



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2025 – 05:02 PM JST

PDB ID : 8KAH / pdb_00008kah
Title : Crystal structure of SpyCas9-crRNA-tracrRNA complex bound to 18nt target DNA
Authors : Chen, Y.; Chen, J.; Liu, L.
Deposited on : 2023-08-03
Resolution : 3.36 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	:	4.02b-467
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

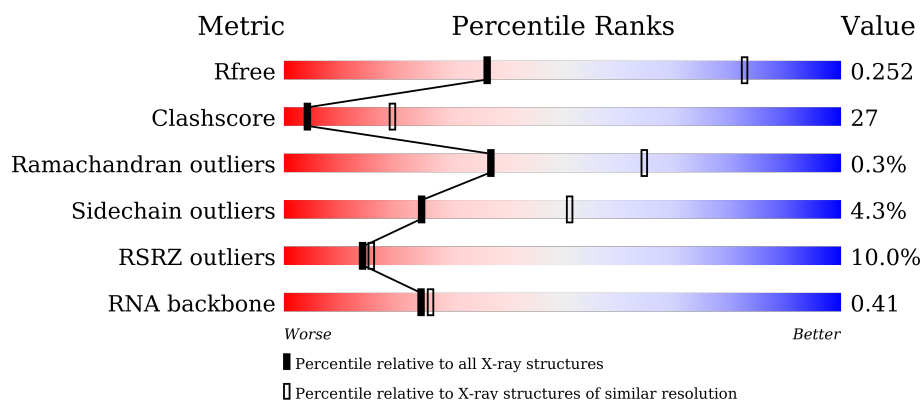
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.36 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}	164625	1012 (3.40-3.32)
Clashscore	180529	1035 (3.40-3.32)
Ramachandran outliers	177936	1037 (3.40-3.32)
Sidechain outliers	177891	1037 (3.40-3.32)
RSRZ outliers	164620	1012 (3.40-3.32)
RNA backbone	3690	1010 (3.74-2.98)

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	34	<div> <div>15%</div> <div>41%</div> <div>32%</div> <div>12%</div> </div>
1	E	34	<div> <div>3%</div> <div>12%</div> <div>41%</div> <div>38%</div> <div>6%</div> </div>
2	B	1368	<div> <div>7%</div> <div>53%</div> <div>42%</div> <div>• •</div> </div>
2	F	1368	<div> <div>14%</div> <div>50%</div> <div>43%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	26	<div><div></div><div>4%</div><div>23%</div><div>69%</div><div>8%</div></div>
3	G	26	<div><div></div><div>4%</div><div>31%</div><div>62%</div><div>8%</div></div>
4	D	11	<div><div></div><div>18%</div><div>36%</div><div>55%</div><div>9%</div></div>
4	H	11	<div><div></div><div>9%</div><div>36%</div><div>55%</div><div>9%</div></div>
5	I	65	<div><div></div><div>2%</div><div>20%</div><div>43%</div><div>23%</div><div>11%</div><div></div></div>
5	J	65	<div><div></div><div>5%</div><div>18%</div><div>42%</div><div>31%</div><div>6%</div><div></div></div>



2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27025 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 (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	34	Total	C	N	O	P	0	0	0
			725	325	127	239	34			
1	E	32	Total	C	N	O	P	0	0	0
			685	307	123	223	32			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1322	Total	C	N	O	S	0	0	0
			10732	6827	1864	2019	22			
2	F	1327	Total	C	N	O	S	0	0	0
			10695	6814	1845	2014	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	26	Total	C	N	O	P	0	0	0
			521	254	85	157	25			
3	G	26	Total	C	N	O	P	0	0	0
			521	254	85	157	25			

- 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 225	C 110	N 37	O 68	P 10	0	0	0
4	H	11	Total 225	C 110	N 37	O 68	P 10	0	0	0

- Molecule 5 is a RNA chain called RNA (65-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	63	Total 1348	C 603	N 245	O 437	P 63	0	0	0
5	J	63	Total 1348	C 603	N 245	O 437	P 63	0	0	0

3 Residue-property plots [i](#)

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.

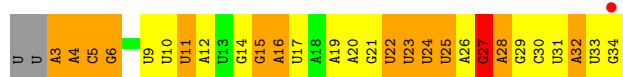
- Molecule 1: RNA (34-MER)

Chain A: 15% 41% 32% 12%



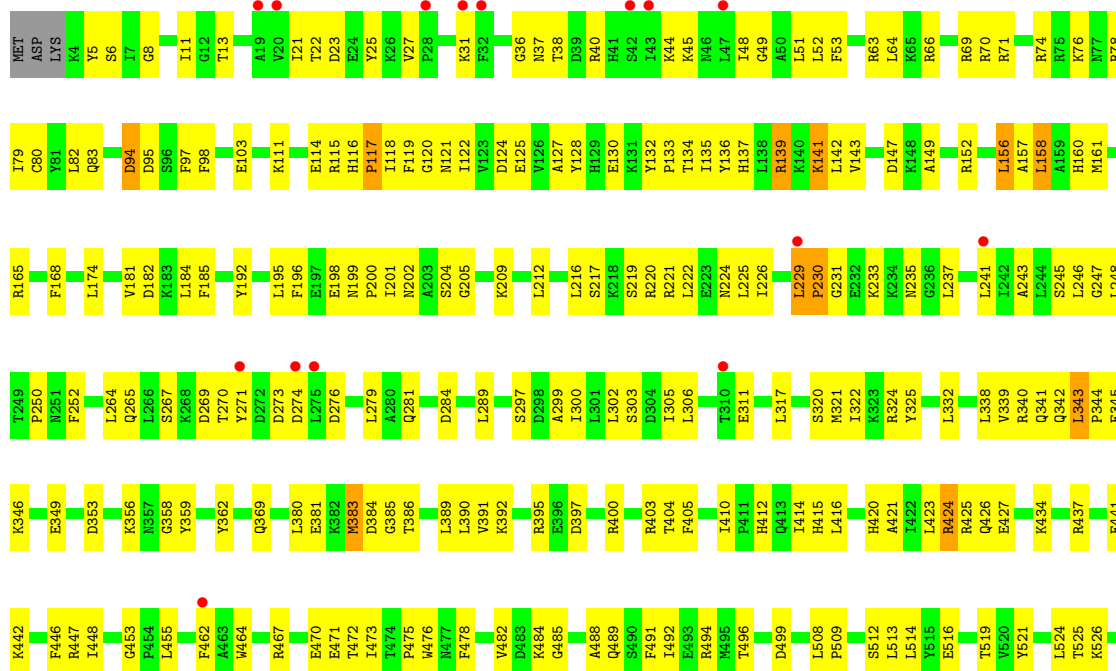
- Molecule 1: RNA (34-MER)

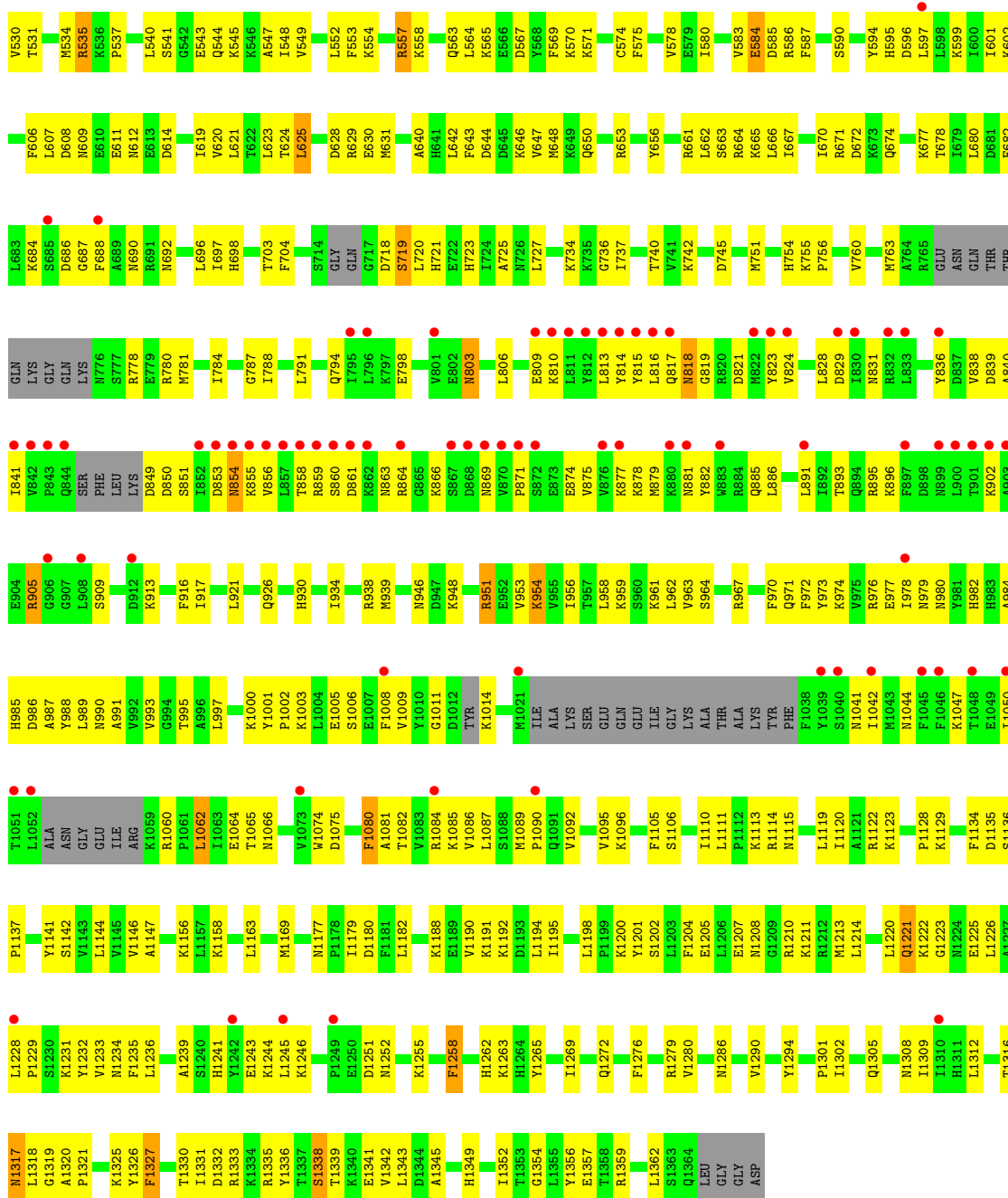
Chain E: 3% 12% 41% 38% 6%



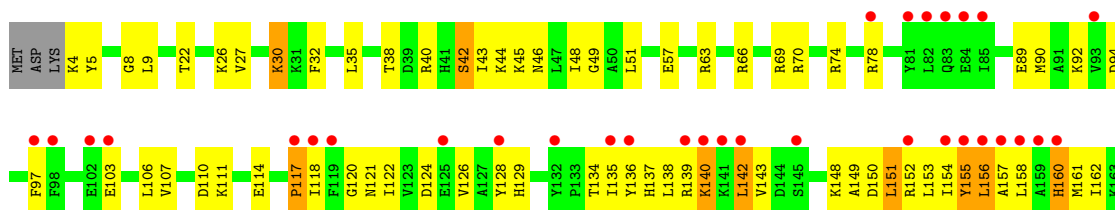
- Molecule 2: CRISPR-associated endonuclease Cas9/Csn1

Chain B: 7% 53% 42%

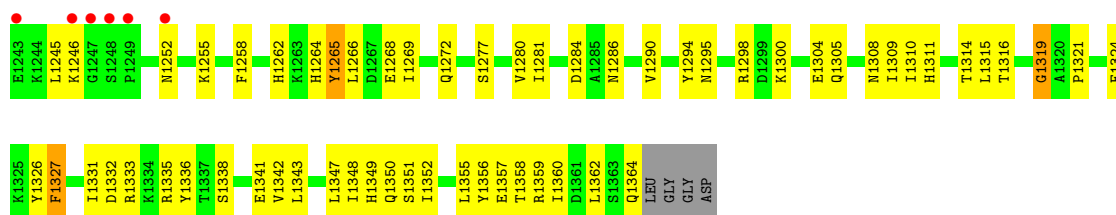




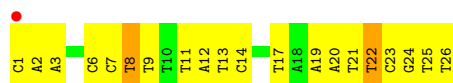
- Molecule 2: CRISPR-associated endonuclease Cas9/Csn1



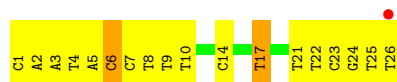




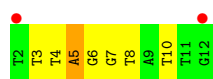
• Molecule 3: DNA (26-MER)



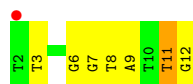
• Molecule 3: DNA (26-MER)



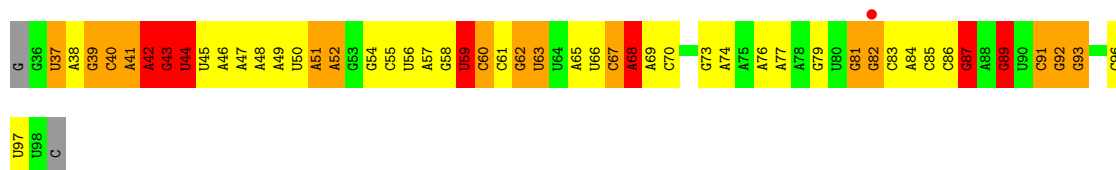
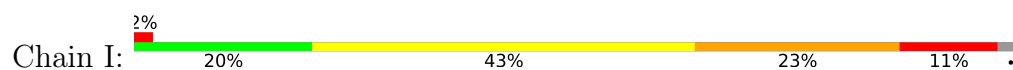
• Molecule 4: DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP*G)-3')



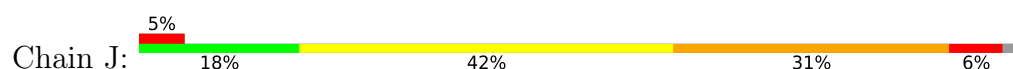
• Molecule 4: DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP*G)-3')

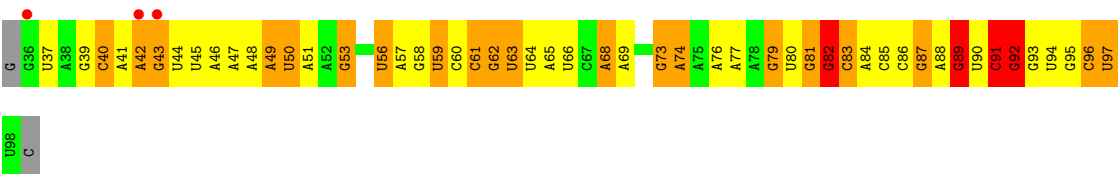


• Molecule 5: RNA (65-MER)



• Molecule 5: RNA (65-MER)





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	145.21Å 130.60Å 148.73Å 90.00° 104.08° 90.00°	Depositor
Resolution (Å)	48.23 – 3.36 48.23 – 3.36	Depositor EDS
% Data completeness (in resolution range)	59.4 (48.23-3.36) 73.8 (48.23-3.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.230 , 0.255 0.229 , 0.252	Depositor DCC
R_{free} test set	75003 reflections (3.44%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.069 for l,-k,h	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	27025	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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](#)

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	1.01	1/811 (0.1%)	1.81	32/1261 (2.5%)
1	E	0.87	0/767	1.73	23/1193 (1.9%)
2	B	0.58	1/10915 (0.0%)	0.80	11/14673 (0.1%)
2	F	0.58	2/10879 (0.0%)	0.78	4/14636 (0.0%)
3	C	1.42	6/581 (1.0%)	1.36	6/893 (0.7%)
3	G	1.25	1/581 (0.2%)	1.34	4/893 (0.4%)
4	D	1.51	1/251 (0.4%)	1.41	3/387 (0.8%)
4	H	1.49	1/251 (0.4%)	1.36	2/387 (0.5%)
5	I	1.03	1/1509 (0.1%)	1.90	61/2350 (2.6%)
5	J	0.93	0/1509	1.80	55/2350 (2.3%)
All	All	0.73	14/28054 (0.0%)	1.10	201/39023 (0.5%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5	DA	C3'-O3'	-10.11	1.30	1.44
4	H	3	DT	C1'-N1	6.85	1.58	1.49
3	C	8	DT	C3'-O3'	-6.36	1.35	1.44
5	I	41	A	N9-C4	-6.20	1.34	1.37
2	F	1319	GLY	C-N	-5.73	1.20	1.34
3	C	19	DA	C3'-O3'	-5.61	1.36	1.44
1	A	20	A	C6-N1	-5.48	1.31	1.35
3	C	12	DA	C5'-C4'	5.46	1.57	1.51
3	C	9	DT	N1-C2	-5.35	1.33	1.38
3	C	12	DA	N3-C4	-5.16	1.31	1.34
2	B	1321	PRO	N-CD	5.14	1.55	1.47
3	G	21	DT	P-O5'	5.08	1.64	1.59
2	F	1089	MET	C-N	-5.06	1.24	1.34
3	C	6	DC	C3'-O3'	5.01	1.50	1.44

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	91	C	C4-C5-C6	-9.82	112.49	117.40
5	J	76	A	C8-N9-C4	-9.81	101.88	105.80
3	C	14	DC	O4'-C4'-C3'	-9.62	100.23	106.00
5	J	92	G	C5-C6-O6	-9.36	122.99	128.60
5	I	59	U	O5'-P-OP2	-9.32	97.31	105.70
5	J	89	G	N3-C4-N9	9.12	131.47	126.00
1	A	26	A	C8-N9-C4	9.09	109.44	105.80
5	I	49	A	C5-C6-N1	8.96	122.18	117.70
5	J	91	C	N3-C2-O2	8.75	128.03	121.90
5	I	96	C	C6-N1-C2	-8.64	116.84	120.30
5	I	45	U	C6-N1-C2	-8.63	115.82	121.00
1	A	25	U	C2-N1-C1'	-8.57	107.41	117.70
1	E	15	G	C5-C6-N1	8.56	115.78	111.50
5	I	67	C	C6-N1-C2	8.46	123.69	120.30
5	J	49	A	N1-C6-N6	-8.37	113.58	118.60
2	F	246	LEU	CA-CB-CG	8.30	134.39	115.30
5	J	89	G	C6-C5-N7	-8.27	125.44	130.40
5	I	43	G	N9-C4-C5	8.19	108.67	105.40
3	G	14	DC	O4'-C4'-C3'	-8.17	101.10	106.00
1	E	17	U	C6-N1-C2	-7.99	116.20	121.00
1	E	16	A	C8-N9-C4	7.99	109.00	105.80
5	I	62	G	C5-C6-O6	7.99	133.39	128.60
5	J	66	U	N3-C4-O4	7.93	124.95	119.40
1	A	21	G	C8-N9-C4	-7.92	103.23	106.40
5	I	45	U	C5-C6-N1	7.86	126.63	122.70
5	J	91	C	C5-C4-N4	-7.83	114.72	120.20
5	I	41	A	C2-N3-C4	-7.80	106.70	110.60
1	A	14	G	C8-N9-C4	7.80	109.52	106.40
1	A	20	A	N1-C6-N6	-7.75	113.95	118.60
5	J	97	U	C6-N1-C2	-7.65	116.41	121.00
5	J	92	G	N1-C6-O6	7.64	124.48	119.90
5	I	43	G	C4-C5-N7	-7.63	107.75	110.80
1	E	15	G	C2-N3-C4	7.60	115.70	111.90
5	J	68	A	C8-N9-C4	-7.55	102.78	105.80
3	G	10	DT	O4'-C1'-N1	7.43	113.20	108.00
2	B	82	LEU	CB-CG-CD2	-7.38	98.45	111.00
5	J	73	G	C8-N9-C4	-7.32	103.47	106.40
5	I	54	G	N1-C6-O6	7.27	124.26	119.90
1	A	2	U	C2-N1-C1'	7.20	126.34	117.70
1	E	11	U	N3-C2-O2	-7.17	117.18	122.20
5	I	48	A	C5-C6-N6	-7.09	118.03	123.70
5	I	89	G	C2-N3-C4	7.06	115.43	111.90
1	A	26	A	N1-C6-N6	7.04	122.83	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	343	LEU	CA-CB-CG	7.03	131.46	115.30
5	I	46	A	OP2-P-O3'	7.01	120.62	105.20
5	J	59	U	O5'-P-OP2	-7.01	99.39	105.70
5	J	91	C	N3-C4-C5	7.00	124.70	121.90
5	I	65	A	C8-N9-C4	-6.94	103.03	105.80
5	J	89	G	N3-C4-C5	-6.91	125.15	128.60
1	E	11	U	C5-C4-O4	6.90	130.04	125.90
5	I	58	G	N1-C6-O6	6.88	124.03	119.90
5	I	48	A	N1-C6-N6	6.87	122.72	118.60
5	I	62	G	C8-N9-C4	-6.86	103.66	106.40
1	E	24	U	C5-C6-N1	6.79	126.09	122.70
5	I	79	G	N1-C6-O6	6.77	123.96	119.90
5	I	42	A	C8-N9-C4	-6.70	103.12	105.80
5	J	62	G	C8-N9-C4	-6.62	103.75	106.40
5	J	83	C	C6-N1-C2	-6.59	117.67	120.30
5	I	42	A	N9-C4-C5	6.57	108.43	105.80
5	I	62	G	N3-C2-N2	6.57	124.50	119.90
5	I	62	G	N3-C4-C5	-6.48	125.36	128.60
5	J	76	A	N9-C4-C5	6.48	108.39	105.80
1	A	17	U	O5'-P-OP1	-6.48	99.87	105.70
1	E	15	G	O5'-P-OP1	-6.43	99.91	105.70
5	J	73	G	C6-C5-N7	-6.37	126.58	130.40
1	A	21	G	N7-C8-N9	6.37	116.28	113.10
5	I	55	C	C4-C5-C6	6.34	120.57	117.40
5	I	62	G	N1-C6-O6	-6.34	116.10	119.90
4	D	5	DA	OP1-P-OP2	6.33	129.09	119.60
5	J	86	C	N3-C4-N4	6.31	122.42	118.00
5	J	49	A	N9-C4-C5	6.31	108.32	105.80
3	C	13	DT	O4'-C4'-C3'	-6.29	101.98	104.50
4	H	11	DT	O4'-C1'-N1	6.28	112.39	108.00
5	I	87	G	C2-N3-C4	6.27	115.03	111.90
1	E	11	U	C6-N1-C2	-6.24	117.25	121.00
1	E	15	G	N1-C6-O6	-6.23	116.16	119.90
5	I	43	G	C8-N9-C4	-6.23	103.91	106.40
5	I	60	C	N3-C4-C5	-6.21	119.41	121.90
5	J	61	C	C6-N1-C2	-6.21	117.81	120.30
5	I	45	U	N3-C4-O4	6.21	123.75	119.40
1	A	13	U	O5'-P-OP2	-6.20	100.12	105.70
5	J	79	G	C8-N9-C4	6.20	108.88	106.40
5	I	96	C	C5-C6-N1	6.19	124.10	121.00
1	A	26	A	N7-C8-N9	-6.19	110.71	113.80
5	J	89	G	C8-N9-C1'	-6.17	118.97	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	45	U	O5'-P-OP1	-6.14	100.17	105.70
5	I	49	A	C2-N3-C4	6.13	113.67	110.60
1	A	23	U	N3-C4-O4	6.10	123.67	119.40
1	E	25	U	C5-C6-N1	6.09	125.75	122.70
5	I	43	G	C2-N3-C4	6.08	114.94	111.90
1	A	21	G	C2-N3-C4	6.07	114.94	111.90
5	I	43	G	C6-C5-N7	6.06	134.04	130.40
5	J	91	C	C6-N1-C2	6.06	122.72	120.30
5	J	68	A	N7-C8-N9	6.05	116.83	113.80
5	I	67	C	N3-C2-O2	6.04	126.13	121.90
5	I	87	G	N1-C2-N3	-6.04	120.27	123.90
1	E	16	A	N7-C8-N9	-6.04	110.78	113.80
2	B	1245	LEU	CB-CG-CD1	6.02	121.24	111.00
5	I	47	A	N1-C2-N3	-6.02	126.29	129.30
5	J	91	C	N1-C2-N3	-6.02	114.99	119.20
2	B	158	LEU	CB-CG-CD1	-6.01	100.79	111.00
1	A	18	A	C4-C5-C6	6.00	120.00	117.00
5	J	89	G	C4-C5-C6	5.99	122.39	118.80
1	E	22	U	N3-C2-O2	-5.98	118.01	122.20
5	J	48	A	C5-C6-N1	-5.96	114.72	117.70
5	I	68	A	OP1-P-OP2	-5.95	110.67	119.60
5	J	91	C	C5-C6-N1	5.95	123.98	121.00
1	E	10	U	C6-N1-C2	-5.94	117.43	121.00
2	B	139	ARG	NE-CZ-NH1	-5.94	117.33	120.30
5	J	66	U	N3-C2-O2	5.93	126.36	122.20
1	A	25	U	C5-C6-N1	-5.91	119.74	122.70
1	A	21	G	N3-C4-C5	-5.89	125.65	128.60
5	I	87	G	C5-C6-O6	-5.87	125.08	128.60
1	A	14	G	N7-C8-N9	-5.87	110.17	113.10
5	J	89	G	C4-N9-C1'	5.87	134.13	126.50
5	I	63	U	C2-N3-C4	-5.86	123.49	127.00
1	E	10	U	C5-C4-O4	5.83	129.40	125.90
5	I	81	G	C2-N3-C4	5.82	114.81	111.90
2	F	30	LYS	CD-CE-NZ	5.77	124.98	111.70
5	J	50	U	C6-N1-C2	5.77	124.46	121.00
2	B	1320	ALA	C-N-CD	5.77	140.52	128.40
5	I	62	G	C4-C5-N7	-5.76	108.50	110.80
5	J	66	U	N1-C2-O2	-5.75	118.78	122.80
5	I	62	G	N1-C2-N2	-5.73	111.05	116.20
5	I	54	G	C6-C5-N7	-5.72	126.97	130.40
5	J	89	G	N1-C6-O6	5.72	123.33	119.90
1	A	28	A	O4'-C1'-N9	-5.69	103.65	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	17	U	N3-C2-O2	-5.65	118.25	122.20
5	J	73	G	N1-C6-O6	5.64	123.28	119.90
5	J	89	G	C5-C6-O6	-5.64	125.22	128.60
5	I	58	G	C5-C6-O6	-5.63	125.22	128.60
5	I	59	U	N3-C2-O2	-5.62	118.27	122.20
1	A	26	A	N9-C4-C5	-5.58	103.57	105.80
5	J	49	A	C5-C6-N6	5.58	128.16	123.70
1	E	34	G	C8-N9-C4	-5.56	104.18	106.40
5	J	49	A	C4-C5-N7	-5.53	107.93	110.70
5	I	47	A	C5-C6-N1	5.52	120.46	117.70
3	C	11	DT	O4'-C4'-C3'	-5.51	102.30	104.50
5	I	96	C	N3-C4-C5	-5.49	119.70	121.90
2	B	156	LEU	CB-CG-CD2	-5.46	101.71	111.00
5	J	81	G	C5-C6-O6	-5.46	125.33	128.60
1	A	21	G	O5'-P-OP1	5.43	117.22	110.70
1	A	21	G	C4-N9-C1'	5.40	133.52	126.50
4	D	8	DT	OP1-P-OP2	-5.40	111.50	119.60
5	I	46	A	C8-N9-C4	-5.39	103.64	105.80
2	F	241	LEU	CA-CB-CG	5.38	127.66	115.30
5	J	48	A	C4-C5-C6	5.37	119.68	117.00
5	I	55	C	N1-C2-O2	-5.36	115.69	118.90
5	I	62	G	N9-C4-C5	5.35	107.54	105.40
3	G	6	DC	O4'-C1'-N1	5.35	111.74	108.00
1	E	11	U	OP2-P-O3'	5.33	116.94	105.20
1	A	23	U	N1-C2-O2	-5.33	119.07	122.80
1	A	23	U	C5-C4-O4	-5.32	122.71	125.90
5	J	77	A	C4-C5-C6	-5.32	114.34	117.00
5	J	77	A	C4-C5-N7	5.32	113.36	110.70
1	A	2	U	C6-N1-C1'	-5.31	113.76	121.20
5	J	76	A	N7-C8-N9	5.30	116.45	113.80
4	D	10	DT	OP1-P-OP2	5.30	127.55	119.60
3	G	17	DT	N3-C4-O4	5.29	123.08	119.90
2	F	306	LEU	CB-CG-CD1	5.28	119.98	111.00
5	I	79	G	N3-C2-N2	-5.26	116.22	119.90
1	A	22	U	C5-C6-N1	5.25	125.32	122.70
2	B	1245	LEU	CA-CB-CG	5.24	127.34	115.30
5	J	86	C	C5-C4-N4	-5.23	116.54	120.20
5	I	51	A	C2-N3-C4	-5.21	107.99	110.60
1	E	17	U	C5-C6-N1	5.21	125.31	122.70
1	A	25	U	C6-N1-C1'	5.20	128.48	121.20
5	J	81	G	N3-C4-N9	5.20	129.12	126.00
5	J	82	G	N9-C4-C5	-5.20	103.32	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	229	LEU	CA-CB-CG	5.20	127.25	115.30
3	C	22	DT	O4'-C1'-N1	5.20	111.64	108.00
5	J	48	A	N1-C2-N3	5.19	131.89	129.30
5	J	89	G	N9-C4-C5	-5.17	103.33	105.40
1	E	22	U	C6-N1-C2	-5.17	117.90	121.00
5	I	42	A	C2'-C3'-O3'	5.17	121.97	113.70
2	B	52	LEU	CA-CB-CG	-5.16	103.43	115.30
5	J	90	U	C2-N1-C1'	-5.16	111.50	117.70
1	A	25	U	C6-N1-C2	5.16	124.10	121.00
1	A	31	U	N1-C2-O2	5.16	126.41	122.80
1	A	26	A	C5-C6-N6	-5.15	119.58	123.70
2	B	625	LEU	CA-CB-CG	5.14	127.12	115.30
1	A	8	A	P-O3'-C3'	5.13	125.86	119.70
5	J	64	U	N3-C2-O2	-5.13	118.61	122.20
5	J	96	C	N3-C4-N4	5.12	121.59	118.00
1	A	25	U	N1-C2-O2	-5.12	119.22	122.80
1	E	15	G	OP2-P-O3'	5.12	116.46	105.20
5	I	44	U	OP2-P-O3'	5.11	116.44	105.20
5	I	52	A	N1-C6-N6	-5.10	115.54	118.60
5	I	89	G	N1-C6-O6	-5.10	116.84	119.90
1	E	27	G	P-O3'-C3'	5.09	125.81	119.70
5	I	66	U	N3-C2-O2	5.09	125.77	122.20
5	J	53	G	O5'-P-OP1	-5.08	101.12	105.70
5	I	55	C	N3-C4-N4	5.07	121.55	118.00
5	I	91	C	N3-C2-O2	5.06	125.44	121.90
1	E	23	U	OP2-P-O3'	5.06	116.33	105.20
4	H	11	DT	N3-C4-O4	5.05	122.93	119.90
1	A	25	U	N3-C2-O2	5.05	125.73	122.20
5	I	93	G	C8-N9-C4	-5.04	104.38	106.40
3	C	13	DT	OP2-P-O3'	5.04	116.28	105.20
5	J	92	G	C4-C5-N7	5.02	112.81	110.80
3	C	17	DT	N3-C4-O4	5.02	122.91	119.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	725	0	362	40	0
1	E	685	0	342	44	0
2	B	10732	0	10828	517	1
2	F	10695	0	10736	702	0
3	C	521	0	299	19	0
3	G	521	0	299	20	0
4	D	225	0	129	3	0
4	H	225	0	129	10	0
5	I	1348	0	678	38	0
5	J	1348	0	678	61	0
All	All	27025	0	24480	1373	1

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 27.

All (1373) 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:142:LEU:CD1	2:F:154:ILE:HG12	1.37	1.54
2:F:142:LEU:HD11	2:F:154:ILE:CG1	1.39	1.51
2:F:142:LEU:CD2	2:F:154:ILE:HD11	1.41	1.48
2:F:142:LEU:CD2	2:F:154:ILE:CD1	1.94	1.45
2:B:1222:LYS:O	2:B:1318:LEU:CD2	1.66	1.42
2:F:142:LEU:HD21	2:F:154:ILE:CD1	1.49	1.38
2:F:212:LEU:CD1	2:F:300:ILE:HG12	1.55	1.35
2:F:139:ARG:CG	2:F:157:ALA:HB1	1.56	1.34
2:F:138:LEU:CD1	2:F:153:LEU:HD21	1.58	1.32
2:F:165:ARG:HD2	2:F:168:PHE:CE1	1.65	1.31
2:F:138:LEU:CD1	2:F:153:LEU:CD2	2.10	1.30
1:E:4:A:C2	1:E:5:C:C5	2.20	1.27
2:F:139:ARG:HG2	2:F:157:ALA:CB	1.63	1.27
2:F:208:ALA:CA	2:F:211:ILE:HD12	1.63	1.26
2:F:138:LEU:HD11	2:F:153:LEU:CD2	1.66	1.25
2:F:921:LEU:HD12	2:F:1008:PHE:CE2	1.71	1.22
2:F:208:ALA:HA	2:F:211:ILE:CD1	1.71	1.21
2:F:142:LEU:HD21	2:F:154:ILE:CG1	1.72	1.19
2:F:249:THR:HG1	2:F:267:SER:N	1.43	1.17
2:B:392:LYS:HG2	2:B:395:ARG:NH1	1.61	1.14
2:F:207:ASP:O	2:F:211:ILE:HG13	1.49	1.12
2:F:142:LEU:HD13	2:F:154:ILE:HG23	1.21	1.11
2:F:142:LEU:HD22	2:F:154:ILE:CD1	1.71	1.11
2:F:90:MET:CE	2:F:151:LEU:HD21	1.80	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:138:LEU:CD2	2:F:153:LEU:HD21	1.80	1.10
2:F:142:LEU:HD11	2:F:154:ILE:CB	1.81	1.10
2:F:164:PHE:O	2:F:415:HIS:CD2	2.03	1.10
2:F:165:ARG:HD2	2:F:168:PHE:CZ	1.90	1.06
2:B:392:LYS:HG2	2:B:395:ARG:HH12	0.91	1.05
2:F:212:LEU:HD12	2:F:300:ILE:HG12	1.29	1.05
2:F:142:LEU:CG	2:F:154:ILE:HG12	1.86	1.05
3:G:24:DG:H2'	3:G:25:DT:H5'	1.10	1.04
2:B:545:LYS:NZ	2:B:690:ASN:OD1	1.92	1.03
2:B:558:LYS:HE3	2:B:590:SER:HB3	1.36	1.03
2:F:142:LEU:CD1	2:F:154:ILE:CG1	2.11	1.03
2:B:1221:GLN:HG2	2:B:1319:GLY:O	1.59	1.02
2:F:151:LEU:HD13	2:F:152:ARG:H	1.22	1.02
2:F:180:ASP:HB3	2:F:183:LYS:HB2	1.39	1.02
2:B:1222:LYS:O	2:B:1318:LEU:HD21	1.60	1.00
2:F:138:LEU:CG	2:F:153:LEU:HD21	1.93	0.99
2:F:139:ARG:HD3	2:F:157:ALA:O	1.63	0.99
2:F:1210:ARG:NH2	2:F:1341:GLU:OE1	1.95	0.99
2:F:138:LEU:HD13	2:F:153:LEU:HD21	1.42	0.99
2:B:1222:LYS:O	2:B:1318:LEU:HD23	1.59	0.99
2:B:381:GLU:HG2	2:B:390:LEU:HD11	1.43	0.98
2:F:139:ARG:HD3	2:F:157:ALA:C	1.84	0.98
2:F:138:LEU:CD2	2:F:153:LEU:CD2	2.42	0.98
2:B:951:ARG:NH2	2:B:1011:GLY:HA2	1.80	0.97
2:F:90:MET:CE	2:F:151:LEU:CD2	2.42	0.97
2:F:142:LEU:HD22	2:F:154:ILE:HD13	1.45	0.97
2:F:142:LEU:CD2	2:F:154:ILE:CG1	2.39	0.96
3:G:24:DG:C2'	3:G:25:DT:H5'	1.96	0.96
2:B:1211:LYS:O	2:B:1223:GLY:HA3	1.65	0.95
2:B:137:HIS:HA	2:B:322:ILE:HD11	1.47	0.95
2:F:212:LEU:CD1	2:F:300:ILE:CG1	2.44	0.95
2:B:1222:LYS:O	2:B:1318:LEU:HD22	1.67	0.94
2:F:921:LEU:HD12	2:F:1008:PHE:HE2	1.15	0.94
1:A:4:A:O2'	1:A:5:C:O5'	1.83	0.94
3:G:24:DG:H2'	3:G:25:DT:C5'	1.97	0.94
2:B:220:ARG:O	2:B:224:ASN:ND2	2.00	0.94
2:F:142:LEU:HD13	2:F:154:ILE:CG2	1.97	0.94
2:F:212:LEU:HD11	2:F:300:ILE:HG12	1.48	0.94
2:F:165:ARG:HD2	2:F:168:PHE:HE1	1.15	0.93
2:F:142:LEU:CD1	2:F:154:ILE:HG23	1.98	0.93
1:A:3:A:O2'	1:A:4:A:O5'	1.85	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:142:LEU:HD22	2:F:154:ILE:HD11	1.38	0.93
2:F:626:PHE:O	2:F:655:ARG:NH1	2.01	0.93
1:E:4:A:N3	1:E:5:C:C6	2.38	0.92
2:F:149:ALA:HB3	2:F:154:ILE:CD1	2.00	0.92
2:F:138:LEU:HD13	2:F:153:LEU:CD2	1.97	0.91
2:F:90:MET:HE1	2:F:151:LEU:HD21	1.53	0.91
2:F:777:SER:HA	2:F:807:GLN:HE21	1.35	0.91
2:F:138:LEU:HD11	2:F:153:LEU:HD22	1.51	0.91
2:F:485:GLY:HA3	2:F:631:MET:HG3	1.52	0.91
2:F:90:MET:HE1	2:F:151:LEU:CD2	2.00	0.90
2:F:142:LEU:HD21	2:F:154:ILE:HD11	1.00	0.90
2:F:686:ASP:CG	2:F:690:ASN:HA	1.91	0.90
2:B:601:ILE:HD11	2:B:607:LEU:HD21	1.53	0.90
2:F:142:LEU:HD11	2:F:154:ILE:CA	2.02	0.90
2:F:978:ILE:HD12	2:F:1233:VAL:HG22	1.53	0.90
2:F:686:ASP:CB	2:F:690:ASN:HA	2.02	0.89
2:F:138:LEU:HD21	2:F:153:LEU:CD2	2.03	0.89
2:F:142:LEU:HD11	2:F:154:ILE:HA	1.54	0.89
2:F:138:LEU:CD1	2:F:153:LEU:HD22	2.02	0.88
1:E:4:A:N3	1:E:5:C:C5	2.40	0.88
2:F:380:LEU:HD11	2:F:390:LEU:HG	1.53	0.88
2:F:328:HIS:HE2	2:F:359:TYR:HH	1.20	0.88
2:B:392:LYS:CG	2:B:395:ARG:HH12	1.84	0.87
1:E:4:A:C2	1:E:5:C:C6	2.63	0.87
2:F:142:LEU:CD2	2:F:154:ILE:HG12	2.04	0.87
2:F:467:ARG:HA	2:F:482:VAL:HG22	1.57	0.87
2:F:249:THR:OG1	2:F:267:SER:N	2.08	0.86
2:F:142:LEU:CD1	2:F:154:ILE:HA	2.06	0.85
2:B:921:LEU:HD21	2:B:1042:ILE:HG21	1.57	0.85
2:B:967:ARG:HE	2:B:974:LYS:HB2	1.42	0.85
2:F:893:THR:HG23	2:F:896:LYS:H	1.40	0.84
2:F:279:LEU:HD21	2:F:287:ALA:HB2	1.59	0.84
2:F:226:ILE:HG13	2:F:232:GLU:HG2	1.59	0.84
2:F:139:ARG:HH21	2:F:160:HIS:CD2	1.95	0.84
2:F:208:ALA:HA	2:F:211:ILE:HD12	0.88	0.84
2:B:455:LEU:HD23	2:B:473:ILE:HD12	1.60	0.84
2:F:451:TYR:O	2:F:464:TRP:NE1	2.10	0.84
5:J:46:A:H2'	5:J:47:A:C8	2.13	0.83
1:A:2:U:H3	1:A:4:A:H3'	1.42	0.83
3:G:1:DC:N4	4:H:12:DG:O6	2.11	0.83
2:F:1045:PHE:HA	2:F:1060:ARG:HH11	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1110:ILE:HD12	2:B:1122:ARG:HD2	1.60	0.83
2:F:151:LEU:HD13	2:F:152:ARG:N	1.93	0.82
1:A:14:G:OP2	2:B:63:ARG:NH1	2.12	0.82
2:B:1236:LEU:HD11	2:B:1269:ILE:HD13	1.62	0.82
2:B:384:ASP:OD1	2:B:385:GLY:N	2.12	0.82
2:F:1045:PHE:HB2	2:F:1064:GLU:HG2	1.62	0.82
3:G:25:DT:H2"	3:G:26:DT:OP2	1.80	0.81
2:F:138:LEU:HD21	2:F:153:LEU:HD23	1.59	0.81
2:F:151:LEU:HD22	2:F:152:ARG:N	1.95	0.81
2:F:164:PHE:O	2:F:415:HIS:HD2	1.58	0.81
1:E:4:A:C2	1:E:5:C:C4	2.68	0.81
2:F:1120:ILE:HD11	2:F:1137:PRO:HD3	1.62	0.81
2:B:212:LEU:O	2:B:221:ARG:NH1	2.14	0.81
2:F:165:ARG:CD	2:F:168:PHE:CE1	2.56	0.81
2:F:1212:ARG:NH2	2:F:1280:VAL:O	2.15	0.80
2:F:142:LEU:CD1	2:F:154:ILE:CB	2.52	0.80
2:F:1041:ASN:O	2:F:1043:MET:N	2.13	0.80
2:F:425:ARG:HG3	2:F:426:GLN:HG2	1.63	0.79
2:F:139:ARG:CD	2:F:157:ALA:O	2.29	0.79
2:F:165:ARG:CD	2:F:168:PHE:HE1	1.92	0.79
2:F:135:ILE:HD11	2:F:156:LEU:HB3	1.64	0.79
2:F:686:ASP:HB3	2:F:690:ASN:HA	1.63	0.79
2:B:823:TYR:HA	2:B:875:VAL:HG11	1.64	0.79
2:F:89:GLU:OE2	2:F:92:LYS:NZ	2.15	0.79
2:F:90:MET:SD	2:F:151:LEU:HD21	2.22	0.79
2:B:116:HIS:CE1	2:B:122:ILE:HG12	2.17	0.78
2:F:166:GLY:HA3	2:F:410:ILE:HG22	1.64	0.78
2:B:404:THR:HG22	2:B:405:PHE:CD1	2.19	0.78
2:F:886:LEU:HA	2:F:891:LEU:HD21	1.64	0.78
2:F:142:LEU:CD1	2:F:154:ILE:CG2	2.59	0.78
2:B:442:LYS:HE3	2:B:476:TRP:HA	1.65	0.78
2:B:725:ALA:O	2:B:734:LYS:NZ	2.17	0.77
2:F:522:ASN:OD1	2:F:692:ASN:ND2	2.16	0.77
2:B:1222:LYS:HE3	2:B:1317:ASN:O	1.85	0.77
2:F:94:ASP:HB3	2:F:97:PHE:HB2	1.65	0.77
2:F:846:PHE:O	2:F:1040:SER:OG	2.02	0.77
2:F:70:ARG:NH2	5:J:61:C:OP1	2.16	0.77
2:F:63:ARG:HA	2:F:66:ARG:HG3	1.65	0.77
1:A:27:G:H5'	1:A:28:A:H5"	1.67	0.77
2:F:649:LYS:O	2:F:653:ARG:NE	2.17	0.77
2:B:1147:ALA:HB2	2:B:1190:VAL:HA	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:6:DC:N4	4:H:7:DG:O6	2.18	0.77
2:B:279:LEU:HD11	2:B:284:ASP:HA	1.68	0.76
2:F:142:LEU:HD11	2:F:154:ILE:HG12	0.76	0.76
2:B:913:LYS:HA	2:B:916:PHE:HD2	1.50	0.76
2:B:201:ILE:HG22	2:B:202:ASN:H	1.51	0.76
2:B:524:LEU:HD12	2:B:587:PHE:HE2	1.50	0.76
1:E:15:G:OP1	2:F:66:ARG:NH2	2.19	0.76
2:F:921:LEU:HD21	2:F:1042:ILE:HG21	1.67	0.76
2:B:586:ARG:NH1	3:C:26:DT:O2	2.19	0.76
2:F:128:TYR:CE1	2:F:153:LEU:HD11	2.21	0.76
2:F:1045:PHE:HA	2:F:1060:ARG:NH1	2.01	0.76
2:F:999:LYS:HB3	2:F:1073:VAL:HG12	1.66	0.75
2:F:139:ARG:HG2	2:F:157:ALA:HB1	0.79	0.75
2:F:139:ARG:CG	2:F:157:ALA:CB	2.40	0.75
2:F:149:ALA:CB	2:F:154:ILE:CD1	2.65	0.74
2:F:446:PHE:HZ	2:F:478:PHE:HD1	1.34	0.74
2:B:45:LYS:NZ	2:B:1357:GLU:OE2	2.15	0.74
2:B:864:ARG:NH2	2:B:869:ASN:O	2.19	0.74
2:F:1215:ALA:HB2	2:F:1221:GLN:HG3	1.68	0.74
2:F:168:PHE:HB2	2:F:447:ARG:HH11	1.52	0.74
2:F:844:GLN:OE1	2:F:848:LYS:NZ	2.15	0.74
2:B:74:ARG:HH21	5:I:60:C:P	2.10	0.74
2:B:1211:LYS:O	2:B:1223:GLY:CA	2.34	0.74
2:F:842:VAL:HG12	2:F:854:ASN:OD1	1.87	0.74
2:F:148:LYS:CB	2:F:429:PHE:CD2	2.70	0.73
2:F:446:PHE:CZ	2:F:478:PHE:HD1	2.06	0.73
1:A:20:A:OP2	2:B:403:ARG:NH1	2.21	0.73
2:F:199:ASN:O	2:F:201:ILE:HD11	1.87	0.73
2:F:138:LEU:HD22	2:F:153:LEU:HD21	1.69	0.73
2:F:142:LEU:HD21	2:F:149:ALA:CB	2.17	0.73
2:F:149:ALA:CB	2:F:154:ILE:HG13	2.18	0.73
2:F:913:LYS:HG3	2:F:1040:SER:HB3	1.69	0.73
3:C:25:DT:C2	3:C:26:DT:H72	2.24	0.73
1:E:27:G:N2	5:J:44:U:OP2	2.22	0.73
2:F:149:ALA:CB	2:F:154:ILE:HD11	2.18	0.73
2:F:370:GLU:OE2	2:F:374:LYS:NZ	2.22	0.72
2:B:279:LEU:CD1	2:B:284:ASP:HA	2.19	0.72
2:B:1210:ARG:NH2	2:B:1341:GLU:OE1	2.22	0.72
2:F:923:GLU:HG2	2:F:928:THR:HG21	1.72	0.72
2:B:619:ILE:O	2:B:623:LEU:HB2	1.90	0.72
2:F:530:VAL:HG22	2:F:537:PRO:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:A:O2'	2:F:405:PHE:O	2.07	0.72
2:F:253:LYS:HG3	2:F:261:ASP:HA	1.72	0.72
2:B:1210:ARG:HB2	2:B:1280:VAL:HG13	1.72	0.71
2:F:90:MET:HE2	2:F:151:LEU:CD2	2.20	0.71
2:F:1205:GLU:OE1	2:F:1359:ARG:NH2	2.22	0.71
2:B:21:ILE:HD11	2:B:995:THR:HG21	1.71	0.71
2:B:217:SER:HB2	2:B:220:ARG:H	1.56	0.71
2:B:1220:LEU:HD11	2:B:1339:THR:HA	1.70	0.71
2:F:128:TYR:HE1	2:F:153:LEU:HD11	1.55	0.71
2:B:165:ARG:NH2	2:B:446:PHE:O	2.24	0.71
2:B:787:GLY:HA3	2:B:891:LEU:HD21	1.71	0.71
2:B:299:ALA:O	2:B:303:SER:OG	2.07	0.71
2:F:527:VAL:HA	2:F:582:GLY:HA3	1.73	0.71
3:C:25:DT:N3	3:C:26:DT:C4	2.59	0.70
2:F:505:GLU:HG3	2:F:665:LYS:HB2	1.72	0.70
2:F:1207:GLU:OE2	2:F:1210:ARG:NH1	2.24	0.70
2:B:530:VAL:HG22	2:B:537:PRO:HB3	1.72	0.70
2:F:139:ARG:CD	2:F:157:ALA:HB1	2.21	0.70
2:F:921:LEU:HD21	2:F:1042:ILE:HD13	1.73	0.70
2:B:874:GLU:HA	2:B:877:LYS:HE3	1.74	0.70
2:B:1135:ASP:OD1	2:B:1136:SER:N	2.24	0.70
2:B:650:GLN:OE1	2:B:653:ARG:NH2	2.25	0.70
2:B:951:ARG:CZ	2:B:1011:GLY:HA2	2.21	0.70
2:F:128:TYR:CE1	2:F:153:LEU:CD1	2.75	0.70
3:G:24:DG:C2'	3:G:25:DT:C5'	2.65	0.70
2:B:69:ARG:HD3	5:I:62:G:N7	2.07	0.70
2:F:936:ASP:OD1	2:F:940:ASN:ND2	2.24	0.70
2:B:1119:LEU:HD23	2:B:1128:PRO:HB2	1.73	0.69
2:B:1333:ARG:NH1	2:B:1335:ARG:HD2	2.06	0.69
2:F:921:LEU:HD12	2:F:1008:PHE:CZ	2.25	0.69
2:F:1206:LEU:HD11	2:F:1210:ARG:CZ	2.21	0.69
2:B:51:LEU:HD13	2:B:1095:VAL:HG23	1.74	0.69
2:F:199:ASN:O	2:F:201:ILE:CD1	2.41	0.69
2:F:446:PHE:HZ	2:F:478:PHE:CD1	2.11	0.69
2:F:892:ILE:HB	2:F:896:LYS:HE3	1.74	0.69
2:B:345:GLU:N	2:B:345:GLU:OE1	2.26	0.69
5:J:40:C:H2'	5:J:41:A:C8	2.28	0.68
2:B:243:ALA:O	2:B:248:LEU:HB2	1.93	0.68
2:F:471:GLU:OE1	2:F:477:ASN:ND2	2.26	0.68
2:F:1091:GLN:HG3	5:J:91:C:H5''	1.76	0.68
2:F:1219:GLU:OE1	2:F:1335:ARG:NH2	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:745:ASP:OD2	2:B:938:ARG:NH2	2.27	0.68
2:F:151:LEU:HD22	2:F:151:LEU:C	2.14	0.68
2:B:369:GLN:HE22	2:B:400:ARG:HD2	1.57	0.68
2:F:697:ILE:HD11	2:F:708:ILE:HG13	1.76	0.67
5:J:40:C:H2'	5:J:41:A:H8	1.59	0.67
2:B:557:ARG:NH2	2:B:596:ASP:OD1	2.27	0.67
2:F:686:ASP:OD2	2:F:690:ASN:HA	1.93	0.67
2:B:565:LYS:HE2	2:B:580:ILE:HG12	1.77	0.67
2:B:818:ASN:O	2:B:818:ASN:ND2	2.28	0.67
2:B:860:SER:OG	2:B:863:ASN:OD1	2.11	0.67
2:F:208:ALA:HA	2:F:211:ILE:CG1	2.24	0.67
2:F:148:LYS:HB3	2:F:429:PHE:CD2	2.30	0.67
2:B:229:LEU:HB2	2:B:230:PRO:HD2	1.76	0.67
2:B:1241:HIS:CE1	2:B:1244:LYS:HA	2.29	0.67
2:F:870:VAL:HG12	2:F:871:PRO:HD2	1.77	0.67
2:B:1318:LEU:HD13	2:B:1319:GLY:N	2.09	0.67
2:F:153:LEU:HD23	2:F:153:LEU:C	2.16	0.67
2:F:791:LEU:HD23	2:F:818:ASN:OD1	1.94	0.67
2:F:826:GLN:OE1	2:F:859:ARG:NH1	2.28	0.67
1:A:27:G:H5'	1:A:28:A:C5'	2.25	0.66
2:B:70:ARG:NH2	5:I:61:C:OP1	2.28	0.66
2:F:70:ARG:NE	5:J:61:C:OP2	2.19	0.66
2:F:967:ARG:NH1	2:F:986:ASP:OD1	2.27	0.66
2:B:585:ASP:OD1	2:B:586:ARG:N	2.28	0.66
2:F:672:ASP:OD1	2:F:703:THR:HG22	1.95	0.66
2:B:5:TYR:CE2	2:B:756:PRO:HB3	2.30	0.66
2:F:139:ARG:NE	2:F:157:ALA:O	2.28	0.66
2:F:165:ARG:CD	2:F:168:PHE:CZ	2.73	0.66
2:B:967:ARG:NE	2:B:974:LYS:HB2	2.09	0.66
2:F:46:ASN:HD21	5:J:88:A:H61	1.44	0.66
2:F:892:ILE:HB	2:F:896:LYS:CE	2.25	0.66
2:F:40:ARG:NE	2:F:43:ILE:HD11	2.11	0.66
2:F:633:GLU:O	2:F:637:LYS:N	2.27	0.66
2:B:317:LEU:HD22	2:B:414:ILE:HD11	1.78	0.66
2:F:1206:LEU:HD11	2:F:1210:ARG:NH2	2.11	0.66
2:B:5:TYR:OH	2:B:754:HIS:O	2.13	0.66
2:F:340:ARG:HG3	2:F:347:TYR:CE1	2.31	0.66
2:F:686:ASP:HB3	2:F:690:ASN:OD1	1.96	0.66
2:B:544:GLN:O	2:B:548:ILE:N	2.18	0.65
2:F:90:MET:HE2	2:F:151:LEU:HD23	1.79	0.65
2:F:142:LEU:HD21	2:F:154:ILE:HG12	1.64	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:524:LEU:HD12	2:B:587:PHE:CE2	2.30	0.65
2:B:549:VAL:HA	2:B:553:PHE:HD2	1.61	0.65
2:B:989:LEU:HD21	2:B:1087:LEU:HD21	1.78	0.65
2:B:404:THR:HG22	2:B:405:PHE:H	1.61	0.65
2:F:853:ASP:HB3	2:F:895:ARG:HH11	1.61	0.65
2:B:823:TYR:HD2	2:B:858:THR:HG21	1.61	0.65
2:F:212:LEU:O	2:F:221:ARG:CB	2.45	0.65
2:F:686:ASP:HB3	2:F:690:ASN:CA	2.26	0.65
2:F:867:SER:HB2	2:F:1054:ASN:N	2.11	0.65
2:B:181:VAL:O	2:B:185:PHE:N	2.28	0.65
3:C:22:DT:H2''	3:C:23:DC:O5'	1.95	0.65
2:F:986:ASP:O	2:F:990:ASN:ND2	2.30	0.65
2:B:939:MET:HE2	2:B:953:VAL:HG21	1.79	0.65
3:C:25:DT:N3	3:C:26:DT:O4	2.29	0.65
2:F:153:LEU:HD23	2:F:153:LEU:O	1.96	0.65
2:F:422:ILE:O	2:F:425:ARG:HG2	1.97	0.65
2:F:978:ILE:CD1	2:F:1233:VAL:HG22	2.25	0.65
2:F:1197:LYS:O	2:F:1199:PRO:HD3	1.97	0.65
2:F:1304:GLU:O	2:F:1308:ASN:ND2	2.29	0.65
2:B:516:GLU:O	2:B:519:THR:HG22	1.98	0.64
2:B:824:VAL:HG22	2:B:863:ASN:HD22	1.61	0.64
2:F:167:HIS:HD2	2:F:169:LEU:HB2	1.60	0.64
2:F:221:ARG:O	2:F:225:LEU:N	2.22	0.64
1:A:5:C:O2'	1:A:6:G:O5'	2.16	0.64
2:B:879:MET:HG3	2:B:882:TYR:HB3	1.78	0.64
2:F:887:LEU:HD21	2:F:894:GLN:HG2	1.80	0.64
2:F:1357:GLU:O	5:J:81:G:N2	2.29	0.64
2:F:923:GLU:OE2	2:F:925:ARG:NH1	2.29	0.64
1:E:3:A:C4	1:E:4:A:N7	2.66	0.64
2:F:149:ALA:HB3	2:F:154:ILE:HG13	1.80	0.64
2:F:760:VAL:HG22	2:F:956:ILE:HD12	1.79	0.64
2:B:1120:ILE:HD11	2:B:1137:PRO:HG3	1.79	0.64
2:F:149:ALA:HB3	2:F:154:ILE:CG1	2.28	0.64
2:F:1110:ILE:HD13	2:F:1122:ARG:CZ	2.28	0.64
2:F:1286:ASN:ND2	2:F:1332:ASP:O	2.31	0.64
2:F:89:GLU:HG3	2:F:432:PHE:HD2	1.62	0.63
2:F:165:ARG:HG2	2:F:166:GLY:O	1.98	0.63
2:F:184:LEU:HD13	2:F:295:ASN:HB3	1.79	0.63
2:F:853:ASP:HB3	2:F:895:ARG:NH1	2.12	0.63
2:F:1147:ALA:HB2	2:F:1190:VAL:HA	1.79	0.63
2:B:1312:LEU:HD21	2:B:1326:TYR:HD1	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:U:O2	1:A:3:A:H2'	1.97	0.63
2:F:135:ILE:HG21	5:J:46:A:H5'	1.80	0.63
2:F:189:VAL:HG13	2:F:201:ILE:HG22	1.80	0.63
1:A:2:U:O2	1:A:3:A:C2'	2.46	0.63
2:F:168:PHE:HB2	2:F:447:ARG:NH1	2.14	0.63
2:F:373:TYR:OH	2:F:398:LEU:N	2.30	0.63
2:B:121:ASN:OD1	2:B:124:ASP:HB2	1.99	0.63
2:B:270:THR:O	2:B:274:ASP:HB2	1.98	0.63
1:E:19:A:OP1	2:F:164:PHE:HD1	1.82	0.63
2:B:103:GLU:OE2	2:B:111:LYS:HG2	1.99	0.62
2:F:121:ASN:OD1	2:F:124:ASP:N	2.31	0.62
2:F:601:ILE:CD1	2:F:607:LEU:HD21	2.28	0.62
2:F:646:LYS:O	2:F:650:GLN:NE2	2.22	0.62
2:F:921:LEU:CD1	2:F:1008:PHE:HE2	2.02	0.62
2:F:963:VAL:HG21	2:F:990:ASN:OD1	1.99	0.62
2:B:70:ARG:HH22	2:B:462:PHE:HD2	1.47	0.62
2:F:89:GLU:HG3	2:F:432:PHE:CD2	2.34	0.62
2:F:139:ARG:HH21	2:F:160:HIS:HD2	1.45	0.62
2:F:168:PHE:CB	2:F:447:ARG:HH11	2.12	0.62
2:F:182:ASP:O	2:F:186:ILE:HD12	1.99	0.62
1:E:3:A:H2'	1:E:4:A:H8	1.64	0.62
2:F:918:LYS:O	2:F:922:VAL:HG22	2.00	0.62
2:F:1266:LEU:HB3	2:F:1294:TYR:OH	1.99	0.62
2:F:1294:TYR:HE1	2:F:1305:GLN:HE21	1.45	0.62
2:F:1311:HIS:O	2:F:1314:THR:HG22	2.00	0.62
1:A:5:C:H2'	1:A:6:G:H8	1.64	0.62
2:F:114:GLU:HG2	2:F:120:GLY:HA2	1.81	0.62
2:B:893:THR:HG23	2:B:896:LYS:H	1.63	0.62
2:F:841:ILE:HD12	2:F:854:ASN:HA	1.82	0.62
2:B:823:TYR:HA	2:B:875:VAL:CG1	2.30	0.62
2:F:189:VAL:HG13	2:F:201:ILE:CG2	2.30	0.62
2:F:207:ASP:O	2:F:211:ILE:CG1	2.39	0.62
2:F:977:GLU:HG3	2:F:1310:ILE:CG2	2.30	0.62
2:F:1300:LYS:NZ	2:F:1304:GLU:OE1	2.33	0.62
2:B:118:ILE:HD13	2:B:128:TYR:CD2	2.35	0.62
2:F:184:LEU:O	2:F:187:GLN:OE1	2.18	0.62
2:B:233:LYS:HG2	2:B:235:ASN:H	1.65	0.61
2:B:247:GLY:O	2:B:248:LEU:HG	2.00	0.61
2:B:810:LYS:HG2	2:B:838:VAL:HG23	1.82	0.61
2:B:184:LEU:HD12	2:B:299:ALA:HB2	1.82	0.61
2:F:183:LYS:H	2:F:183:LYS:HD2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:LEU:HD23	2:B:302:LEU:HD23	1.81	0.61
1:E:19:A:H4'	2:F:407:ASN:C	2.20	0.61
2:F:208:ALA:N	2:F:211:ILE:HD12	2.15	0.61
2:B:332:LEU:HD13	2:B:359:TYR:CE1	2.35	0.61
2:F:212:LEU:HD11	2:F:300:ILE:CG1	2.19	0.61
5:J:83:C:H2'	5:J:84:A:H8	1.65	0.61
5:I:83:C:H2'	5:I:84:A:H8	1.64	0.61
2:B:1318:LEU:HD13	2:B:1318:LEU:C	2.20	0.61
2:F:1064:GLU:OE1	2:F:1065:THR:N	2.31	0.61
2:B:525:THR:HA	2:B:545:LYS:HE2	1.83	0.61
2:B:1000:LYS:HE2	2:B:1066:ASN:HA	1.83	0.61
2:F:35:LEU:HB2	2:F:1358:THR:HG22	1.83	0.61
2:F:841:ILE:CD1	2:F:896:LYS:HG3	2.30	0.61
2:F:275:LEU:O	2:F:279:LEU:N	2.34	0.61
2:F:818:ASN:ND2	2:F:818:ASN:O	2.32	0.61
5:J:44:U:O2'	5:J:45:U:H5'	1.99	0.61
2:B:168:PHE:CD2	2:B:447:ARG:HD3	2.35	0.61
2:B:114:GLU:HG2	2:B:120:GLY:HA2	1.83	0.60
1:A:31:U:H1'	5:I:39:G:N2	2.15	0.60
2:F:1062:LEU:O	2:F:1062:LEU:HG	2.01	0.60
2:F:1206:LEU:CD1	2:F:1210:ARG:NH1	2.64	0.60
2:B:1123:LYS:NZ	5:I:52:A:OP1	2.34	0.60
2:F:70:ARG:HH21	5:J:61:C:P	2.24	0.60
2:F:149:ALA:CB	2:F:154:ILE:CG1	2.79	0.60
1:A:2:U:O2	1:A:4:A:H8	1.83	0.60
2:B:917:ILE:HD11	2:B:1042:ILE:HG22	1.82	0.60
2:F:692:ASN:O	2:F:696:LEU:HG	2.01	0.60
2:B:909:SER:O	2:B:913:LYS:N	2.26	0.60
2:F:737:ILE:O	2:F:740:THR:HG22	2.01	0.60
2:F:1120:ILE:HB	2:F:1134:PHE:HB2	1.84	0.60
2:B:27:VAL:HG12	2:B:1086:VAL:HG22	1.83	0.60
2:B:250:PRO:HD2	2:B:264:LEU:O	2.01	0.60
2:B:420:HIS:ND1	2:B:441:GLU:OE2	2.35	0.60
2:F:69:ARG:NH2	5:J:63:U:OP2	2.35	0.60
2:F:545:LYS:NZ	2:F:683:LEU:O	2.35	0.60
2:F:142:LEU:HD21	2:F:149:ALA:HB2	1.83	0.60
2:B:541:SER:N	2:B:544:GLN:OE1	2.34	0.59
2:B:670:ILE:HG22	2:B:704:PHE:HE1	1.67	0.59
2:B:1305:GLN:O	2:B:1309:ILE:HG13	2.02	0.59
2:F:821:ASP:HB2	2:F:828:LEU:HD21	1.83	0.59
2:B:902:LYS:HA	2:B:905:ARG:HE	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:138:LEU:HD11	2:F:153:LEU:HD23	1.74	0.59
2:B:158:LEU:HD11	2:B:423:LEU:HD21	1.84	0.59
2:B:386:THR:O	2:B:386:THR:HG22	2.01	0.59
2:B:1062:LEU:HD23	2:B:1062:LEU:H	1.67	0.59
2:F:137:HIS:HA	2:F:322:ILE:HD11	1.83	0.59
2:F:138:LEU:HD21	2:F:153:LEU:O	2.01	0.59
2:F:149:ALA:HB2	2:F:154:ILE:HD11	1.82	0.59
2:F:677:LYS:HB3	2:F:682:PHE:CD2	2.36	0.59
1:A:10:U:H2'	1:A:11:U:C6	2.37	0.59
3:C:25:DT:H2'	3:C:25:DT:O2	2.01	0.59
2:B:979:ASN:OD1	2:B:980:ASN:N	2.35	0.59
2:B:358:GLY:O	2:B:362:TYR:N	2.33	0.59
2:B:644:ASP:HB3	2:B:647:VAL:HG23	1.85	0.59
2:F:253:LYS:HB2	2:F:262:ALA:H	1.66	0.59
2:F:686:ASP:OD2	2:F:691:ARG:N	2.35	0.59
2:B:1252:ASN:HD22	2:B:1255:LYS:HD2	1.66	0.59
2:F:531:THR:HG21	2:F:575:PHE:CE1	2.38	0.59
2:B:828:LEU:HD22	2:B:836:TYR:CE2	2.37	0.59
2:F:943:TYR:CE2	2:F:949:LEU:HD13	2.38	0.59
2:B:971:GLN:O	2:B:971:GLN:HG2	2.01	0.59
2:B:1308:ASN:HD22	2:B:1327:PHE:H	1.51	0.59
2:F:601:ILE:HD11	2:F:607:LEU:HD21	1.83	0.59
2:B:1258:PHE:HE1	2:B:1262:HIS:CD2	2.21	0.59
2:B:1290:VAL:HG22	2:B:1331:ILE:HD13	1.85	0.59
2:F:1326:TYR:CE2	2:F:1327:PHE:HD2	2.21	0.58
2:B:565:LYS:HA	2:B:569:PHE:HB2	1.84	0.58
2:F:1206:LEU:HD11	2:F:1210:ARG:NH1	2.16	0.58
2:B:563:GLN:O	2:B:567:ASP:HB2	2.03	0.58
2:B:971:GLN:O	2:B:1234:ASN:ND2	2.35	0.58
2:B:671:ARG:HG3	2:B:678:THR:HG22	1.84	0.58
2:B:1146:VAL:HG11	2:B:1194:LEU:HD12	1.86	0.58
2:F:466:THR:O	2:F:482:VAL:HG13	2.04	0.58
2:B:135:ILE:HG21	2:B:160:HIS:CD2	2.39	0.58
5:J:53:G:C4	5:J:62:G:N2	2.72	0.58
2:F:208:ALA:O	2:F:211:ILE:HB	2.04	0.58
2:F:448:ILE:HD12	2:F:455:LEU:HD11	1.86	0.58
2:F:135:ILE:HD13	2:F:156:LEU:HD23	1.85	0.58
2:F:139:ARG:NH1	2:F:418:GLU:OE2	2.37	0.58
2:B:243:ALA:O	2:B:246:LEU:O	2.21	0.58
2:F:844:GLN:HA	2:F:847:LEU:O	2.04	0.58
2:B:119:PHE:HD1	2:B:152:ARG:NH1	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1041:ASN:O	2:B:1044:ASN:ND2	2.36	0.58
2:F:149:ALA:HB3	2:F:154:ILE:HD12	1.82	0.58
2:F:226:ILE:CG1	2:F:232:GLU:HG2	2.30	0.58
2:B:544:GLN:HA	2:B:547:ALA:HB3	1.86	0.57
2:F:305:ILE:HG13	2:F:306:LEU:HD13	1.86	0.57
2:F:499:ASP:HB2	2:F:663:SER:HB3	1.85	0.57
2:B:245:SER:HA	2:B:297:SER:HB2	1.85	0.57
2:B:687:GLY:O	2:B:690:ASN:ND2	2.38	0.57
2:F:677:LYS:HB3	2:F:682:PHE:CE2	2.39	0.57
1:E:3:A:N6	1:E:4:A:H62	2.01	0.57
2:F:78:ARG:CZ	2:F:165:ARG:NH2	2.67	0.57
2:F:1286:ASN:O	2:F:1290:VAL:HG23	2.04	0.57
2:F:135:ILE:CG2	5:J:46:A:H5'	2.33	0.57
2:F:962:LEU:HB3	2:F:1043:MET:CE	2.35	0.57
2:F:1019:ARG:O	2:F:1021:MET:N	2.31	0.57
2:B:76:LYS:HE3	2:B:80:CYS:SG	2.44	0.57
2:B:229:LEU:O	2:B:231:GLY:N	2.38	0.57
2:B:485:GLY:HA3	2:B:631:MET:SD	2.44	0.57
2:B:954:LYS:HG3	2:B:1009:VAL:HG11	1.86	0.57
1:E:14:G:OP2	2:F:63:ARG:HD3	2.04	0.57
1:E:4:A:O2'	1:E:5:C:O5'	2.21	0.57
2:F:886:LEU:HD22	2:F:891:LEU:HD11	1.87	0.57
2:B:11:ILE:HB	2:B:763:MET:HG2	1.87	0.57
2:B:70:ARG:HH21	5:I:61:C:P	2.27	0.57
2:B:51:LEU:CD1	2:B:1095:VAL:HG23	2.35	0.57
2:B:338:LEU:O	2:B:383:MET:CE	2.53	0.57
2:B:816:LEU:HD12	2:B:891:LEU:HA	1.86	0.57
4:H:11:DT:H2''	4:H:12:DG:C8	2.39	0.57
2:F:212:LEU:HA	2:F:221:ARG:CB	2.35	0.57
2:F:921:LEU:HD21	2:F:1042:ILE:CD1	2.35	0.57
2:F:1179:ILE:O	2:F:1183:GLU:HG3	2.05	0.57
2:B:22:THR:HG22	2:B:23:ASP:H	1.69	0.56
2:B:45:LYS:NZ	2:B:1354:GLY:O	2.34	0.56
2:B:756:PRO:O	2:B:953:VAL:HG22	2.05	0.56
2:F:514:LEU:H	2:F:514:LEU:HD12	1.70	0.56
2:B:40:ARG:NH2	5:I:92:G:OP1	2.37	0.56
2:B:127:ALA:HA	2:B:130:GLU:HB2	1.87	0.56
2:B:1220:LEU:CD1	2:B:1338:SER:O	2.53	0.56
2:F:272:ASP:HA	2:F:275:LEU:HB3	1.86	0.56
2:F:1114:ARG:HD2	2:F:1116:SER:HB2	1.88	0.56
2:B:139:ARG:O	2:B:143:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:583:VAL:HG22	2:B:584:GLU:N	2.19	0.56
2:B:1000:LYS:O	2:B:1000:LYS:HD3	2.05	0.56
2:B:1349:HIS:HB3	5:I:68:A:N3	2.20	0.56
2:F:149:ALA:HB1	2:F:154:ILE:HG13	1.86	0.56
2:F:167:HIS:CD2	2:F:169:LEU:HB2	2.40	0.56
2:F:258:LEU:HD22	2:F:260:GLU:H	1.69	0.56
2:F:925:ARG:HB3	2:F:928:THR:HG22	1.87	0.56
5:J:94:U:H2'	5:J:95:G:C8	2.40	0.56
2:B:6:SER:HB2	2:B:21:ILE:HG13	1.86	0.56
2:B:1228:LEU:HD12	2:B:1229:PRO:HD2	1.86	0.56
2:F:94:ASP:CB	2:F:97:PHE:HB2	2.36	0.56
2:F:551:LEU:O	2:F:555:THR:OG1	2.14	0.56
2:F:870:VAL:HG11	2:F:899:ASN:O	2.05	0.56
2:F:1326:TYR:HE2	2:F:1327:PHE:HD2	1.54	0.56
5:J:91:C:O2'	5:J:92:G:P	2.64	0.56
2:B:114:GLU:HG3	2:B:116:HIS:H	1.70	0.56
2:B:489:GLN:HG3	2:B:625:LEU:HD21	1.88	0.56
2:F:135:ILE:HG21	2:F:160:HIS:ND1	2.21	0.56
2:F:332:LEU:HD21	2:F:336:LYS:HE3	1.85	0.56
2:F:681:ASP:HA	2:F:684:LYS:NZ	2.20	0.56
2:B:543:GLU:O	2:B:547:ALA:N	2.38	0.56
2:B:956:ILE:HG12	2:B:1009:VAL:HG22	1.88	0.56
2:F:820:ARG:HG3	2:F:826:GLN:O	2.06	0.56
2:B:369:GLN:NE2	2:B:400:ARG:HD2	2.21	0.56
2:B:755:LYS:NZ	2:B:939:MET:O	2.19	0.56
2:F:829:ASP:OD1	2:F:831:ASN:N	2.39	0.56
2:F:1114:ARG:NH1	4:H:9:DA:OP1	2.38	0.56
1:A:5:C:C2'	1:A:6:G:O5'	2.54	0.56
2:B:321:MET:O	2:B:324:ARG:N	2.39	0.56
2:B:8:GLY:HA3	2:B:991:ALA:HB2	1.88	0.55
2:B:38:THR:HG22	2:B:40:ARG:H	1.71	0.55
2:B:395:ARG:NH2	2:B:397:ASP:OD2	2.38	0.55
2:F:185:PHE:O	2:F:189:VAL:HG23	2.07	0.55
2:F:1266:LEU:HG	2:F:1309:ILE:CD1	2.36	0.55
2:B:620:VAL:O	2:B:624:THR:HG22	2.06	0.55
2:B:875:VAL:HA	2:B:878:LYS:HD2	1.88	0.55
4:D:5:DA:H1'	4:D:6:DG:C8	2.41	0.55
2:F:51:LEU:HD13	2:F:1352:ILE:HG13	1.87	0.55
2:F:162:ILE:HG12	2:F:444:LEU:HD12	1.88	0.55
2:F:516:GLU:O	2:F:519:THR:HG22	2.06	0.55
2:B:1041:ASN:HB2	2:B:1044:ASN:HD21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:U:H5'	2:F:107:VAL:HG12	1.87	0.55
2:F:478:PHE:HE2	2:F:482:VAL:HB	1.71	0.55
2:F:336:LYS:HE2	2:F:351:PHE:CE1	2.41	0.55
2:F:243:ALA:HB3	2:F:250:PRO:HG3	1.88	0.55
2:F:671:ARG:HD3	2:F:671:ARG:N	2.21	0.55
2:B:1207:GLU:HG2	2:B:1210:ARG:HH11	1.72	0.55
2:F:122:ILE:O	2:F:126:VAL:HG23	2.05	0.55
2:F:1224:ASN:HB2	2:F:1280:VAL:HG11	1.87	0.55
2:F:106:LEU:HD22	2:F:1131:TYR:OH	2.06	0.55
2:F:46:ASN:HD22	2:F:1089:MET:CE	2.20	0.55
2:F:151:LEU:HD13	2:F:151:LEU:N	2.21	0.55
2:F:853:ASP:CG	2:F:893:THR:HG21	2.27	0.55
2:B:325:TYR:HD1	5:I:44:U:C2	2.24	0.55
2:B:595:HIS:HB3	2:B:599:LYS:NZ	2.22	0.55
2:F:234:LYS:H	2:F:234:LYS:HD3	1.71	0.55
2:F:309:ASN:OD1	2:F:312:ILE:HG23	2.07	0.55
2:F:1349:HIS:CE1	5:J:69:A:H5'	2.41	0.55
2:B:824:VAL:HG11	2:B:859:ARG:HH12	1.72	0.55
2:B:1120:ILE:HB	2:B:1134:PHE:HB2	1.89	0.55
2:F:427:GLU:HA	2:F:433:LEU:HB2	1.87	0.55
2:F:523:GLU:OE1	2:F:589:ALA:N	2.38	0.55
2:F:672:ASP:HB3	2:F:675:SER:HB2	1.89	0.55
2:F:921:LEU:HD11	2:F:1042:ILE:HD13	1.89	0.55
2:F:1262:HIS:HB3	2:F:1265:TYR:CD2	2.41	0.55
2:B:971:GLN:HA	2:B:973:TYR:CE2	2.42	0.54
2:F:583:VAL:HG22	2:F:584:GLU:H	1.72	0.54
2:B:212:LEU:HD21	2:B:225:LEU:HD12	1.90	0.54
2:B:1318:LEU:HD22	2:B:1319:GLY:H	1.72	0.54
2:F:328:HIS:NE2	2:F:359:TYR:OH	2.24	0.54
3:G:3:DA:N6	4:H:9:DA:H61	2.04	0.54
4:H:11:DT:H2''	4:H:12:DG:H8	1.72	0.54
2:B:117:PRO:HD2	2:B:125:GLU:OE2	2.07	0.54
2:B:930:HIS:O	2:B:934:ILE:HG13	2.06	0.54
2:B:217:SER:O	2:B:221:ARG:HG3	2.08	0.54
2:B:545:LYS:CE	2:B:690:ASN:OD1	2.55	0.54
2:B:212:LEU:O	2:B:221:ARG:HD2	2.08	0.54
2:F:662:LEU:HD22	2:F:666:LEU:HD23	1.89	0.54
2:F:962:LEU:HB3	2:F:1043:MET:HE1	1.89	0.54
2:B:824:VAL:HG22	2:B:863:ASN:ND2	2.23	0.54
2:F:140:LYS:HD3	2:F:319:ALA:HB2	1.90	0.54
2:F:1108:GLU:HB2	3:G:9:DT:H5''	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:GLN:HG2	2:B:267:SER:H	1.72	0.54
2:B:980:ASN:HB2	2:B:1225:GLU:CD	2.28	0.54
5:J:96:C:C4	5:J:97:U:C4	2.96	0.54
2:B:219:SER:O	2:B:222:LEU:HB3	2.08	0.54
2:B:302:LEU:HA	2:B:305:ILE:HG12	1.90	0.54
2:F:869:ASN:HD21	2:F:907:GLY:HA3	1.72	0.54
2:F:922:VAL:CG1	2:F:1007:GLU:HG3	2.38	0.54
2:B:339:VAL:HA	2:B:383:MET:HE1	1.90	0.54
2:F:750:VAL:HG21	2:F:1355:LEU:HD12	1.90	0.54
2:B:137:HIS:HE1	2:B:325:TYR:CD2	2.25	0.54
2:B:521:TYR:CE2	2:B:549:VAL:HG21	2.43	0.54
2:B:621:LEU:O	2:B:625:LEU:HB2	2.08	0.54
1:E:27:G:H5'	1:E:28:A:O5'	2.07	0.54
2:F:343:LEU:HD11	2:F:383:MET:HB2	1.90	0.54
2:F:489:GLN:HG3	2:F:625:LEU:HD21	1.89	0.54
2:F:1019:ARG:C	2:F:1021:MET:H	2.11	0.54
2:B:464:TRP:CZ2	2:B:491:PHE:HD1	2.26	0.53
2:F:362:TYR:OH	2:F:401:LYS:HG3	2.08	0.53
1:A:3:A:H2'	1:A:3:A:N3	2.23	0.53
2:B:94:ASP:OD2	2:B:152:ARG:HD3	2.08	0.53
2:B:1207:GLU:HG3	2:B:1208:ASN:N	2.22	0.53
1:E:27:G:H5'	1:E:28:A:C5'	2.39	0.53
2:F:5:TYR:CE2	2:F:751:MET:HG3	2.44	0.53
2:F:212:LEU:CD1	2:F:300:ILE:CD1	2.87	0.53
5:I:37:U:H2'	5:I:38:A:C8	2.43	0.53
5:J:45:U:C2	5:J:46:A:C8	2.97	0.53
2:B:742:LYS:NZ	5:I:67:C:OP1	2.21	0.53
2:F:32:PHE:O	2:F:42:SER:HA	2.08	0.53
2:F:220:ARG:O	2:F:224:ASN:N	2.37	0.53
2:F:841:ILE:HD11	2:F:896:LYS:HG3	1.89	0.53
2:F:1124:LYS:N	5:J:53:G:OP1	2.33	0.53
3:G:3:DA:H61	4:H:9:DA:N6	2.07	0.53
2:B:1147:ALA:HB1	2:B:1188:LYS:O	2.08	0.53
2:B:1207:GLU:HG3	2:B:1208:ASN:H	1.74	0.53
1:E:27:G:H1'	2:F:129:HIS:CD2	2.44	0.53
2:F:1295:ASN:HA	2:F:1298:ARG:NH1	2.24	0.53
1:A:2:U:N3	1:A:4:A:H3'	2.19	0.53
2:B:1232:TYR:HA	2:B:1235:PHE:HB3	1.89	0.53
2:F:468:LYS:HE3	2:F:483:ASP:HB3	1.91	0.53
2:F:976:ARG:HA	2:F:982:HIS:CD2	2.43	0.53
2:B:642:LEU:HB2	2:B:643:PHE:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:972:PHE:HE1	2:B:1084:ARG:HB2	1.73	0.53
2:F:48:ILE:HG12	2:F:984:ALA:HB1	1.90	0.53
2:F:137:HIS:HA	2:F:322:ILE:CD1	2.39	0.53
2:F:271:TYR:O	2:F:275:LEU:N	2.34	0.53
2:B:118:ILE:HD13	2:B:128:TYR:HD2	1.71	0.53
2:B:672:ASP:HA	2:B:703:THR:HG22	1.91	0.53
2:B:849:ASP:OD2	2:B:895:ARG:NH1	2.40	0.53
3:C:25:DT:C2	3:C:26:DT:C5	2.96	0.53
2:F:649:LYS:HB3	2:F:653:ARG:HH21	1.74	0.53
5:I:69:A:H2'	5:I:70:C:C6	2.44	0.53
2:B:273:ASP:N	2:B:273:ASP:OD1	2.36	0.53
2:F:226:ILE:HD11	2:F:232:GLU:CD	2.30	0.53
2:F:312:ILE:HG13	2:F:313:THR:N	2.24	0.53
2:F:1048:THR:HA	2:F:1076:LYS:HD3	1.91	0.53
2:B:672:ASP:HA	2:B:703:THR:CG2	2.39	0.53
2:F:164:PHE:O	2:F:415:HIS:NE2	2.41	0.53
2:F:860:SER:OG	2:F:863:ASN:OD1	2.27	0.53
2:B:380:LEU:O	2:B:386:THR:HG21	2.07	0.52
2:B:1211:LYS:C	2:B:1223:GLY:HA3	2.28	0.52
2:F:66:ARG:HA	2:F:69:ARG:NH1	2.24	0.52
2:B:1047:LYS:HB2	2:B:1050:ILE:HG22	1.90	0.52
2:B:1106:SER:HB2	2:B:1135:ASP:O	2.09	0.52
2:B:1241:HIS:ND1	2:B:1244:LYS:HA	2.25	0.52
2:F:139:ARG:O	2:F:143:VAL:HG23	2.09	0.52
2:F:977:GLU:HG3	2:F:1310:ILE:HG21	1.90	0.52
2:F:1351:SER:OG	2:F:1356:TYR:HB2	2.09	0.52
3:G:3:DA:H61	4:H:9:DA:H61	1.57	0.52
2:B:233:LYS:HG2	2:B:235:ASN:N	2.25	0.52
2:B:1002:PRO:HA	2:B:1005:GLU:HG3	1.90	0.52
2:F:167:HIS:HD2	2:F:169:LEU:CB	2.23	0.52
2:F:1050:ILE:HG13	2:F:1050:ILE:O	2.09	0.52
1:A:2:U:O2	1:A:3:A:O2'	2.27	0.52
1:A:10:U:H2'	1:A:11:U:H6	1.75	0.52
2:F:38:THR:HG22	2:F:40:ARG:H	1.74	0.52
2:F:140:LYS:HB3	2:F:322:ILE:CD1	2.40	0.52
2:F:922:VAL:HG11	2:F:1007:GLU:HG3	1.90	0.52
2:B:391:VAL:O	2:B:395:ARG:HG3	2.09	0.52
2:B:427:GLU:OE1	2:B:437:ARG:NH1	2.42	0.52
2:F:151:LEU:HD22	2:F:152:ARG:CA	2.40	0.52
4:H:6:DG:H2''	4:H:7:DG:H5''	1.91	0.52
2:B:1231:LYS:HD2	2:B:1265:TYR:OH	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:844:GLN:HG3	2:F:848:LYS:HD2	1.91	0.52
2:F:867:SER:HB2	2:F:1053:ALA:C	2.30	0.52
2:F:151:LEU:N	2:F:151:LEU:CD1	2.73	0.52
2:F:531:THR:HG1	2:F:575:PHE:HD1	1.57	0.52
2:F:776:ASN:O	2:F:780:ARG:HG2	2.08	0.52
2:F:980:ASN:HB2	2:F:1225:GLU:OE2	2.10	0.52
5:I:39:G:H5'	5:I:40:C:OP2	2.10	0.52
2:B:737:ILE:O	2:B:740:THR:HG22	2.09	0.51
2:B:1074:TRP:HZ2	2:B:1080:PHE:CD2	2.28	0.51
2:B:1243:GLU:HG3	2:B:1246:LYS:NZ	2.26	0.51
2:F:262:ALA:HB1	2:F:278:LEU:HG	1.91	0.51
2:F:867:SER:HB2	2:F:1054:ASN:CA	2.40	0.51
2:F:1000:LYS:HG3	2:F:1001:TYR:CD2	2.46	0.51
1:A:5:C:O2'	1:A:6:G:C5'	2.58	0.51
2:B:201:ILE:HG22	2:B:202:ASN:N	2.22	0.51
2:B:849:ASP:OD1	2:B:851:SER:OG	2.25	0.51
2:F:40:ARG:HE	2:F:43:ILE:HD11	1.75	0.51
2:F:542:GLY:HA3	2:F:685:SER:HA	1.92	0.51
2:F:878:LYS:HB3	2:F:879:MET:SD	2.51	0.51
2:F:1167:THR:HG23	2:F:1170:GLU:H	1.74	0.51
5:J:45:U:H2'	5:J:46:A:C8	2.45	0.51
2:F:551:LEU:HD23	2:F:568:TYR:HD1	1.75	0.51
1:A:29:G:N3	5:I:41:A:C2	2.78	0.51
2:F:134:THR:O	2:F:137:HIS:HB2	2.11	0.51
2:F:650:GLN:O	2:F:653:ARG:HG2	2.11	0.51
2:B:686:ASP:HB3	2:B:690:ASN:HA	1.92	0.51
2:B:921:LEU:HB3	2:B:1008:PHE:CZ	2.45	0.51
2:F:349:GLU:O	2:F:353:ASP:HB3	2.11	0.51
3:G:22:DT:H2''	3:G:23:DC:O5'	2.09	0.51
2:B:492:ILE:O	2:B:496:THR:HG23	2.10	0.51
2:B:1060:ARG:NH1	2:B:1064:GLU:OE2	2.42	0.51
2:B:1074:TRP:HZ2	2:B:1080:PHE:CE2	2.28	0.51
2:F:142:LEU:CD1	2:F:154:ILE:CD1	2.85	0.51
2:B:338:LEU:O	2:B:383:MET:HE1	2.10	0.51
2:B:353:ASP:CG	2:B:356:LYS:HG2	2.30	0.51
2:F:44:LYS:NZ	5:J:92:G:O6	2.21	0.51
2:F:410:ILE:HG21	2:F:415:HIS:NE2	2.26	0.51
2:F:755:LYS:HD3	2:F:939:MET:HE3	1.93	0.51
1:A:25:U:H2'	1:A:26:A:C8	2.46	0.51
2:B:325:TYR:CD1	5:I:44:U:C2	2.99	0.51
2:B:677:LYS:HD3	2:B:682:PHE:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1232:TYR:O	2:B:1236:LEU:N	2.29	0.51
2:B:1308:ASN:HD22	2:B:1327:PHE:N	2.07	0.51
2:F:167:HIS:N	2:F:410:ILE:O	2.41	0.51
2:F:1051:THR:HG22	2:F:1053:ALA:H	1.76	0.51
2:B:66:ARG:HD2	2:B:462:PHE:CE2	2.46	0.51
2:F:465:MET:SD	2:F:482:VAL:HG21	2.51	0.51
5:J:83:C:H2'	5:J:84:A:C8	2.46	0.51
2:F:137:HIS:HA	2:F:322:ILE:CG1	2.41	0.51
2:F:226:ILE:CG2	2:F:231:GLY:H	2.24	0.51
2:F:971:GLN:HG2	2:F:973:TYR:CE2	2.47	0.51
2:B:509:PRO:HB3	2:B:624:THR:HG21	1.93	0.50
2:B:977:GLU:N	2:B:977:GLU:OE1	2.44	0.50
1:A:1:U:H5	2:B:661:ARG:HH12	1.59	0.50
2:B:823:TYR:CD2	2:B:858:THR:HG21	2.45	0.50
2:B:1081:ALA:O	2:B:1085:LYS:HG3	2.11	0.50
2:F:148:LYS:HB2	2:F:429:PHE:CD2	2.46	0.50
2:F:1205:GLU:CD	2:F:1359:ARG:HH22	2.13	0.50
2:B:281:GLN:OE1	2:B:281:GLN:N	2.38	0.50
2:B:1356:TYR:HB3	5:I:81:G:N1	2.27	0.50
2:F:128:TYR:CE1	2:F:153:LEU:HD12	2.45	0.50
2:F:601:ILE:HD11	2:F:607:LEU:HD11	1.93	0.50
2:F:1045:PHE:CA	2:F:1060:ARG:NH1	2.73	0.50
2:F:1046:PHE:O	2:F:1076:LYS:NZ	2.45	0.50
2:B:448:ILE:HD13	2:B:455:LEU:HD13	1.93	0.50
2:B:1105:PHE:CG	2:B:1169:MET:HG3	2.46	0.50
3:C:24:DG:H5''	3:C:25:DT:OP2	2.11	0.50
2:F:43:ILE:HG22	2:F:45:LYS:HG3	1.91	0.50
2:B:69:ARG:HD3	5:I:62:G:C8	2.47	0.50
2:B:1047:LYS:CB	2:B:1050:ILE:HG22	2.42	0.50
1:E:23:U:H5''	2:F:1112:PRO:HG3	1.93	0.50
2:F:762:GLU:OE1	2:F:990:ASN:ND2	2.39	0.50
5:J:95:G:C6	5:J:96:C:N4	2.79	0.50
2:B:670:ILE:HG22	2:B:704:PHE:CE1	2.45	0.50
2:F:1333:ARG:CZ	2:F:1335:ARG:HD2	2.41	0.50
2:B:195:LEU:HB3	2:B:196:PHE:HD1	1.77	0.50
2:B:813:LEU:O	2:B:817:GLN:HG3	2.11	0.50
2:B:1207:GLU:CG	2:B:1208:ASN:H	2.25	0.50
2:F:8:GLY:O	2:F:987:ALA:HB1	2.11	0.50
2:F:74:ARG:O	2:F:78:ARG:HG3	2.12	0.50
2:F:160:HIS:CD2	2:F:160:HIS:C	2.85	0.50
2:B:595:HIS:HB3	2:B:599:LYS:HZ2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:606:PHE:O	2:B:612:ASN:ND2	2.44	0.50
2:B:913:LYS:O	2:B:916:PHE:HB2	2.12	0.50
2:B:1226:LEU:HB2	2:B:1276:PHE:CE2	2.47	0.50
2:F:155:TYR:C	2:F:155:TYR:CD1	2.84	0.50
2:F:237:LEU:HD12	2:F:238:PHE:N	2.27	0.50
2:B:1220:LEU:HD12	2:B:1338:SER:O	2.12	0.50
2:F:27:VAL:HG12	2:F:1086:VAL:HG22	1.92	0.50
2:F:616:LEU:HA	2:F:619:ILE:HG22	1.93	0.50
2:B:74:ARG:NH2	5:I:60:C:OP1	2.44	0.49
2:B:514:LEU:HD11	2:B:667:ILE:HG21	1.94	0.49
2:B:1096:LYS:HG2	2:B:1201:TYR:CD2	2.47	0.49
2:F:427:GLU:OE1	2:F:434:LYS:HA	2.12	0.49
2:F:981:TYR:O	2:F:983:HIS:N	2.45	0.49
2:B:1235:PHE:O	2:B:1239:ALA:N	2.33	0.49
2:F:410:ILE:HD13	2:F:415:HIS:NE2	2.27	0.49
2:F:695:GLN:O	2:F:699:ASP:HB2	2.12	0.49
2:F:985:HIS:CD2	2:F:1087:LEU:HD22	2.47	0.49
2:F:1147:ALA:HB1	2:F:1188:LYS:O	2.11	0.49
2:F:1206:LEU:HD12	2:F:1210:ARG:HH12	1.76	0.49
2:F:1228:LEU:HD12	2:F:1229:PRO:HD2	1.94	0.49
2:B:961:LYS:HA	2:B:964:SER:HB3	1.94	0.49
2:F:628:ASP:O	2:F:632:ILE:HG13	2.12	0.49
2:F:918:LYS:CE	2:F:1018:VAL:HG11	2.43	0.49
2:B:784:ILE:HG21	2:B:815:TYR:HD2	1.77	0.49
2:F:139:ARG:HD3	2:F:157:ALA:CA	2.43	0.49
2:F:334:LEU:O	2:F:338:LEU:HG	2.12	0.49
2:F:566:GLU:O	2:F:570:LYS:HB3	2.11	0.49
2:F:583:VAL:HG22	2:F:584:GLU:N	2.26	0.49
2:B:809:GLU:OE1	2:B:855:LYS:HE2	2.12	0.49
2:B:850:ASP:HB3	2:B:855:LYS:NZ	2.27	0.49
2:F:433:LEU:O	2:F:437:ARG:HB2	2.12	0.49
2:F:795:ILE:HA	2:F:798:GLU:HB2	1.94	0.49
2:F:1114:ARG:HG2	2:F:1115:ASN:N	2.28	0.49
5:J:88:A:C6	5:J:91:C:N4	2.76	0.49
2:F:253:LYS:CG	2:F:261:ASP:HA	2.43	0.49
2:F:268:LYS:O	2:F:271:TYR:HD2	1.95	0.49
2:F:794:GLN:H	2:F:794:GLN:CD	2.15	0.49
2:F:850:ASP:O	2:F:855:LYS:HD2	2.11	0.49
2:F:1300:LYS:HG3	2:F:1327:PHE:CZ	2.48	0.49
2:B:1111:LEU:HD12	2:B:1135:ASP:HB2	1.95	0.49
2:B:1252:ASN:ND2	2:B:1255:LYS:HD2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:158:LEU:O	2:F:161:MET:N	2.46	0.49
2:F:324:ARG:O	2:F:327:GLU:HB2	2.12	0.49
2:F:981:TYR:O	2:F:984:ALA:N	2.45	0.49
2:F:1206:LEU:CD1	2:F:1210:ARG:HH12	2.25	0.49
2:B:252:PHE:CE1	2:B:264:LEU:HD13	2.47	0.49
2:F:784:ILE:HG21	2:F:815:TYR:HD1	1.78	0.49
2:F:791:LEU:CD2	2:F:818:ASN:OD1	2.59	0.49
2:B:149:ALA:H	2:B:426:GLN:HE22	1.59	0.49
2:B:455:LEU:HD12	2:B:455:LEU:N	2.28	0.49
2:B:512:SER:O	2:B:516:GLU:HG2	2.13	0.49
2:B:1204:PHE:CG	2:B:1342:VAL:HG13	2.48	0.49
2:B:1357:GLU:O	5:I:81:G:N2	2.46	0.49
2:F:758:ASN:HD22	2:F:995:THR:HG22	1.78	0.49
5:J:79:G:C2'	5:J:80:U:H5'	2.43	0.49
2:B:478:PHE:HE2	2:B:484:LYS:HE2	1.78	0.49
1:E:3:A:N6	1:E:4:A:N6	2.60	0.49
2:F:411:PRO:HB2	2:F:413:GLN:OE1	2.13	0.49
2:F:632:ILE:O	2:F:636:LEU:HD13	2.13	0.49
2:F:843:PRO:HG3	2:F:864:ARG:HH22	1.77	0.49
2:F:1002:PRO:HD2	2:F:1036:TYR:OH	2.13	0.49
2:F:1314:THR:HG21	2:F:1324:PHE:HB3	1.94	0.49
5:J:94:U:H2'	5:J:95:G:H8	1.77	0.49
2:B:83:GLN:HG2	2:B:98:PHE:CE1	2.48	0.48
2:B:850:ASP:O	2:B:855:LYS:HD2	2.13	0.48
2:B:1062:LEU:O	2:B:1075:ASP:HA	2.13	0.48
3:C:25:DT:C2	3:C:26:DT:C7	2.94	0.48
2:F:923:GLU:CG	2:F:928:THR:HG21	2.40	0.48
2:B:241:LEU:HD11	2:B:289:LEU:HD11	1.96	0.48
2:B:531:THR:HG21	2:B:575:PHE:HE2	1.78	0.48
2:F:140:LYS:HB3	2:F:322:ILE:HD12	1.96	0.48
2:B:736:GLY:O	2:B:740:THR:HB	2.14	0.48
2:F:346:LYS:O	2:F:350:ILE:N	2.42	0.48
1:A:3:A:H2'	1:A:4:A:H8	1.78	0.48
2:B:83:GLN:HG2	2:B:98:PHE:CZ	2.49	0.48
2:B:525:THR:CG2	2:B:690:ASN:HB3	2.43	0.48
2:B:540:LEU:HD12	2:B:540:LEU:HA	1.52	0.48
2:F:844:GLN:HG3	2:F:848:LYS:HA	1.95	0.48
2:F:1162:GLU:OE2	2:F:1187:TYR:OH	2.16	0.48
2:B:157:ALA:O	2:B:161:MET:HG3	2.14	0.48
2:F:138:LEU:HD22	2:F:153:LEU:CD2	2.34	0.48
2:F:142:LEU:HD12	2:F:154:ILE:HA	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:563:GLN:O	2:F:567:ASP:HB2	2.14	0.48
5:J:95:G:H2'	5:J:96:C:C6	2.49	0.48
2:B:472:THR:HG23	5:I:59:U:OP2	2.14	0.48
2:B:697:ILE:HG22	2:B:698:HIS:ND1	2.29	0.48
2:B:985:HIS:O	2:B:989:LEU:HG	2.13	0.48
2:F:208:ALA:CA	2:F:211:ILE:CD1	2.53	0.48
2:F:373:TYR:HE1	2:F:398:LEU:HB3	1.77	0.48
2:F:780:ARG:HB2	2:F:806:LEU:HD12	1.95	0.48
5:J:49:A:O5'	5:J:49:A:H8	1.96	0.48
2:B:525:THR:HG23	2:B:690:ASN:HB3	1.95	0.48
2:B:531:THR:HG1	2:B:575:PHE:HD2	1.59	0.48
2:F:361:GLY:HA2	2:F:365:GLY:HA3	1.96	0.48
2:F:446:PHE:CZ	2:F:478:PHE:CD1	2.92	0.48
2:F:467:ARG:HD3	2:F:470:GLU:HA	1.95	0.48
2:F:1038:PHE:CD2	2:F:1039:TYR:HE1	2.31	0.48
1:A:2:U:O2	1:A:4:A:C8	2.67	0.48
2:F:44:LYS:HD3	5:J:92:G:N7	2.29	0.48
2:F:151:LEU:CD1	2:F:151:LEU:H	2.27	0.48
2:F:404:THR:HG22	2:F:405:PHE:CD1	2.48	0.48
2:F:1119:LEU:HD23	2:F:1128:PRO:HB2	1.94	0.48
2:F:1205:GLU:CB	2:F:1348:ILE:HD11	2.44	0.48
2:F:1272:GLN:CD	5:J:89:G:H1	2.18	0.48
2:B:63:ARG:O	2:B:66:ARG:N	2.47	0.48
2:B:181:VAL:HG21	2:B:209:LYS:HA	1.96	0.48
2:B:597:LEU:O	2:B:601:ILE:HG12	2.14	0.48
2:B:980:ASN:HB2	2:B:1225:GLU:OE1	2.14	0.48
2:F:143:VAL:HG21	2:F:315:ALA:HB2	1.96	0.48
2:F:1115:ASN:OD1	2:F:1129:LYS:HE3	2.14	0.48
2:F:1200:LYS:HG2	2:F:1201:TYR:CD1	2.49	0.48
2:B:530:VAL:CG2	2:B:537:PRO:HB3	2.42	0.47
1:E:19:A:O3'	2:F:407:ASN:HB2	2.14	0.47
2:F:137:HIS:HA	2:F:322:ILE:HG12	1.95	0.47
2:F:373:TYR:CE1	2:F:398:LEU:HB3	2.49	0.47
2:F:1266:LEU:HG	2:F:1309:ILE:HD12	1.96	0.47
2:B:66:ARG:HD2	2:B:462:PHE:HE2	1.78	0.47
2:B:269:ASP:O	2:B:271:TYR:N	2.41	0.47
2:B:531:THR:HG23	2:B:534:MET:HG3	1.96	0.47
2:B:644:ASP:OD2	2:B:646:LYS:HB2	2.14	0.47
2:B:1179:ILE:HD11	2:B:1192:LYS:HD2	1.94	0.47
2:B:1208:ASN:OD1	2:B:1279:ARG:HG3	2.14	0.47
2:B:1333:ARG:CZ	2:B:1335:ARG:HD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:G:C2	3:G:24:DG:N2	2.82	0.47
2:F:282:ILE:HG22	2:F:286:TYR:CD1	2.49	0.47
2:F:795:ILE:HG13	2:F:795:ILE:O	2.15	0.47
2:B:1006:SER:HG	2:B:1014:LYS:N	2.12	0.47
3:G:6:DC:H2''	3:G:7:DC:O5'	2.14	0.47
2:B:1122:ARG:O	5:I:52:A:H5''	2.14	0.47
2:B:1251:ASP:O	2:B:1255:LYS:HG3	2.13	0.47
2:F:853:ASP:OD1	2:F:893:THR:HG21	2.14	0.47
1:A:25:U:H2'	1:A:26:A:H8	1.78	0.47
2:B:136:TYR:CG	2:B:321:MET:HG3	2.49	0.47
2:B:217:SER:HB2	2:B:220:ARG:HG2	1.96	0.47
2:B:985:HIS:ND1	2:B:1087:LEU:HD13	2.29	0.47
2:B:1235:PHE:CE1	2:B:1239:ALA:HB2	2.50	0.47
1:E:31:U:N3	1:E:32:A:N7	2.62	0.47
2:F:167:HIS:ND1	2:F:410:ILE:O	2.39	0.47
2:F:455:LEU:O	5:J:60:C:H5'	2.15	0.47
2:F:671:ARG:HD3	2:F:671:ARG:H	1.78	0.47
2:F:1326:TYR:CE2	2:F:1327:PHE:CD2	3.03	0.47
2:B:48:ILE:HG12	2:B:984:ALA:HB1	1.97	0.47
2:B:121:ASN:H	2:B:121:ASN:ND2	2.12	0.47
2:B:570:LYS:NZ	2:B:571:LYS:HG2	2.30	0.47
2:B:620:VAL:HG13	2:B:656:TYR:HD2	1.80	0.47
2:B:1000:LYS:HB3	2:B:1001:TYR:CE2	2.50	0.47
2:B:1110:ILE:HD13	2:B:1134:PHE:HE1	1.79	0.47
2:B:1286:ASN:ND2	2:B:1332:ASP:O	2.47	0.47
1:E:3:A:C5	1:E:4:A:N7	2.83	0.47
1:E:15:G:P	2:F:66:ARG:HH22	2.37	0.47
2:F:180:ASP:CB	2:F:183:LYS:HB2	2.28	0.47
2:F:258:LEU:HD23	2:F:259:ALA:H	1.80	0.47
2:B:49:GLY:HA2	2:B:1092:VAL:CG1	2.45	0.47
2:B:114:GLU:HG2	2:B:120:GLY:CA	2.45	0.47
2:B:939:MET:HG3	2:B:953:VAL:HG11	1.97	0.47
1:E:21:G:H2'	1:E:22:U:O4'	2.15	0.47
2:B:721:HIS:O	2:B:725:ALA:N	2.39	0.47
2:B:1114:ARG:O	2:B:1129:LYS:HA	2.15	0.47
2:B:1177:ASN:ND2	2:B:1180:ASP:OD2	2.47	0.47
2:F:424:ARG:HH12	2:F:437:ARG:NE	2.13	0.47
2:F:103:GLU:OE2	2:F:111:LYS:HG2	2.14	0.47
2:F:237:LEU:HD12	2:F:238:PHE:H	1.80	0.47
2:F:1205:GLU:HB2	2:F:1348:ILE:HD11	1.96	0.47
5:J:73:G:H5'	5:J:74:A:OP2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:LEU:HD21	2:B:346:LYS:HG3	1.98	0.46
2:B:478:PHE:CE1	2:B:482:VAL:HG21	2.51	0.46
2:B:1089:MET:HA	2:B:1090:PRO:HD3	1.64	0.46
2:B:1163:LEU:HG	2:B:1343:LEU:HD21	1.97	0.46
2:F:832:ARG:HD2	2:F:835:ASP:OD2	2.15	0.46
2:B:74:ARG:O	2:B:78:ARG:HG3	2.15	0.46
2:B:143:VAL:HG13	2:B:421:ALA:HB1	1.97	0.46
2:B:970:PHE:HZ	2:B:1047:LYS:HG2	1.80	0.46
5:I:37:U:H2'	5:I:38:A:H8	1.79	0.46
2:B:133:PRO:HD2	2:B:137:HIS:CG	2.50	0.46
2:B:453:GLY:O	2:B:455:LEU:HD12	2.15	0.46
3:C:7:DC:H2'	3:C:8:DT:C6	2.50	0.46
2:F:553:PHE:HZ	2:F:587:PHE:CD2	2.34	0.46
1:A:11:U:C2	1:A:12:A:C8	3.03	0.46
1:E:16:A:H5''	2:F:74:ARG:HH12	1.79	0.46
2:F:521:TYR:CE2	2:F:549:VAL:HG21	2.49	0.46
2:F:1232:TYR:CE1	2:F:1265:TYR:CD1	3.04	0.46
2:B:1294:TYR:HE1	2:B:1305:GLN:HE21	1.62	0.46
1:E:27:G:H5'	1:E:28:A:H5''	1.97	0.46
2:F:142:LEU:CD1	2:F:154:ILE:CA	2.72	0.46
2:F:142:LEU:CD2	2:F:149:ALA:HB2	2.46	0.46
2:F:258:LEU:HB3	2:F:260:GLU:O	2.16	0.46
2:F:404:THR:HG22	2:F:405:PHE:H	1.80	0.46
2:F:842:VAL:CG1	2:F:854:ASN:OD1	2.61	0.46
2:F:1038:PHE:CD2	2:F:1039:TYR:CE1	3.04	0.46
2:F:1045:PHE:O	2:F:1076:LYS:NZ	2.49	0.46
3:G:25:DT:C2'	3:G:26:DT:OP2	2.55	0.46
2:B:221:ARG:NH1	2:B:246:LEU:HD22	2.30	0.46
1:E:3:A:H8	1:E:3:A:O5'	1.99	0.46
2:F:22:THR:HG23	2:F:26:LYS:O	2.15	0.46
2:F:468:LYS:HD2	2:F:483:ASP:N	2.29	0.46
2:F:1232:TYR:HE1	2:F:1265:TYR:CD1	2.33	0.46
2:B:718:ASP:H	2:B:723:HIS:HE1	1.64	0.46
2:F:151:LEU:CD1	2:F:152:ARG:N	2.73	0.46
2:F:600:ILE:HD13	2:F:651:LEU:HA	1.97	0.46
5:I:42:A:O3'	5:I:43:G:C8	2.69	0.46
1:A:3:A:H2'	1:A:4:A:C8	2.51	0.46
1:A:11:U:N3	1:A:12:A:N7	2.63	0.46
2:B:448:ILE:HD13	2:B:455:LEU:CD1	2.46	0.46
2:B:780:ARG:HB2	2:B:806:LEU:HD12	1.97	0.46
2:B:963:VAL:HG21	2:B:990:ASN:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1:DC:H2'	3:C:2:DA:C8	2.51	0.46
2:F:828:LEU:HD22	2:F:836:TYR:CE2	2.51	0.46
5:J:79:G:O2'	5:J:80:U:H5'	2.15	0.46
2:B:128:TYR:CE1	2:B:132:TYR:HB2	2.50	0.46
2:B:139:ARG:HH12	2:B:415:HIS:CD2	2.34	0.46
2:B:143:VAL:HG13	2:B:421:ALA:CB	2.46	0.46
2:B:343:LEU:HD13	2:B:383:MET:SD	2.56	0.46
2:B:818:ASN:HB3	2:B:882:TYR:OH	2.16	0.46
2:F:241:LEU:HD23	2:F:241:LEU:H	1.81	0.46
2:F:971:GLN:OE1	2:F:1255:LYS:HE3	2.16	0.46
2:F:978:ILE:HD13	2:F:1228:LEU:HD23	1.98	0.46
1:A:20:A:P	2:B:403:ARG:NH1	2.89	0.46
2:B:317:LEU:O	2:B:320:SER:HB3	2.16	0.46
2:B:692:ASN:O	2:B:696:LEU:HD23	2.16	0.46
2:B:978:ILE:HD12	2:B:1233:VAL:HG22	1.98	0.46
2:B:1115:ASN:HA	2:B:1129:LYS:HG2	1.98	0.46
2:F:1151:LYS:HD2	2:F:1158:LYS:HB3	1.97	0.46
2:B:548:ILE:HG23	2:B:552:LEU:CD1	2.46	0.45
2:B:1357:GLU:OE1	2:B:1359:ARG:NH1	2.49	0.45
2:F:238:PHE:O	2:F:242:ILE:HG12	2.15	0.45
2:F:1245:LEU:HD23	2:F:1245:LEU:HA	1.63	0.45
2:B:513:LEU:HD11	2:B:597:LEU:HD12	1.97	0.45
2:B:881:ASN:OD1	2:B:885:GLN:NE2	2.48	0.45
2:B:1146:VAL:HG13	2:B:1191:LYS:HB2	1.97	0.45
2:F:138:LEU:HD13	2:F:153:LEU:HD22	1.82	0.45
2:F:166:GLY:HA3	2:F:410:ILE:CG2	2.41	0.45
2:F:1096:LYS:HG2	2:F:1201:TYR:CD2	2.51	0.45
2:B:340:ARG:HA	2:B:344:PRO:HB3	1.97	0.45
2:B:640:ALA:HA	2:B:648:MET:CE	2.47	0.45
2:B:976:ARG:HB2	2:B:977:GLU:OE1	2.17	0.45
2:F:554:LYS:HB3	2:F:594:TYR:CE2	2.51	0.45
2:F:615:ILE:HG23	2:F:639:TYR:CD1	2.51	0.45
2:B:204:SER:HB2	2:B:205:GLY:H	1.47	0.45
2:B:392:LYS:CG	2:B:395:ARG:NH1	2.54	0.45
2:F:177:ASP:OD1	2:F:177:ASP:N	2.50	0.45
2:F:328:HIS:ND1	5:J:44:U:C2	2.85	0.45
5:J:82:G:N7	5:J:97:U:O2	2.50	0.45
2:B:853:ASP:CG	2:B:893:THR:HG21	2.36	0.45
2:B:1144:LEU:O	2:B:1195:ILE:HA	2.17	0.45
2:B:1204:PHE:HE2	2:B:1214:LEU:HB2	1.80	0.45
3:C:25:DT:N1	3:C:26:DT:H72	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:90:MET:CE	2:F:151:LEU:HD23	2.33	0.45
2:F:151:LEU:CD2	2:F:152:ARG:N	2.75	0.45
2:F:506:LYS:H	2:F:506:LYS:HG2	1.52	0.45
2:F:795:ILE:HA	2:F:798:GLU:OE1	2.15	0.45
2:F:855:LYS:NZ	2:F:1246:LYS:O	2.32	0.45
5:J:87:G:N3	5:J:87:G:H2'	2.31	0.45
2:B:1308:ASN:ND2	2:B:1327:PHE:H	2.15	0.45
3:C:25:DT:N3	3:C:26:DT:C5	2.85	0.45
3:C:25:DT:N3	3:C:26:DT:C7	2.80	0.45
2:F:139:ARG:HD3	2:F:157:ALA:HB1	1.97	0.45
2:F:1079:ASP:HA	2:F:1082:THR:HG23	1.98	0.45
5:J:91:C:O2'	5:J:92:G:O5'	2.34	0.45
5:J:92:G:H2'	5:J:93:G:C8	2.51	0.45
2:B:269:ASP:OD1	2:B:270:THR:N	2.50	0.45
2:B:760:VAL:HG11	2:B:958:LEU:HD12	1.99	0.45
2:B:1243:GLU:HG3	2:B:1246:LYS:HZ1	1.80	0.45
2:F:247:GLY:O	2:F:267:SER:HB3	2.16	0.45
2:F:551:LEU:HD12	2:F:551:LEU:HA	1.80	0.45
2:F:565:LYS:HD2	2:F:580:ILE:HG12	1.99	0.45
2:F:622:THR:HG21	2:F:635:ARG:CB	2.46	0.45
2:F:844:GLN:CG	2:F:848:LYS:HD2	2.47	0.45
2:B:36:GLY:HA3	2:B:1359:ARG:O	2.17	0.45
2:B:226:ILE:HA	2:B:229:LEU:HG	1.99	0.45
2:B:317:LEU:HD21	2:B:410:ILE:HD13	1.99	0.45
2:B:525:THR:HA	2:B:545:LYS:CE	2.47	0.45
2:F:137:HIS:HE1	2:F:325:TYR:CG	2.34	0.45
2:F:329:HIS:HB2	5:J:44:U:O4	2.17	0.45
2:F:913:LYS:O	2:F:916:PHE:HB2	2.17	0.45
2:F:1349:HIS:ND1	5:J:69:A:H5'	2.31	0.45
5:J:45:U:H2'	5:J:46:A:O4'	2.17	0.45
2:B:6:SER:HB2	2:B:21:ILE:CG1	2.47	0.45
2:B:94:ASP:HB3	2:B:97:PHE:HB2	1.99	0.45
2:B:116:HIS:NE2	2:B:122:ILE:HG23	2.32	0.45
2:B:165:ARG:O	2:B:412:HIS:HA	2.17	0.45
2:B:414:ILE:HG21	2:B:414:ILE:HD13	1.74	0.45
2:B:531:THR:HG21	2:B:575:PHE:CE2	2.52	0.45
2:F:328:HIS:CG	5:J:44:U:C2	3.05	0.45
2:F:909:SER:N	2:F:912:ASP:HB2	2.32	0.45
5:I:83:C:H2'	5:I:84:A:C8	2.49	0.45
2:B:467:ARG:NH2	2:B:471:GLU:O	2.50	0.45
2:B:1111:LEU:HD23	2:B:1111:LEU:HA	1.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:546:LYS:HE3	2:F:546:LYS:HB3	1.79	0.45
1:A:3:A:C2'	1:A:4:A:H8	2.30	0.44
2:B:719:SER:OG	2:B:720:LEU:N	2.49	0.44
2:B:864:ARG:HB2	2:B:871:PRO:HA	1.97	0.44
2:B:1113:LYS:HB2	2:B:1129:LYS:O	2.17	0.44
2:F:681:ASP:HA	2:F:684:LYS:HZ3	1.81	0.44
2:F:788:ILE:HA	2:F:791:LEU:HB2	1.98	0.44
2:F:879:MET:HB3	2:F:882:TYR:HB3	1.99	0.44
2:F:954:LYS:NZ	2:F:998:ILE:HD13	2.32	0.44
2:F:1284:ASP:OD1	2:F:1284:ASP:N	2.43	0.44
2:B:115:ARG:HG3	2:B:116:HIS:CE1	2.53	0.44
2:B:118:ILE:HD12	2:B:125:GLU:OE2	2.17	0.44
2:B:662:LEU:HD23	2:B:666:LEU:HD22	1.98	0.44
2:B:958:LEU:HD22	2:B:962:LEU:HD12	1.99	0.44
2:B:1272:GLN:NE2	5:I:89:G:O6	2.31	0.44
1:E:3:A:O5'	1:E:3:A:C8	2.70	0.44
2:F:151:LEU:CD2	2:F:151:LEU:C	2.86	0.44
2:F:208:ALA:N	2:F:211:ILE:CD1	2.78	0.44
2:F:410:ILE:HD13	2:F:415:HIS:HE2	1.82	0.44
2:F:509:PRO:HG2	2:F:621:LEU:HA	1.98	0.44
2:F:615:ILE:HG23	2:F:639:TYR:CE1	2.52	0.44
2:F:1290:VAL:HG22	2:F:1331:ILE:HD13	2.00	0.44
2:B:264:LEU:HD23	2:B:271:TYR:CE1	2.52	0.44
2:B:390:LEU:HD23	2:B:390:LEU:HA	1.63	0.44
2:F:164:PHE:O	2:F:164:PHE:CD1	2.70	0.44
2:F:167:HIS:HD1	2:F:167:HIS:H	1.65	0.44
5:J:88:A:C2	5:J:91:C:N3	2.85	0.44
2:B:37:ASN:OD1	2:B:37:ASN:N	2.46	0.44
2:B:51:LEU:HD22	2:B:1352:ILE:HG13	1.98	0.44
2:B:192:TYR:HE1	2:B:237:LEU:HD23	1.82	0.44
2:B:548:ILE:HD13	2:B:564:LEU:HD11	1.98	0.44
2:F:233:LYS:HB3	2:F:236:GLY:H	1.82	0.44
2:F:300:ILE:O	2:F:303:SER:OG	2.24	0.44
2:F:883:TRP:HB3	2:F:897:PHE:HD1	1.82	0.44
2:F:1167:THR:OG1	2:F:1168:ILE:N	2.50	0.44
1:A:5:C:H2'	1:A:6:G:C8	2.47	0.44
2:B:147:ASP:O	2:B:426:GLN:NE2	2.51	0.44
2:F:30:LYS:HB2	2:F:30:LYS:HE3	1.81	0.44
2:F:821:ASP:HA	2:F:828:LEU:HD11	2.00	0.44
2:F:1212:ARG:HD2	2:F:1336:TYR:HD2	1.83	0.44
1:A:8:A:H2'	1:A:9:U:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:720:LEU:HD13	2:B:938:ARG:HH11	1.82	0.44
2:B:1241:HIS:HD1	2:B:1244:LYS:HA	1.83	0.44
2:F:867:SER:HB2	2:F:1054:ASN:HA	1.99	0.44
5:J:58:G:C6	5:J:60:C:C2	3.06	0.44
2:B:565:LYS:HD3	2:B:578:VAL:HG13	1.99	0.44
2:B:643:PHE:CD2	2:B:643:PHE:N	2.86	0.44
2:B:781:MET:HG3	2:B:803:ASN:ND2	2.33	0.44
1:E:4:A:C4	1:E:5:C:C5	3.05	0.44
2:F:158:LEU:HB2	2:F:419:LEU:HD12	1.99	0.44
2:F:328:HIS:CE1	2:F:359:TYR:HH	2.33	0.44
2:F:823:TYR:HB3	2:F:863:ASN:HB3	1.99	0.44
2:F:1073:VAL:HG23	2:F:1074:TRP:N	2.32	0.44
2:B:141:LYS:HD3	2:B:142:LEU:HD23	2.00	0.44
2:B:558:LYS:HA	2:B:558:LYS:HD3	1.68	0.44
2:B:601:ILE:HG21	2:B:643:PHE:HE1	1.83	0.44
2:B:628:ASP:OD1	2:B:630:GLU:HB3	2.17	0.44
2:B:829:ASP:OD1	2:B:831:ASN:N	2.50	0.44
2:B:939:MET:CE	2:B:953:VAL:HG21	2.47	0.44
2:B:1208:ASN:CG	2:B:1208:ASN:O	2.55	0.44
1:E:25:U:H6	1:E:25:U:O5'	2.01	0.44
2:F:243:ALA:O	2:F:246:LEU:HB3	2.17	0.44
2:F:671:ARG:H	2:F:671:ARG:CD	2.30	0.44
2:F:1222:LYS:NZ	2:F:1315:LEU:O	2.47	0.44
2:B:13:THR:O	2:B:53:PHE:HE1	2.00	0.44
2:B:1276:PHE:CE2	2:B:1316:THR:HB	2.53	0.44
2:F:1095:VAL:HG13	2:F:1350:GLN:OE1	2.18	0.44
2:B:51:LEU:HD13	2:B:1095:VAL:CG2	2.44	0.43
2:B:134:THR:OG1	2:B:137:HIS:N	2.49	0.43
3:C:25:DT:C4	3:C:26:DT:O4	2.71	0.43
2:F:637:LYS:HB2	2:F:637:LYS:HE3	1.68	0.43
2:F:1212:ARG:CZ	2:F:1336:TYR:HE2	2.31	0.43
2:F:1347:LEU:HD22	2:F:1349:HIS:CD2	2.53	0.43
5:J:91:C:HO2'	5:J:92:G:P	2.41	0.43
1:A:3:A:O2'	1:A:4:A:H8	2.00	0.43
2:B:921:LEU:HB3	2:B:1008:PHE:CE1	2.53	0.43
2:B:1200:LYS:HG2	2:B:1201:TYR:CD1	2.52	0.43
2:F:46:ASN:HD21	5:J:88:A:N6	2.13	0.43
2:F:63:ARG:HG3	2:F:66:ARG:NH1	2.32	0.43
2:B:156:LEU:HA	2:B:156:LEU:HD23	1.62	0.43
2:B:416:LEU:HD11	2:B:441:GLU:HG2	2.00	0.43
2:B:1345:ALA:O	2:B:1362:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:57:GLU:HB2	5:J:65:A:OP1	2.18	0.43
2:F:1010:TYR:O	2:F:1012:ASP:N	2.51	0.43
2:F:1035:LYS:HD3	2:F:1035:LYS:HA	1.57	0.43
2:F:1123:LYS:HG3	5:J:53:G:OP1	2.18	0.43
5:J:84:A:C2	5:J:85:C:C2	3.06	0.43
2:B:79:ILE:HA	2:B:79:ILE:HD13	1.77	0.43
2:B:136:TYR:CD2	2:B:321:MET:HG3	2.53	0.43
2:B:220:ARG:HD3	2:B:220:ARG:HA	1.77	0.43
2:B:958:LEU:HA	2:B:958:LEU:HD23	1.63	0.43
2:B:978:ILE:CD1	2:B:1233:VAL:HG22	2.48	0.43
2:B:1325:LYS:HB3	2:B:1330:THR:HG22	2.00	0.43
2:F:631:MET:O	2:F:635:ARG:N	2.43	0.43
2:F:1126:TRP:N	2:F:1126:TRP:CD1	2.86	0.43
5:I:76:A:H2'	5:I:77:A:O4'	2.19	0.43
2:B:184:LEU:HD23	2:B:184:LEU:HA	1.78	0.43
2:F:465:MET:HE1	2:F:482:VAL:HG21	2.01	0.43
2:B:64:LEU:HD13	2:B:64:LEU:HA	1.71	0.43
2:B:305:ILE:HG13	2:B:306:LEU:N	2.33	0.43
2:B:341:GLN:HG2	2:B:342:GLN:HG3	1.99	0.43
2:B:345:GLU:H	2:B:345:GLU:CD	2.21	0.43
2:B:926:GLN:HG2	3:C:20:DA:P	2.58	0.43
2:B:1120:ILE:HG21	2:B:1120:ILE:HD13	1.61	0.43
2:F:918:LYS:HZ1	2:F:1018:VAL:HG11	1.84	0.43
2:F:1166:ILE:HG13	2:F:1174:PHE:CE2	2.54	0.43
2:F:1356:TYR:HB3	5:J:81:G:C2	2.54	0.43
2:B:122:ILE:H	2:B:122:ILE:HG13	1.66	0.43
2:B:499:ASP:OD2	2:B:663:SER:N	2.37	0.43
2:B:839:ASP:N	2:B:856:VAL:O	2.33	0.43
2:B:886:LEU:HB3	2:B:891:LEU:HB2	2.01	0.43
2:F:1277:SER:HA	2:F:1281:ILE:HG12	2.00	0.43
5:I:73:G:C2	5:I:77:A:C6	3.05	0.43
1:A:15:G:O5'	1:A:15:G:H8	2.02	0.43
2:B:508:LEU:HD21	2:B:664:ARG:HB2	2.00	0.43
2:B:524:LEU:CD2	2:B:545:LYS:HA	2.48	0.43
2:F:51:LEU:CD1	2:F:1352:ILE:HG13	2.49	0.43
2:F:777:SER:CA	2:F:807:GLN:HE21	2.18	0.43
1:E:5:C:O2	1:E:5:C:H2'	2.18	0.43
2:F:9:LEU:HD11	2:F:744:VAL:CG2	2.48	0.43
2:F:110:ASP:OD2	2:F:1130:LYS:HE3	2.18	0.43
2:F:212:LEU:HD13	2:F:300:ILE:CD1	2.49	0.43
2:F:226:ILE:CD1	2:F:232:GLU:HG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:561:VAL:HG12	2:F:565:LYS:HG3	2.00	0.43
2:F:597:LEU:O	2:F:601:ILE:HG12	2.19	0.43
2:F:627:GLU:HA	2:F:655:ARG:NH1	2.34	0.43
2:F:1052:LEU:HD12	2:F:1052:LEU:HA	1.86	0.43
2:B:216:LEU:HA	2:B:216:LEU:HD23	1.77	0.43
2:B:570:LYS:HE3	2:B:570:LYS:HB3	1.69	0.43
2:B:623:LEU:HD12	2:B:623:LEU:HA	1.70	0.43
2:B:946:ASN:HB3	2:B:948:LYS:HD2	2.00	0.43
1:E:15:G:H4'	2:F:454:PRO:HD3	2.01	0.43
2:F:137:HIS:CD2	2:F:322:ILE:HG23	2.54	0.43
2:F:339:VAL:HG12	2:F:347:TYR:HB2	2.00	0.43
2:F:829:ASP:OD1	2:F:832:ARG:N	2.36	0.43
5:J:96:C:H2'	5:J:97:U:O4'	2.19	0.43
2:F:5:TYR:CZ	2:F:751:MET:HG3	2.54	0.42
2:F:136:TYR:CZ	2:F:160:HIS:NE2	2.85	0.42
2:F:199:ASN:O	2:F:201:ILE:HD12	2.18	0.42
2:F:684:LYS:O	2:F:685:SER:OG	2.31	0.42
2:F:686:ASP:CB	2:F:690:ASN:CA	2.85	0.42
2:F:817:GLN:HB3	2:F:820:ARG:O	2.19	0.42
2:F:843:PRO:O	2:F:846:PHE:HB2	2.19	0.42
5:I:85:C:H42	5:I:93:G:H1	1.67	0.42
5:I:85:C:H2'	5:I:86:C:C6	2.54	0.42
1:A:3:A:O2'	1:A:4:A:P	2.77	0.42
2:B:814:TYR:CE2	2:B:819:GLY:HA2	2.54	0.42
1:E:26:A:C6	1:E:27:G:N7	2.87	0.42
2:F:484:LYS:H	2:F:484:LYS:CE	2.32	0.42
2:F:686:ASP:HB3	2:F:689:ALA:O	2.19	0.42
2:F:802:GLU:H	2:F:805:GLN:HG3	1.84	0.42
2:F:1019:ARG:C	2:F:1021:MET:N	2.73	0.42
5:J:96:C:H2'	5:J:97:U:C6	2.54	0.42
2:B:594:TYR:OH	2:B:608:ASP:OD1	2.37	0.42
2:B:727:LEU:HD11	2:B:934:ILE:HD11	2.01	0.42
2:B:1163:LEU:HD23	2:B:1163:LEU:HA	1.71	0.42
2:B:1301:PRO:O	2:B:1305:GLN:HB2	2.20	0.42
2:B:1336:TYR:N	2:B:1336:TYR:CD1	2.87	0.42
1:E:19:A:OP1	2:F:164:PHE:CD1	2.68	0.42
2:F:165:ARG:CD	2:F:168:PHE:HZ	2.29	0.42
2:F:183:LYS:HD2	2:F:183:LYS:N	2.34	0.42
2:F:213:SER:O	2:F:213:SER:OG	2.32	0.42
2:F:350:ILE:O	2:F:359:TYR:N	2.52	0.42
2:F:848:LYS:HB3	2:F:848:LYS:HE3	1.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1228:LEU:HD12	2:F:1228:LEU:HA	1.82	0.42
2:B:424:ARG:NE	2:B:427:GLU:OE2	2.52	0.42
2:B:913:LYS:HA	2:B:916:PHE:CD2	2.41	0.42
2:B:1110:ILE:CD1	2:B:1134:PHE:HE1	2.31	0.42
2:B:1246:LYS:HB2	2:B:1246:LYS:HE2	1.86	0.42
4:D:3:DT:H1'	4:D:4:DT:H5'	2.00	0.42
2:F:891:LEU:H	2:F:891:LEU:HD23	1.84	0.42
2:F:1266:LEU:HG	2:F:1309:ILE:HD11	2.00	0.42
3:G:23:DC:H2'	3:G:24:DG:O4'	2.19	0.42
2:B:609:ASN:ND2	2:B:611:GLU:OE1	2.45	0.42
2:B:840:ALA:HA	2:B:854:ASN:O	2.19	0.42
2:B:1082:THR:O	2:B:1086:VAL:HG23	2.19	0.42
1:E:15:G:H2'	1:E:16:A:O4'	2.19	0.42
2:F:824:VAL:HG12	2:F:825:ASP:H	1.83	0.42
2:F:1135:ASP:OD1	4:H:8:DT:H5''	2.20	0.42
1:A:4:A:O2'	1:A:5:C:C5'	2.68	0.42
2:B:665:LYS:O	2:B:670:ILE:HG12	2.19	0.42
2:B:986:ASP:O	2:B:990:ASN:ND2	2.52	0.42
2:B:1213:MET:O	2:B:1221:GLN:N	2.48	0.42
2:B:1244:LYS:HB2	2:B:1244:LYS:HE2	1.80	0.42
2:F:381:GLU:H	2:F:381:GLU:HG2	1.72	0.42
2:F:424:ARG:HH22	2:F:437:ARG:NH1	2.17	0.42
2:F:679:ILE:HG12	2:F:704:PHE:CZ	2.54	0.42
2:F:981:TYR:HE1	2:F:1225:GLU:HG3	1.84	0.42
2:F:985:HIS:CG	2:F:1087:LEU:HD22	2.55	0.42
2:F:988:TYR:CZ	2:F:1086:VAL:HG11	2.54	0.42
2:F:1111:LEU:HD23	2:F:1111:LEU:HA	1.64	0.42
2:F:1264:HIS:ND1	2:F:1268:GLU:OE2	2.49	0.42
5:J:42:A:O2'	5:J:43:G:OP1	2.30	0.42
2:B:25:TYR:O	2:B:988:TYR:OH	2.36	0.42
2:B:997:LEU:HD23	2:B:997:LEU:HA	1.87	0.42
1:E:11:U:C2	1:E:12:A:C8	3.07	0.42
2:F:165:ARG:CG	2:F:168:PHE:HE1	2.33	0.42
2:F:1089:MET:HA	2:F:1090:PRO:HD3	1.66	0.42
2:F:1178:PRO:O	2:F:1182:LEU:HG	2.19	0.42
2:B:8:GLY:O	2:B:987:ALA:HB1	2.20	0.42
2:B:1182:LEU:HD13	2:B:1190:VAL:HG11	2.01	0.42
2:F:226:ILE:HG22	2:F:230:PRO:HA	2.01	0.42
2:F:813:LEU:O	2:F:817:GLN:HG3	2.20	0.42
2:F:1321:PRO:HG2	2:F:1335:ARG:HA	2.02	0.42
2:B:1141:TYR:C	2:B:1141:TYR:CD1	2.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:170:ILE:HG22	2:F:413:GLN:NE2	2.35	0.42
2:F:495:MET:HB3	3:G:17:DT:H1'	2.02	0.42
2:F:521:TYR:HE1	2:F:684:LYS:HD2	1.85	0.42
2:F:1096:LYS:HE2	2:F:1201:TYR:CE2	2.55	0.42
2:B:1142:SER:O	2:B:1198:LEU:N	2.35	0.42
2:F:441:GLU:O	2:F:445:THR:HG22	2.20	0.42
2:F:591:LEU:O	2:F:595:HIS:ND1	2.48	0.42
2:F:644:ASP:HB3	2:F:647:VAL:HG23	2.02	0.42
2:F:823:TYR:CD2	2:F:863:ASN:HB2	2.55	0.42
2:B:570:LYS:O	2:B:574:CYS:HA	2.20	0.41
2:B:794:GLN:HG2	2:B:798:GLU:HG3	2.01	0.41
2:B:1191:LYS:HD2	2:B:1194:LEU:HD12	2.01	0.41
2:B:1229:PRO:HB2	2:B:1232:TYR:CE2	2.55	0.41
2:B:1258:PHE:CE1	2:B:1262:HIS:CD2	3.06	0.41
3:C:25:DT:N3	3:C:26:DT:H72	2.35	0.41
2:F:201:ILE:HD12	2:F:201:ILE:N	2.35	0.41
2:F:522:ASN:HA	2:F:683:LEU:HD13	2.01	0.41
2:F:523:GLU:OE1	2:F:588:ASN:HB2	2.20	0.41
2:F:910:GLU:OE1	2:F:910:GLU:N	2.51	0.41
2:F:1236:LEU:HD11	2:F:1269:ILE:HD13	2.01	0.41
5:J:53:G:C2	5:J:62:G:C2	3.08	0.41
2:B:40:ARG:HH22	5:I:92:G:P	2.43	0.41
2:B:300:ILE:HA	2:B:303:SER:OG	2.20	0.41
2:B:349:GLU:HG3	2:B:356:LYS:HG3	2.01	0.41
2:B:599:LYS:O	2:B:602:LYS:HG3	2.19	0.41
1:E:5:C:C2	1:E:6:G:C8	3.08	0.41
1:E:22:U:O2	2:F:1110:ILE:HD12	2.20	0.41
2:F:164:PHE:CD1	2:F:164:PHE:C	2.94	0.41
2:F:758:ASN:ND2	2:F:995:THR:HG22	2.36	0.41
2:F:794:GLN:HE21	2:F:798:GLU:CD	2.24	0.41
2:F:1221:GLN:HB3	2:F:1319:GLY:O	2.20	0.41
1:A:18:A:OP2	2:B:71:ARG:HD2	2.20	0.41
1:A:18:A:OP1	2:B:165:ARG:HD3	2.19	0.41
2:B:325:TYR:HA	5:I:44:U:O2	2.20	0.41
2:F:143:VAL:HG22	2:F:422:ILE:CG1	2.50	0.41
2:F:174:LEU:CD2	2:F:413:GLN:HB2	2.50	0.41
2:B:31:LYS:HG3	2:B:44:LYS:HG3	2.02	0.41
2:B:212:LEU:HD21	2:B:225:LEU:CD1	2.50	0.41
2:B:742:LYS:HB3	2:B:1352:ILE:HD13	2.02	0.41
2:B:1000:LYS:HE2	2:B:1065:THR:O	2.20	0.41
2:F:268:LYS:O	2:F:271:TYR:CD2	2.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:918:LYS:NZ	2:F:1007:GLU:OE2	2.41	0.41
2:F:1087:LEU:HD23	2:F:1087:LEU:HA	1.76	0.41
2:F:1204:PHE:CE1	2:F:1347:LEU:HG	2.56	0.41
2:F:1245:LEU:HD13	2:F:1252:ASN:ND2	2.35	0.41
5:I:87:G:C2	5:I:92:G:C6	3.09	0.41
1:A:4:A:O2'	1:A:5:C:P	2.77	0.41
2:B:475:PRO:HG3	5:I:59:U:O4	2.21	0.41
2:B:680:LEU:HD12	2:B:680:LEU:HA	1.76	0.41
2:B:1003:LYS:H	2:B:1003:LYS:HG2	1.54	0.41
2:B:1179:ILE:HD11	2:B:1192:LYS:CE	2.50	0.41
2:B:1207:GLU:HG2	2:B:1210:ARG:NH1	2.35	0.41
2:F:49:GLY:HA2	2:F:1092:VAL:CG1	2.50	0.41
2:F:174:LEU:HD22	2:F:413:GLN:HB2	2.02	0.41
2:F:289:LEU:O	2:F:292:ALA:HB3	2.19	0.41
2:F:302:LEU:HD23	2:F:305:ILE:HD11	2.02	0.41
2:F:409:SER:O	2:F:411:PRO:HD3	2.20	0.41
2:F:442:LYS:HE3	2:F:446:PHE:CD1	2.55	0.41
2:F:1228:LEU:HD12	2:F:1229:PRO:CD	2.51	0.41
2:F:1281:ILE:HG13	2:F:1316:THR:HG22	2.02	0.41
3:G:2:DA:H2''	3:G:3:DA:OP1	2.21	0.41
2:B:554:LYS:HG2	2:B:594:TYR:CE2	2.56	0.41
2:B:784:ILE:HD13	2:B:815:TYR:CB	2.51	0.41
2:B:841:ILE:HD11	2:B:896:LYS:HG3	2.02	0.41
2:B:1084:ARG:O	2:B:1084:ARG:HG2	2.18	0.41
2:F:143:VAL:HG21	2:F:315:ALA:CB	2.50	0.41
2:F:424:ARG:O	2:F:427:GLU:HG2	2.19	0.41
2:F:662:LEU:HD22	2:F:666:LEU:CD2	2.50	0.41
2:B:25:TYR:HE2	2:B:1074:TRP:CE3	2.38	0.41
2:B:1220:LEU:HD21	2:B:1342:VAL:HG21	2.02	0.41
2:B:1318:LEU:HD22	2:B:1319:GLY:N	2.35	0.41
2:F:137:HIS:CD2	2:F:322:ILE:HG12	2.55	0.41
2:F:348:LYS:HA	2:F:352:PHE:HD2	1.85	0.41
2:F:583:VAL:HG21	2:F:587:PHE:CD1	2.54	0.41
2:F:636:LEU:HA	2:F:639:TYR:HD2	1.84	0.41
2:F:649:LYS:CB	2:F:653:ARG:HH21	2.34	0.41
3:G:4:DT:H2''	3:G:5:DA:C5'	2.51	0.41
2:B:959:LYS:HB3	2:B:962:LEU:HG	2.02	0.41
3:C:2:DA:H2'	3:C:3:DA:C8	2.55	0.41
2:F:1061:PRO:O	2:F:1076:LYS:HE2	2.21	0.41
2:F:1203:LEU:HD23	2:F:1348:ILE:HD12	2.02	0.41
2:F:1343:LEU:O	2:F:1362:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:ILE:HG12	2:B:156:LEU:HD11	2.03	0.41
2:B:248:LEU:HA	2:B:248:LEU:HD23	1.72	0.41
2:B:447:ARG:HD3	2:B:447:ARG:HH11	1.76	0.41
2:B:524:LEU:HD23	2:B:545:LYS:HG2	2.02	0.41
2:B:535:ARG:HE	2:B:535:ARG:HB3	1.70	0.41
2:B:544:GLN:O	2:B:548:ILE:HG13	2.21	0.41
2:B:861:ASP:O	2:B:864:ARG:HG2	2.21	0.41
2:B:1119:LEU:HD12	2:B:1119:LEU:HA	1.93	0.41
2:B:1205:GLU:O	2:B:1345:ALA:HB1	2.21	0.41
1:E:4:A:HO2'	1:E:5:C:C5'	2.33	0.41
2:F:4:LYS:HE2	2:F:4:LYS:HB2	1.54	0.41
2:F:97:PHE:CE1	2:F:118:ILE:HA	2.56	0.41
2:F:117:PRO:HD2	2:F:118:ILE:HD12	2.03	0.41
2:F:336:LYS:HG2	2:F:351:PHE:CZ	2.55	0.41
2:F:513:LEU:HA	2:F:513:LEU:HD23	1.80	0.41
2:F:525:THR:OG1	2:F:545:LYS:NZ	2.30	0.41
2:F:546:LYS:NZ	2:F:550:ASP:OD2	2.53	0.41
2:F:553:PHE:CD2	2:F:559:VAL:HG21	2.56	0.41
2:F:632:ILE:O	2:F:636:LEU:N	2.39	0.41
2:F:852:ILE:O	2:F:896:LYS:HD3	2.21	0.41
2:F:853:ASP:OD2	2:F:895:ARG:HD3	2.21	0.41
2:F:878:LYS:HE3	2:F:878:LYS:HB2	1.84	0.41
2:F:897:PHE:CZ	2:F:901:THR:HG21	2.56	0.41
2:F:949:LEU:HD23	2:F:951:ARG:HH22	1.85	0.41
2:F:1163:LEU:HD23	2:F:1163:LEU:HA	1.91	0.41
2:F:1207:GLU:CG	2:F:1208:ASN:H	2.34	0.41
5:I:52:A:OP2	5:I:62:G:N2	2.51	0.41
5:I:82:G:N7	5:I:97:U:O2	2.53	0.41
5:I:92:G:H2'	5:I:93:G:C8	2.56	0.41
5:J:45:U:H2'	5:J:46:A:H8	1.86	0.41
5:J:56:U:O2	5:J:58:G:N2	2.46	0.41
2:B:198:GLU:C	2:B:200:PRO:HD3	2.41	0.41
2:B:423:LEU:HA	2:B:423:LEU:HD23	1.70	0.41
2:B:982:HIS:HA	2:B:985:HIS:HB2	2.02	0.41
2:B:1302:ILE:H	2:B:1302:ILE:HG13	1.71	0.41
2:F:318:SER:O	2:F:321:MET:HB2	2.21	0.41
2:F:1360:ILE:HD13	2:F:1360:ILE:HA	1.92	0.41
2:B:338:LEU:C	2:B:383:MET:HE1	2.42	0.40
2:B:455:LEU:O	5:I:60:C:H5'	2.21	0.40
2:B:485:GLY:O	2:B:488:ALA:N	2.54	0.40
2:B:526:LYS:HD3	2:B:526:LYS:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:788:ILE:HA	2:B:791:LEU:HB2	2.03	0.40
3:C:20:DA:C8	3:C:21:DT:H72	2.57	0.40
2:F:324:ARG:HB3	2:F:402:GLN:HE21	1.86	0.40
2:F:360:ALA:O	2:F:364:ASP:N	2.53	0.40
2:F:492:ILE:O	2:F:496:THR:HG23	2.21	0.40
5:J:46:A:H2'	5:J:47:A:H8	1.80	0.40
2:B:198:GLU:HG2	2:B:199:ASN:N	2.35	0.40
2:B:455:LEU:N	2:B:455:LEU:CD1	2.84	0.40
2:B:1156:LYS:HE3	2:B:1156:LYS:HB2	1.91	0.40
1:E:15:G:O5'	1:E:15:G:H8	2.04	0.40
2:F:139:ARG:CG	2:F:157:ALA:CA	2.99	0.40
2:F:148:LYS:HA	2:F:429:PHE:CD2	2.56	0.40
2:F:451:TYR:CD1	2:F:488:ALA:HB2	2.56	0.40
2:F:967:ARG:NH1	2:F:974:LYS:HE3	2.36	0.40
2:F:1093:ASN:O	2:F:1094:ILE:HD13	2.22	0.40
2:F:1114:ARG:HG2	2:F:1115:ASN:H	1.85	0.40
2:B:424:ARG:CZ	2:B:437:ARG:NH1	2.85	0.40
2:B:821:ASP:OD2	2:B:828:LEU:HG	2.22	0.40
2:F:526:LYS:HA	2:F:526:LYS:HD3	1.68	0.40
2:F:927:ILE:O	2:F:930:HIS:N	2.54	0.40
2:F:1210:ARG:HB2	2:F:1280:VAL:HA	2.03	0.40
2:F:1236:LEU:O	2:F:1240:SER:OG	2.27	0.40
4:D:6:DG:H2''	4:D:7:DG:H5''	2.03	0.40
2:F:160:HIS:HE2	2:F:164:PHE:HD2	1.68	0.40
2:F:1107:LYS:HE2	3:G:8:DT:H1'	2.03	0.40
2:F:1146:VAL:O	2:F:1191:LYS:HG3	2.21	0.40
2:F:1204:PHE:CE2	2:F:1342:VAL:HG11	2.56	0.40
2:B:514:LEU:HD11	2:B:667:ILE:CG2	2.51	0.40
2:B:558:LYS:HD2	2:B:586:ARG:HD2	2.04	0.40
2:B:642:LEU:HB2	2:B:643:PHE:HD2	1.83	0.40
2:B:967:ARG:HH11	2:B:989:LEU:HD12	1.86	0.40
2:B:989:LEU:O	2:B:993:VAL:HG23	2.22	0.40
2:B:1228:LEU:HD12	2:B:1229:PRO:CD	2.51	0.40
1:E:14:G:O2'	1:E:15:G:H5'	2.22	0.40
2:F:57:GLU:HB2	5:J:65:A:P	2.62	0.40
2:F:1206:LEU:HD12	2:F:1210:ARG:NH1	2.35	0.40
2:F:1280:VAL:HG12	2:F:1281:ILE:HD13	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:ASN:OD1	2:B:541:SER:OG[2_545]	2.07	0.13

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	1308/1368 (96%)	1268 (97%)	36 (3%)	4 (0%)	37	65
2	F	1313/1368 (96%)	1267 (96%)	41 (3%)	5 (0%)	30	59
All	All	2621/2736 (96%)	2535 (97%)	77 (3%)	9 (0%)	37	65

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	1042	ILE
2	F	585	ASP
2	F	1011	GLY
2	F	1020	LYS
2	B	1327	PHE
2	B	470	GLU
2	B	117	PRO
2	F	117	PRO
2	B	230	PRO

5.3.2 Protein sidechains [i](#)

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	1170/1225 (96%)	1131 (97%)	39 (3%)	33	59
2	F	1155/1225 (94%)	1093 (95%)	62 (5%)	18	45
All	All	2325/2450 (95%)	2224 (96%)	101 (4%)	25	51

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	94	ASP
2	B	95	ASP
2	B	141	LYS
2	B	182	ASP
2	B	276	ASP
2	B	311	GLU
2	B	383	MET
2	B	389	LEU
2	B	424	ARG
2	B	425	ARG
2	B	434	LYS
2	B	494	ARG
2	B	535	ARG
2	B	557	ARG
2	B	584	GLU
2	B	614	ASP
2	B	629	ARG
2	B	674	GLN
2	B	684	LYS
2	B	688	PHE
2	B	719	SER
2	B	751	MET
2	B	778	ARG
2	B	803	ASN
2	B	818	ASN
2	B	854	ASN
2	B	866	LYS
2	B	905	ARG
2	B	951	ARG
2	B	954	LYS
2	B	1062	LEU
2	B	1080	PHE
2	B	1158	LYS
2	B	1202	SER
2	B	1221	GLN

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Mol	Chain	Res	Type
2	B	1258	PHE
2	B	1263	LYS
2	B	1317	ASN
2	B	1338	SER
2	F	42	SER
2	F	140	LYS
2	F	142	LEU
2	F	150	ASP
2	F	151	LEU
2	F	155	TYR
2	F	156	LEU
2	F	160	HIS
2	F	164	PHE
2	F	183	LYS
2	F	229	LEU
2	F	234	LYS
2	F	237	LEU
2	F	267	SER
2	F	271	TYR
2	F	284	ASP
2	F	295	ASN
2	F	383	MET
2	F	384	ASP
2	F	423	LEU
2	F	425	ARG
2	F	451	TYR
2	F	476	TRP
2	F	478	PHE
2	F	484	LYS
2	F	494	ARG
2	F	532	GLU
2	F	535	ARG
2	F	546	LYS
2	F	567	ASP
2	F	598	LEU
2	F	629	ARG
2	F	631	MET
2	F	650	GLN
2	F	654	ARG
2	F	663	SER
2	F	671	ARG
2	F	682	PHE

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Mol	Chain	Res	Type
2	F	686	ASP
2	F	688	PHE
2	F	704	PHE
2	F	705	LYS
2	F	753	ARG
2	F	803	ASN
2	F	818	ASN
2	F	820	ARG
2	F	822	MET
2	F	891	LEU
2	F	976	ARG
2	F	977	GLU
2	F	1008	PHE
2	F	1037	PHE
2	F	1080	PHE
2	F	1118	LYS
2	F	1202	SER
2	F	1206	LEU
2	F	1208	ASN
2	F	1258	PHE
2	F	1265	TYR
2	F	1327	PHE
2	F	1338	SER
2	F	1364	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	137	HIS
2	B	920	GLN
2	B	1044	ASN
2	B	1252	ASN
2	B	1262	HIS
2	B	1308	ASN
2	B	1350	GLN
2	F	46	ASN
2	F	178	ASN
2	F	295	ASN
2	F	329	HIS
2	F	758	ASN
2	F	794	GLN
2	F	807	GLN

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Mol	Chain	Res	Type
2	F	920	GLN
2	F	1252	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	33/34 (97%)	11 (33%)	4 (12%)
1	E	32/34 (94%)	11 (34%)	2 (6%)
5	I	62/65 (95%)	19 (30%)	1 (1%)
5	J	62/65 (95%)	18 (29%)	1 (1%)
All	All	189/198 (95%)	59 (31%)	8 (4%)

All (59) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	3	A
1	A	4	A
1	A	6	G
1	A	9	U
1	A	20	A
1	A	24	U
1	A	28	A
1	A	29	G
1	A	32	A
1	A	33	U
1	E	4	A
1	E	5	C
1	E	6	G
1	E	9	U
1	E	20	A
1	E	24	U
1	E	28	A
1	E	29	G
1	E	30	C
1	E	32	A
1	E	33	U
5	I	37	U
5	I	39	G
5	I	40	C
5	I	42	A

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Mol	Chain	Res	Type
5	I	43	G
5	I	44	U
5	I	50	U
5	I	51	A
5	I	56	U
5	I	57	A
5	I	59	U
5	I	63	U
5	I	68	A
5	I	74	A
5	I	82	G
5	I	87	G
5	I	89	G
5	I	91	C
5	I	92	G
5	J	37	U
5	J	39	G
5	J	40	C
5	J	42	A
5	J	43	G
5	J	50	U
5	J	51	A
5	J	56	U
5	J	57	A
5	J	59	U
5	J	63	U
5	J	68	A
5	J	74	A
5	J	82	G
5	J	87	G
5	J	89	G
5	J	91	C
5	J	92	G

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	3	A
1	A	8	A
1	A	27	G
1	A	28	A
1	E	3	A

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Mol	Chain	Res	Type
1	E	27	G
5	I	42	A
5	J	42	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	34/34 (100%)	-0.27	0 100 100	18, 45, 134, 169	0
1	E	32/34 (94%)	0.47	1 (3%) 51 44	38, 77, 181, 216	0
2	B	1322/1368 (96%)	0.36	95 (7%) 23 22	14, 71, 195, 218	0
2	F	1327/1368 (97%)	0.72	186 (14%) 7 10	13, 92, 149, 193	0
3	C	26/26 (100%)	-0.20	1 (3%) 44 37	27, 50, 107, 115	0
3	G	26/26 (100%)	-0.03	1 (3%) 44 37	45, 63, 112, 124	0
4	D	11/11 (100%)	0.27	2 (18%) 4 6	41, 53, 134, 168	0
4	H	11/11 (100%)	0.50	1 (9%) 16 17	41, 59, 110, 175	0
5	I	63/65 (96%)	-0.20	1 (1%) 70 62	20, 74, 126, 157	0
5	J	63/65 (96%)	-0.10	3 (4%) 36 32	36, 56, 156, 192	0
All	All	2915/3008 (96%)	0.49	291 (9%) 14 16	13, 77, 168, 218	0

All (291) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	305	ILE	9.6
2	F	1243	GLU	8.9
1	E	34	G	8.6
2	F	362	TYR	7.4
2	B	900	LEU	6.6
2	F	306	LEU	6.6
2	F	301	LEU	6.4
2	F	416	LEU	6.2
2	B	876	VAL	5.8
2	F	796	LEU	5.8
2	F	443	ILE	5.4
2	B	822	MET	5.3
2	F	815	TYR	5.3

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Mol	Chain	Res	Type	RSRZ
2	F	135	ILE	5.2
2	B	868	ASP	5.2
2	B	842	VAL	5.1
2	B	1051	THR	5.0
2	B	870	VAL	4.9
5	J	36	G	4.9
2	F	247	GLY	4.8
2	B	841	ILE	4.7
2	B	1052	LEU	4.7
2	F	224	ASN	4.7
2	B	1045	PHE	4.6
2	F	818	ASN	4.5
2	B	685	SER	4.5
2	B	42	SER	4.5
2	F	1246	LYS	4.5
2	B	867	SER	4.3
2	B	1046	PHE	4.3
2	F	102	GLU	4.1
2	F	1247	GLY	4.1
2	F	244	LEU	4.0
2	F	249	THR	4.0
2	B	861	ASP	3.9
2	F	400	ARG	3.9
2	F	181	VAL	3.9
2	F	557	ARG	3.9
2	F	103	GLU	3.9
2	F	367	ALA	3.8
2	B	843	PRO	3.8
4	H	2	DT	3.8
2	F	621	LEU	3.8
2	B	815	TYR	3.8
2	B	871	PRO	3.8
2	F	81	TYR	3.7
2	F	267	SER	3.7
2	F	528	LYS	3.7
2	B	872	SER	3.7
2	F	1242	TYR	3.7
2	F	795	ILE	3.6
2	B	801	VAL	3.6
2	F	213	SER	3.6
2	F	581	SER	3.6
2	F	207	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	688	PHE	3.6
2	F	587	PHE	3.6
2	F	262	ALA	3.5
2	F	152	ARG	3.5
2	F	157	ALA	3.5
2	B	859	ARG	3.5
2	B	813	LEU	3.5
2	F	156	LEU	3.5
2	B	462	PHE	3.5
2	B	31	LYS	3.5
2	B	1040	SER	3.4
2	F	413	GLN	3.4
2	B	1039	TYR	3.4
2	B	883	TRP	3.4
2	F	597	LEU	3.4
2	B	811	LEU	3.3
2	F	335	LEU	3.3
2	F	613	GLU	3.3
2	F	359	TYR	3.3
2	F	136	TYR	3.3
2	B	810	LYS	3.3
2	F	154	ILE	3.3
2	F	415	HIS	3.3
2	F	229	LEU	3.2
2	F	412	HIS	3.2
2	B	809	GLU	3.2
2	B	1228	LEU	3.2
2	B	906	GLY	3.2
2	F	538	ALA	3.2
2	B	858	THR	3.2
2	F	142	LEU	3.2
2	F	697	ILE	3.2
2	F	334	LEU	3.1
2	B	817	GLN	3.1
2	F	119	PHE	3.1
2	B	32	PHE	3.1
2	B	897	PHE	3.1
2	F	246	LEU	3.1
2	F	524	LEU	3.1
2	F	220	ARG	3.1
2	F	402	GLN	3.1
4	D	2	DT	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	679	ILE	3.1
2	B	824	VAL	3.0
2	F	98	PHE	3.0
2	B	823	TYR	3.0
2	F	145	SER	3.0
2	B	1050	ILE	3.0
2	F	164	PHE	3.0
2	F	1252	ASN	3.0
2	B	902	LYS	3.0
2	F	369	GLN	2.9
2	F	132	TYR	2.9
2	F	232	GLU	2.9
2	F	440	ILE	2.9
2	F	558	LYS	2.9
2	F	83	GLN	2.8
2	F	408	GLY	2.8
2	F	537	PRO	2.8
2	F	118	ILE	2.8
2	F	243	ALA	2.8
2	F	488	ALA	2.8
2	F	419	LEU	2.8
2	F	886	LEU	2.8
2	B	852	ILE	2.8
2	F	389	LEU	2.8
2	F	788	ILE	2.8
2	B	814	TYR	2.8
2	F	128	TYR	2.8
2	B	833	LEU	2.8
2	F	225	LEU	2.8
2	F	703	THR	2.8
2	B	869	ASN	2.8
2	F	784	ILE	2.8
2	F	159	ALA	2.7
2	B	796	LEU	2.7
2	F	478	PHE	2.7
2	F	302	LEU	2.7
2	B	901	THR	2.7
2	F	208	ALA	2.7
2	F	702	LEU	2.7
2	F	189	VAL	2.7
2	B	597	LEU	2.7
2	F	237	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	269	ASP	2.6
2	F	321	MET	2.6
2	F	530	VAL	2.6
2	F	365	GLY	2.6
2	F	777	SER	2.6
2	F	240	ASN	2.6
2	B	812	TYR	2.6
2	B	28	PRO	2.6
2	B	899	ASN	2.6
2	F	227	ALA	2.6
2	F	1249	PRO	2.6
2	F	155	TYR	2.6
2	F	317	LEU	2.6
2	F	304	ASP	2.6
2	F	202	ASN	2.6
2	F	811	LEU	2.5
2	F	688	PHE	2.5
2	B	903	ALA	2.5
2	F	689	ALA	2.5
2	F	141	LYS	2.5
2	F	800	PRO	2.5
2	B	1084	ARG	2.5
2	F	160	HIS	2.5
2	B	857	LEU	2.5
2	F	407	ASN	2.5
2	F	248	LEU	2.5
2	B	1048	THR	2.5
2	F	919	ARG	2.5
2	F	792	GLY	2.5
2	F	85	ILE	2.4
2	F	125	GLU	2.4
2	F	525	THR	2.4
2	F	804	THR	2.4
2	B	854	ASN	2.4
2	F	363	ILE	2.4
2	F	313	THR	2.4
2	B	1242	TYR	2.4
2	B	860	SER	2.4
2	B	908	LEU	2.4
2	F	253	LYS	2.4
2	B	1073	VAL	2.4
2	B	855	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	863	ASN	2.4
2	F	539	PHE	2.4
2	F	781	MET	2.4
2	F	158	LEU	2.3
2	F	594	TYR	2.3
2	F	1111	LEU	2.3
2	F	257	ASP	2.3
2	B	830	ILE	2.3
2	B	836	TYR	2.3
2	F	117	PRO	2.3
2	F	836	TYR	2.3
2	F	575	PHE	2.3
5	J	43	G	2.3
2	F	694	MET	2.3
2	B	856	VAL	2.3
2	F	307	ARG	2.3
2	B	844	GLN	2.3
2	F	372	PHE	2.3
2	F	139	ARG	2.3
2	B	816	LEU	2.3
4	D	12	DG	2.3
2	F	140	LYS	2.3
2	B	912	ASP	2.3
2	B	43	ILE	2.3
2	F	1120	ILE	2.3
2	F	545	LYS	2.3
2	F	222	LEU	2.3
2	F	399	LEU	2.3
2	F	798	GLU	2.3
2	F	816	LEU	2.3
2	F	78	ARG	2.2
2	F	93	VAL	2.2
5	I	82	G	2.2
2	B	853	ASP	2.2
2	B	881	ASN	2.2
2	F	588	ASN	2.2
2	F	97	PHE	2.2
2	F	238	PHE	2.2
2	B	880	LYS	2.2
2	F	515	TYR	2.2
2	F	1248	SER	2.2
2	B	829	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	1090	PRO	2.2
2	F	209	LYS	2.2
2	B	241	LEU	2.2
2	B	1245	LEU	2.2
2	F	212	LEU	2.2
2	B	1310	ILE	2.2
3	C	1	DC	2.2
2	F	698	HIS	2.2
2	B	862	LYS	2.2
2	B	47	LEU	2.2
2	F	271	TYR	2.2
2	F	423	LEU	2.2
2	B	795	ILE	2.2
2	F	84	GLU	2.2
2	F	420	HIS	2.2
2	B	877	LYS	2.2
2	F	230	PRO	2.2
2	F	803	ASN	2.2
2	F	391	VAL	2.2
2	F	853	ASP	2.2
2	F	312	ILE	2.1
2	F	376	ILE	2.1
2	F	619	ILE	2.1
2	B	832	ARG	2.1
2	B	864	ARG	2.1
2	F	1112	PRO	2.1
2	F	631	MET	2.1
2	F	833	LEU	2.1
2	B	310	THR	2.1
2	F	192	TYR	2.1
2	F	712	GLN	2.1
2	B	1042	ILE	2.1
2	B	229	LEU	2.1
2	B	1021	MET	2.1
2	F	308	VAL	2.1
2	F	421	ALA	2.1
2	F	670	ILE	2.1
2	F	861	ASP	2.1
2	F	1218	GLY	2.1
3	G	26	DT	2.1
2	B	978	ILE	2.1
2	F	805	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	20	VAL	2.1
2	B	19	ALA	2.1
2	B	271	TYR	2.1
2	F	256	PHE	2.1
2	F	432	PHE	2.1
2	B	275	LEU	2.1
2	F	887	LEU	2.1
2	F	620	VAL	2.1
2	F	799	HIS	2.1
2	F	856	VAL	2.1
5	J	42	A	2.0
2	B	1008	PHE	2.0
2	F	309	ASN	2.0
2	F	82	LEU	2.0
2	F	822	MET	2.0
2	B	1249	PRO	2.0
2	F	883	TRP	2.0
2	F	166	GLY	2.0
2	F	446	PHE	2.0
2	B	891	LEU	2.0
2	F	1238	LEU	2.0
2	F	648	MET	2.0
2	B	274	ASP	2.0
2	F	578	VAL	2.0
2	F	250	PRO	2.0
2	F	314	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.