA	2.08	0.53
2:B:114:GLU:HG2	2:B:120:GLY:C	2.34	0.53
2:B:212:LEU:CD1	2:B:246:LEU:HD11	2.38	0.53
2:B:270:THR:OG1	2:B:629:ARG:NH1	2.41	0.53
2:B:530:VAL:HG22	2:B:537:PRO:HA	1.90	0.53
2:B:1284:ASP:OD1	2:B:1284:ASP:N	2.35	0.53
2:F:665:LYS:C	2:F:669:GLY:H	2.17	0.53
2:F:665:LYS:O	2:F:669:GLY:C	2.51	0.53
2:B:275:LEU:CD1	2:B:279:LEU:CG	2.86	0.53
2:B:755:LYS:CD	2:B:939:MET:HE3	2.38	0.53
2:F:128:TYR:CD1	2:F:132:TYR:HD2	2.27	0.53
2:F:275:LEU:HD11	2:F:279:LEU:CD1	2.38	0.53
2:F:569:PHE:CD1	2:F:575:PHE:CE2	2.97	0.53
2:F:570:LYS:HA	2:F:574:CYS:HA	1.91	0.53
2:F:755:LYS:CD	2:F:939:MET:HE3	2.38	0.53
2:F:870:VAL:CG1	2:F:871:PRO:CD	2.85	0.53
2:F:963:VAL:HG21	2:F:990:ASN:OD1	2.08	0.53
2:F:1284:ASP:OD1	2:F:1284:ASP:N	2.35	0.53
2:B:128:TYR:CD1	2:B:132:TYR:HD2	2.27	0.53
2:B:220:ARG:HG3	2:B:220:ARG:NH1	2.14	0.53
2:B:569:PHE:CD1	2:B:575:PHE:CE2	2.97	0.53
2:B:665:LYS:C	2:B:669:GLY:H	2.17	0.53
2:B:1135:ASP:OD2	4:D:8:DT:H5''	2.09	0.53
2:B:1304:GLU:C	2:B:1327:PHE:CE1	2.87	0.53
2:F:66:ARG:CZ	2:F:462:PHE:CZ	2.78	0.53
2:F:114:GLU:HG2	2:F:120:GLY:C	2.34	0.53
2:F:275:LEU:CD1	2:F:279:LEU:CG	2.86	0.53
2:B:570:LYS:HA	2:B:574:CYS:HA	1.91	0.53
2:B:762:GLU:OE1	2:B:990:ASN:ND2	2.41	0.53
2:B:911:LEU:HA	2:B:1032:ALA:CB	2.39	0.53
2:F:7:ILE:O	2:F:759:ILE:HA	2.08	0.53
2:F:386:THR:OG1	2:F:389:LEU:HD12	2.09	0.53
2:F:911:LEU:HA	2:F:1032:ALA:CB	2.39	0.53
2:F:1304:GLU:C	2:F:1327:PHE:CE1	2.87	0.53
1:A:42:A:O2'	1:A:43:G:OP1	2.23	0.52
2:B:249:THR:HG22	2:B:265:GLN:HE21	1.70	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:553:PHE:CD1	2:B:559:VAL:HG21	2.44	0.52
2:F:277:ASN:O	2:F:281:GLN:NE2	2.42	0.52
2:F:553:PHE:CD1	2:F:559:VAL:HG21	2.44	0.52
2:F:1210:ARG:HA	2:F:1280:VAL:HG13	1.90	0.52
2:F:1287:LEU:HD12	2:F:1287:LEU:C	2.32	0.52
2:B:594:TYR:OH	2:B:608:ASP:OD1	2.20	0.52
2:B:1045:PHE:HD1	2:B:1045:PHE:N	2.06	0.52
2:F:37:ASN:OD1	2:F:37:ASN:N	2.39	0.52
2:B:561:VAL:CG2	2:B:584:GLU:O	2.57	0.52
2:B:1210:ARG:HA	2:B:1280:VAL:HG13	1.90	0.52
2:B:1262:HIS:O	2:B:1265:TYR:HB2	2.10	0.52
2:B:1287:LEU:HD12	2:B:1287:LEU:C	2.32	0.52
2:F:1262:HIS:O	2:F:1265:TYR:HB2	2.10	0.52
2:B:81:TYR:O	2:B:85:ILE:HG13	2.09	0.52
2:B:277:ASN:O	2:B:281:GLN:NE2	2.42	0.52
2:B:665:LYS:C	2:B:669:GLY:N	2.66	0.52
2:B:830:ILE:CD1	2:B:831:ASN:N	2.73	0.52
2:F:40:ARG:NE	2:F:43:ILE:CD1	2.73	0.52
2:F:244:LEU:HD13	2:F:250:PRO:CG	2.40	0.52
2:F:561:VAL:CG2	2:F:584:GLU:O	2.57	0.52
2:F:830:ILE:CD1	2:F:831:ASN:N	2.73	0.52
2:F:1284:ASP:O	2:F:1287:LEU:N	2.43	0.52
3:G:24:DG:C2'	3:G:25:DG:C5'	2.85	0.52
2:B:696:LEU:CD1	2:B:702:LEU:HD13	2.19	0.52
2:B:1284:ASP:O	2:B:1287:LEU:N	2.43	0.52
2:F:167:HIS:ND1	2:F:167:HIS:O	2.41	0.52
2:F:635:ARG:HH11	2:F:635:ARG:CG	2.20	0.52
2:F:694:MET:SD	2:F:698:HIS:NE2	2.82	0.52
2:F:1045:PHE:HD1	2:F:1045:PHE:N	2.06	0.52
2:B:37:ASN:OD1	2:B:37:ASN:N	2.39	0.52
2:B:40:ARG:NE	2:B:43:ILE:CD1	2.73	0.52
2:B:244:LEU:HD13	2:B:250:PRO:CG	2.40	0.52
2:B:647:VAL:O	2:B:651:LEU:N	2.43	0.52
2:B:1216:SER:CB	4:D:6:DG:H3'	2.38	0.52
2:F:58:THR:CG2	2:F:731:PRO:HG3	2.21	0.52
2:B:207:ASP:HB2	2:B:210:ALA:HB3	1.84	0.52
2:B:963:VAL:CG2	2:B:990:ASN:OD1	2.57	0.52
2:F:165:ARG:O	2:F:415:HIS:ND1	2.42	0.52
2:F:212:LEU:O	2:F:221:ARG:NH1	2.40	0.52
2:F:594:TYR:OH	2:F:608:ASP:OD1	2.20	0.52
2:F:1203:LEU:HD21	2:F:1211:LYS:CD	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1216:SER:CB	4:H:6:DG:H3'	2.38	0.52
2:B:393:LEU:HD23	2:B:393:LEU:O	2.10	0.52
2:B:523:GLU:OE1	2:B:588:ASN:HB2	2.09	0.52
2:B:694:MET:SD	2:B:698:HIS:NE2	2.82	0.52
2:F:81:TYR:O	2:F:85:ILE:HG13	2.09	0.52
2:F:400:ARG:HD3	2:F:401:LYS:H	1.74	0.52
2:F:492:ILE:CD1	2:F:625:LEU:O	2.58	0.52
2:F:1272:GLN:NE2	2:F:1272:GLN:CA	2.73	0.52
2:B:58:THR:CG2	2:B:731:PRO:HG3	2.22	0.52
2:B:212:LEU:O	2:B:221:ARG:NH1	2.39	0.52
2:B:340:ARG:CA	2:B:344:PRO:HG3	2.40	0.52
2:B:523:GLU:OE2	2:B:588:ASN:N	2.35	0.52
2:B:635:ARG:HH11	2:B:635:ARG:CG	2.20	0.52
2:B:1045:PHE:N	2:B:1045:PHE:CD1	2.73	0.52
2:F:531:THR:CG2	2:F:534:MET:SD	2.94	0.52
2:F:963:VAL:CG2	2:F:990:ASN:OD1	2.57	0.52
2:B:165:ARG:O	2:B:415:HIS:ND1	2.42	0.52
2:B:167:HIS:ND1	2:B:167:HIS:O	2.41	0.52
2:B:226:ILE:HA	2:B:229:LEU:HG	1.92	0.52
2:B:275:LEU:CD1	2:B:279:LEU:CB	2.87	0.52
2:B:429:PHE:N	2:B:429:PHE:HD2	2.08	0.52
2:B:981:TYR:CE1	2:B:1092:VAL:CG1	2.88	0.52
2:B:1203:LEU:HD21	2:B:1211:LYS:CD	2.40	0.52
3:C:24:DG:C2'	3:C:25:DG:C5'	2.86	0.52
2:F:275:LEU:CD1	2:F:279:LEU:CB	2.87	0.52
2:F:429:PHE:HD2	2:F:429:PHE:N	2.08	0.52
2:F:647:VAL:O	2:F:651:LEU:N	2.43	0.52
2:B:66:ARG:CZ	2:B:462:PHE:CZ	2.78	0.51
2:B:123:VAL:HG13	2:B:124:ASP:N	2.25	0.51
2:B:274:ASP:O	2:B:278:LEU:HB3	2.10	0.51
2:B:492:ILE:CD1	2:B:625:LEU:O	2.58	0.51
2:B:1272:GLN:NE2	2:B:1272:GLN:CA	2.73	0.51
2:F:246:LEU:CD1	2:F:246:LEU:N	2.73	0.51
2:B:1250:GLU:O	2:B:1254:GLN:OE1	2.28	0.51
2:F:123:VAL:HG13	2:F:124:ASP:N	2.25	0.51
2:F:245:SER:HB3	2:F:296:LEU:HD22	1.91	0.51
2:F:340:ARG:CA	2:F:344:PRO:HG3	2.40	0.51
2:F:523:GLU:OE1	2:F:588:ASN:HB2	2.09	0.51
2:F:981:TYR:OH	2:F:1092:VAL:HG12	2.00	0.51
2:F:1216:SER:HB2	4:H:6:DG:H5''	1.90	0.51
2:F:40:ARG:NE	2:F:43:ILE:HD11	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:226:ILE:HA	2:F:229:LEU:HG	1.92	0.51
2:F:275:LEU:HD12	2:F:279:LEU:CB	2.26	0.51
2:F:341:GLN:NE2	2:F:342:GLN:CG	2.73	0.51
2:F:759:ILE:HG21	2:F:935:LEU:HD23	1.92	0.51
2:B:520:VAL:HG21	2:B:591:LEU:CD2	2.40	0.51
2:B:759:ILE:HG21	2:B:935:LEU:HD23	1.92	0.51
2:B:788:ILE:HG13	2:B:796:LEU:HG	1.93	0.51
2:B:1048:THR:HA	2:B:1076:LYS:HZ2	1.75	0.51
2:B:1351:SER:OG	2:B:1356:TYR:HB2	2.10	0.51
2:F:274:ASP:O	2:F:278:LEU:HB3	2.11	0.51
2:F:801:VAL:HG11	2:F:815:TYR:CE2	2.46	0.51
2:F:1000:LYS:HZ1	2:F:1064:GLU:CG	2.20	0.51
2:F:1250:GLU:O	2:F:1254:GLN:OE1	2.28	0.51
2:B:341:GLN:NE2	2:B:342:GLN:CG	2.73	0.51
2:B:531:THR:CG2	2:B:534:MET:SD	2.94	0.51
2:B:655:ARG:HH11	2:B:655:ARG:HG3	1.76	0.51
2:B:801:VAL:HG11	2:B:815:TYR:CE2	2.46	0.51
2:B:1216:SER:HB2	4:D:6:DG:H5''	1.90	0.51
2:F:788:ILE:HG13	2:F:796:LEU:HG	1.93	0.51
2:F:1351:SER:OG	2:F:1356:TYR:HB2	2.10	0.51
2:B:40:ARG:NE	2:B:43:ILE:HD11	2.25	0.51
2:B:302:LEU:O	2:B:305:ILE:HD12	2.11	0.51
2:B:827:GLU:O	2:B:828:LEU:HD23	2.10	0.51
2:B:1048:THR:HA	2:B:1076:LYS:NZ	2.25	0.51
2:B:1145:VAL:CG1	2:B:1182:LEU:CD1	2.89	0.51
2:B:1204:PHE:CD1	2:B:1347:LEU:HG	2.45	0.51
2:F:373:TYR:HA	2:F:376:ILE:CD1	2.40	0.51
2:F:393:LEU:HD23	2:F:393:LEU:O	2.10	0.51
2:F:520:VAL:HG21	2:F:591:LEU:CD2	2.40	0.51
2:F:1145:VAL:CG1	2:F:1182:LEU:CD1	2.89	0.51
1:A:14:A:H5''	2:B:66:ARG:NH1	2.26	0.51
2:B:1314:THR:HG23	2:B:1324:PHE:CD1	2.46	0.51
2:F:114:GLU:CD	2:F:120:GLY:O	2.50	0.51
2:F:362:TYR:CD2	2:F:362:TYR:C	2.89	0.51
2:F:655:ARG:HH11	2:F:655:ARG:HG3	1.76	0.51
2:F:708:ILE:HD13	2:F:708:ILE:N	2.25	0.51
2:F:870:VAL:CG2	2:F:908:LEU:HD21	2.40	0.51
2:F:1314:THR:HG23	2:F:1324:PHE:CD1	2.46	0.51
1:A:97:U:H2'	1:A:98:C:O4'	2.11	0.51
2:B:558:LYS:HD2	2:B:586:ARG:HD2	1.93	0.51
2:B:708:ILE:HD13	2:B:708:ILE:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:121:ASN:HD21	2:F:124:ASP:CG	2.19	0.51
2:F:429:PHE:HB2	2:F:430:TYR:CE1	2.46	0.51
2:F:665:LYS:C	2:F:669:GLY:N	2.67	0.51
2:F:827:GLU:O	2:F:828:LEU:HD23	2.10	0.51
1:A:91:C:H6	2:B:44:LYS:O	1.94	0.51
2:B:121:ASN:HD21	2:B:124:ASP:CG	2.19	0.51
2:B:429:PHE:HB2	2:B:430:TYR:CE1	2.46	0.51
2:B:975:VAL:HG23	2:B:1233:VAL:HG12	1.92	0.51
1:E:97:U:H2'	1:E:98:C:O4'	2.11	0.51
2:F:905:ARG:NH1	2:F:905:ARG:CG	2.73	0.51
2:F:981:TYR:CE1	2:F:1092:VAL:CG1	2.88	0.51
2:F:1255:LYS:N	2:F:1255:LYS:CE	2.73	0.51
2:B:78:ARG:CZ	2:B:165:ARG:HH11	2.24	0.51
2:B:110:ASP:O	2:B:110:ASP:OD1	2.29	0.51
2:B:244:LEU:CG	2:B:266:LEU:CD1	2.78	0.51
2:B:573:GLU:C	2:B:574:CYS:SG	2.94	0.51
1:E:14:A:H5''	2:F:66:ARG:NH1	2.26	0.51
2:F:78:ARG:CZ	2:F:165:ARG:HH11	2.24	0.51
2:F:302:LEU:O	2:F:305:ILE:HD12	2.11	0.51
2:F:359:TYR:C	2:F:359:TYR:CD2	2.88	0.51
2:F:359:TYR:CD1	2:F:399:LEU:CD2	2.94	0.51
2:F:558:LYS:HD2	2:F:586:ARG:HD2	1.93	0.51
2:F:573:GLU:C	2:F:574:CYS:SG	2.94	0.51
2:F:910:GLU:HG2	2:F:1033:THR:HG22	1.91	0.51
2:F:1204:PHE:CD1	2:F:1347:LEU:HG	2.45	0.51
3:G:1:DC:H42	4:H:12:DG:H1	1.57	0.51
2:B:186:ILE:CD1	2:B:203:ALA:HB1	2.42	0.50
2:B:275:LEU:HD12	2:B:279:LEU:CB	2.26	0.50
2:B:429:PHE:N	2:B:429:PHE:CD2	2.78	0.50
2:B:553:PHE:CD1	2:B:559:VAL:CG2	2.94	0.50
2:B:625:LEU:HD13	2:B:659:TRP:CZ2	2.46	0.50
2:B:1203:LEU:HD21	2:B:1211:LYS:HD2	1.92	0.50
1:E:91:C:H6	2:F:44:LYS:O	1.94	0.50
2:F:1203:LEU:HD21	2:F:1211:LYS:HD2	1.93	0.50
2:B:153:LEU:HD23	2:B:156:LEU:HD12	1.93	0.50
2:B:398:LEU:O	2:B:398:LEU:HD23	2.11	0.50
2:B:905:ARG:NH1	2:B:905:ARG:CG	2.73	0.50
3:C:1:DC:H42	4:D:12:DG:H1	1.57	0.50
2:F:244:LEU:CG	2:F:266:LEU:CD1	2.78	0.50
2:F:398:LEU:O	2:F:398:LEU:HD23	2.11	0.50
2:F:625:LEU:HD13	2:F:659:TRP:CZ2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:844:GLN:HA	2:F:847:LEU:O	2.11	0.50
2:F:1048:THR:HA	2:F:1076:LYS:NZ	2.25	0.50
1:A:83:C:H2'	1:A:84:A:C8	2.46	0.50
2:B:981:TYR:CG	2:B:1092:VAL:HG11	2.46	0.50
2:B:1255:LYS:N	2:B:1255:LYS:CE	2.73	0.50
2:F:153:LEU:HD23	2:F:156:LEU:HD12	1.93	0.50
2:F:186:ILE:CD1	2:F:203:ALA:HB1	2.42	0.50
2:F:359:TYR:O	2:F:362:TYR:HB3	2.11	0.50
2:F:429:PHE:N	2:F:429:PHE:CD2	2.78	0.50
2:F:492:ILE:HD12	2:F:625:LEU:O	2.11	0.50
2:F:553:PHE:CD1	2:F:559:VAL:CG2	2.94	0.50
2:B:114:GLU:CG	2:B:120:GLY:O	2.60	0.50
2:B:844:GLN:HA	2:B:847:LEU:O	2.11	0.50
1:E:59:U:O4	2:F:475:PRO:HG3	2.12	0.50
2:F:114:GLU:CG	2:F:120:GLY:O	2.60	0.50
2:F:313:THR:HG23	2:F:313:THR:O	2.10	0.50
1:A:59:U:O4	2:B:475:PRO:HG3	2.12	0.50
2:B:97:PHE:HD2	2:B:98:PHE:CD1	2.30	0.50
2:B:220:ARG:NH1	2:B:220:ARG:CG	2.73	0.50
2:B:492:ILE:HD12	2:B:625:LEU:O	2.11	0.50
1:E:83:C:H2'	1:E:84:A:C8	2.46	0.50
2:F:723:HIS:CD2	2:F:727:LEU:HD21	2.47	0.50
2:F:1033:THR:O	2:F:1036:TYR:HB3	2.12	0.50
2:B:723:HIS:CD2	2:B:727:LEU:HD21	2.46	0.50
2:B:910:GLU:HG2	2:B:1033:THR:HG22	1.91	0.50
2:B:1038:PHE:C	2:B:1038:PHE:HD1	2.20	0.50
2:F:97:PHE:HD2	2:F:98:PHE:CD1	2.30	0.50
2:F:738:LEU:HD23	2:F:738:LEU:O	2.12	0.50
2:F:1038:PHE:C	2:F:1038:PHE:HD1	2.20	0.50
2:B:296:LEU:HD23	2:B:296:LEU:O	2.11	0.50
2:B:870:VAL:CG2	2:B:908:LEU:HD21	2.40	0.50
2:B:1033:THR:O	2:B:1036:TYR:HB3	2.12	0.50
2:B:1145:VAL:CG1	2:B:1182:LEU:HD13	2.42	0.50
2:F:139:ARG:HD3	2:F:161:MET:HE2	1.94	0.50
2:F:296:LEU:HD23	2:F:296:LEU:O	2.11	0.50
2:B:114:GLU:HG3	2:B:120:GLY:HA2	1.92	0.50
2:B:313:THR:O	2:B:313:THR:HG23	2.10	0.50
2:B:738:LEU:HD23	2:B:738:LEU:O	2.12	0.50
2:B:926:GLN:HA	2:B:929:LYS:HE3	1.93	0.50
1:E:39:G:H5'	1:E:40:C:OP2	2.12	0.50
2:F:849:ASP:CG	2:F:854:ASN:HB3	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:926:GLN:HA	2:F:929:LYS:HE3	1.93	0.50
2:F:981:TYR:CG	2:F:1092:VAL:HG11	2.46	0.50
2:F:1145:VAL:CG1	2:F:1182:LEU:HD13	2.42	0.50
1:A:74:A:H3'	1:A:75:A:C8	2.47	0.50
2:B:568:TYR:O	2:B:572:ILE:HB	2.12	0.50
1:E:44:U:N3	2:F:328:HIS:HB3	2.27	0.50
1:E:74:A:H3'	1:E:75:A:C8	2.47	0.50
2:F:568:TYR:O	2:F:572:ILE:HB	2.12	0.50
2:F:644:ASP:HB3	2:F:647:VAL:HG23	1.94	0.50
1:A:44:U:N3	2:B:328:HIS:HB3	2.27	0.49
2:B:139:ARG:HD3	2:B:161:MET:HE2	1.94	0.49
2:B:644:ASP:HB3	2:B:647:VAL:HG23	1.94	0.49
2:F:220:ARG:NH1	2:F:220:ARG:CG	2.73	0.49
2:F:362:TYR:HE1	2:F:372:PHE:HD2	1.54	0.49
2:F:655:ARG:CG	2:F:655:ARG:NH1	2.73	0.49
2:F:897:PHE:CZ	2:F:901:THR:HG21	2.46	0.49
1:A:39:G:H5'	1:A:40:C:OP2	2.12	0.49
2:B:338:LEU:HD22	2:B:341:GLN:HG2	1.95	0.49
2:B:841:ILE:HD11	2:B:900:LEU:HD21	1.95	0.49
2:B:849:ASP:CG	2:B:854:ASN:HB3	2.37	0.49
2:F:296:LEU:C	2:F:296:LEU:CD2	2.85	0.49
2:F:338:LEU:HD22	2:F:341:GLN:HG2	1.95	0.49
2:F:974:LYS:HZ3	2:F:976:ARG:HH11	1.60	0.49
2:B:379:ILE:O	2:B:383:MET:HG2	2.12	0.49
2:B:658:GLY:C	2:B:659:TRP:CD1	2.90	0.49
2:B:897:PHE:CZ	2:B:901:THR:HG21	2.46	0.49
2:F:62:THR:O	2:F:65:LYS:HB2	2.13	0.49
2:F:658:GLY:C	2:F:659:TRP:CD1	2.90	0.49
2:F:841:ILE:HD11	2:F:900:LEU:HD21	1.95	0.49
2:B:178:ASN:CB	2:B:299:ALA:HA	2.30	0.49
2:B:708:ILE:O	2:B:711:ALA:N	2.44	0.49
2:B:234:LYS:C	2:B:234:LYS:CD	2.85	0.49
2:B:379:ILE:O	2:B:383:MET:HG3	2.13	0.49
2:B:1031:LYS:O	2:B:1031:LYS:HD3	2.13	0.49
2:F:114:GLU:HG3	2:F:120:GLY:HA2	1.92	0.49
2:F:508:LEU:CD1	2:F:663:SER:O	2.61	0.49
2:F:849:ASP:CB	2:F:854:ASN:HD22	2.13	0.49
2:F:1141:TYR:OH	2:F:1175:GLU:OE2	2.21	0.49
2:B:373:TYR:CA	2:B:376:ILE:HD11	2.40	0.49
2:B:410:ILE:HD12	2:B:410:ILE:N	2.27	0.49
2:B:508:LEU:CD1	2:B:663:SER:O	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:655:ARG:CG	2:B:655:ARG:NH1	2.73	0.49
2:B:844:GLN:NE2	2:B:848:LYS:CD	2.76	0.49
2:B:974:LYS:HZ3	2:B:976:ARG:NH1	2.06	0.49
2:F:974:LYS:NZ	2:F:976:ARG:HH11	2.09	0.49
1:A:16:U:O2	2:B:447:ARG:NH2	2.45	0.49
2:B:910:GLU:CG	2:B:1033:THR:HG22	2.43	0.49
2:B:926:GLN:C	2:B:929:LYS:HG3	2.38	0.49
2:B:1121:ALA:HB2	2:B:1128:PRO:HD3	1.95	0.49
2:F:234:LYS:CD	2:F:234:LYS:C	2.85	0.49
2:F:321:MET:CE	2:F:324:ARG:HD2	2.43	0.49
2:F:410:ILE:N	2:F:410:ILE:HD12	2.27	0.49
2:F:414:ILE:O	2:F:418:GLU:N	2.40	0.49
2:F:583:VAL:HG13	2:F:584:GLU:O	2.13	0.49
2:F:708:ILE:O	2:F:711:ALA:N	2.44	0.49
2:F:844:GLN:NE2	2:F:848:LYS:CD	2.76	0.49
2:F:926:GLN:C	2:F:929:LYS:HG3	2.38	0.49
2:F:1121:ALA:HB2	2:F:1128:PRO:HD3	1.95	0.49
2:B:414:ILE:O	2:B:418:GLU:N	2.40	0.49
2:B:746:GLU:O	2:B:750:VAL:N	2.33	0.49
2:B:840:ALA:O	2:B:864:ARG:NH1	2.45	0.49
2:B:933:GLN:OE1	2:B:934:ILE:N	2.46	0.49
2:B:971:GLN:HA	2:B:973:TYR:CE2	2.47	0.49
2:B:1286:ASN:O	2:B:1289:LYS:HB3	2.12	0.49
2:F:432:PHE:CE1	2:F:433:LEU:HG	2.48	0.49
2:F:507:VAL:HG11	2:F:660:GLY:C	2.37	0.49
2:F:910:GLU:CG	2:F:1033:THR:HG22	2.43	0.49
2:F:933:GLN:OE1	2:F:934:ILE:N	2.46	0.49
2:F:971:GLN:HA	2:F:973:TYR:CE2	2.47	0.49
2:F:1286:ASN:O	2:F:1289:LYS:HB3	2.12	0.49
2:B:106:LEU:HD23	2:B:110:ASP:CB	2.41	0.49
2:B:321:MET:HE3	2:B:321:MET:HA	1.95	0.49
2:B:583:VAL:HG13	2:B:584:GLU:O	2.13	0.49
1:E:16:U:O2	2:F:447:ARG:NH2	2.45	0.49
2:F:373:TYR:CA	2:F:376:ILE:HD11	2.40	0.49
2:B:90:MET:HE3	2:B:98:PHE:CZ	2.48	0.49
2:F:358:GLY:O	2:F:361:GLY:N	2.45	0.49
2:B:432:PHE:CE1	2:B:433:LEU:HG	2.48	0.48
2:B:440:ILE:HA	2:B:443:ILE:HD12	1.94	0.48
2:F:90:MET:HE3	2:F:98:PHE:CZ	2.48	0.48
2:F:234:LYS:HD3	2:F:234:LYS:C	2.38	0.48
2:F:341:GLN:CG	2:F:342:GLN:HG2	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:840:ALA:O	2:F:864:ARG:NH1	2.45	0.48
2:F:969:ASP:C	2:F:970:PHE:HD2	2.21	0.48
2:F:1224:ASN:N	2:F:1224:ASN:ND2	2.60	0.48
2:B:340:ARG:HA	2:B:344:PRO:HG3	1.95	0.48
2:B:507:VAL:HG11	2:B:660:GLY:C	2.37	0.48
2:B:583:VAL:HG22	2:B:584:GLU:H	1.77	0.48
2:B:776:ASN:N	2:B:776:ASN:ND2	2.60	0.48
2:F:106:LEU:HD23	2:F:110:ASP:CB	2.41	0.48
2:F:299:ALA:O	2:F:302:LEU:HD21	2.12	0.48
2:F:340:ARG:HA	2:F:344:PRO:HG3	1.95	0.48
2:F:440:ILE:HA	2:F:443:ILE:HD12	1.94	0.48
2:F:776:ASN:N	2:F:776:ASN:ND2	2.60	0.48
1:A:26:A:H2'	1:A:27:G:H8	1.78	0.48
2:B:94:ASP:HB2	2:B:152:ARG:HD3	1.95	0.48
2:B:226:ILE:CD1	2:F:574:CYS:SG	2.95	0.48
2:B:234:LYS:HD3	2:B:234:LYS:C	2.38	0.48
2:B:1224:ASN:N	2:B:1224:ASN:ND2	2.60	0.48
1:E:26:A:H2'	1:E:27:G:H8	1.78	0.48
2:F:181:VAL:HG12	2:F:300:ILE:CG1	2.43	0.48
2:B:299:ALA:O	2:B:302:LEU:HD21	2.12	0.48
2:B:341:GLN:CG	2:B:342:GLN:HG2	2.41	0.48
2:B:419:LEU:HD21	2:B:440:ILE:HG22	1.94	0.48
2:B:758:ASN:ND2	2:B:995:THR:HG22	2.29	0.48
2:B:969:ASP:C	2:B:970:PHE:HD2	2.21	0.48
2:B:975:VAL:HB	2:B:978:ILE:HD12	1.95	0.48
2:F:94:ASP:HB2	2:F:152:ARG:HD3	1.94	0.48
2:F:143:VAL:HG13	2:F:421:ALA:CB	2.44	0.48
2:F:1089:MET:HE2	2:F:1089:MET:HB2	1.65	0.48
2:B:201:ILE:HG22	2:B:202:ASN:N	2.28	0.48
2:B:419:LEU:HD13	2:B:444:LEU:HD12	1.95	0.48
2:B:779:GLU:O	2:B:783:ARG:HG3	2.13	0.48
2:B:849:ASP:CB	2:B:854:ASN:HD22	2.13	0.48
2:F:5:TYR:HD2	2:F:20:VAL:HG13	1.77	0.48
2:F:324:ARG:CG	2:F:400:ARG:CG	2.89	0.48
2:F:419:LEU:HD13	2:F:444:LEU:HD12	1.95	0.48
2:F:758:ASN:ND2	2:F:995:THR:HG22	2.29	0.48
2:F:977:GLU:HG3	2:F:1310:ILE:HG23	1.94	0.48
2:F:978:ILE:HG12	2:F:1313:PHE:CD2	2.44	0.48
2:B:78:ARG:HD3	2:B:165:ARG:NH1	2.27	0.48
2:B:143:VAL:HG13	2:B:421:ALA:CB	2.44	0.48
2:B:181:VAL:HG12	2:B:300:ILE:CG1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:ALA:O	2:B:248:LEU:HB2	2.13	0.48
2:B:410:ILE:N	2:B:410:ILE:CD1	2.77	0.48
2:B:448:ILE:HG22	2:B:452:VAL:HB	1.96	0.48
2:F:28:PRO:HB2	2:F:47:LEU:HG	1.96	0.48
2:F:118:ILE:HB	2:F:119:PHE:CD2	2.48	0.48
2:F:178:ASN:CB	2:F:299:ALA:HA	2.30	0.48
2:F:321:MET:CE	2:F:321:MET:CA	2.86	0.48
2:F:404:THR:O	2:F:407:ASN:ND2	2.43	0.48
2:F:448:ILE:HG22	2:F:452:VAL:HB	1.96	0.48
2:F:705:LYS:HE2	2:F:705:LYS:HB3	1.60	0.48
2:F:779:GLU:O	2:F:783:ARG:HG3	2.13	0.48
2:F:821:ASP:CB	2:F:824:VAL:HB	2.43	0.48
2:B:5:TYR:HD2	2:B:20:VAL:HG13	1.77	0.48
2:B:28:PRO:HB2	2:B:47:LEU:HG	1.96	0.48
2:B:687:GLY:CA	2:B:688:PHE:C	2.85	0.48
2:B:692:ASN:H	2:B:695:GLN:HB2	1.78	0.48
2:B:699:ASP:HB3	2:B:702:LEU:CB	2.44	0.48
2:B:1302:ILE:HG22	2:B:1306:ALA:HB2	1.96	0.48
2:F:321:MET:HE1	2:F:324:ARG:HD2	1.95	0.48
2:F:410:ILE:N	2:F:410:ILE:CD1	2.77	0.48
2:F:419:LEU:HD21	2:F:440:ILE:HG22	1.94	0.48
2:F:699:ASP:HB3	2:F:702:LEU:CB	2.44	0.48
2:F:1302:ILE:HG22	2:F:1306:ALA:HB2	1.96	0.48
1:A:68:A:C4	2:B:1350:GLN:O	2.67	0.48
2:B:225:LEU:HD13	2:B:242:ILE:HG21	1.95	0.48
3:C:1:DC:N4	3:C:2:DA:N1	2.60	0.48
2:F:78:ARG:HD3	2:F:165:ARG:NH1	2.27	0.48
2:F:201:ILE:HG22	2:F:202:ASN:N	2.28	0.48
2:F:225:LEU:HD13	2:F:242:ILE:HG21	1.95	0.48
2:F:432:PHE:HD1	2:F:433:LEU:N	2.12	0.48
2:F:583:VAL:HG22	2:F:584:GLU:H	1.77	0.48
3:G:1:DC:N4	3:G:2:DA:N1	2.61	0.48
1:A:13:A:H2'	1:A:14:A:H8	1.78	0.48
2:B:432:PHE:HD1	2:B:433:LEU:N	2.11	0.48
2:B:821:ASP:CB	2:B:824:VAL:HB	2.43	0.48
2:B:988:TYR:OH	2:B:1086:VAL:HG21	2.14	0.48
2:F:351:PHE:CD2	2:F:351:PHE:N	2.82	0.48
2:F:842:VAL:CG1	2:F:847:LEU:HD22	2.44	0.48
2:F:1242:TYR:CD1	2:F:1242:TYR:N	2.72	0.48
2:B:27:VAL:HG11	2:B:1086:VAL:CG1	2.43	0.48
2:B:38:THR:HG22	2:B:39:ASP:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1135:ASP:CG	2:B:1136:SER:N	2.72	0.48
2:B:1242:TYR:CD1	2:B:1242:TYR:N	2.72	0.48
2:F:972:PHE:CE1	2:F:1083:VAL:HG11	2.48	0.48
2:B:118:ILE:HB	2:B:119:PHE:CD2	2.48	0.47
2:B:151:LEU:O	2:B:154:ILE:N	2.47	0.47
2:B:358:GLY:O	2:B:361:GLY:N	2.47	0.47
2:B:705:LYS:HB3	2:B:705:LYS:HE2	1.60	0.47
2:B:821:ASP:HB3	2:B:824:VAL:HB	1.95	0.47
1:E:13:A:H2'	1:E:14:A:H8	1.78	0.47
1:E:68:A:C4	2:F:1350:GLN:O	2.67	0.47
2:F:838:VAL:HG11	2:F:855:LYS:HE3	1.95	0.47
2:F:1135:ASP:CG	2:F:1136:SER:N	2.72	0.47
2:F:1219:GLU:CG	2:F:1220:LEU:N	2.77	0.47
2:B:336:LYS:HG2	2:B:347:TYR:HE2	1.79	0.47
2:B:351:PHE:CD2	2:B:351:PHE:N	2.82	0.47
2:B:972:PHE:CE1	2:B:1083:VAL:HG11	2.48	0.47
2:B:1251:ASP:O	2:B:1254:GLN:HB2	2.14	0.47
2:F:151:LEU:O	2:F:154:ILE:N	2.47	0.47
2:F:336:LYS:HG2	2:F:347:TYR:HE2	1.79	0.47
2:F:362:TYR:C	2:F:362:TYR:HD2	2.22	0.47
2:F:386:THR:OG1	2:F:389:LEU:CD1	2.62	0.47
2:F:821:ASP:HB3	2:F:824:VAL:HB	1.95	0.47
2:F:988:TYR:OH	2:F:1086:VAL:HG21	2.14	0.47
1:A:58:G:H5''	1:A:59:U:OP2	2.14	0.47
1:A:77:A:OP1	2:B:721:HIS:NE2	2.47	0.47
2:B:75:ARG:HA	2:B:78:ARG:NH2	2.29	0.47
2:B:404:THR:O	2:B:407:ASN:ND2	2.43	0.47
2:B:842:VAL:CG1	2:B:847:LEU:HD22	2.44	0.47
2:B:1219:GLU:CG	2:B:1220:LEU:N	2.77	0.47
2:F:297:SER:CA	2:F:301:LEU:HD12	2.44	0.47
2:F:692:ASN:H	2:F:695:GLN:HB2	1.78	0.47
2:F:978:ILE:CG1	2:F:1313:PHE:CE2	2.83	0.47
2:B:79:ILE:HG13	2:B:163:LYS:HG3	1.96	0.47
2:B:297:SER:CA	2:B:301:LEU:HD12	2.44	0.47
2:B:830:ILE:HD13	2:B:831:ASN:H	1.79	0.47
2:B:849:ASP:OD2	2:B:854:ASN:HB2	2.15	0.47
2:F:181:VAL:CG2	2:F:209:LYS:HA	2.33	0.47
2:F:1251:ASP:O	2:F:1254:GLN:HB2	2.14	0.47
2:B:250:PRO:HD2	2:B:264:LEU:O	2.15	0.47
2:B:529:TYR:CD1	2:B:538:ALA:O	2.68	0.47
2:B:838:VAL:HG11	2:B:855:LYS:HE3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:844:GLN:NE2	2:B:848:LYS:CG	2.73	0.47
2:B:979:ASN:ND2	2:B:981:TYR:CG	2.81	0.47
2:B:1076:LYS:O	2:B:1080:PHE:HD2	1.97	0.47
2:F:27:VAL:HG11	2:F:1086:VAL:CG1	2.43	0.47
2:F:45:LYS:HE2	2:F:1093:ASN:OD1	2.13	0.47
2:F:75:ARG:HA	2:F:78:ARG:NH2	2.29	0.47
2:F:178:ASN:HB2	2:F:299:ALA:CA	2.29	0.47
2:F:341:GLN:NE2	2:F:341:GLN:C	2.73	0.47
2:B:341:GLN:NE2	2:B:341:GLN:C	2.73	0.47
2:B:412:HIS:CD2	2:B:413:GLN:HE21	2.33	0.47
2:B:516:GLU:OE1	2:B:593:THR:N	2.33	0.47
1:E:58:G:H5"	1:E:59:U:OP2	2.14	0.47
1:E:77:A:OP1	2:F:721:HIS:NE2	2.47	0.47
2:F:362:TYR:HE2	2:F:401:LYS:CE	2.27	0.47
2:F:529:TYR:CD1	2:F:538:ALA:O	2.68	0.47
2:F:765:ARG:HH22	2:F:848:LYS:HE3	1.79	0.47
2:F:849:ASP:OD2	2:F:854:ASN:HB2	2.14	0.47
2:F:1347:LEU:HB3	2:F:1360:ILE:HB	1.96	0.47
1:A:49:A:OP2	2:B:76:LYS:HE2	2.15	0.47
2:B:6:SER:HB3	2:B:758:ASN:HB2	1.96	0.47
2:B:45:LYS:HE2	2:B:1093:ASN:OD1	2.13	0.47
2:B:167:HIS:CE1	2:B:411:PRO:CA	2.98	0.47
2:B:212:LEU:HD21	2:B:225:LEU:CD1	2.41	0.47
2:B:311:GLU:H	2:B:311:GLU:CD	2.21	0.47
2:B:318:SER:HG	2:B:418:GLU:CD	2.16	0.47
2:B:432:PHE:CD1	2:B:432:PHE:C	2.91	0.47
2:B:509:PRO:HG2	2:B:621:LEU:HA	1.97	0.47
2:B:746:GLU:HA	2:B:749:LYS:HB3	1.96	0.47
2:B:796:LEU:HD23	2:B:796:LEU:HA	1.80	0.47
2:B:840:ALA:HA	2:B:854:ASN:O	2.15	0.47
2:B:1000:LYS:HZ1	2:B:1064:GLU:HB2	1.79	0.47
2:B:1206:LEU:HD11	2:B:1210:ARG:CZ	2.44	0.47
2:B:1232:TYR:CE1	2:B:1268:GLU:HB3	2.49	0.47
1:E:51:A:C6	2:F:1105:PHE:CZ	3.02	0.47
2:F:6:SER:HB3	2:F:758:ASN:HB2	1.96	0.47
2:F:79:ILE:HG13	2:F:163:LYS:HG3	1.96	0.47
2:F:212:LEU:HD21	2:F:225:LEU:CD1	2.41	0.47
2:F:250:PRO:HD2	2:F:264:LEU:O	2.15	0.47
2:F:297:SER:O	2:F:301:LEU:CB	2.63	0.47
2:F:324:ARG:HG2	2:F:400:ARG:CB	2.44	0.47
2:F:412:HIS:CD2	2:F:413:GLN:HE21	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:516:GLU:OE1	2:F:593:THR:N	2.33	0.47
2:F:557:ARG:NH1	2:F:557:ARG:CG	2.73	0.47
2:F:830:ILE:HD13	2:F:831:ASN:H	1.79	0.47
2:F:1076:LYS:O	2:F:1080:PHE:HD2	1.97	0.47
2:B:297:SER:O	2:B:301:LEU:CB	2.63	0.47
2:B:963:VAL:HG13	2:B:989:LEU:HB2	1.97	0.47
2:B:1206:LEU:HD11	2:B:1210:ARG:NE	2.30	0.47
1:E:49:A:OP2	2:F:76:LYS:HE2	2.15	0.47
2:F:311:GLU:H	2:F:311:GLU:CD	2.21	0.47
2:F:746:GLU:HA	2:F:749:LYS:HB3	1.96	0.47
2:F:795:ILE:HG23	2:F:796:LEU:N	2.30	0.47
2:F:838:VAL:CG2	2:F:857:LEU:HD12	2.45	0.47
2:F:840:ALA:HA	2:F:854:ASN:O	2.15	0.47
2:F:963:VAL:HG13	2:F:989:LEU:HB2	1.97	0.47
1:A:51:A:C6	2:B:1105:PHE:CZ	3.02	0.47
2:B:491:PHE:CE2	3:C:16:DT:H1'	2.50	0.47
2:B:765:ARG:HH22	2:B:848:LYS:HE3	1.79	0.47
2:B:838:VAL:CG2	2:B:857:LEU:HD12	2.45	0.47
2:B:945:GLU:CD	2:B:946:ASN:N	2.73	0.47
2:B:1302:ILE:O	2:B:1306:ALA:HB2	2.12	0.47
2:F:167:HIS:CE1	2:F:411:PRO:CA	2.98	0.47
2:F:350:ILE:O	2:F:359:TYR:N	2.48	0.47
2:F:416:LEU:HD13	2:F:444:LEU:HD13	1.97	0.47
2:F:509:PRO:HG2	2:F:621:LEU:HA	1.97	0.47
2:F:627:GLU:N	2:F:627:GLU:CD	2.73	0.47
2:F:655:ARG:HH11	2:F:655:ARG:CB	2.27	0.47
2:B:143:VAL:HG13	2:B:421:ALA:HB1	1.97	0.47
2:B:207:ASP:O	2:B:211:ILE:HG13	2.15	0.47
2:B:373:TYR:HA	2:B:376:ILE:CD1	2.40	0.47
2:B:795:ILE:HG23	2:B:796:LEU:N	2.30	0.47
2:B:1108:GLU:HB2	3:C:9:DC:H5''	1.96	0.47
2:B:1347:LEU:HB3	2:B:1360:ILE:HB	1.96	0.47
2:F:38:THR:HG22	2:F:39:ASP:H	1.79	0.47
2:F:143:VAL:HG13	2:F:421:ALA:HB1	1.97	0.47
2:F:207:ASP:O	2:F:211:ILE:HG13	2.15	0.47
2:F:270:THR:O	2:F:274:ASP:HB2	2.15	0.47
2:F:1108:GLU:HB2	3:G:9:DC:H5''	1.96	0.47
2:F:1179:ILE:HD11	2:F:1192:LYS:HD3	1.97	0.47
2:F:1204:PHE:CG	2:F:1342:VAL:HG13	2.50	0.47
2:F:1206:LEU:HD11	2:F:1210:ARG:CZ	2.44	0.47
1:A:63:U:H3'	2:B:62:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ARG:NH2	2:B:168:PHE:HZ	2.06	0.46
2:B:181:VAL:CG2	2:B:209:LYS:HA	2.33	0.46
2:B:416:LEU:HD13	2:B:444:LEU:HD13	1.97	0.46
2:B:557:ARG:NH1	2:B:557:ARG:CG	2.73	0.46
2:B:655:ARG:HH11	2:B:655:ARG:CB	2.27	0.46
2:B:897:PHE:CE2	2:B:901:THR:HG21	2.50	0.46
2:B:980:ASN:HB2	2:B:1225:GLU:OE2	2.15	0.46
2:B:1177:ASN:ND2	2:B:1180:ASP:CG	2.73	0.46
2:B:1204:PHE:CG	2:B:1342:VAL:HG13	2.50	0.46
2:F:190:GLN:O	2:F:194:GLN:HG2	2.16	0.46
2:F:491:PHE:CE2	3:G:16:DT:H1'	2.50	0.46
2:F:897:PHE:CE2	2:F:901:THR:HG21	2.50	0.46
2:F:940:ASN:N	2:F:940:ASN:ND2	2.60	0.46
2:F:945:GLU:CD	2:F:946:ASN:N	2.73	0.46
2:F:1206:LEU:HD11	2:F:1210:ARG:NE	2.30	0.46
2:B:270:THR:O	2:B:274:ASP:HB2	2.15	0.46
2:B:627:GLU:N	2:B:627:GLU:CD	2.73	0.46
2:B:1042:ILE:HG23	2:B:1043:MET:SD	2.55	0.46
2:B:1145:VAL:HG23	2:B:1145:VAL:O	2.15	0.46
2:B:1179:ILE:HD11	2:B:1192:LYS:HD3	1.97	0.46
2:B:1312:LEU:HD21	2:B:1326:TYR:HD1	1.80	0.46
1:E:63:U:H3'	2:F:62:THR:HG21	1.97	0.46
2:F:432:PHE:CD1	2:F:432:PHE:C	2.91	0.46
1:A:59:U:P	2:B:467:ARG:HH22	2.37	0.46
2:B:190:GLN:O	2:B:194:GLN:HG2	2.16	0.46
2:B:253:LYS:HD2	2:B:261:ASP:HA	1.98	0.46
2:B:271:TYR:C	2:B:271:TYR:CD2	2.93	0.46
2:B:737:ILE:O	2:B:740:THR:HG23	2.15	0.46
2:B:925:ARG:C	2:B:929:LYS:HE3	2.41	0.46
2:B:1236:LEU:HD13	2:B:1310:ILE:HG12	1.97	0.46
1:E:43:G:H22	2:F:360:ALA:CB	2.28	0.46
1:E:59:U:P	2:F:467:ARG:HH22	2.37	0.46
1:E:87:G:H1	1:E:91:C:H42	1.63	0.46
2:F:148:LYS:HD2	2:F:429:PHE:CD1	2.48	0.46
2:F:229:LEU:CD2	2:F:232:GLU:HB2	2.43	0.46
2:F:253:LYS:HD2	2:F:261:ASP:HA	1.98	0.46
2:F:342:GLN:OE1	2:F:384:ASP:N	2.47	0.46
2:F:925:ARG:C	2:F:929:LYS:HE3	2.41	0.46
2:F:970:PHE:CD1	2:F:1080:PHE:CZ	3.02	0.46
2:F:1031:LYS:H	2:F:1031:LYS:CD	2.22	0.46
2:F:1042:ILE:HG23	2:F:1043:MET:SD	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1177:ASN:ND2	2:F:1180:ASP:CG	2.73	0.46
2:F:1312:LEU:HD21	2:F:1326:TYR:HD1	1.80	0.46
2:B:719:SER:O	2:B:722:GLU:HB2	2.15	0.46
2:B:1091:GLN:NE2	2:B:1091:GLN:C	2.73	0.46
2:F:719:SER:O	2:F:722:GLU:HB2	2.15	0.46
2:F:1236:LEU:HD13	2:F:1310:ILE:HG12	1.97	0.46
1:A:27:G:H5'	1:A:28:A:C5'	2.45	0.46
2:B:27:VAL:CG1	2:B:1086:VAL:CG1	2.88	0.46
2:B:62:THR:O	2:B:66:ARG:HG3	2.15	0.46
2:B:148:LYS:HD2	2:B:429:PHE:CD1	2.48	0.46
2:B:178:ASN:HB2	2:B:299:ALA:CA	2.29	0.46
2:B:970:PHE:CD1	2:B:1080:PHE:CZ	3.02	0.46
2:B:1204:PHE:CZ	2:B:1214:LEU:CD1	2.99	0.46
2:B:1336:TYR:N	2:B:1336:TYR:CD1	2.83	0.46
1:E:27:G:H5'	1:E:28:A:C5'	2.45	0.46
1:E:78:A:H2'	1:E:79:G:C8	2.47	0.46
2:F:62:THR:O	2:F:66:ARG:HG3	2.15	0.46
2:F:271:TYR:CD2	2:F:271:TYR:C	2.93	0.46
2:F:737:ILE:O	2:F:740:THR:HG23	2.15	0.46
2:F:963:VAL:HG21	2:F:990:ASN:HD21	1.76	0.46
2:F:1091:GLN:NE2	2:F:1091:GLN:C	2.73	0.46
2:F:1145:VAL:O	2:F:1145:VAL:HG23	2.15	0.46
2:F:1204:PHE:CZ	2:F:1214:LEU:CD1	2.99	0.46
1:A:87:G:H1	1:A:91:C:H42	1.63	0.46
2:B:637:LYS:O	2:B:640:ALA:HB3	2.15	0.46
1:E:17:G:HO2'	2:F:168:PHE:HE1	1.59	0.46
2:F:1302:ILE:O	2:F:1306:ALA:HB2	2.12	0.46
2:B:107:VAL:HG23	2:B:110:ASP:HB3	1.98	0.46
2:B:244:LEU:HD12	2:B:250:PRO:CG	2.45	0.46
2:B:940:ASN:N	2:B:940:ASN:ND2	2.60	0.46
2:B:1092:VAL:HG13	2:B:1094:ILE:HG12	1.96	0.46
2:F:469:SER:HB3	2:F:471:GLU:HG2	1.96	0.46
2:F:1298:ARG:HH11	2:F:1298:ARG:HG3	1.81	0.46
1:A:78:A:H2'	1:A:79:G:C8	2.47	0.46
2:B:229:LEU:CD2	2:B:232:GLU:HB2	2.43	0.46
2:B:992:VAL:HA	2:B:995:THR:OG1	2.16	0.46
2:B:1252:ASN:HD22	2:B:1252:ASN:H	1.61	0.46
2:B:1298:ARG:HG3	2:B:1298:ARG:HH11	1.81	0.46
1:E:27:G:N2	1:E:44:U:OP2	2.49	0.46
2:F:32:PHE:O	2:F:42:SER:HB2	2.15	0.46
2:F:324:ARG:CZ	2:F:400:ARG:HG2	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:477:ASN:ND2	2:F:481:VAL:HG21	2.30	0.46
2:F:679:ILE:HG12	2:F:704:PHE:HE1	1.71	0.46
2:F:844:GLN:NE2	2:F:848:LYS:CG	2.73	0.46
2:F:1092:VAL:HG13	2:F:1094:ILE:HG12	1.96	0.46
2:F:1252:ASN:HD22	2:F:1252:ASN:H	1.61	0.46
1:A:65:A:C5	1:A:66:U:C4	3.04	0.46
2:B:477:ASN:ND2	2:B:481:VAL:HG21	2.30	0.46
2:B:687:GLY:HA3	2:B:689:ALA:O	2.16	0.46
2:F:165:ARG:NH2	2:F:168:PHE:HZ	2.06	0.46
2:F:1122:ARG:HD3	2:F:1134:PHE:CZ	2.50	0.46
2:F:1336:TYR:N	2:F:1336:TYR:CD1	2.83	0.46
1:A:27:G:N2	1:A:44:U:OP2	2.49	0.46
2:B:32:PHE:O	2:B:42:SER:HB2	2.15	0.46
2:B:272:ASP:O	2:B:276:ASP:HB2	2.16	0.46
2:B:469:SER:HB3	2:B:471:GLU:HG2	1.96	0.46
2:B:923:GLU:OE2	2:B:925:ARG:NH2	2.46	0.46
2:B:1122:ARG:HD3	2:B:1134:PHE:CZ	2.50	0.46
2:B:1257:LEU:N	2:B:1257:LEU:CD1	2.73	0.46
2:F:338:LEU:CD1	2:F:384:ASP:O	2.64	0.46
2:F:637:LYS:O	2:F:640:ALA:HB3	2.15	0.46
2:F:992:VAL:HA	2:F:995:THR:OG1	2.16	0.46
2:B:393:LEU:HB2	2:B:398:LEU:CD1	2.46	0.45
2:B:531:THR:OG1	2:B:532:GLU:N	2.49	0.45
2:B:655:ARG:H	2:B:655:ARG:HG2	1.46	0.45
2:B:864:ARG:O	2:B:875:VAL:HG21	2.16	0.45
2:B:1100:VAL:HG13	2:B:1140:ALA:O	2.16	0.45
2:F:165:ARG:C	2:F:415:HIS:ND1	2.74	0.45
2:F:393:LEU:HB2	2:F:398:LEU:CD1	2.46	0.45
2:F:393:LEU:HA	2:F:398:LEU:HB2	1.98	0.45
2:F:531:THR:OG1	2:F:532:GLU:N	2.49	0.45
2:F:864:ARG:O	2:F:875:VAL:HG21	2.16	0.45
2:F:1257:LEU:CD1	2:F:1257:LEU:N	2.73	0.45
2:B:963:VAL:HG21	2:B:990:ASN:HD21	1.76	0.45
1:E:65:A:C5	1:E:66:U:C4	3.04	0.45
2:F:223:GLU:HA	2:F:226:ILE:HG12	1.98	0.45
2:F:272:ASP:O	2:F:276:ASP:HB2	2.16	0.45
2:F:350:ILE:CG2	2:F:351:PHE:CD2	2.99	0.45
2:F:1206:LEU:CD1	2:F:1210:ARG:CZ	2.94	0.45
3:G:6:DC:H2''	3:G:7:DC:O5'	2.15	0.45
2:B:154:ILE:O	2:B:155:TYR:C	2.58	0.45
2:B:165:ARG:C	2:B:415:HIS:ND1	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:ILE:CG2	2:B:351:PHE:CD2	2.99	0.45
2:B:691:ARG:HB2	2:B:691:ARG:HE	1.62	0.45
2:B:1335:ARG:C	2:B:1336:TYR:HD1	2.24	0.45
2:F:78:ARG:CD	2:F:165:ARG:HH11	2.26	0.45
2:F:320:SER:O	2:F:323:LYS:HB3	2.17	0.45
2:F:457:ARG:HB2	2:F:467:ARG:NH1	2.32	0.45
2:F:603:ASP:OD1	2:F:606:PHE:HB2	2.16	0.45
2:F:680:LEU:HD12	2:F:680:LEU:HA	1.76	0.45
2:F:923:GLU:OE2	2:F:925:ARG:NH2	2.46	0.45
2:F:1100:VAL:HG13	2:F:1140:ALA:O	2.16	0.45
1:A:64:U:OP1	2:B:1102:THR:OG1	2.26	0.45
2:B:393:LEU:HA	2:B:398:LEU:HB2	1.98	0.45
2:B:452:VAL:HG13	2:B:482:VAL:HG11	1.98	0.45
2:B:457:ARG:HB2	2:B:467:ARG:NH1	2.32	0.45
2:B:568:TYR:HD2	2:B:569:PHE:CD2	2.35	0.45
2:B:603:ASP:OD1	2:B:606:PHE:HB2	2.15	0.45
2:B:679:ILE:HA	2:B:682:PHE:HB2	1.99	0.45
2:B:839:ASP:O	2:B:856:VAL:N	2.47	0.45
2:B:1206:LEU:CD1	2:B:1210:ARG:CZ	2.94	0.45
2:B:1304:GLU:C	2:B:1327:PHE:HE1	2.24	0.45
3:C:6:DC:H2''	3:C:7:DC:O5'	2.15	0.45
4:D:7:DG:C2	4:D:8:DT:C2	3.04	0.45
2:F:27:VAL:CG1	2:F:1086:VAL:CG1	2.88	0.45
2:F:184:LEU:HD12	2:F:296:LEU:CA	2.34	0.45
2:F:452:VAL:HG13	2:F:482:VAL:HG11	1.98	0.45
2:F:679:ILE:HA	2:F:682:PHE:HB2	1.99	0.45
2:F:1304:GLU:C	2:F:1327:PHE:HE1	2.24	0.45
1:A:53:G:C4	1:A:62:G:N2	2.84	0.45
2:B:223:GLU:HA	2:B:226:ILE:HG12	1.98	0.45
2:B:234:LYS:HD3	2:B:235:ASN:CG	2.41	0.45
2:B:277:ASN:ND2	2:B:653:ARG:CD	2.75	0.45
2:B:596:ASP:CG	2:B:656:TYR:OH	2.53	0.45
2:F:94:ASP:CB	2:F:152:ARG:HD3	2.47	0.45
2:F:492:ILE:O	2:F:496:THR:HG23	2.16	0.45
2:F:568:TYR:HD2	2:F:569:PHE:CD2	2.35	0.45
4:H:7:DG:C2	4:H:8:DT:C2	3.04	0.45
2:B:94:ASP:CB	2:B:152:ARG:HD3	2.47	0.45
2:B:520:VAL:HG21	2:B:591:LEU:HD23	1.98	0.45
2:B:949:LEU:HD23	2:B:951:ARG:NH2	2.32	0.45
2:F:311:GLU:N	2:F:311:GLU:CD	2.73	0.45
2:F:341:GLN:HE21	2:F:341:GLN:C	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:655:ARG:H	2:F:655:ARG:HG2	1.46	0.45
2:F:740:THR:O	2:F:743:VAL:HB	2.17	0.45
2:F:838:VAL:HG23	2:F:857:LEU:CD1	2.46	0.45
2:F:1335:ARG:C	2:F:1336:TYR:HD1	2.25	0.45
1:A:17:G:HO2'	2:B:168:PHE:HE1	1.60	0.45
2:B:78:ARG:CD	2:B:165:ARG:HH11	2.26	0.45
2:B:184:LEU:CD1	2:B:295:ASN:C	2.90	0.45
2:B:311:GLU:N	2:B:311:GLU:CD	2.73	0.45
2:B:341:GLN:HE21	2:B:341:GLN:C	2.25	0.45
2:B:740:THR:O	2:B:743:VAL:HB	2.17	0.45
2:B:838:VAL:HG23	2:B:857:LEU:CD1	2.46	0.45
2:B:1113:LYS:O	2:B:1113:LYS:HG3	2.16	0.45
2:B:1257:LEU:O	2:B:1261:GLN:N	2.43	0.45
2:F:184:LEU:CD1	2:F:295:ASN:C	2.90	0.45
2:F:244:LEU:O	2:F:246:LEU:O	2.35	0.45
2:F:520:VAL:HG21	2:F:591:LEU:HD23	1.97	0.45
2:F:949:LEU:HD23	2:F:951:ARG:NH2	2.32	0.45
2:B:118:ILE:HG22	2:B:119:PHE:CE2	2.52	0.45
2:B:492:ILE:O	2:B:496:THR:HG23	2.16	0.45
2:B:514:LEU:O	2:B:515:TYR:C	2.58	0.45
2:B:756:PRO:HD2	2:B:953:VAL:CG2	2.47	0.45
2:B:1062:LEU:HD21	2:B:1063:ILE:CG1	2.39	0.45
1:E:53:G:C4	1:E:62:G:N2	2.84	0.45
2:F:93:VAL:CG2	2:F:151:LEU:HD23	2.47	0.45
2:F:154:ILE:O	2:F:155:TYR:C	2.58	0.45
2:F:841:ILE:CD1	2:F:900:LEU:HD21	2.47	0.45
2:F:1113:LYS:HG3	2:F:1113:LYS:O	2.16	0.45
2:F:1210:ARG:NH2	2:F:1341:GLU:OE1	2.17	0.45
2:B:184:LEU:HD12	2:B:296:LEU:CA	2.34	0.45
2:B:473:ILE:HG12	2:B:481:VAL:HG11	1.98	0.45
2:B:474:THR:O	2:B:475:PRO:C	2.59	0.45
2:B:825:ASP:HB2	2:B:879:MET:HE3	1.02	0.45
2:B:830:ILE:HD13	2:B:831:ASN:N	2.31	0.45
2:B:841:ILE:CD1	2:B:900:LEU:HD21	2.46	0.45
2:B:847:LEU:O	2:B:847:LEU:HD23	2.17	0.45
2:F:207:ASP:CB	2:F:210:ALA:CB	2.56	0.45
2:F:277:ASN:ND2	2:F:653:ARG:CD	2.75	0.45
2:F:525:THR:HG23	2:F:545:LYS:HZ1	1.82	0.45
2:F:610:GLU:O	2:F:613:GLU:HB3	2.17	0.45
2:F:756:PRO:HD2	2:F:953:VAL:CG2	2.47	0.45
2:F:784:ILE:O	2:F:788:ILE:CG1	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:839:ASP:O	2:F:856:VAL:N	2.47	0.45
2:B:977:GLU:HG3	2:B:1310:ILE:HG21	1.95	0.45
2:B:1108:GLU:HG3	3:C:9:DC:H5''	1.99	0.45
2:F:118:ILE:HG22	2:F:119:PHE:CE2	2.52	0.45
2:B:186:ILE:HD13	2:B:186:ILE:HA	1.86	0.44
2:B:450:TYR:OH	2:B:627:GLU:HG3	2.17	0.44
2:B:610:GLU:O	2:B:613:GLU:HB3	2.17	0.44
2:B:782:LYS:O	2:B:786:GLU:HG3	2.17	0.44
2:B:1210:ARG:NH2	2:B:1341:GLU:OE1	2.17	0.44
2:F:49:GLY:HA2	2:F:1092:VAL:CG2	2.47	0.44
2:F:234:LYS:HD3	2:F:235:ASN:CG	2.41	0.44
2:F:519:THR:OG1	2:F:589:ALA:HB2	2.16	0.44
2:F:553:PHE:CE1	2:F:559:VAL:CG2	3.00	0.44
2:F:596:ASP:CG	2:F:656:TYR:OH	2.53	0.44
2:F:812:TYR:CD1	2:F:812:TYR:O	2.71	0.44
2:F:945:GLU:N	2:F:945:GLU:CD	2.73	0.44
2:F:979:ASN:OD1	2:F:981:TYR:HD1	1.98	0.44
2:F:1108:GLU:HG3	3:G:9:DC:H5''	1.99	0.44
1:A:63:U:HO2'	2:B:62:THR:HG23	1.73	0.44
2:B:812:TYR:O	2:B:812:TYR:CD1	2.71	0.44
2:B:945:GLU:N	2:B:945:GLU:CD	2.73	0.44
2:B:1108:GLU:CG	3:C:9:DC:H5''	2.47	0.44
2:F:206:VAL:O	2:F:206:VAL:HG23	2.17	0.44
2:F:473:ILE:HG12	2:F:481:VAL:HG11	1.98	0.44
2:F:606:PHE:CE2	2:F:612:ASN:OD1	2.70	0.44
2:F:830:ILE:HD13	2:F:831:ASN:N	2.31	0.44
2:F:838:VAL:HG23	2:F:857:LEU:HD12	1.99	0.44
2:F:847:LEU:O	2:F:847:LEU:HD23	2.17	0.44
2:F:1143:VAL:HG22	2:F:1197:LYS:HA	1.98	0.44
2:B:49:GLY:HA2	2:B:1092:VAL:CG2	2.47	0.44
2:B:207:ASP:CB	2:B:210:ALA:CB	2.56	0.44
2:B:553:PHE:CE1	2:B:559:VAL:CG2	3.00	0.44
2:B:784:ILE:O	2:B:788:ILE:CG1	2.64	0.44
2:B:838:VAL:HG23	2:B:857:LEU:HD12	2.00	0.44
2:B:874:GLU:C	2:B:877:LYS:HG3	2.41	0.44
2:B:902:LYS:HE3	2:B:907:GLY:O	2.17	0.44
2:F:45:LYS:HE3	2:F:45:LYS:HB3	1.78	0.44
2:F:474:THR:O	2:F:475:PRO:C	2.59	0.44
2:F:514:LEU:O	2:F:515:TYR:C	2.58	0.44
2:F:746:GLU:O	2:F:750:VAL:N	2.33	0.44
2:F:782:LYS:O	2:F:786:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1062:LEU:HD21	2:F:1063:ILE:CG1	2.39	0.44
2:F:1076:LYS:O	2:F:1080:PHE:CD2	2.70	0.44
2:F:1257:LEU:O	2:F:1261:GLN:N	2.43	0.44
2:B:20:VAL:O	2:B:27:VAL:HG23	2.18	0.44
2:B:206:VAL:O	2:B:206:VAL:HG23	2.18	0.44
2:B:256:PHE:CE2	2:B:282:ILE:HD13	2.53	0.44
2:B:519:THR:OG1	2:B:589:ALA:HB2	2.16	0.44
2:B:606:PHE:CE2	2:B:612:ASN:OD1	2.70	0.44
2:B:923:GLU:HG2	2:B:928:THR:OG1	2.17	0.44
2:B:1076:LYS:O	2:B:1080:PHE:CD2	2.70	0.44
2:B:1143:VAL:HG22	2:B:1197:LYS:HA	1.98	0.44
2:F:20:VAL:O	2:F:27:VAL:HG23	2.18	0.44
2:F:249:THR:HG23	2:F:265:GLN:HE22	1.81	0.44
2:F:265:GLN:O	2:F:271:TYR:HD1	2.00	0.44
2:F:450:TYR:OH	2:F:627:GLU:HG3	2.17	0.44
2:F:623:LEU:HD12	2:F:623:LEU:HA	1.51	0.44
2:F:974:LYS:HE2	2:F:982:HIS:CD2	2.53	0.44
2:F:979:ASN:ND2	2:F:981:TYR:CB	2.80	0.44
2:B:666:LEU:HA	2:B:666:LEU:HD23	1.63	0.44
2:B:678:THR:O	2:B:682:PHE:N	2.42	0.44
2:B:974:LYS:HE2	2:B:982:HIS:CD2	2.53	0.44
2:B:1122:ARG:CG	2:B:1134:PHE:HE2	2.31	0.44
3:C:2:DA:H1'	3:C:3:DA:OP1	2.18	0.44
1:E:78:A:C5	1:E:79:G:N7	2.85	0.44
2:F:89:GLU:OE1	2:F:92:LYS:HD2	2.16	0.44
2:F:550:ASP:HA	2:F:554:LYS:HG3	1.98	0.44
2:F:691:ARG:HB2	2:F:691:ARG:HE	1.62	0.44
2:F:692:ASN:CB	2:F:695:GLN:HG3	2.45	0.44
2:F:902:LYS:HE3	2:F:907:GLY:O	2.17	0.44
2:F:1250:GLU:C	2:F:1254:GLN:OE1	2.60	0.44
3:G:2:DA:H1'	3:G:3:DA:OP1	2.18	0.44
2:B:692:ASN:CB	2:B:695:GLN:HG3	2.45	0.44
2:F:256:PHE:CE2	2:F:282:ILE:HD13	2.53	0.44
2:F:874:GLU:C	2:F:877:LYS:HG3	2.41	0.44
2:F:923:GLU:HG2	2:F:928:THR:OG1	2.17	0.44
2:F:1108:GLU:CG	3:G:9:DC:H5''	2.47	0.44
2:F:1122:ARG:CG	2:F:1134:PHE:HE2	2.31	0.44
1:A:24:U:O2	2:B:105:PHE:CE1	2.63	0.44
2:B:106:LEU:HD23	2:B:110:ASP:HB3	1.99	0.44
2:B:156:LEU:HD23	2:B:156:LEU:HA	1.80	0.44
2:B:265:GLN:O	2:B:271:TYR:HD1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:780:ARG:NH1	2:B:812:TYR:CE2	2.66	0.44
2:B:1243:GLU:C	2:B:1244:LYS:CD	2.86	0.44
2:B:1250:GLU:C	2:B:1254:GLN:OE1	2.60	0.44
2:B:1291:LEU:HD23	2:B:1291:LEU:HA	1.82	0.44
2:F:186:ILE:HD13	2:F:186:ILE:HA	1.86	0.44
2:F:386:THR:OG1	2:F:389:LEU:HB2	2.18	0.44
2:F:431:PRO:O	2:F:434:LYS:HG2	2.17	0.44
2:F:513:LEU:O	2:F:516:GLU:HB2	2.18	0.44
2:F:568:TYR:CZ	2:F:573:GLU:OE2	2.70	0.44
2:F:1185:LYS:HA	2:F:1185:LYS:HD2	1.77	0.44
2:F:1292:SER:CA	2:F:1296:LYS:HE3	2.48	0.44
1:A:45:U:C5'	2:B:402:GLN:HG2	2.43	0.44
1:A:61:C:OP1	2:B:70:ARG:CZ	2.66	0.44
1:A:94:U:H2'	1:A:95:G:C8	2.53	0.44
2:B:393:LEU:C	2:B:393:LEU:CD2	2.85	0.44
2:B:530:VAL:O	2:B:578:VAL:HG23	2.18	0.44
2:B:550:ASP:HA	2:B:554:LYS:HG3	1.99	0.44
2:B:568:TYR:CZ	2:B:573:GLU:OE2	2.70	0.44
2:B:1203:LEU:HD13	2:B:1213:MET:HG3	1.97	0.44
1:E:61:C:OP1	2:F:70:ARG:CZ	2.66	0.44
1:E:63:U:HO2'	2:F:62:THR:HG23	1.73	0.44
2:F:351:PHE:N	2:F:351:PHE:HD2	2.16	0.44
2:F:678:THR:O	2:F:682:PHE:N	2.42	0.44
2:F:975:VAL:HG23	2:F:1233:VAL:HG12	2.00	0.44
2:F:1203:LEU:HD13	2:F:1213:MET:HG3	1.97	0.44
2:F:1243:GLU:C	2:F:1244:LYS:CD	2.86	0.44
2:F:1291:LEU:HD23	2:F:1291:LEU:HA	1.82	0.44
1:A:53:G:OP1	2:B:1123:LYS:HG3	2.18	0.44
1:A:78:A:C5	1:A:79:G:N7	2.85	0.44
2:B:89:GLU:OE1	2:B:92:LYS:HD2	2.16	0.44
2:B:248:LEU:HD13	2:B:248:LEU:HA	1.77	0.44
2:B:513:LEU:O	2:B:516:GLU:HB2	2.18	0.44
1:E:45:U:C5'	2:F:402:GLN:HG2	2.43	0.44
1:E:94:U:H2'	1:E:95:G:C8	2.53	0.44
2:F:10:ALA:O	2:F:17:GLY:N	2.45	0.44
2:F:342:GLN:OE1	2:F:384:ASP:CA	2.66	0.44
2:F:530:VAL:O	2:F:578:VAL:HG23	2.18	0.44
2:F:1360:ILE:HG22	2:F:1362:LEU:HD23	2.00	0.44
1:A:64:U:O5'	1:A:64:U:H6	2.01	0.43
2:B:70:ARG:HH11	2:B:454:PRO:HG3	1.78	0.43
2:B:317:LEU:CD2	2:B:414:ILE:CD1	2.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:PRO:O	2:B:434:LYS:HG2	2.17	0.43
2:B:679:ILE:HG12	2:B:704:PHE:HE1	1.71	0.43
2:B:1235:PHE:CE2	2:B:1266:LEU:CD1	3.01	0.43
2:B:1292:SER:CA	2:B:1296:LYS:HE3	2.48	0.43
2:B:1360:ILE:HG22	2:B:1362:LEU:HD23	2.00	0.43
2:F:184:LEU:CD1	2:F:295:ASN:O	2.67	0.43
2:F:317:LEU:CD2	2:F:414:ILE:CD1	2.95	0.43
2:F:342:GLN:HB2	2:F:383:MET:HE3	1.98	0.43
2:F:825:ASP:HB2	2:F:879:MET:HE3	1.02	0.43
2:F:1219:GLU:HG3	2:F:1220:LEU:H	1.83	0.43
2:B:184:LEU:CD1	2:B:295:ASN:O	2.67	0.43
2:B:568:TYR:CD2	2:B:569:PHE:CD2	3.06	0.43
2:B:649:LYS:HA	2:B:652:LYS:HD3	2.00	0.43
2:B:874:GLU:HA	2:B:877:LYS:CD	2.42	0.43
2:B:1219:GLU:HG3	2:B:1220:LEU:H	1.84	0.43
1:E:64:U:H6	1:E:64:U:O5'	2.01	0.43
2:F:341:GLN:HE21	2:F:342:GLN:N	2.16	0.43
2:F:345:GLU:HG2	2:F:346:LYS:H	1.83	0.43
2:F:568:TYR:CD2	2:F:569:PHE:CD2	3.06	0.43
2:F:1235:PHE:CE2	2:F:1266:LEU:CD1	3.01	0.43
1:A:24:U:C1'	2:B:105:PHE:HE1	2.27	0.43
2:B:94:ASP:HB2	2:B:152:ARG:HH11	1.83	0.43
2:B:345:GLU:HG2	2:B:346:LYS:H	1.83	0.43
2:B:541:SER:H	2:B:544:GLN:CD	2.26	0.43
2:B:944:ASP:OD1	2:B:948:LYS:O	2.36	0.43
2:B:1031:LYS:NZ	2:B:1031:LYS:HB2	2.32	0.43
2:F:248:LEU:HD22	2:F:248:LEU:HA	1.83	0.43
2:F:291:LEU:HD23	2:F:292:ALA:N	2.33	0.43
2:F:374:LYS:O	2:F:374:LYS:HG2	2.18	0.43
2:F:641:HIS:CD2	2:F:642:LEU:N	2.87	0.43
2:F:882:TYR:CD2	2:F:882:TYR:C	2.96	0.43
2:F:944:ASP:OD1	2:F:948:LYS:O	2.36	0.43
2:F:1216:SER:CB	4:H:6:DG:C3'	2.96	0.43
1:A:15:U:H5''	2:B:70:ARG:NH1	2.33	0.43
2:B:45:LYS:HE3	2:B:45:LYS:HB3	1.77	0.43
2:B:291:LEU:HD23	2:B:292:ALA:N	2.33	0.43
2:B:328:HIS:O	2:B:332:LEU:N	2.51	0.43
2:B:374:LYS:HG2	2:B:374:LYS:O	2.18	0.43
2:B:383:MET:HE3	2:B:383:MET:HB3	1.65	0.43
2:B:451:TYR:HA	2:B:491:PHE:CD1	2.53	0.43
2:B:623:LEU:HD12	2:B:623:LEU:HA	1.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:641:HIS:CD2	2:B:642:LEU:N	2.87	0.43
1:E:53:G:OP1	2:F:1123:LYS:HG3	2.18	0.43
2:F:27:VAL:HG11	2:F:1089:MET:HE1	2.01	0.43
2:F:1251:ASP:CA	2:F:1254:GLN:OE1	2.60	0.43
2:B:27:VAL:HG11	2:B:1089:MET:HE1	2.01	0.43
2:B:882:TYR:CD2	2:B:882:TYR:C	2.96	0.43
2:B:1216:SER:CB	4:D:6:DG:C3'	2.96	0.43
2:F:94:ASP:HB2	2:F:152:ARG:HH11	1.83	0.43
2:F:212:LEU:HD13	2:F:212:LEU:HA	1.79	0.43
2:F:541:SER:H	2:F:544:GLN:CD	2.26	0.43
2:F:649:LYS:HA	2:F:652:LYS:HD3	2.00	0.43
1:A:49:A:P	2:B:76:LYS:HE2	2.58	0.43
1:A:70:C:H2'	1:A:71:U:H6	1.82	0.43
2:B:341:GLN:HE21	2:B:342:GLN:N	2.16	0.43
2:B:594:TYR:OH	2:B:604:LYS:NZ	2.48	0.43
2:B:686:ASP:OD2	2:B:691:ARG:CB	2.63	0.43
2:B:737:ILE:HD13	2:B:931:VAL:HG22	2.00	0.43
2:B:1185:LYS:HA	2:B:1185:LYS:HD2	1.77	0.43
2:B:1325:LYS:HB3	2:B:1330:THR:HA	1.99	0.43
1:E:49:A:P	2:F:76:LYS:HE2	2.58	0.43
2:F:328:HIS:O	2:F:332:LEU:N	2.51	0.43
2:F:541:SER:O	2:F:545:LYS:HG3	2.18	0.43
2:F:780:ARG:NH1	2:F:812:TYR:CE2	2.66	0.43
2:F:1325:LYS:HB3	2:F:1330:THR:HA	1.99	0.43
2:B:212:LEU:HD13	2:B:212:LEU:HA	1.79	0.43
2:B:233:LYS:HG3	2:F:543:GLU:OE1	2.19	0.43
2:B:556:ASN:O	2:B:595:HIS:NE2	2.51	0.43
2:B:851:SER:H	2:B:851:SER:HG	1.48	0.43
1:E:15:U:H5''	2:F:70:ARG:NH1	2.33	0.43
2:F:451:TYR:HA	2:F:491:PHE:CD1	2.53	0.43
2:F:464:TRP:HD1	2:F:490:SER:HB3	1.84	0.43
2:F:708:ILE:O	2:F:709:GLN:C	2.60	0.43
2:F:780:ARG:H	2:F:780:ARG:HG2	1.66	0.43
2:B:296:LEU:C	2:B:296:LEU:CD2	2.85	0.43
2:B:541:SER:O	2:B:545:LYS:HG3	2.18	0.43
2:F:138:LEU:HD21	2:F:153:LEU:HD22	2.00	0.43
2:F:216:LEU:HD23	2:F:216:LEU:H	1.82	0.43
2:F:395:ARG:O	2:F:396:GLU:CB	2.54	0.43
2:B:138:LEU:HD21	2:B:153:LEU:HD22	2.00	0.43
2:B:464:TRP:HD1	2:B:490:SER:HB3	1.84	0.43
2:B:516:GLU:O	2:B:520:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:321:MET:HA	2:F:321:MET:HE2	1.97	0.43
2:F:488:ALA:O	2:F:491:PHE:HB3	2.19	0.43
2:F:556:ASN:O	2:F:595:HIS:NE2	2.51	0.43
2:F:737:ILE:HD13	2:F:931:VAL:HG22	2.00	0.43
2:B:10:ALA:O	2:B:17:GLY:N	2.45	0.43
2:B:167:HIS:ND1	2:B:167:HIS:C	2.77	0.43
2:B:380:LEU:HD11	2:B:398:LEU:HD11	2.00	0.43
2:B:402:GLN:OE1	2:B:402:GLN:HA	2.19	0.43
2:F:156:LEU:HD23	2:F:156:LEU:HA	1.80	0.43
2:F:874:GLU:HA	2:F:877:LYS:CD	2.42	0.43
1:A:36:A:C5	1:A:37:U:H1'	2.54	0.42
2:B:216:LEU:HD23	2:B:216:LEU:H	1.82	0.42
2:B:233:LYS:HE3	2:F:547:ALA:HB2	2.01	0.42
2:B:488:ALA:O	2:B:491:PHE:HB3	2.19	0.42
2:B:625:LEU:HD13	2:B:659:TRP:CH2	2.53	0.42
2:B:708:ILE:O	2:B:709:GLN:C	2.60	0.42
2:B:1292:SER:CB	2:B:1296:LYS:NZ	2.80	0.42
2:B:1324:PHE:O	2:B:1331:ILE:N	2.41	0.42
2:F:256:PHE:CE2	2:F:282:ILE:HG21	2.54	0.42
2:F:1062:LEU:CD2	2:F:1063:ILE:N	2.73	0.42
2:F:1292:SER:CB	2:F:1296:LYS:NZ	2.80	0.42
2:F:1295:ASN:O	2:F:1298:ARG:HG3	2.19	0.42
2:B:256:PHE:CE2	2:B:282:ILE:HG21	2.54	0.42
2:B:765:ARG:HH22	2:B:848:LYS:CE	2.32	0.42
2:B:846:PHE:CZ	2:B:913:LYS:HD3	2.55	0.42
2:B:1235:PHE:CZ	2:B:1266:LEU:HD13	2.53	0.42
2:B:1251:ASP:CA	2:B:1254:GLN:OE1	2.60	0.42
2:B:1295:ASN:O	2:B:1298:ARG:HG3	2.19	0.42
1:E:12:U:H2'	1:E:13:A:H8	1.84	0.42
1:E:36:A:C5	1:E:37:U:H1'	2.54	0.42
1:E:70:C:H2'	1:E:71:U:H6	1.82	0.42
2:F:70:ARG:HH11	2:F:454:PRO:HG3	1.78	0.42
2:F:167:HIS:ND1	2:F:167:HIS:C	2.77	0.42
2:F:207:ASP:O	2:F:208:ALA:C	2.61	0.42
2:F:234:LYS:CD	2:F:235:ASN:ND2	2.79	0.42
2:F:324:ARG:CZ	2:F:400:ARG:CD	2.97	0.42
2:F:594:TYR:OH	2:F:604:LYS:NZ	2.48	0.42
2:F:846:PHE:CZ	2:F:913:LYS:HD3	2.55	0.42
2:F:856:VAL:HG12	2:F:857:LEU:N	2.34	0.42
2:F:1265:TYR:O	2:F:1268:GLU:HB2	2.18	0.42
1:A:27:G:H1'	2:B:129:HIS:ND1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:U:H2'	1:A:32:A:O4'	2.20	0.42
1:A:48:A:H2'	1:A:49:A:C8	2.55	0.42
2:B:207:ASP:O	2:B:208:ALA:C	2.61	0.42
2:B:312:ILE:H	2:B:312:ILE:HG13	1.68	0.42
2:B:359:TYR:CZ	2:B:363:ILE:HD11	2.54	0.42
2:B:388:GLU:O	2:B:391:VAL:N	2.52	0.42
2:B:398:LEU:C	2:B:398:LEU:CD2	2.92	0.42
2:B:849:ASP:OD2	2:B:854:ASN:CB	2.67	0.42
2:B:856:VAL:HG12	2:B:857:LEU:N	2.34	0.42
2:B:1002:PRO:O	2:B:1005:GLU:HB2	2.19	0.42
2:F:380:LEU:HD11	2:F:398:LEU:HD11	2.00	0.42
2:F:393:LEU:C	2:F:393:LEU:CD2	2.85	0.42
2:F:402:GLN:OE1	2:F:402:GLN:HA	2.20	0.42
2:F:516:GLU:O	2:F:520:VAL:HG23	2.18	0.42
2:F:625:LEU:HD13	2:F:659:TRP:CH2	2.53	0.42
2:F:849:ASP:OD2	2:F:854:ASN:CB	2.67	0.42
2:F:1002:PRO:O	2:F:1005:GLU:HB2	2.19	0.42
2:F:1235:PHE:CZ	2:F:1266:LEU:HD13	2.53	0.42
1:A:12:U:H2'	1:A:13:A:H8	1.84	0.42
2:B:234:LYS:CD	2:B:235:ASN:ND2	2.79	0.42
2:B:423:LEU:HD12	2:B:437:ARG:HG3	2.00	0.42
2:B:979:ASN:CG	2:B:981:TYR:HB2	2.44	0.42
2:B:1062:LEU:CD2	2:B:1063:ILE:N	2.73	0.42
2:B:1105:PHE:O	2:B:1137:PRO:HA	2.20	0.42
2:B:1114:ARG:HH12	4:D:9:DA:P	2.41	0.42
1:E:27:G:H1'	2:F:129:HIS:ND1	2.34	0.42
1:E:31:U:H2'	1:E:32:A:O4'	2.20	0.42
2:F:63:ARG:HA	2:F:66:ARG:HD3	2.01	0.42
2:F:148:LYS:N	2:F:429:PHE:CZ	2.81	0.42
2:F:380:LEU:O	2:F:386:THR:HG21	2.20	0.42
2:F:423:LEU:HD12	2:F:437:ARG:HG3	2.00	0.42
2:F:765:ARG:HH22	2:F:848:LYS:CE	2.32	0.42
2:F:1105:PHE:O	2:F:1137:PRO:HA	2.20	0.42
2:B:333:THR:O	2:B:337:ALA:CB	2.67	0.42
2:B:451:TYR:O	2:B:464:TRP:NE1	2.51	0.42
2:B:499:ASP:HB3	2:B:502:LEU:O	2.19	0.42
1:E:45:U:HO2'	2:F:135:ILE:H	1.67	0.42
1:E:48:A:H2'	1:E:49:A:C8	2.55	0.42
2:F:224:ASN:O	2:F:228:GLN:NE2	2.52	0.42
2:F:253:LYS:HB2	2:F:262:ALA:H	1.84	0.42
2:F:398:LEU:C	2:F:398:LEU:CD2	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:U:HO2'	2:B:135:ILE:H	1.67	0.42
2:B:63:ARG:HA	2:B:66:ARG:HD3	2.01	0.42
2:B:448:ILE:H	2:B:448:ILE:HG13	1.69	0.42
1:E:24:U:C1'	2:F:105:PHE:HE1	2.27	0.42
2:F:173:ASP:O	2:F:174:LEU:HD12	2.19	0.42
2:F:451:TYR:O	2:F:464:TRP:NE1	2.51	0.42
2:F:756:PRO:O	2:F:953:VAL:HG22	2.20	0.42
2:F:796:LEU:HD23	2:F:796:LEU:HA	1.80	0.42
2:F:1221:GLN:HE21	2:F:1320:ALA:HB2	1.79	0.42
2:F:1324:PHE:O	2:F:1331:ILE:N	2.41	0.42
2:B:224:ASN:O	2:B:228:GLN:NE2	2.52	0.42
2:F:78:ARG:HG2	2:F:443:ILE:HG23	2.01	0.42
2:F:499:ASP:HB3	2:F:502:LEU:O	2.19	0.42
2:F:883:TRP:CZ3	2:F:900:LEU:HB3	2.54	0.42
2:F:974:LYS:NZ	2:F:976:ARG:NH1	2.68	0.42
2:F:1232:TYR:OH	2:F:1268:GLU:HB3	2.20	0.42
2:F:1245:LEU:HD13	2:F:1252:ASN:OD1	2.20	0.42
2:B:249:THR:CG2	2:B:265:GLN:HE21	2.28	0.42
2:B:253:LYS:HB2	2:B:262:ALA:H	1.84	0.42
2:B:756:PRO:O	2:B:953:VAL:HG22	2.20	0.42
2:F:139:ARG:HH22	2:F:415:HIS:CD2	2.37	0.42
2:F:155:TYR:C	2:F:155:TYR:CD2	2.98	0.42
2:F:324:ARG:CZ	2:F:400:ARG:CG	2.98	0.42
2:F:333:THR:O	2:F:337:ALA:CB	2.67	0.42
2:F:448:ILE:H	2:F:448:ILE:HG13	1.69	0.42
2:F:1000:LYS:CE	2:F:1045:PHE:CD2	2.96	0.42
2:F:1114:ARG:HH12	4:H:9:DA:P	2.41	0.42
1:A:42:A:HO2'	1:A:43:G:P	2.42	0.42
1:A:43:G:O2'	2:B:363:ILE:HG13	2.19	0.42
2:B:48:ILE:HD11	2:B:984:ALA:O	2.19	0.42
2:B:119:PHE:CD2	2:B:119:PHE:N	2.87	0.42
2:B:155:TYR:C	2:B:155:TYR:CD2	2.98	0.42
2:B:351:PHE:N	2:B:351:PHE:HD2	2.16	0.42
2:F:48:ILE:HD11	2:F:984:ALA:O	2.19	0.42
2:F:66:ARG:NH2	2:F:462:PHE:CE2	2.61	0.42
2:F:255:ASN:HD22	2:F:256:PHE:HE1	1.65	0.42
2:F:829:ASP:OD1	2:F:831:ASN:N	2.53	0.42
2:F:1295:ASN:OD1	2:F:1298:ARG:NH2	2.53	0.42
2:B:78:ARG:HG2	2:B:443:ILE:HG23	2.02	0.42
2:B:139:ARG:HH22	2:B:415:HIS:CD2	2.37	0.42
2:B:173:ASP:O	2:B:174:LEU:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:ARG:O	2:B:396:GLU:CB	2.53	0.42
2:B:429:PHE:HD2	2:B:429:PHE:H	1.68	0.42
2:B:739:GLN:OE1	2:B:1352:ILE:HD11	2.19	0.42
2:B:883:TRP:CZ3	2:B:900:LEU:HB3	2.54	0.42
2:B:1205:GLU:HB2	2:B:1211:LYS:HG3	2.02	0.42
2:B:1220:LEU:CD2	2:B:1342:VAL:HG21	2.50	0.42
2:B:1245:LEU:HD13	2:B:1252:ASN:OD1	2.20	0.42
2:B:1295:ASN:OD1	2:B:1298:ARG:NH2	2.53	0.42
3:C:3:DA:H2''	3:C:4:DT:O5'	2.20	0.42
2:F:421:ALA:O	2:F:425:ARG:HB2	2.19	0.42
2:F:423:LEU:N	2:F:423:LEU:CD2	2.82	0.42
2:F:503:PRO:CD	2:F:711:ALA:HB1	2.50	0.42
2:F:506:LYS:H	2:F:506:LYS:HG2	1.65	0.42
2:F:683:LEU:HA	2:F:683:LEU:HD23	1.70	0.42
2:F:1240:SER:OG	2:F:1310:ILE:HD12	2.20	0.42
2:B:86:PHE:CE2	2:B:155:TYR:HB2	2.55	0.41
2:B:421:ALA:O	2:B:425:ARG:HB2	2.19	0.41
2:B:760:VAL:HG11	2:B:990:ASN:O	2.20	0.41
2:B:829:ASP:OD1	2:B:831:ASN:N	2.53	0.41
2:B:1000:LYS:CE	2:B:1045:PHE:CD2	2.96	0.41
2:B:1154:SER:O	2:B:1155:LYS:HB2	2.20	0.41
2:B:1212:ARG:CZ	2:B:1336:TYR:CE2	3.01	0.41
2:B:1213:MET:O	2:B:1221:GLN:N	2.52	0.41
1:E:10:U:H2'	1:E:11:C:C6	2.55	0.41
1:E:43:G:O2'	2:F:363:ILE:HG13	2.19	0.41
2:F:1212:ARG:NH2	2:F:1280:VAL:O	2.53	0.41
3:G:3:DA:H2''	3:G:4:DT:O5'	2.20	0.41
1:A:10:U:H2'	1:A:11:C:C6	2.55	0.41
1:A:92:G:C2	1:A:93:G:C4	3.08	0.41
2:B:244:LEU:HD11	2:B:264:LEU:O	2.19	0.41
2:B:256:PHE:CD2	2:B:282:ILE:HG21	2.54	0.41
2:B:780:ARG:H	2:B:780:ARG:HG2	1.67	0.41
2:B:1204:PHE:CE2	2:B:1342:VAL:HG11	2.55	0.41
2:F:119:PHE:CD2	2:F:119:PHE:N	2.87	0.41
2:F:336:LYS:CG	2:F:347:TYR:HE2	2.32	0.41
2:F:429:PHE:HD2	2:F:429:PHE:H	1.68	0.41
2:F:739:GLN:OE1	2:F:1352:ILE:HD11	2.19	0.41
2:B:423:LEU:N	2:B:423:LEU:CD2	2.82	0.41
2:B:447:ARG:HG2	2:B:448:ILE:O	2.20	0.41
2:B:535:ARG:HG2	2:B:536:LYS:H	1.86	0.41
2:B:1000:LYS:CG	2:B:1073:VAL:HG11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:G:C2	1:E:93:G:C4	3.08	0.41
2:F:86:PHE:CE2	2:F:155:TYR:HB2	2.55	0.41
2:F:286:TYR:O	2:F:289:LEU:HB2	2.21	0.41
2:F:760:VAL:HG11	2:F:990:ASN:O	2.20	0.41
2:F:1000:LYS:HE2	2:F:1064:GLU:CB	2.44	0.41
2:F:1118:LYS:HA	2:F:1118:LYS:HD3	1.79	0.41
2:F:1154:SER:O	2:F:1155:LYS:HB2	2.20	0.41
2:F:1220:LEU:CD2	2:F:1342:VAL:HG21	2.50	0.41
2:B:286:TYR:O	2:B:289:LEU:HB2	2.20	0.41
2:B:1000:LYS:HE2	2:B:1064:GLU:CB	2.44	0.41
2:B:1141:TYR:OH	2:B:1175:GLU:OE2	2.21	0.41
2:B:1153:LYS:O	2:B:1155:LYS:HG3	2.20	0.41
2:B:1178:PRO:O	2:B:1182:LEU:N	2.42	0.41
2:B:1212:ARG:NH2	2:B:1280:VAL:O	2.53	0.41
2:B:1240:SER:OG	2:B:1310:ILE:HD12	2.20	0.41
3:C:5:DA:C2	4:D:9:DA:C2	3.08	0.41
4:D:4:DT:C4	4:D:5:DA:N1	2.88	0.41
4:D:8:DT:H2''	4:D:9:DA:H5'	2.02	0.41
1:E:8:G:C2	3:G:22:DA:C2	3.09	0.41
2:F:256:PHE:CD2	2:F:282:ILE:HG21	2.54	0.41
2:F:290:PHE:O	2:F:293:ALA:HB3	2.20	0.41
2:F:535:ARG:HG2	2:F:536:LYS:H	1.86	0.41
2:F:1000:LYS:HZ3	2:F:1064:GLU:CG	2.19	0.41
2:F:1205:GLU:HB2	2:F:1211:LYS:HG3	2.02	0.41
4:H:8:DT:H2''	4:H:9:DA:H5'	2.02	0.41
1:A:8:G:C2	3:C:22:DA:C2	3.09	0.41
2:B:252:PHE:CE1	2:B:278:LEU:HD21	2.55	0.41
2:B:290:PHE:O	2:B:293:ALA:HB3	2.20	0.41
2:B:336:LYS:CG	2:B:347:TYR:HE2	2.32	0.41
2:B:1302:ILE:O	2:B:1306:ALA:CA	2.69	0.41
2:F:82:LEU:HB3	2:F:155:TYR:HE1	1.85	0.41
2:F:122:ILE:O	2:F:126:VAL:HG23	2.21	0.41
2:F:244:LEU:CD2	2:F:266:LEU:CD1	2.97	0.41
2:F:244:LEU:HD11	2:F:264:LEU:O	2.19	0.41
2:F:525:THR:CG2	2:F:690:ASN:HB3	2.31	0.41
2:F:641:HIS:CD2	2:F:642:LEU:H	2.38	0.41
2:F:1178:PRO:O	2:F:1182:LEU:N	2.43	0.41
2:F:1204:PHE:CE2	2:F:1342:VAL:HG11	2.55	0.41
2:F:1213:MET:O	2:F:1221:GLN:N	2.52	0.41
2:F:1302:ILE:O	2:F:1306:ALA:CA	2.69	0.41
4:H:4:DT:C4	4:H:5:DA:N1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:LEU:HB3	2:B:155:TYR:HE1	1.85	0.41
2:B:186:ILE:CD1	2:B:203:ALA:CB	2.99	0.41
2:B:255:ASN:HD22	2:B:256:PHE:HE1	1.65	0.41
2:B:536:LYS:HB2	2:B:536:LYS:HE2	1.83	0.41
2:B:852:ILE:CG1	5:B:1401:SO4:O1	2.60	0.41
2:B:1000:LYS:CD	2:B:1045:PHE:CE2	3.04	0.41
2:B:1221:GLN:HE21	2:B:1320:ALA:HB2	1.79	0.41
2:F:252:PHE:CE1	2:F:278:LEU:HD21	2.55	0.41
2:F:447:ARG:HG2	2:F:448:ILE:O	2.20	0.41
2:F:812:TYR:CD1	2:F:812:TYR:C	2.97	0.41
2:F:1000:LYS:CG	2:F:1073:VAL:HG11	2.50	0.41
2:F:1244:LYS:NZ	2:F:1244:LYS:HB2	2.36	0.41
2:F:1314:THR:CG2	2:F:1324:PHE:CD2	3.03	0.41
2:B:122:ILE:O	2:B:126:VAL:HG23	2.21	0.41
2:B:600:ILE:O	2:B:647:VAL:CG1	2.58	0.41
2:B:758:ASN:OD1	2:B:954:LYS:NZ	2.44	0.41
1:E:74:A:H3'	1:E:75:A:H8	1.86	0.41
2:F:40:ARG:CZ	2:F:43:ILE:HD13	2.50	0.41
2:F:186:ILE:CD1	2:F:203:ALA:CB	2.99	0.41
2:F:390:LEU:HA	2:F:390:LEU:HD23	1.81	0.41
2:F:896:LYS:O	2:F:900:LEU:HG	2.19	0.41
2:F:1000:LYS:CD	2:F:1045:PHE:CE2	3.04	0.41
3:G:5:DA:C2	4:H:9:DA:C2	3.08	0.41
1:A:74:A:H3'	1:A:75:A:H8	1.86	0.41
2:B:641:HIS:HD2	2:B:642:LEU:CG	2.16	0.41
2:B:683:LEU:HA	2:B:683:LEU:HD23	1.70	0.41
2:B:896:LYS:O	2:B:900:LEU:HG	2.20	0.41
2:B:939:MET:C	2:B:940:ASN:HD22	2.27	0.41
2:B:1244:LYS:NZ	2:B:1244:LYS:HB2	2.36	0.41
1:E:64:U:OP1	2:F:1102:THR:OG1	2.26	0.41
2:F:1153:LYS:O	2:F:1155:LYS:HG3	2.20	0.41
2:B:40:ARG:CZ	2:B:43:ILE:HD13	2.50	0.41
2:B:107:VAL:O	2:B:111:LYS:N	2.54	0.41
2:B:244:LEU:CD2	2:B:266:LEU:CD1	2.97	0.41
2:B:256:PHE:N	2:B:256:PHE:CD1	2.89	0.41
2:B:393:LEU:O	2:B:396:GLU:N	2.44	0.41
2:B:451:TYR:HB2	2:B:488:ALA:HA	2.03	0.41
2:B:505:GLU:CD	2:B:665:LYS:HG3	2.46	0.41
2:B:641:HIS:CD2	2:B:642:LEU:H	2.38	0.41
2:B:777:SER:OG	4:D:2:DT:O5'	2.01	0.41
2:B:812:TYR:CD1	2:B:812:TYR:C	2.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1314:THR:CG2	2:B:1324:PHE:CD2	3.03	0.41
2:B:1321:PRO:HB2	2:B:1333:ARG:HD2	2.02	0.41
2:F:256:PHE:N	2:F:256:PHE:CD1	2.89	0.41
2:F:393:LEU:O	2:F:396:GLU:N	2.44	0.41
2:F:444:LEU:HD23	2:F:444:LEU:C	2.44	0.41
2:F:536:LYS:HB2	2:F:536:LYS:HE2	1.83	0.41
2:F:685:SER:O	2:F:685:SER:OG	2.26	0.41
2:F:758:ASN:OD1	2:F:954:LYS:NZ	2.44	0.41
2:F:923:GLU:CD	2:F:925:ARG:HH21	2.28	0.41
2:F:1321:PRO:HB2	2:F:1333:ARG:HD2	2.02	0.41
2:B:294:LYS:O	2:B:297:SER:HB3	2.21	0.41
2:B:436:ASN:ND2	2:B:436:ASN:N	2.69	0.41
2:B:923:GLU:CD	2:B:925:ARG:HH21	2.29	0.41
2:B:1122:ARG:HG3	2:B:1134:PHE:HE2	1.86	0.41
1:E:43:G:N2	2:F:360:ALA:HA	2.35	0.41
2:F:107:VAL:O	2:F:111:LYS:N	2.54	0.41
2:F:246:LEU:N	2:F:246:LEU:HD12	2.36	0.41
2:F:841:ILE:CD1	2:F:900:LEU:HG	2.51	0.41
2:F:939:MET:C	2:F:940:ASN:HD22	2.28	0.41
2:F:1122:ARG:HG3	2:F:1134:PHE:HE2	1.86	0.41
1:A:26:A:H2'	1:A:27:G:C8	2.56	0.40
2:B:355:SER:OG	2:B:356:LYS:HG2	2.21	0.40
2:B:1203:LEU:HD13	2:B:1213:MET:CG	2.51	0.40
2:F:436:ASN:ND2	2:F:436:ASN:N	2.69	0.40
2:F:616:LEU:O	2:F:619:ILE:HG22	2.21	0.40
2:B:249:THR:CG2	2:B:265:GLN:HE22	2.29	0.40
2:B:534:MET:H	2:B:534:MET:HG2	1.58	0.40
2:B:841:ILE:CD1	2:B:900:LEU:HG	2.51	0.40
2:F:291:LEU:C	2:F:291:LEU:CD2	2.90	0.40
2:F:350:ILE:CG2	2:F:351:PHE:HE2	2.34	0.40
2:F:1139:VAL:HA	2:F:1167:THR:HA	2.03	0.40
2:F:1246:LYS:HZ2	2:F:1246:LYS:CB	2.29	0.40
2:B:454:PRO:HD2	2:B:463:ALA:HA	2.02	0.40
2:B:575:PHE:O	2:B:576:ASP:C	2.61	0.40
2:B:616:LEU:O	2:B:619:ILE:HG22	2.21	0.40
2:B:784:ILE:O	2:B:788:ILE:CD1	2.69	0.40
2:B:924:THR:O	2:B:929:LYS:CE	2.69	0.40
2:B:979:ASN:OD1	2:B:981:TYR:CD1	2.62	0.40
2:B:1246:LYS:NZ	2:B:1246:LYS:CB	2.73	0.40
1:E:54:G:H22	1:E:61:C:H1'	1.87	0.40
2:F:294:LYS:O	2:F:297:SER:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:355:SER:OG	2:F:356:LYS:HG2	2.21	0.40
2:F:451:TYR:HB2	2:F:488:ALA:HA	2.03	0.40
2:F:505:GLU:CD	2:F:665:LYS:HG3	2.46	0.40
2:F:561:VAL:HG23	2:F:585:ASP:O	2.21	0.40
2:B:6:SER:O	2:B:21:ILE:HG12	2.22	0.40
2:B:38:THR:CG2	2:B:39:ASP:N	2.84	0.40
2:B:51:LEU:HD13	2:B:1352:ILE:O	2.22	0.40
2:B:70:ARG:NH1	2:B:454:PRO:HG2	2.35	0.40
2:B:842:VAL:HG13	2:B:847:LEU:HD22	2.03	0.40
2:B:1139:VAL:HA	2:B:1167:THR:HA	2.03	0.40
2:B:1286:ASN:O	2:B:1289:LYS:CB	2.69	0.40
1:E:26:A:H2'	1:E:27:G:C8	2.56	0.40
1:E:67:C:P	2:F:739:GLN:HE22	2.43	0.40
2:F:38:THR:CG2	2:F:39:ASP:N	2.84	0.40
2:F:40:ARG:C	2:F:41:HIS:ND1	2.79	0.40
2:F:51:LEU:HD13	2:F:1352:ILE:O	2.22	0.40
2:F:245:SER:CB	2:F:296:LEU:HD22	2.51	0.40
2:F:255:ASN:C	2:F:256:PHE:HD1	2.29	0.40
2:F:575:PHE:O	2:F:576:ASP:C	2.61	0.40
2:F:842:VAL:HG13	2:F:847:LEU:HD22	2.02	0.40
2:F:1203:LEU:HD13	2:F:1213:MET:CG	2.51	0.40
1:A:67:C:P	2:B:739:GLN:HE22	2.43	0.40
2:B:81:TYR:CE2	2:B:475:PRO:HD3	2.56	0.40
2:B:291:LEU:C	2:B:291:LEU:CD2	2.90	0.40
2:B:350:ILE:CG2	2:B:351:PHE:HE2	2.33	0.40
2:B:406:ASP:OD1	2:B:407:ASN:ND2	2.54	0.40
2:B:561:VAL:HG23	2:B:585:ASP:O	2.21	0.40
2:B:568:TYR:HD2	2:B:569:PHE:CE2	2.40	0.40
2:B:678:THR:O	2:B:681:ASP:HB2	2.21	0.40
2:B:710:LYS:HE2	2:B:710:LYS:HB2	1.81	0.40
2:B:979:ASN:OD1	2:B:981:TYR:N	2.55	0.40
2:B:1207:GLU:C	2:B:1209:GLY:H	2.29	0.40
2:F:244:LEU:HD12	2:F:250:PRO:CG	2.45	0.40
2:F:454:PRO:HD2	2:F:463:ALA:HA	2.02	0.40
2:F:534:MET:H	2:F:534:MET:HG2	1.58	0.40
2:F:600:ILE:O	2:F:647:VAL:CG1	2.58	0.40
2:F:641:HIS:HD2	2:F:642:LEU:CG	2.16	0.40
2:F:811:LEU:O	2:F:814:TYR:HB3	2.22	0.40
2:F:924:THR:O	2:F:929:LYS:CE	2.69	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	
2	B	1318/1368 (96%)	1279 (97%)	39 (3%)	0	100	100
2	F	1318/1368 (96%)	1281 (97%)	37 (3%)	0	100	100
All	All	2636/2736 (96%)	2560 (97%)	76 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	B	1186/1225 (97%)	919 (78%)	267 (22%)	1	6
2	F	1186/1225 (97%)	916 (77%)	270 (23%)	1	6
All	All	2372/2450 (97%)	1835 (77%)	537 (23%)	1	6

All (537) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	4	LYS
2	B	9	LEU
2	B	40	ARG
2	B	43	ILE
2	B	47	LEU
2	B	48	ILE
2	B	57	GLU
2	B	62	THR

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Mol	Chain	Res	Type
2	B	71	ARG
2	B	72	TYR
2	B	74	ARG
2	B	75	ARG
2	B	76	LYS
2	B	93	VAL
2	B	96	SER
2	B	101	LEU
2	B	104	SER
2	B	106	LEU
2	B	107	VAL
2	B	111	LYS
2	B	114	GLU
2	B	121	ASN
2	B	122	ILE
2	B	162	ILE
2	B	165	ARG
2	B	167	HIS
2	B	177	ASP
2	B	181	VAL
2	B	183	LYS
2	B	184	LEU
2	B	195	LEU
2	B	198	GLU
2	B	204	SER
2	B	209	LYS
2	B	211	ILE
2	B	212	LEU
2	B	216	LEU
2	B	218	LYS
2	B	220	ARG
2	B	233	LYS
2	B	234	LYS
2	B	245	SER
2	B	246	LEU
2	B	248	LEU
2	B	268	LYS
2	B	270	THR
2	B	274	ASP
2	B	275	LEU
2	B	278	LEU
2	B	279	LEU

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Mol	Chain	Res	Type
2	B	289	LEU
2	B	291	LEU
2	B	294	LYS
2	B	301	LEU
2	B	302	LEU
2	B	304	ASP
2	B	305	ILE
2	B	307	ARG
2	B	308	VAL
2	B	309	ASN
2	B	311	GLU
2	B	317	LEU
2	B	318	SER
2	B	321	MET
2	B	323	LYS
2	B	338	LEU
2	B	339	VAL
2	B	341	GLN
2	B	342	GLN
2	B	345	GLU
2	B	348	LYS
2	B	352	PHE
2	B	376	ILE
2	B	377	LYS
2	B	379	ILE
2	B	380	LEU
2	B	382	LYS
2	B	383	MET
2	B	384	ASP
2	B	387	GLU
2	B	388	GLU
2	B	390	LEU
2	B	397	ASP
2	B	398	LEU
2	B	404	THR
2	B	405	PHE
2	B	407	ASN
2	B	419	LEU
2	B	423	LEU
2	B	425	ARG
2	B	429	PHE
2	B	432	PHE

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Mol	Chain	Res	Type
2	B	436	ASN
2	B	442	LYS
2	B	445	THR
2	B	455	LEU
2	B	460	SER
2	B	461	ARG
2	B	468	LYS
2	B	469	SER
2	B	479	GLU
2	B	502	LEU
2	B	506	LYS
2	B	508	LEU
2	B	510	LYS
2	B	513	LEU
2	B	514	LEU
2	B	531	THR
2	B	532	GLU
2	B	536	LYS
2	B	540	LEU
2	B	543	GLU
2	B	544	GLN
2	B	546	LYS
2	B	550	ASP
2	B	555	THR
2	B	556	ASN
2	B	557	ARG
2	B	571	LYS
2	B	573	GLU
2	B	574	CYS
2	B	577	SER
2	B	580	ILE
2	B	583	VAL
2	B	585	ASP
2	B	598	LEU
2	B	601	ILE
2	B	602	LYS
2	B	610	GLU
2	B	627	GLU
2	B	629	ARG
2	B	631	MET
2	B	632	ILE
2	B	636	LEU

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Mol	Chain	Res	Type
2	B	642	LEU
2	B	653	ARG
2	B	655	ARG
2	B	671	ARG
2	B	673	LYS
2	B	675	SER
2	B	677	LYS
2	B	691	ARG
2	B	701	SER
2	B	703	THR
2	B	708	ILE
2	B	709	GLN
2	B	710	LYS
2	B	719	SER
2	B	730	SER
2	B	740	THR
2	B	751	MET
2	B	753	ARG
2	B	776	ASN
2	B	777	SER
2	B	778	ARG
2	B	779	GLU
2	B	780	ARG
2	B	781	MET
2	B	782	LYS
2	B	785	GLU
2	B	788	ILE
2	B	791	LEU
2	B	795	ILE
2	B	796	LEU
2	B	814	TYR
2	B	828	LEU
2	B	830	ILE
2	B	833	LEU
2	B	834	SER
2	B	837	ASP
2	B	844	GLN
2	B	845	SER
2	B	847	LEU
2	B	850	ASP
2	B	851	SER
2	B	857	LEU

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Mol	Chain	Res	Type
2	B	866	LYS
2	B	867	SER
2	B	877	LYS
2	B	885	GLN
2	B	887	LEU
2	B	893	THR
2	B	905	ARG
2	B	910	GLU
2	B	911	LEU
2	B	938	ARG
2	B	940	ASN
2	B	945	GLU
2	B	963	VAL
2	B	964	SER
2	B	968	LYS
2	B	969	ASP
2	B	977	GLU
2	B	980	ASN
2	B	1006	SER
2	B	1007	GLU
2	B	1031	LYS
2	B	1035	LYS
2	B	1038	PHE
2	B	1041	ASN
2	B	1042	ILE
2	B	1045	PHE
2	B	1047	LYS
2	B	1060	ARG
2	B	1062	LEU
2	B	1082	THR
2	B	1086	VAL
2	B	1087	LEU
2	B	1089	MET
2	B	1091	GLN
2	B	1106	SER
2	B	1110	ILE
2	B	1135	ASP
2	B	1136	SER
2	B	1146	VAL
2	B	1148	LYS
2	B	1150	GLU
2	B	1151	LYS

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Mol	Chain	Res	Type
2	B	1153	LYS
2	B	1154	SER
2	B	1156	LYS
2	B	1171	ARG
2	B	1175	GLU
2	B	1182	LEU
2	B	1191	LYS
2	B	1195	ILE
2	B	1197	LYS
2	B	1202	SER
2	B	1206	LEU
2	B	1207	GLU
2	B	1214	LEU
2	B	1220	LEU
2	B	1224	ASN
2	B	1226	LEU
2	B	1230	SER
2	B	1231	LYS
2	B	1233	VAL
2	B	1242	TYR
2	B	1243	GLU
2	B	1244	LYS
2	B	1246	LYS
2	B	1250	GLU
2	B	1252	ASN
2	B	1253	GLU
2	B	1254	GLN
2	B	1255	LYS
2	B	1257	LEU
2	B	1266	LEU
2	B	1268	GLU
2	B	1270	ILE
2	B	1272	GLN
2	B	1274	SER
2	B	1277	SER
2	B	1278	LYS
2	B	1282	LEU
2	B	1284	ASP
2	B	1288	ASP
2	B	1291	LEU
2	B	1292	SER
2	B	1296	LYS

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Mol	Chain	Res	Type
2	B	1307	GLU
2	B	1311	HIS
2	B	1315	LEU
2	B	1325	LYS
2	B	1329	THR
2	B	1337	THR
2	B	1344	ASP
2	F	4	LYS
2	F	9	LEU
2	F	23	ASP
2	F	40	ARG
2	F	43	ILE
2	F	47	LEU
2	F	48	ILE
2	F	57	GLU
2	F	62	THR
2	F	71	ARG
2	F	72	TYR
2	F	74	ARG
2	F	75	ARG
2	F	76	LYS
2	F	93	VAL
2	F	96	SER
2	F	101	LEU
2	F	104	SER
2	F	106	LEU
2	F	107	VAL
2	F	111	LYS
2	F	114	GLU
2	F	121	ASN
2	F	122	ILE
2	F	162	ILE
2	F	165	ARG
2	F	167	HIS
2	F	177	ASP
2	F	181	VAL
2	F	183	LYS
2	F	184	LEU
2	F	195	LEU
2	F	198	GLU
2	F	204	SER
2	F	209	LYS

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Mol	Chain	Res	Type
2	F	211	ILE
2	F	212	LEU
2	F	216	LEU
2	F	218	LYS
2	F	220	ARG
2	F	233	LYS
2	F	234	LYS
2	F	245	SER
2	F	246	LEU
2	F	248	LEU
2	F	268	LYS
2	F	270	THR
2	F	274	ASP
2	F	275	LEU
2	F	278	LEU
2	F	279	LEU
2	F	289	LEU
2	F	291	LEU
2	F	294	LYS
2	F	301	LEU
2	F	302	LEU
2	F	304	ASP
2	F	305	ILE
2	F	307	ARG
2	F	308	VAL
2	F	309	ASN
2	F	311	GLU
2	F	317	LEU
2	F	318	SER
2	F	320	SER
2	F	321	MET
2	F	323	LYS
2	F	338	LEU
2	F	339	VAL
2	F	341	GLN
2	F	342	GLN
2	F	345	GLU
2	F	348	LYS
2	F	352	PHE
2	F	376	ILE
2	F	377	LYS
2	F	379	ILE

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Mol	Chain	Res	Type
2	F	380	LEU
2	F	382	LYS
2	F	383	MET
2	F	384	ASP
2	F	387	GLU
2	F	388	GLU
2	F	390	LEU
2	F	397	ASP
2	F	398	LEU
2	F	404	THR
2	F	405	PHE
2	F	407	ASN
2	F	419	LEU
2	F	423	LEU
2	F	425	ARG
2	F	429	PHE
2	F	432	PHE
2	F	436	ASN
2	F	442	LYS
2	F	445	THR
2	F	455	LEU
2	F	460	SER
2	F	461	ARG
2	F	468	LYS
2	F	469	SER
2	F	479	GLU
2	F	502	LEU
2	F	506	LYS
2	F	508	LEU
2	F	510	LYS
2	F	513	LEU
2	F	514	LEU
2	F	531	THR
2	F	532	GLU
2	F	536	LYS
2	F	540	LEU
2	F	543	GLU
2	F	544	GLN
2	F	546	LYS
2	F	550	ASP
2	F	555	THR
2	F	556	ASN

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Mol	Chain	Res	Type
2	F	557	ARG
2	F	571	LYS
2	F	573	GLU
2	F	574	CYS
2	F	577	SER
2	F	580	ILE
2	F	583	VAL
2	F	585	ASP
2	F	598	LEU
2	F	601	ILE
2	F	602	LYS
2	F	610	GLU
2	F	627	GLU
2	F	629	ARG
2	F	631	MET
2	F	632	ILE
2	F	636	LEU
2	F	642	LEU
2	F	653	ARG
2	F	655	ARG
2	F	671	ARG
2	F	673	LYS
2	F	675	SER
2	F	677	LYS
2	F	685	SER
2	F	691	ARG
2	F	701	SER
2	F	703	THR
2	F	708	ILE
2	F	709	GLN
2	F	719	SER
2	F	730	SER
2	F	740	THR
2	F	751	MET
2	F	753	ARG
2	F	776	ASN
2	F	777	SER
2	F	778	ARG
2	F	779	GLU
2	F	781	MET
2	F	782	LYS
2	F	785	GLU

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Mol	Chain	Res	Type
2	F	788	ILE
2	F	791	LEU
2	F	795	ILE
2	F	796	LEU
2	F	814	TYR
2	F	828	LEU
2	F	830	ILE
2	F	833	LEU
2	F	834	SER
2	F	837	ASP
2	F	844	GLN
2	F	845	SER
2	F	847	LEU
2	F	850	ASP
2	F	851	SER
2	F	857	LEU
2	F	866	LYS
2	F	867	SER
2	F	877	LYS
2	F	885	GLN
2	F	887	LEU
2	F	893	THR
2	F	905	ARG
2	F	910	GLU
2	F	911	LEU
2	F	938	ARG
2	F	940	ASN
2	F	945	GLU
2	F	963	VAL
2	F	964	SER
2	F	968	LYS
2	F	969	ASP
2	F	975	VAL
2	F	976	ARG
2	F	977	GLU
2	F	980	ASN
2	F	1006	SER
2	F	1007	GLU
2	F	1031	LYS
2	F	1035	LYS
2	F	1038	PHE
2	F	1041	ASN

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Mol	Chain	Res	Type
2	F	1042	ILE
2	F	1045	PHE
2	F	1047	LYS
2	F	1060	ARG
2	F	1062	LEU
2	F	1082	THR
2	F	1086	VAL
2	F	1087	LEU
2	F	1089	MET
2	F	1091	GLN
2	F	1106	SER
2	F	1110	ILE
2	F	1130	LYS
2	F	1135	ASP
2	F	1136	SER
2	F	1146	VAL
2	F	1148	LYS
2	F	1150	GLU
2	F	1151	LYS
2	F	1153	LYS
2	F	1154	SER
2	F	1156	LYS
2	F	1171	ARG
2	F	1175	GLU
2	F	1182	LEU
2	F	1191	LYS
2	F	1195	ILE
2	F	1197	LYS
2	F	1202	SER
2	F	1206	LEU
2	F	1207	GLU
2	F	1214	LEU
2	F	1220	LEU
2	F	1224	ASN
2	F	1226	LEU
2	F	1230	SER
2	F	1231	LYS
2	F	1233	VAL
2	F	1242	TYR
2	F	1243	GLU
2	F	1244	LYS
2	F	1246	LYS

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Mol	Chain	Res	Type
2	F	1250	GLU
2	F	1252	ASN
2	F	1253	GLU
2	F	1254	GLN
2	F	1255	LYS
2	F	1257	LEU
2	F	1266	LEU
2	F	1270	ILE
2	F	1272	GLN
2	F	1274	SER
2	F	1277	SER
2	F	1278	LYS
2	F	1282	LEU
2	F	1284	ASP
2	F	1288	ASP
2	F	1291	LEU
2	F	1292	SER
2	F	1296	LYS
2	F	1307	GLU
2	F	1311	HIS
2	F	1315	LEU
2	F	1325	LYS
2	F	1329	THR
2	F	1337	THR
2	F	1344	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	178	ASN
2	B	228	GLN
2	B	235	ASN
2	B	265	GLN
2	B	277	ASN
2	B	281	GLN
2	B	295	ASN
2	B	341	GLN
2	B	394	ASN
2	B	407	ASN
2	B	412	HIS
2	B	413	GLN
2	B	522	ASN

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Mol	Chain	Res	Type
2	B	641	HIS
2	B	650	GLN
2	B	690	ASN
2	B	776	ASN
2	B	844	GLN
2	B	854	ASN
2	B	980	ASN
2	B	1221	GLN
2	B	1241	HIS
2	B	1252	ASN
2	B	1256	GLN
2	B	1272	GLN
2	B	1317	ASN
2	F	178	ASN
2	F	228	GLN
2	F	235	ASN
2	F	265	GLN
2	F	277	ASN
2	F	281	GLN
2	F	295	ASN
2	F	341	GLN
2	F	369	GLN
2	F	394	ASN
2	F	407	ASN
2	F	412	HIS
2	F	413	GLN
2	F	522	ASN
2	F	641	HIS
2	F	650	GLN
2	F	690	ASN
2	F	776	ASN
2	F	844	GLN
2	F	854	ASN
2	F	1221	GLN
2	F	1241	HIS
2	F	1252	ASN
2	F	1256	GLN
2	F	1272	GLN
2	F	1317	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	93/98 (94%)	31 (33%)	4 (4%)
1	E	93/98 (94%)	31 (33%)	4 (4%)
All	All	186/196 (94%)	62 (33%)	8 (4%)

All (62) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	11	C
1	A	20	G
1	A	24	U
1	A	27	G
1	A	28	A
1	A	29	G
1	A	34	A
1	A	35	A
1	A	37	U
1	A	38	A
1	A	39	G
1	A	40	C
1	A	42	A
1	A	43	G
1	A	44	U
1	A	51	A
1	A	54	G
1	A	56	U
1	A	57	A
1	A	59	U
1	A	68	A
1	A	69	A
1	A	73	G
1	A	74	A
1	A	82	G
1	A	87	G
1	A	88	A
1	A	89	G
1	A	91	C
1	A	92	G
1	E	9	U
1	E	11	C
1	E	20	G
1	E	24	U
1	E	27	G

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Mol	Chain	Res	Type
1	E	28	A
1	E	29	G
1	E	34	A
1	E	35	A
1	E	37	U
1	E	38	A
1	E	39	G
1	E	40	C
1	E	42	A
1	E	43	G
1	E	44	U
1	E	51	A
1	E	54	G
1	E	56	U
1	E	57	A
1	E	59	U
1	E	68	A
1	E	69	A
1	E	73	G
1	E	74	A
1	E	82	G
1	E	87	G
1	E	88	A
1	E	89	G
1	E	91	C
1	E	92	G

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	8	G
1	A	27	G
1	A	42	A
1	A	68	A
1	E	8	G
1	E	27	G
1	E	42	A
1	E	68	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
5	SO4	F	1401	-	4,4,4	1.04	0	6,6,6	1.39	1 (16%)
5	SO4	B	1401	-	4,4,4	1.04	0	6,6,6	1.39	1 (16%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	B	1401	SO4	O4-S-O3	3.06	125.39	108.54
5	F	1401	SO4	O4-S-O3	3.06	125.39	108.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1401	SO4	1	0
5	B	1401	SO4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	94/98 (95%)	-1.64	0	100	100	7, 25, 69, 93	0
1	E	94/98 (95%)	-1.61	0	100	100	11, 39, 87, 112	0
2	B	1326/1368 (96%)	-1.09	1 (0%)	92	85	5, 26, 65, 117	0
2	F	1326/1368 (96%)	-1.03	8 (0%)	85	64	11, 40, 74, 131	0
3	C	25/26 (96%)	-1.08	0	100	100	9, 17, 64, 79	0
3	G	25/26 (96%)	-0.75	0	100	100	19, 29, 78, 84	0
4	D	11/11 (100%)	-1.17	0	100	100	18, 32, 95, 99	0
4	H	11/11 (100%)	-0.84	0	100	100	27, 56, 102, 112	0
All	All	2912/3006 (96%)	-1.10	9 (0%)	90	75	5, 33, 74, 131	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	543	GLU	4.1
2	F	29	SER	3.6
2	F	31	LYS	3.2
2	F	896	LYS	2.7
2	F	46	ASN	2.5
2	F	899	ASN	2.5
2	F	895	ARG	2.4
2	F	30	LYS	2.2
2	F	76	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	F	1401	5/5	0.99	0.03	30,30,30,30	0
5	SO4	B	1401	5/5	1.00	0.03	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.