



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2025 – 04:53 PM JST

PDB ID : 8KAI / pdb\_00008kai  
Title : Crystal structure of SpyCas9-crRNA-tracrRNA complex bound to 17nt target DNA  
Authors : Chen, Y.; Chen, J.; Liu, L.  
Deposited on : 2023-08-03  
Resolution : 3.49 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](mailto: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>.

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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

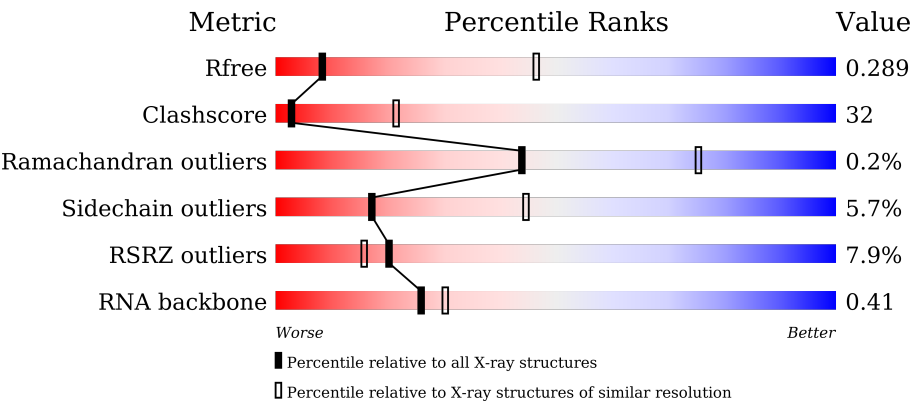
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.49 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 <sub>free</sub>	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)
RNA backbone	3690	1089 (4.00-3.00)

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  $\geq 3$ , 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>3%</div><div>9%</div><div>38%</div><div>32%</div><div>21%</div></div>
1	E	34	<div><div>3%</div><div>24%</div><div>26%</div><div>38%</div><div>9%</div></div>
2	B	1368	<div><div>6%</div><div>45%</div><div>48%</div><div>•</div></div>
2	F	1368	<div><div>11%</div><div>44%</div><div>48%</div><div>5%</div><div>•</div></div>

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Mol	Chain	Length	Quality of chain
3	C	25	<div><div></div><div>20%60%20%</div></div>
3	G	25	<div><div></div><div>20%44%36%</div></div>
4	D	11	<div><div></div><div>9%64%36%</div></div>
4	H	11	<div><div></div><div>9%27%55%18%</div></div>
5	I	65	<div><div></div><div>8%35%38%15%. </div></div>
5	J	65	<div><div></div><div>2%17%32%38%9%. </div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27007 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	31	Total	C	N	O	P	0	0	0
			663	297	118	217	31			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1326	Total	C	N	O	S	0	0	0
			10769	6854	1869	2024	22			
2	F	1327	Total	C	N	O	S	0	0	0
			10698	6816	1845	2014	23			

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 (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	25	Total	C	N	O	P	0	0	0
			501	244	83	150	24			
3	G	25	Total	C	N	O	P	0	0	0
			501	244	83	150	24			

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

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

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	O	0	0
			1	1		
6	F	3	Total	O	0	0
			3	3		

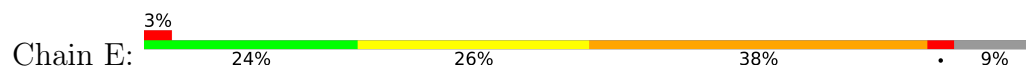
### 3 Residue-property plots

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

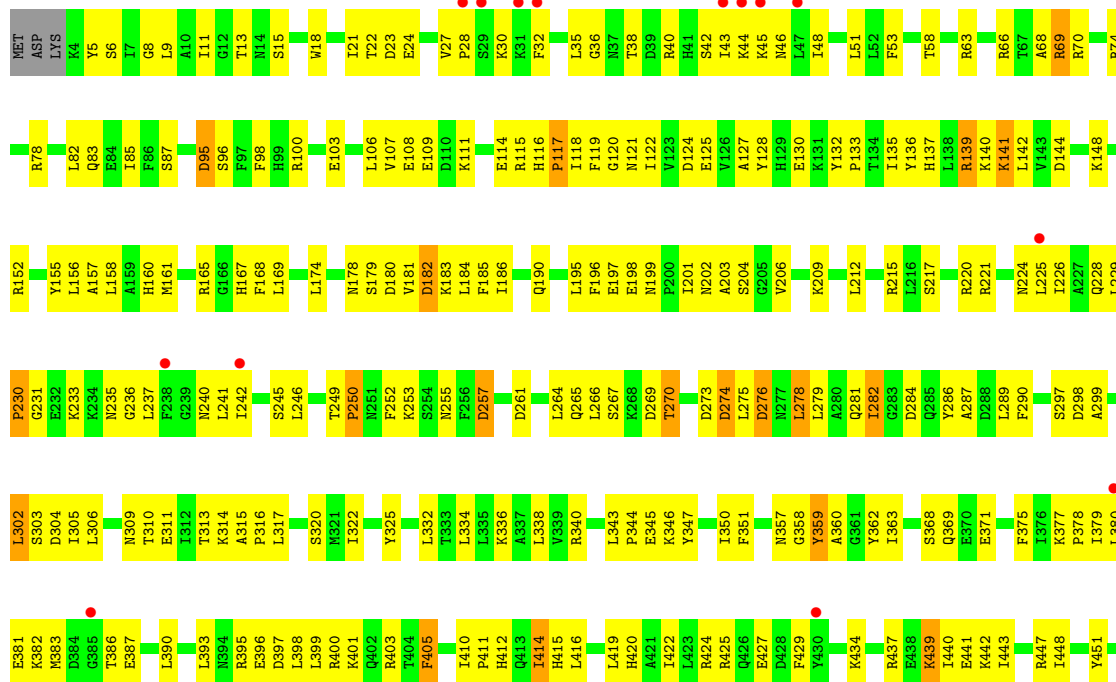
- Molecule 1: RNA (34-MER)

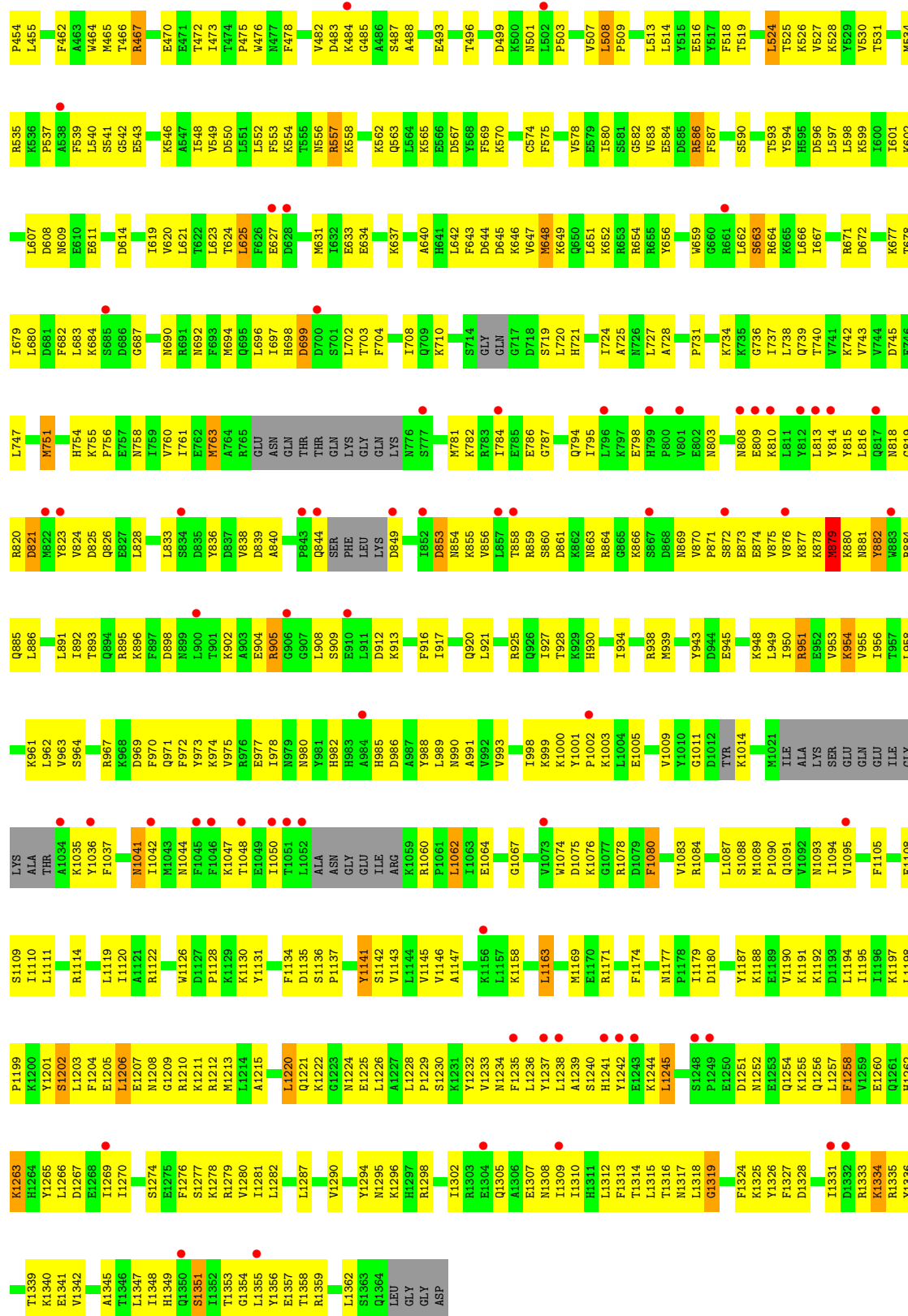


- Molecule 1: RNA (34-MER)

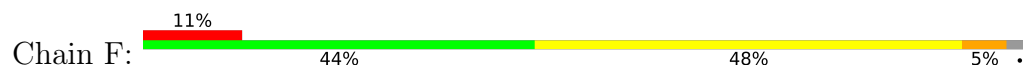


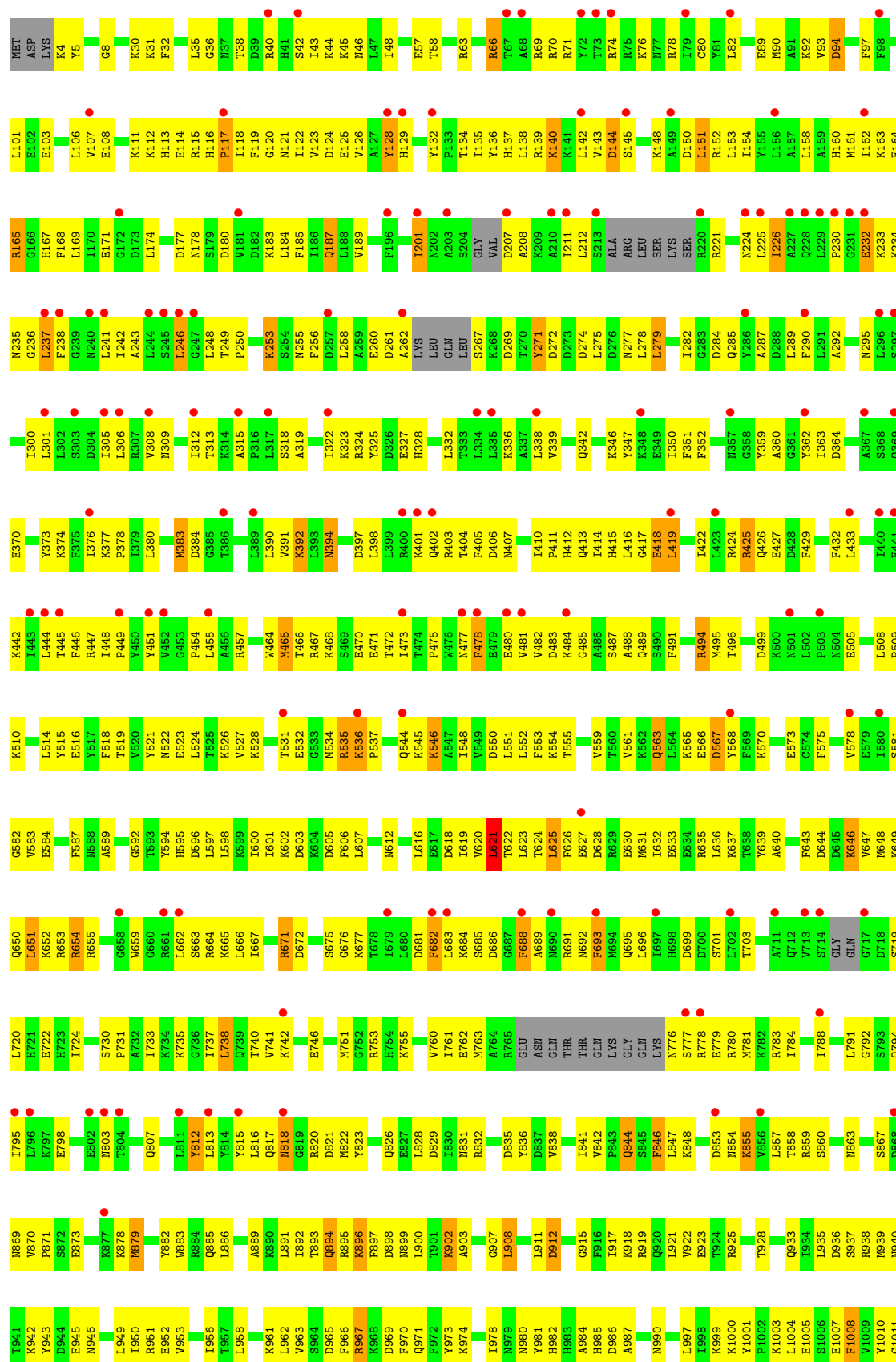
- Molecule 2: CRISPR-associated endonuclease Cas9/Csn1



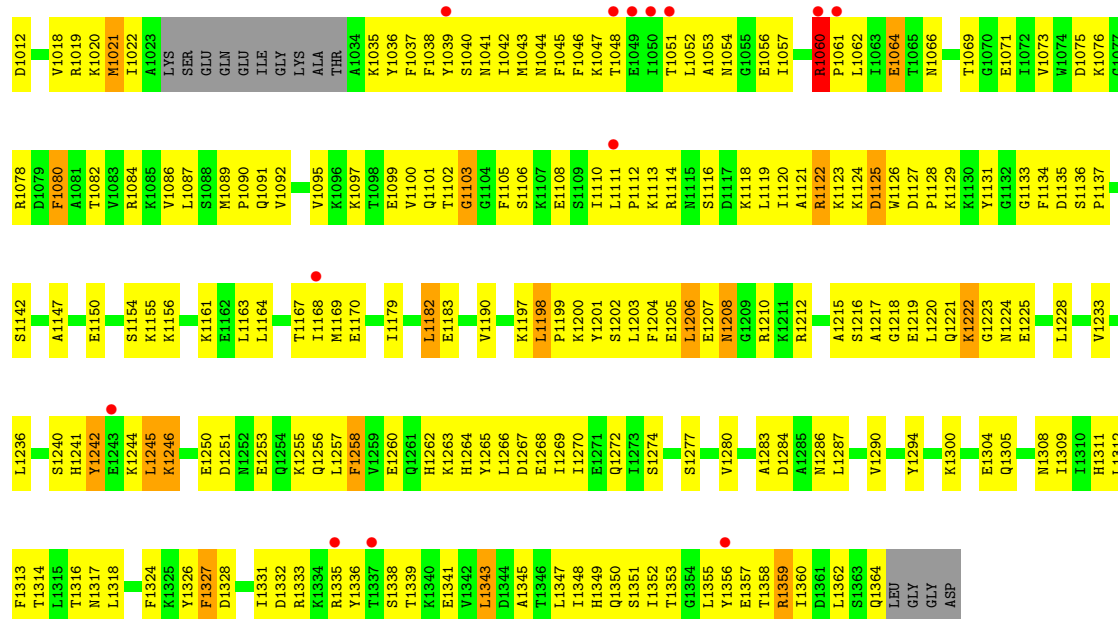


- Molecule 2: CRISPR-associated endonuclease Cas9/Csn1

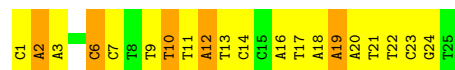




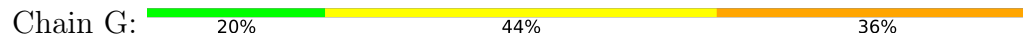




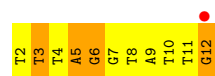
• Molecule 3: DNA (25-MER)



• Molecule 3: DNA (25-MER)



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

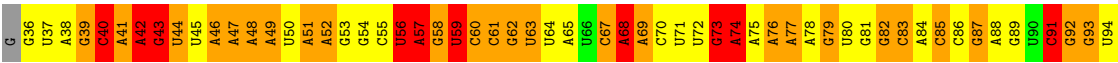


• Molecule 4: DNA (5'-D(\*TP\*TP\*TP\*AP\*GP\*GP\*TP\*AP\*TP\*TP\*G)-3')

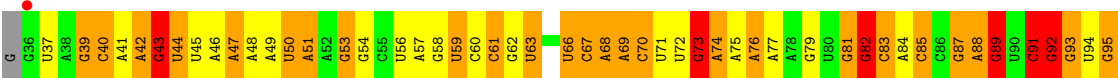


• Molecule 5: RNA (65-MER)





● 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, $\alpha$ , $\beta$ , $\gamma$	144.30Å 130.19Å 146.41Å 90.00° 104.02° 90.00°	Depositor
Resolution (Å)	48.57 – 3.49 48.57 – 3.49	Depositor EDS
% Data completeness (in resolution range)	79.0 (48.57-3.49) 79.0 (48.57-3.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.225 , 0.294 0.224 , 0.289	Depositor DCC
$R_{free}$ test set	3301 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.1	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 76.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.087 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	27007	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	1.18	2/811 (0.2%)	2.15	52/1261 (4.1%)
1	E	1.03	1/742 (0.1%)	1.89	24/1154 (2.1%)
2	B	0.68	5/10954 (0.0%)	0.89	26/14725 (0.2%)
2	F	0.69	7/10882 (0.1%)	0.90	23/14639 (0.2%)
3	C	1.69	8/559 (1.4%)	1.64	14/859 (1.6%)
3	G	1.60	8/559 (1.4%)	1.53	12/859 (1.4%)
4	D	1.81	4/251 (1.6%)	1.44	2/387 (0.5%)
4	H	1.56	1/251 (0.4%)	1.57	4/387 (1.0%)
5	I	1.19	3/1509 (0.2%)	2.11	93/2350 (4.0%)
5	J	1.09	2/1509 (0.1%)	1.98	66/2350 (2.8%)
All	All	0.85	41/28027 (0.1%)	1.23	316/38971 (0.8%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	16	DA	C3'-O3'	-9.28	1.31	1.44
5	I	47	A	C6-N1	-8.44	1.29	1.35
4	D	3	DT	C3'-O3'	-8.17	1.33	1.44
3	G	1	DC	C3'-O3'	8.03	1.54	1.44
2	F	425	ARG	CG-CD	-7.73	1.32	1.51
2	B	627	GLU	CG-CD	7.48	1.63	1.51
4	H	5	DA	C3'-O3'	-7.42	1.34	1.44
5	J	66	U	C2-N3	7.25	1.42	1.37
3	G	19	DA	C3'-O3'	-7.12	1.34	1.44
2	F	418	GLU	CB-CG	-6.84	1.39	1.52
2	B	627	GLU	CB-CG	6.73	1.65	1.52
3	C	12	DA	N7-C5	-6.67	1.35	1.39
2	B	1126	TRP	CB-CG	6.56	1.62	1.50
3	C	1	DC	C1'-N1	6.36	1.57	1.49
5	J	91	C	N3-C4	6.33	1.38	1.33
5	I	43	G	N9-C4	6.25	1.43	1.38
2	F	232	GLU	CB-CG	6.21	1.64	1.52
3	G	17	DT	C1'-N1	6.16	1.57	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	12	DA	C5'-C4'	5.94	1.57	1.51
3	G	1	DC	C1'-N1	5.92	1.56	1.49
3	C	19	DA	C3'-O3'	-5.86	1.36	1.44
5	I	60	C	N1-C6	-5.82	1.33	1.37
3	C	1	DC	N1-C2	5.81	1.46	1.40
1	A	21	G	N7-C5	-5.81	1.35	1.39
3	G	12	DA	C5-C6	5.77	1.46	1.41
3	G	24	DG	C3'-O3'	5.71	1.51	1.44
2	F	1103	GLY	C-O	-5.68	1.14	1.23
2	B	464	TRP	CB-CG	-5.61	1.40	1.50
4	D	8	DT	C3'-O3'	5.55	1.51	1.44
3	C	1	DC	C2'-C1'	5.41	1.57	1.52
1	E	16	A	N9-C4	-5.38	1.34	1.37
3	C	6	DC	C3'-O3'	5.34	1.50	1.44
4	D	5	DA	N9-C4	5.29	1.41	1.37
2	F	1064	GLU	CG-CD	5.21	1.59	1.51
2	B	1319	GLY	C-N	-5.18	1.22	1.34
4	D	12	DG	N7-C5	5.15	1.42	1.39
3	G	1	DC	N1-C2	5.14	1.45	1.40
1	A	18	A	N3-C4	-5.08	1.31	1.34
2	F	1005	GLU	CB-CG	-5.08	1.42	1.52
3	G	16	DA	C3'-O3'	-5.01	1.37	1.44
2	F	57	GLU	CG-CD	5.01	1.59	1.51

All (316) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	59	U	O5'-P-OP2	-14.53	92.62	105.70
5	J	91	C	C5-C4-N4	-13.11	111.02	120.20
5	I	48	A	C8-N9-C4	12.70	110.88	105.80
5	I	62	G	C5-C6-O6	12.51	136.11	128.60
5	J	91	C	C5-C6-N1	10.97	126.48	121.00
5	J	53	G	O5'-P-OP1	-10.55	96.21	105.70
5	J	91	C	N3-C4-N4	10.51	125.35	118.00
5	J	91	C	C4-C5-C6	-10.50	112.15	117.40
5	I	54	G	N1-C6-O6	10.20	126.02	119.90
5	J	91	C	N3-C2-O2	10.12	128.99	121.90
5	I	62	G	C4-C5-N7	-9.60	106.96	110.80
1	A	17	U	C6-N1-C2	9.53	126.72	121.00
5	I	62	G	N1-C6-O6	-9.21	114.37	119.90
1	A	17	U	N3-C4-C5	9.19	120.12	114.60
2	F	1060	ARG	NE-CZ-NH1	9.17	124.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	43	G	N3-C4-C5	-9.06	124.07	128.60
1	A	18	A	C4-C5-C6	9.05	121.52	117.00
2	B	343	LEU	CA-CB-CG	8.81	135.57	115.30
5	I	93	G	C8-N9-C4	-8.74	102.90	106.40
2	B	1319	GLY	C-N-CA	-8.69	99.96	121.70
5	I	48	A	N7-C8-N9	-8.67	109.47	113.80
5	I	53	G	N1-C6-O6	8.56	125.04	119.90
1	A	18	A	N1-C6-N6	8.55	123.73	118.60
5	J	66	U	N3-C4-O4	8.48	125.34	119.40
1	A	23	U	C5-C4-O4	-8.44	120.84	125.90
5	I	63	U	C5-C6-N1	-8.44	118.48	122.70
1	A	19	A	C2-N3-C4	-8.42	106.39	110.60
5	I	62	G	N9-C4-C5	8.33	108.73	105.40
1	A	2	U	C2-N1-C1'	8.31	127.67	117.70
5	I	43	G	C8-N9-C4	-8.30	103.08	106.40
5	I	42	A	C5-N7-C8	-8.28	99.76	103.90
2	F	902	LYS	CD-CE-NZ	-8.23	92.78	111.70
4	H	2	DT	O4'-C1'-N1	8.22	113.76	108.00
5	J	81	G	N3-C4-C5	-8.21	124.49	128.60
5	I	48	A	N9-C4-C5	-8.21	102.52	105.80
3	G	14	DC	O4'-C4'-C3'	-8.19	101.08	106.00
5	J	73	G	N1-C6-O6	8.14	124.79	119.90
5	I	73	G	C8-N9-C4	-8.12	103.15	106.40
5	J	66	U	N3-C4-C5	-8.12	109.73	114.60
1	A	11	U	C5-C6-N1	8.10	126.75	122.70
2	F	896	LYS	CD-CE-NZ	-8.05	93.18	111.70
5	I	54	G	C8-N9-C4	-8.02	103.19	106.40
3	C	24	DG	O4'-C1'-N9	7.98	113.58	108.00
1	E	16	A	C8-N9-C4	7.97	108.99	105.80
5	I	47	A	C8-N9-C4	-7.91	102.64	105.80
5	I	63	U	C6-N1-C2	7.89	125.73	121.00
1	E	24	U	C5-C6-N1	7.88	126.64	122.70
5	J	89	G	C6-C5-N7	-7.86	125.69	130.40
5	J	66	U	N1-C2-O2	-7.83	117.32	122.80
2	B	416	LEU	CB-CG-CD2	-7.82	97.70	111.00
1	A	5	C	C6-N1-C2	-7.72	117.21	120.30
5	J	79	G	C8-N9-C4	7.72	109.49	106.40
3	C	6	DC	OP1-P-OP2	7.71	131.16	119.60
5	I	52	A	N9-C4-C5	7.70	108.88	105.80
5	I	53	G	C2-N3-C4	-7.64	108.08	111.90
2	F	967	ARG	NE-CZ-NH1	-7.53	116.53	120.30
3	C	14	DC	O4'-C4'-C3'	-7.49	101.51	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	89	G	N1-C6-O6	7.44	124.36	119.90
5	J	82	G	O5'-P-OP2	-7.41	99.03	105.70
5	I	54	G	C6-C5-N7	-7.40	125.96	130.40
3	G	14	DC	O4'-C1'-N1	7.37	113.16	108.00
5	J	53	G	O5'-P-OP2	7.34	119.51	110.70
4	H	5	DA	O5'-P-OP1	-7.29	99.14	105.70
5	J	73	G	C8-N9-C4	-7.28	103.49	106.40
5	I	42	A	N7-C8-N9	7.24	117.42	113.80
5	J	91	C	N1-C2-N3	-7.21	114.15	119.20
5	I	57	A	O5'-P-OP1	-7.19	99.22	105.70
5	I	53	G	C6-C5-N7	-7.19	126.08	130.40
5	I	67	C	C6-N1-C2	7.19	123.18	120.30
2	F	66	ARG	NE-CZ-NH1	-7.15	116.72	120.30
5	J	73	G	N7-C8-N9	7.15	116.68	113.10
5	I	52	A	N1-C6-N6	-7.12	114.33	118.60
1	A	22	U	C6-N1-C2	-7.12	116.73	121.00
1	A	17	U	N1-C2-O2	7.11	127.78	122.80
5	I	44	U	O5'-P-OP1	-7.09	99.32	105.70
1	A	18	A	C6-C5-N7	-7.05	127.36	132.30
5	I	74	A	N1-C6-N6	7.05	122.83	118.60
1	A	8	A	P-O3'-C3'	7.04	128.15	119.70
1	A	18	A	N1-C2-N3	6.96	132.78	129.30
1	A	33	U	N3-C2-O2	-6.95	117.33	122.20
1	E	9	U	N1-C2-N3	-6.94	110.73	114.90
2	B	82	LEU	CB-CG-CD2	-6.92	99.24	111.00
3	G	6	DC	O4'-C1'-N1	6.88	112.81	108.00
1	E	15	G	C5-C6-N1	6.84	114.92	111.50
2	B	514	LEU	CA-CB-CG	6.83	131.00	115.30
2	B	1282	LEU	CA-CB-CG	6.83	131.00	115.30
2	F	246	LEU	CA-CB-CG	6.80	130.94	115.30
5	J	89	G	O5'-P-OP1	-6.75	99.62	105.70
5	I	93	G	N9-C4-C5	6.72	108.09	105.40
3	C	6	DC	O5'-P-OP2	-6.72	99.66	105.70
5	J	66	U	N3-C2-O2	6.71	126.90	122.20
1	A	8	A	N9-C1'-C2'	-6.68	104.65	112.00
2	F	621	LEU	CA-CB-CG	6.67	130.64	115.30
5	I	47	A	N9-C4-C5	6.66	108.46	105.80
1	A	2	U	O5'-P-OP1	6.64	118.67	110.70
1	A	17	U	N1-C2-N3	-6.63	110.92	114.90
5	J	61	C	C6-N1-C2	-6.62	117.65	120.30
5	J	81	G	C2-N3-C4	6.61	115.21	111.90
2	B	69	ARG	NE-CZ-NH1	-6.56	117.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	47	A	N1-C6-N6	-6.56	114.66	118.60
5	I	46	A	C5-C6-N6	-6.55	118.46	123.70
1	E	15	G	N1-C6-O6	-6.54	115.97	119.90
5	J	47	A	N1-C6-N6	6.54	122.53	118.60
2	B	424	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	A	27	G	C8-N9-C4	-6.51	103.80	106.40
1	A	16	A	N1-C6-N6	-6.50	114.70	118.60
1	A	33	U	N1-C2-O2	6.50	127.35	122.80
4	H	6	DG	O5'-P-OP1	6.47	118.47	110.70
2	B	879	MET	CA-CB-CG	-6.46	102.32	113.30
2	F	651	LEU	CB-CG-CD1	-6.45	100.03	111.00
2	B	625	LEU	CB-CG-CD1	-6.39	100.14	111.00
2	F	425	ARG	NE-CZ-NH1	-6.38	117.11	120.30
5	I	52	A	C4-C5-N7	-6.38	107.51	110.70
5	I	93	G	C4-C5-N7	-6.38	108.25	110.80
5	J	81	G	N3-C4-N9	6.36	129.81	126.00
5	I	62	G	C8-N9-C4	-6.35	103.86	106.40
2	F	201	ILE	CG1-CB-CG2	-6.31	97.53	111.40
1	A	17	U	OP1-P-OP2	-6.30	110.14	119.60
1	A	2	U	C6-N1-C1'	-6.28	112.41	121.20
1	A	2	U	C5-C6-N1	6.25	125.83	122.70
2	B	249	THR	C-N-CD	6.25	141.53	128.40
3	C	2	DA	O5'-P-OP1	-6.21	100.11	105.70
1	E	22	U	N3-C2-O2	-6.21	117.86	122.20
2	B	1257	LEU	CA-CB-CG	6.20	129.57	115.30
1	E	19	A	C8-N9-C4	6.20	108.28	105.80
1	E	13	U	N3-C4-C5	-6.18	110.89	114.60
2	B	278	LEU	CA-CB-CG	6.16	129.47	115.30
5	I	53	G	C4-C5-N7	6.16	113.26	110.80
5	I	46	A	C5-C6-N1	6.15	120.78	117.70
5	J	76	A	N1-C6-N6	-6.15	114.91	118.60
5	J	81	G	C8-N9-C4	-6.15	103.94	106.40
2	B	174	LEU	CA-CB-CG	6.14	129.42	115.30
5	I	41	A	C2-N3-C4	-6.12	107.54	110.60
5	I	46	A	C4-C5-N7	6.12	113.76	110.70
5	I	82	G	N3-C4-N9	6.08	129.65	126.00
5	I	53	G	C5-C6-N1	-6.05	108.48	111.50
5	I	58	G	OP1-P-O3'	6.04	118.48	105.20
5	J	73	G	C5-N7-C8	-6.04	101.28	104.30
5	J	44	U	C5-C6-N1	-6.03	119.68	122.70
2	F	151	LEU	CA-CB-CG	6.02	129.15	115.30
1	A	21	G	OP2-P-O3'	6.02	118.45	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	95	G	C8-N9-C4	-6.02	103.99	106.40
1	A	4	A	C4-C5-N7	6.01	113.71	110.70
5	I	68	A	C5-N7-C8	-6.00	100.90	103.90
5	J	93	G	C5-C6-O6	-6.00	125.00	128.60
5	J	39	G	N3-C4-N9	5.99	129.59	126.00
5	J	85	C	N3-C2-O2	-5.99	117.71	121.90
5	I	46	A	OP2-P-O3'	5.97	118.33	105.20
5	J	69	A	C2-N3-C4	-5.96	107.62	110.60
5	J	70	C	C6-N1-C2	5.96	122.68	120.30
1	E	27	G	P-O3'-C3'	5.96	126.85	119.70
3	G	2	DA	O5'-P-OP1	-5.95	100.34	105.70
1	A	13	U	N3-C4-O4	5.95	123.56	119.40
5	I	63	U	N3-C4-C5	5.95	118.17	114.60
5	I	54	G	N7-C8-N9	5.92	116.06	113.10
1	A	22	U	C5-C6-N1	5.91	125.66	122.70
1	A	26	A	C2-N3-C4	-5.91	107.64	110.60
5	J	87	G	C5-C6-O6	5.88	132.12	128.60
3	C	10	DT	O4'-C1'-N1	5.87	112.11	108.00
5	I	61	C	C5-C6-N1	5.87	123.93	121.00
5	I	60	C	N1-C2-O2	-5.86	115.38	118.90
5	I	56	U	C5-C6-N1	-5.86	119.77	122.70
5	I	40	C	N3-C2-O2	5.85	126.00	121.90
5	J	73	G	C6-C5-N7	-5.83	126.90	130.40
1	A	3	A	C8-N9-C4	-5.82	103.47	105.80
1	A	9	U	N3-C4-C5	5.82	118.09	114.60
2	F	226	ILE	CA-CB-CG1	-5.82	99.95	111.00
2	F	621	LEU	CB-CG-CD2	5.81	120.88	111.00
5	J	87	G	N1-C6-O6	-5.80	116.42	119.90
5	J	67	C	OP1-P-O3'	5.79	117.94	105.20
1	E	21	G	C5-C6-O6	5.79	132.07	128.60
5	I	63	U	C2-N3-C4	-5.79	123.53	127.00
3	G	20	DA	O4'-C1'-N9	-5.78	103.95	108.00
1	A	3	A	OP1-P-O3'	5.76	117.87	105.20
1	A	22	U	N1-C2-O2	-5.76	118.77	122.80
3	G	12	DA	O4'-C1'-N9	5.75	112.03	108.00
1	A	20	A	C6-N1-C2	-5.75	115.15	118.60
5	J	93	G	N1-C6-O6	5.75	123.35	119.90
5	I	42	A	C2'-C3'-O3'	5.73	122.86	113.70
1	A	11	U	C6-N1-C2	-5.72	117.57	121.00
1	A	19	A	N3-C4-C5	5.72	130.80	126.80
5	I	68	A	N7-C8-N9	5.72	116.66	113.80
5	I	54	G	C5-C6-N1	-5.72	108.64	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	17	DT	O4'-C1'-N1	5.71	112.00	108.00
5	I	41	A	C8-N9-C4	5.70	108.08	105.80
5	J	73	G	C5-C6-N1	-5.70	108.65	111.50
1	E	9	U	C4-C5-C6	-5.70	116.28	119.70
1	E	21	G	N1-C6-O6	-5.70	116.48	119.90
5	I	42	A	C4-C5-N7	5.69	113.55	110.70
5	J	43	G	C5-C6-N1	5.69	114.34	111.50
1	E	23	U	OP2-P-O3'	5.68	117.70	105.20
5	I	52	A	OP2-P-O3'	5.68	117.70	105.20
5	I	52	A	C5-C6-N6	5.67	128.24	123.70
1	A	22	U	O5'-P-OP2	-5.66	100.60	105.70
5	J	85	C	N1-C2-O2	5.65	122.29	118.90
4	H	11	DT	O4'-C1'-N1	5.64	111.95	108.00
1	A	4	A	N1-C6-N6	5.64	121.98	118.60
1	A	18	A	OP2-P-O3'	5.61	117.55	105.20
1	A	15	G	C8-N9-C4	5.61	108.64	106.40
2	B	204	SER	N-CA-CB	-5.60	102.10	110.50
1	E	24	U	C6-N1-C2	-5.60	117.64	121.00
3	C	11	DT	O4'-C1'-N1	5.60	111.92	108.00
5	I	78	A	N1-C6-N6	5.59	121.95	118.60
1	A	6	G	C5-C6-O6	-5.58	125.25	128.60
1	A	21	G	C6-C5-N7	-5.57	127.06	130.40
5	I	83	C	C6-N1-C2	-5.55	118.08	120.30
5	J	91	C	C6-N1-C1'	-5.55	114.13	120.80
2	B	1163	LEU	CB-CG-CD1	-5.55	101.57	111.00
3	G	10	DT	N3-C4-O4	5.53	123.22	119.90
5	I	42	A	N1-C6-N6	5.52	121.91	118.60
2	F	1198	LEU	CA-CB-CG	-5.51	102.62	115.30
1	A	24	U	N3-C4-O4	5.51	123.26	119.40
2	B	439	LYS	CD-CE-NZ	-5.51	99.03	111.70
5	I	51	A	C4-C5-C6	5.51	119.75	117.00
1	E	22	U	C5-C4-O4	5.50	129.20	125.90
5	J	68	A	C8-N9-C4	-5.48	103.61	105.80
5	I	93	G	N3-C4-C5	-5.48	125.86	128.60
3	C	7	DC	OP2-P-O3'	5.47	117.24	105.20
1	A	13	U	N1-C2-O2	-5.46	118.98	122.80
5	J	87	G	N3-C4-C5	-5.46	125.87	128.60
5	I	93	G	C5-C6-O6	5.45	131.87	128.60
5	J	89	G	C4-C5-C6	5.45	122.07	118.80
5	I	54	G	C5-C6-O6	-5.44	125.34	128.60
5	I	54	G	C4-C5-C6	5.43	122.06	118.80
3	C	12	DA	O4'-C1'-N9	-5.42	104.20	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	67	C	N1-C2-O2	5.42	122.16	118.90
3	G	14	DC	C4'-C3'-C2'	-5.42	98.22	103.10
5	J	92	G	C8-N9-C1'	5.42	134.04	127.00
1	E	29	G	N3-C4-C5	5.41	131.30	128.60
1	A	4	A	C5-N7-C8	-5.40	101.20	103.90
2	B	1245	LEU	CA-CB-CG	5.40	127.72	115.30
5	J	79	G	N7-C8-N9	-5.40	110.40	113.10
1	E	24	U	OP2-P-O3'	5.39	117.07	105.20
1	E	29	G	O5'-P-OP2	-5.39	100.85	105.70
5	I	60	C	N3-C4-N4	5.39	121.77	118.00
3	G	21	DT	N3-C4-O4	5.39	123.13	119.90
5	I	82	G	N3-C2-N2	5.39	123.67	119.90
5	J	73	G	C4-C5-N7	5.39	112.95	110.80
5	J	66	U	C4-C5-C6	5.38	122.93	119.70
5	I	54	G	N3-C2-N2	-5.38	116.13	119.90
5	I	76	A	C8-N9-C4	5.38	107.95	105.80
2	B	821	ASP	CB-CG-OD2	-5.37	113.47	118.30
2	F	908	LEU	CA-CB-CG	-5.37	102.95	115.30
5	J	76	A	OP1-P-O3'	5.37	117.00	105.20
5	I	47	A	C5-C6-N6	5.36	127.99	123.70
1	E	9	U	N1-C2-O2	5.35	126.54	122.80
5	I	57	A	N1-C6-N6	5.33	121.80	118.60
5	J	44	U	C6-N1-C2	5.33	124.19	121.00
2	F	226	ILE	CB-CA-C	5.32	122.24	111.60
3	C	16	DA	O4'-C4'-C3'	-5.31	102.38	104.50
1	E	15	G	C8-N9-C4	5.31	108.52	106.40
2	F	1182	LEU	CB-CG-CD2	5.30	120.02	111.00
1	A	4	A	C5-C6-N6	-5.30	119.46	123.70
3	C	13	DT	O4'-C4'-C3'	-5.30	102.38	104.50
2	B	524	LEU	CB-CG-CD2	-5.29	102.00	111.00
5	I	40	C	N1-C2-O2	-5.28	115.73	118.90
5	I	91	C	C6-N1-C2	-5.28	118.19	120.30
5	I	43	G	C2-N3-C4	5.27	114.54	111.90
5	J	83	C	OP1-P-OP2	-5.27	111.69	119.60
2	B	414	ILE	CG1-CB-CG2	-5.27	99.80	111.40
5	I	55	C	C6-N1-C2	-5.26	118.20	120.30
1	A	33	U	C2-N1-C1'	5.25	124.00	117.70
1	E	24	U	N1-C1'-C2'	-5.25	106.22	112.00
5	I	73	G	N9-C4-C5	5.25	107.50	105.40
1	A	19	A	C5-C6-N6	5.25	127.90	123.70
1	E	19	A	C4-C5-C6	-5.24	114.38	117.00
2	B	139	ARG	NE-CZ-NH1	-5.23	117.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	508	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	24	U	C5-C4-O4	-5.23	122.76	125.90
1	A	27	G	C2-N3-C4	5.22	114.51	111.90
5	I	58	G	C4-C5-N7	5.21	112.88	110.80
3	C	10	DT	N3-C4-O4	5.20	123.02	119.90
5	J	70	C	C5-C6-N1	-5.20	118.40	121.00
5	I	82	G	N3-C4-C5	-5.19	126.00	128.60
5	I	61	C	OP1-P-OP2	-5.18	111.82	119.60
5	I	42	A	C5-C6-N6	-5.17	119.57	123.70
1	E	25	U	C5-C6-N1	5.16	125.28	122.70
2	F	1343	LEU	CA-CB-CG	-5.16	103.44	115.30
2	F	30	LYS	CD-CE-NZ	5.15	123.55	111.70
5	I	49	A	C8-N9-C4	-5.15	103.74	105.80
3	G	25	DT	O4'-C4'-C3'	5.14	109.08	106.00
1	E	27	G	O4'-C1'-N9	5.13	112.31	108.20
5	I	57	A	O4'-C1'-N9	-5.12	104.10	108.20
5	J	92	G	C4-N9-C1'	-5.12	119.85	126.50
5	J	82	G	C8-N9-C1'	-5.11	120.36	127.00
3	G	15	DC	C4'-C3'-C2'	-5.11	98.50	103.10
5	I	68	A	C8-N9-C4	-5.11	103.76	105.80
5	I	74	A	C4-C5-N7	5.10	113.25	110.70
5	J	75	A	N1-C6-N6	5.10	121.66	118.60
3	G	16	DA	O4'-C1'-N9	5.10	111.57	108.00
3	C	16	DA	OP1-P-OP2	-5.09	111.96	119.60
2	F	383	MET	CG-SD-CE	-5.09	92.05	100.20
5	J	62	G	C4-C5-C6	5.09	121.86	118.80
5	J	95	G	C2-N3-C4	5.09	114.44	111.90
5	I	47	A	C2-N3-C4	-5.09	108.06	110.60
2	F	625	LEU	CA-CB-CG	5.07	126.97	115.30
4	D	6	DG	O5'-P-OP2	5.06	116.77	110.70
4	D	10	DT	O4'-C1'-N1	-5.06	104.46	108.00
2	B	524	LEU	CB-CG-CD1	-5.04	102.43	111.00
5	I	79	G	N1-C6-O6	5.04	122.92	119.90
1	A	2	U	O4'-C1'-N1	-5.04	104.17	108.20
5	J	88	A	N7-C8-N9	5.03	116.32	113.80
2	B	282	ILE	CG1-CB-CG2	-5.03	100.33	111.40
2	B	250	PRO	CA-N-CD	-5.03	104.46	111.50
5	J	54	G	C8-N9-C1'	-5.03	120.47	127.00
2	F	1245	LEU	CB-CG-CD2	-5.02	102.46	111.00
1	A	17	U	N3-C4-O4	-5.02	115.89	119.40
2	F	418	GLU	OE1-CD-OE2	5.02	129.32	123.30
5	I	48	A	C5-C6-N6	-5.02	119.68	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	62	G	N3-C4-C5	-5.01	126.09	128.60
5	J	91	C	C2-N1-C1'	5.01	124.31	118.80
5	I	42	A	C8-N9-C4	-5.01	103.80	105.80
5	I	85	C	C5-C4-N4	5.01	123.71	120.20
5	J	62	G	N3-C4-C5	-5.01	126.09	128.60
5	J	43	G	N1-C6-O6	-5.00	116.90	119.90
5	I	74	A	C5-C6-N6	-5.00	119.70	123.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	725	0	362	29	0
1	E	663	0	331	30	0
2	B	10769	0	10863	701	2
2	F	10698	0	10745	807	0
3	C	501	0	287	13	0
3	G	501	0	287	19	0
4	D	225	0	129	7	0
4	H	225	0	129	11	0
5	I	1348	0	678	70	0
5	J	1348	0	678	68	0
6	B	1	0	0	0	0
6	F	3	0	0	0	0
All	All	27007	0	24489	1634	2

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 32.

All (1634) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:380:LEU:O	2:B:386:THR:CG2	1.70	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1222:LYS:NZ	2:B:1315:LEU:O	1.59	1.33
2:F:878:LYS:HB3	2:F:879:MET:SD	1.74	1.28
2:F:878:LYS:HD2	2:F:879:MET:CE	1.76	1.16
2:B:410:ILE:HG23	2:B:414:ILE:HD11	1.26	1.15
2:B:1258:PHE:CE1	2:B:1262:HIS:CD2	2.38	1.11
2:B:1258:PHE:HE1	2:B:1262:HIS:CD2	1.68	1.11
2:F:878:LYS:CD	2:F:879:MET:HE1	1.81	1.10
2:F:1060:ARG:HE	2:F:1061:PRO:HD2	1.04	1.09
2:F:137:HIS:CD2	2:F:322:ILE:HG12	1.86	1.09
2:F:137:HIS:HD2	2:F:322:ILE:HG12	1.06	1.08
2:B:380:LEU:O	2:B:386:THR:HG21	0.89	1.06
2:B:410:ILE:HG23	2:B:414:ILE:CD1	1.85	1.04
2:F:521:TYR:HD1	2:F:684:LYS:HG2	1.20	1.04
2:F:878:LYS:HB3	2:F:879:MET:CE	1.87	1.04
2:B:1179:ILE:HD11	2:B:1192:LYS:HE2	1.41	1.02
2:F:1108:GLU:HB2	3:G:9:DT:H5"	1.44	1.00
2:B:410:ILE:CG2	2:B:414:ILE:HD11	1.91	0.99
1:E:23:U:H5"	2:F:1112:PRO:HG3	1.44	0.99
2:F:922:VAL:HG11	2:F:1007:GLU:HB3	1.44	0.99
2:B:727:LEU:HD12	2:B:927:ILE:HD12	1.42	0.99
2:F:1205:GLU:OE1	2:F:1359:ARG:NH2	1.97	0.98
2:F:168:PHE:HB2	2:F:447:ARG:HH11	1.26	0.97
2:F:521:TYR:CD1	2:F:684:LYS:CD	2.48	0.96
2:B:1000:LYS:HG3	2:B:1001:TYR:CE1	2.01	0.95
2:F:521:TYR:CE1	2:F:684:LYS:CD	2.48	0.95
2:F:878:LYS:CG	2:F:879:MET:HE3	1.97	0.95
2:F:522:ASN:OD1	2:F:692:ASN:ND2	1.99	0.94
2:B:1109:SER:OG	3:C:9:DT:OP2	1.84	0.94
2:F:165:ARG:HD2	2:F:168:PHE:HE1	1.33	0.93
2:B:46:ASN:ND2	2:B:1091:GLN:OE1	2.01	0.93
2:B:727:LEU:HD12	2:B:927:ILE:CD1	1.97	0.93
2:F:1060:ARG:NE	2:F:1061:PRO:HD2	1.82	0.93
2:B:279:LEU:HD11	2:B:284:ASP:HA	1.51	0.93
2:F:923:GLU:HG2	2:F:928:THR:HG21	1.52	0.92
2:B:70:ARG:NH2	5:I:61:C:OP1	2.03	0.92
2:F:527:VAL:HA	2:F:582:GLY:HA3	1.51	0.92
2:F:138:LEU:HD21	2:F:153:LEU:HD21	1.49	0.92
2:F:140:LYS:NZ	2:F:313:THR:HB	1.84	0.92
2:B:212:LEU:HD21	2:B:225:LEU:HD12	1.50	0.92
2:F:760:VAL:HG22	2:F:956:ILE:HD12	1.52	0.91
2:F:180:ASP:HB3	2:F:183:LYS:HB2	1.48	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:140:LYS:HZ2	2:F:313:THR:HB	1.35	0.91
2:F:521:TYR:CD1	2:F:684:LYS:HG2	2.06	0.91
2:F:90:MET:HA	2:F:151:LEU:HD21	1.51	0.90
2:F:860:SER:OG	2:F:863:ASN:OD1	1.90	0.90
2:F:521:TYR:CE1	2:F:684:LYS:HD2	2.04	0.90
2:F:174:LEU:HD21	2:F:413:GLN:CG	2.02	0.89
2:B:1351:SER:OG	5:I:68:A:N6	2.05	0.89
2:F:1045:PHE:HB2	2:F:1064:GLU:HG2	1.54	0.89
2:F:249:THR:OG1	2:F:267:SER:N	2.06	0.89
2:B:1351:SER:HG	5:I:68:A:N6	1.69	0.89
2:F:521:TYR:CD1	2:F:684:LYS:HD3	2.08	0.89
2:F:855:LYS:NZ	2:F:1246:LYS:O	2.06	0.89
2:F:878:LYS:HD2	2:F:879:MET:HE1	0.91	0.88
2:F:521:TYR:CD1	2:F:684:LYS:CG	2.57	0.88
2:F:44:LYS:NZ	5:J:92:G:O6	2.05	0.88
2:F:521:TYR:HD1	2:F:684:LYS:CG	1.86	0.88
2:B:336:LYS:NZ	5:I:43:G:O6	2.06	0.87
5:J:46:A:H2'	5:J:47:A:C8	2.10	0.87
2:B:1251:ASP:HA	2:B:1254:GLN:HE21	1.39	0.87
2:F:187:GLN:NE2	2:F:292:ALA:HB1	1.90	0.87
3:C:6:DC:O2	4:D:7:DG:N2	2.08	0.86
2:F:451:TYR:O	2:F:464:TRP:NE1	2.08	0.86
2:F:338:LEU:HB3	2:F:383:MET:HE2	1.57	0.86
2:B:1277:SER:HA	2:B:1281:ILE:HG12	1.56	0.85
2:F:139:ARG:HH12	2:F:418:GLU:CD	1.78	0.85
2:B:1003:LYS:HG3	2:B:1036:TYR:HE2	1.41	0.85
2:F:174:LEU:HD21	2:F:413:GLN:CD	1.96	0.85
2:B:220:ARG:O	2:B:224:ASN:ND2	2.10	0.84
2:B:1241:HIS:CE1	2:B:1244:LYS:HA	2.11	0.84
2:F:207:ASP:O	2:F:211:ILE:HD13	1.77	0.84
2:F:249:THR:HG1	2:F:267:SER:N	1.75	0.84
2:F:933:GLN:HG2	2:F:1010:TYR:OH	1.77	0.84
5:I:83:C:H2'	5:I:84:A:H8	1.41	0.84
2:F:1357:GLU:O	5:J:81:G:N2	2.10	0.84
2:B:299:ALA:O	2:B:303:SER:OG	1.94	0.83
2:F:478:PHE:HE2	2:F:482:VAL:HB	1.41	0.83
2:B:1228:LEU:HD12	2:B:1229:PRO:HD2	1.61	0.83
2:B:1245:LEU:HB2	2:B:1252:ASN:ND2	1.93	0.83
2:F:627:GLU:HA	2:F:655:ARG:HH12	1.44	0.83
2:F:1256:GLN:NE2	2:F:1260:GLU:OE2	2.12	0.83
2:B:557:ARG:NH2	2:B:596:ASP:OD1	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:136:TYR:CE1	2:F:139:ARG:NH2	2.45	0.83
2:B:508:LEU:HD21	2:B:664:ARG:HB2	1.61	0.82
2:B:1222:LYS:NZ	2:B:1315:LEU:C	2.33	0.82
2:F:672:ASP:OD1	2:F:703:THR:HG22	1.80	0.82
2:F:878:LYS:HG2	2:F:879:MET:HE3	1.60	0.82
2:B:671:ARG:HG3	2:B:678:THR:HG22	1.61	0.82
2:F:211:ILE:HG22	2:F:212:LEU:HD23	1.61	0.82
2:F:878:LYS:CB	2:F:879:MET:CE	2.57	0.81
2:B:241:LEU:HD13	2:B:289:LEU:HD21	1.60	0.81
2:F:226:ILE:CD1	2:F:232:GLU:HB3	2.09	0.81
2:F:633:GLU:HG2	2:F:652:LYS:HD3	1.60	0.81
2:B:212:LEU:O	2:B:221:ARG:NH1	2.13	0.81
2:F:143:VAL:HG23	2:F:422:ILE:HD11	1.62	0.81
2:F:878:LYS:HB3	2:F:879:MET:HE3	1.62	0.81
2:F:878:LYS:CG	2:F:879:MET:CE	2.58	0.81
2:F:923:GLU:OE2	2:F:925:ARG:NH1	2.12	0.81
2:B:978:ILE:HD12	2:B:1233:VAL:HG22	1.62	0.81
2:F:94:ASP:HB3	2:F:97:PHE:HB2	1.63	0.81
2:F:878:LYS:CB	2:F:879:MET:SD	2.66	0.81
1:A:27:G:H5'	1:A:28:A:H5''	1.60	0.81
2:F:1041:ASN:O	2:F:1042:ILE:HG22	1.81	0.81
1:A:14:G:OP2	2:B:63:ARG:NH1	2.13	0.80
2:B:45:LYS:NZ	2:B:1357:GLU:OE2	2.14	0.80
2:F:165:ARG:HD2	2:F:168:PHE:CE1	2.16	0.80
2:F:1210:ARG:NH2	2:F:1341:GLU:OE1	2.15	0.80
2:F:380:LEU:HD11	2:F:390:LEU:HG	1.62	0.80
2:B:967:ARG:HE	2:B:974:LYS:HB2	1.47	0.80
2:F:878:LYS:CD	2:F:879:MET:CE	2.49	0.80
2:B:395:ARG:NH2	2:B:397:ASP:OD2	2.14	0.80
2:B:524:LEU:HD12	2:B:587:PHE:HE2	1.44	0.79
2:B:525:THR:HG23	2:B:690:ASN:HB3	1.63	0.79
2:B:881:ASN:OD1	2:B:885:GLN:NE2	2.15	0.79
2:B:1211:LYS:H	2:B:1224:ASN:HD21	1.30	0.79
2:F:921:LEU:HD22	2:F:1042:ILE:HD12	1.63	0.79
2:F:921:LEU:HD22	2:F:1042:ILE:CD1	2.13	0.79
2:B:1074:TRP:HZ2	2:B:1080:PHE:HE2	1.31	0.79
2:F:878:LYS:CB	2:F:879:MET:HE3	2.12	0.78
2:F:1119:LEU:HD23	2:F:1128:PRO:HB2	1.65	0.78
2:B:634:GLU:HA	2:B:637:LYS:NZ	1.98	0.78
2:F:184:LEU:HD13	2:F:295:ASN:HB3	1.65	0.78
1:A:20:A:OP2	2:B:403:ARG:NH1	2.15	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:LEU:HB2	2:B:230:PRO:HD2	1.66	0.77
2:F:1290:VAL:HG22	2:F:1331:ILE:HD13	1.66	0.77
2:F:466:THR:O	2:F:482:VAL:HG13	1.84	0.77
2:B:563:GLN:O	2:B:567:ASP:HB2	1.82	0.77
5:I:52:A:OP2	5:I:62:G:N2	2.18	0.77
2:B:1108:GLU:N	3:C:9:DT:OP1	2.13	0.77
2:B:824:VAL:HG11	2:B:859:ARG:HH12	1.48	0.77
2:B:1074:TRP:HZ2	2:B:1080:PHE:CE2	2.03	0.77
2:F:48:ILE:HG12	2:F:984:ALA:HB1	1.66	0.77
2:F:933:GLN:HG2	2:F:1010:TYR:CZ	2.20	0.77
1:E:10:U:O4	3:G:19:DA:N6	2.18	0.77
2:B:1326:TYR:HD2	2:B:1327:PHE:H	1.32	0.77
2:F:140:LYS:HZ2	2:F:313:THR:CB	1.98	0.77
2:F:870:VAL:HG11	2:F:899:ASN:O	1.85	0.77
2:F:1001:TYR:HE2	2:F:1045:PHE:CE1	2.03	0.77
2:F:1286:ASN:ND2	2:F:1332:ASP:O	2.17	0.77
2:F:174:LEU:HG	2:F:413:GLN:HB2	1.66	0.76
2:F:644:ASP:OD2	2:F:646:LYS:N	2.17	0.76
2:B:83:GLN:HG2	2:B:98:PHE:CE1	2.21	0.76
2:F:853:ASP:OD1	2:F:893:THR:HG21	1.85	0.76
2:B:860:SER:OG	2:B:863:ASN:OD1	2.03	0.76
2:B:69:ARG:HD3	5:I:62:G:N7	2.01	0.76
2:F:253:LYS:HB2	2:F:262:ALA:H	1.51	0.76
2:F:921:LEU:HG	2:F:1008:PHE:HE2	1.51	0.76
2:F:89:GLU:OE2	2:F:92:LYS:NZ	2.19	0.75
2:F:413:GLN:O	2:F:417:GLY:N	2.14	0.75
2:B:1147:ALA:HB2	2:B:1190:VAL:HA	1.67	0.75
2:F:733:ILE:HD11	2:F:763:MET:HE2	1.68	0.75
2:F:826:GLN:NE2	2:F:859:ARG:HD3	2.01	0.75
2:B:368:SER:OG	2:B:371:GLU:OE1	2.04	0.75
2:F:826:GLN:HE22	2:F:859:ARG:HD3	1.50	0.75
2:F:1091:GLN:HG3	5:J:91:C:H5"	1.69	0.75
2:B:525:THR:CG2	2:B:690:ASN:HB3	2.16	0.75
2:F:1241:HIS:CE1	2:F:1244:LYS:HA	2.22	0.75
2:F:521:TYR:HE1	2:F:684:LYS:HD2	1.51	0.75
2:B:383:MET:O	2:B:386:THR:HG23	1.87	0.75
1:E:27:G:N2	5:J:44:U:OP2	2.19	0.75
2:F:1236:LEU:O	2:F:1240:SER:OG	2.04	0.75
2:F:643:PHE:HD1	2:F:647:VAL:HG11	1.52	0.74
2:F:921:LEU:HD13	2:F:1042:ILE:HD13	1.69	0.74
2:F:187:GLN:HE21	2:F:292:ALA:HB1	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:978:ILE:HD12	2:F:1233:VAL:HG22	1.68	0.74
2:F:958:LEU:HD22	2:F:962:LEU:HD12	1.68	0.74
2:B:1011:GLY:O	2:B:1014:LYS:N	2.20	0.74
2:B:1356:TYR:HB3	5:I:81:G:N1	2.02	0.74
2:F:411:PRO:HB2	2:F:413:GLN:OE1	1.87	0.74
2:B:531:THR:HG21	2:B:575:PHE:HE2	1.53	0.74
2:B:1119:LEU:HD23	2:B:1128:PRO:HB2	1.69	0.74
2:F:473:ILE:HG12	2:F:481:VAL:HG11	1.69	0.74
2:F:489:GLN:HG3	2:F:625:LEU:HD21	1.69	0.74
2:B:725:ALA:O	2:B:734:LYS:NZ	2.21	0.73
2:F:174:LEU:CD2	2:F:413:GLN:CG	2.66	0.73
2:F:521:TYR:CE1	2:F:684:LYS:HD3	2.22	0.73
2:B:594:TYR:OH	2:B:608:ASP:OD1	2.06	0.73
2:B:38:THR:HG22	2:B:40:ARG:H	1.52	0.73
2:B:114:GLU:HG3	2:B:116:HIS:H	1.52	0.73
2:F:258:LEU:HD22	2:F:260:GLU:H	1.54	0.73
2:B:549:VAL:HA	2:B:553:PHE:HD2	1.54	0.72
2:F:1262:HIS:HB3	2:F:1265:TYR:CD2	2.24	0.72
2:B:1047:LYS:HB2	2:B:1050:ILE:HG22	1.71	0.72
2:F:318:SER:OG	2:F:418:GLU:OE2	2.05	0.72
2:F:649:LYS:O	2:F:653:ARG:NE	2.21	0.72
2:F:886:LEU:HA	2:F:891:LEU:HD21	1.70	0.72
2:F:841:ILE:CD1	2:F:896:LYS:HG3	2.19	0.72
2:F:165:ARG:C	2:F:415:HIS:HD2	1.93	0.72
2:F:969:ASP:HB2	2:F:970:PHE:CE2	2.25	0.72
2:B:181:VAL:O	2:B:185:PHE:N	2.22	0.72
2:B:687:GLY:O	2:B:690:ASN:ND2	2.23	0.72
2:F:499:ASP:HB2	2:F:663:SER:HB3	1.72	0.72
2:F:646:LYS:O	2:F:650:GLN:NE2	2.23	0.72
2:F:481:VAL:HG12	2:F:482:VAL:HG23	1.72	0.72
2:F:178:ASN:ND2	2:F:295:ASN:OD1	2.23	0.71
2:B:229:LEU:HD12	2:B:231:GLY:H	1.55	0.71
2:B:975:VAL:HG11	2:B:1310:ILE:HD11	1.72	0.71
2:F:174:LEU:HD21	2:F:413:GLN:HG2	1.69	0.71
2:B:745:ASP:OD2	2:B:938:ARG:NH2	2.22	0.71
2:B:1177:ASN:ND2	2:B:1180:ASP:OD2	2.23	0.71
2:F:531:THR:HG21	2:F:575:PHE:CE1	2.26	0.71
2:F:1217:ALA:O	2:F:1339:THR:HG21	1.91	0.71
2:F:686:ASP:HB3	2:F:689:ALA:O	1.90	0.71
2:F:1212:ARG:NH2	2:F:1280:VAL:O	2.24	0.71
2:B:1307:GLU:O	2:B:1310:ILE:HG22	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:980:ASN:HB2	2:F:1225:GLU:OE2	1.90	0.71
2:F:413:GLN:HA	2:F:416:LEU:HB3	1.73	0.71
2:F:505:GLU:HG3	2:F:665:LYS:HB2	1.72	0.71
2:F:1167:THR:HG23	2:F:1170:GLU:H	1.54	0.71
2:B:1315:LEU:HB2	2:B:1324:PHE:CZ	2.26	0.71
2:B:184:LEU:HD12	2:B:299:ALA:HB2	1.73	0.71
2:F:820:ARG:HG3	2:F:826:GLN:O	1.91	0.71
2:B:509:PRO:HB3	2:B:624:THR:HG21	1.73	0.70
2:B:1276:PHE:HE2	2:B:1316:THR:HB	1.55	0.70
2:F:838:VAL:HG11	2:F:855:LYS:HE3	1.72	0.70
2:F:903:ALA:HA	2:F:907:GLY:HA2	1.73	0.70
2:F:1060:ARG:HH21	2:F:1061:PRO:HG2	1.56	0.70
2:F:826:GLN:OE1	2:F:859:ARG:NH1	2.22	0.70
2:B:137:HIS:HA	2:B:322:ILE:HD11	1.72	0.70
2:B:448:ILE:HD13	2:B:455:LEU:HD13	1.72	0.70
2:F:185:PHE:O	2:F:189:VAL:HG23	1.90	0.70
2:F:1206:LEU:HD11	2:F:1210:ARG:HH22	1.54	0.70
2:B:925:ARG:HB3	2:B:928:THR:HG23	1.72	0.70
2:F:174:LEU:CD2	2:F:413:GLN:HG2	2.22	0.70
2:F:74:ARG:O	2:F:78:ARG:HG3	1.91	0.70
2:F:889:ALA:HB3	2:F:891:LEU:HD23	1.73	0.70
2:F:967:ARG:NH1	2:F:974:LYS:HE3	2.06	0.70
2:B:114:GLU:HG2	2:B:120:GLY:O	1.91	0.70
2:B:1003:LYS:HG3	2:B:1036:TYR:CE2	2.25	0.70
2:F:338:LEU:HB3	2:F:383:MET:CE	2.22	0.70
2:F:692:ASN:O	2:F:696:LEU:HG	1.91	0.70
2:B:849:ASP:OD2	2:B:895:ARG:NH1	2.25	0.70
2:F:627:GLU:HA	2:F:655:ARG:NH1	2.05	0.70
2:F:632:ILE:O	2:F:636:LEU:N	2.20	0.70
2:F:1221:GLN:NE2	4:H:6:DG:OP2	2.24	0.70
2:B:939:MET:HE2	2:B:953:VAL:HG21	1.74	0.70
2:B:1356:TYR:HB3	5:I:81:G:C6	2.26	0.70
5:J:40:C:H2'	5:J:41:A:C8	2.26	0.70
2:B:524:LEU:HD12	2:B:587:PHE:CE2	2.26	0.69
2:F:1001:TYR:HE2	2:F:1045:PHE:CD1	2.10	0.69
2:B:9:LEU:HD12	2:B:761:ILE:HG22	1.72	0.69
2:B:1147:ALA:HB1	2:B:1188:LYS:O	1.90	0.69
2:F:1045:PHE:HA	2:F:1060:ARG:HH11	1.58	0.69
2:B:1208:ASN:ND2	2:B:1208:ASN:O	2.25	0.69
2:F:1286:ASN:O	2:F:1290:VAL:HG23	1.92	0.69
2:B:107:VAL:HG22	2:B:1131:TYR:OH	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:386:THR:O	2:B:390:LEU:N	2.25	0.69
2:B:672:ASP:HA	2:B:703:THR:HG21	1.72	0.69
2:B:1211:LYS:N	2:B:1224:ASN:HD21	1.91	0.69
2:F:1135:ASP:OD1	2:F:1136:SER:N	2.26	0.69
2:F:446:PHE:HZ	2:F:478:PHE:HD1	1.41	0.69
2:F:1062:LEU:O	2:F:1076:LYS:HG3	1.93	0.69
2:F:1021:MET:HG3	2:F:1036:TYR:HD2	1.57	0.68
2:F:271:TYR:O	2:F:275:LEU:N	2.22	0.68
2:F:823:TYR:CD2	2:F:858:THR:HG21	2.29	0.68
2:F:1167:THR:HG22	2:F:1170:GLU:HG3	1.74	0.68
2:B:526:LYS:HE2	2:B:692:ASN:HB2	1.75	0.68
2:F:832:ARG:HD2	2:F:835:ASP:OD2	1.92	0.68
5:I:83:C:H2'	5:I:84:A:C8	2.26	0.68
2:B:1211:LYS:H	2:B:1224:ASN:ND2	1.92	0.68
2:B:1305:GLN:O	2:B:1309:ILE:HG13	1.93	0.68
2:F:672:ASP:HB3	2:F:675:SER:HB2	1.76	0.68
2:F:114:GLU:OE1	2:F:116:HIS:N	2.24	0.68
2:F:603:ASP:OD1	2:F:606:PHE:N	2.25	0.68
2:F:1219:GLU:OE1	2:F:1335:ARG:NH2	2.26	0.68
2:B:240:ASN:HB3	2:B:252:PHE:CE2	2.28	0.68
2:F:1045:PHE:O	2:F:1060:ARG:NH1	2.25	0.68
2:B:305:ILE:HD13	2:B:411:PRO:HD2	1.74	0.68
2:B:1333:ARG:NH1	2:B:1335:ARG:HD2	2.07	0.68
2:B:1349:HIS:HB3	5:I:68:A:N3	2.09	0.68
2:F:1182:LEU:HD13	2:F:1190:VAL:HG21	1.75	0.68
5:J:48:A:H2'	5:J:49:A:C8	2.28	0.68
2:B:369:GLN:NE2	2:B:405:PHE:HZ	1.90	0.67
2:B:116:HIS:CE1	2:B:122:ILE:HG23	2.30	0.67
2:B:1220:LEU:HD11	2:B:1339:THR:HA	1.76	0.67
2:F:168:PHE:HB2	2:F:447:ARG:NH1	2.06	0.67
2:F:234:LYS:H	2:F:234:LYS:HD3	1.57	0.67
2:F:646:LYS:HG3	2:F:650:GLN:HE21	1.59	0.67
2:B:8:GLY:HA3	2:B:991:ALA:HB2	1.76	0.67
2:F:621:LEU:O	2:F:625:LEU:N	2.26	0.67
2:B:240:ASN:HB3	2:B:252:PHE:HE2	1.58	0.67
2:F:153:LEU:HD23	2:F:153:LEU:O	1.93	0.67
2:B:558:LYS:HE3	2:B:590:SER:HB3	1.76	0.67
2:F:136:TYR:HE1	2:F:139:ARG:NH2	1.92	0.67
2:B:971:GLN:O	2:B:971:GLN:HG2	1.94	0.67
5:I:36:G:H2'	5:I:37:U:H6	1.60	0.67
2:B:565:LYS:HD3	2:B:578:VAL:HG13	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:95:G:H2'	5:J:96:C:C6	2.29	0.67
1:A:15:G:H2'	1:A:16:A:H8	1.58	0.67
2:F:143:VAL:HG21	2:F:315:ALA:HB2	1.76	0.67
2:F:472:THR:O	2:F:477:ASN:ND2	2.27	0.67
2:F:943:TYR:HE2	2:F:949:LEU:HD13	1.60	0.67
2:F:46:ASN:ND2	2:F:1089:MET:SD	2.69	0.66
2:B:1120:ILE:HD11	2:B:1137:PRO:HG3	1.76	0.66
2:B:1226:LEU:HB2	2:B:1276:PHE:CE2	2.31	0.66
2:F:1116:SER:HB3	2:F:1119:LEU:HB2	1.75	0.66
2:B:1262:HIS:O	2:B:1265:TYR:HB2	1.94	0.66
2:F:90:MET:SD	2:F:151:LEU:HD23	2.35	0.66
2:B:233:LYS:HG2	2:B:235:ASN:HB2	1.76	0.66
2:B:526:LYS:NZ	2:B:690:ASN:O	2.27	0.66
2:B:755:LYS:NZ	2:B:939:MET:O	2.22	0.66
2:F:143:VAL:CG2	2:F:422:ILE:HD11	2.24	0.66
2:F:323:LYS:HE3	2:F:327:GLU:OE2	1.94	0.66
2:B:1047:LYS:CB	2:B:1050:ILE:HG22	2.26	0.66
2:F:922:VAL:HG11	2:F:1007:GLU:CB	2.24	0.66
2:B:237:LEU:HA	2:B:255:ASN:HD21	1.60	0.66
2:B:1276:PHE:CE2	2:B:1316:THR:HB	2.30	0.66
1:A:22:U:O2'	2:B:1110:ILE:HB	1.96	0.66
2:F:118:ILE:H	2:F:118:ILE:HD12	1.60	0.66
5:I:39:G:H5'	5:I:40:C:OP2	1.96	0.66
2:F:174:LEU:HD22	2:F:174:LEU:N	2.10	0.66
2:B:117:PRO:HD2	2:B:125:GLU:OE2	1.96	0.66
2:F:163:LYS:HG2	2:F:164:PHE:CE1	2.30	0.66
2:F:566:GLU:O	2:F:570:LYS:HE2	1.95	0.66
2:B:182:ASP:OD1	2:B:209:LYS:HB2	1.96	0.66
2:B:317:LEU:HD11	2:B:410:ILE:HD11	1.77	0.66
2:B:420:HIS:ND1	2:B:441:GLU:OE2	2.28	0.66
2:F:551:LEU:HD23	2:F:568:TYR:HD1	1.60	0.66
2:B:531:THR:HG21	2:B:575:PHE:CE2	2.31	0.65
2:B:971:GLN:HA	2:B:973:TYR:CE2	2.30	0.65
2:B:313:THR:HG23	2:B:315:ALA:H	1.60	0.65
2:F:392:LYS:HD3	2:F:397:ASP:O	1.96	0.65
2:F:986:ASP:O	2:F:990:ASN:ND2	2.29	0.65
1:E:15:G:OP1	2:F:66:ARG:NH2	2.28	0.65
2:F:618:ASP:HA	2:F:621:LEU:HD22	1.79	0.65
2:B:874:GLU:HA	2:B:877:LYS:HE3	1.76	0.65
2:F:1084:ARG:HB3	2:F:1084:ARG:CZ	2.26	0.65
2:B:672:ASP:HA	2:B:703:THR:CG2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:272:ASP:HA	2:F:275:LEU:HB3	1.77	0.65
1:A:27:G:H5'	1:A:28:A:C5'	2.27	0.65
2:B:66:ARG:HD2	2:B:462:PHE:HE2	1.62	0.65
2:B:970:PHE:CD1	2:B:1080:PHE:HZ	2.14	0.65
3:G:6:DC:H2''	3:G:7:DC:O5'	1.97	0.65
2:B:107:VAL:HG13	2:B:1131:TYR:CE1	2.32	0.65
2:F:671:ARG:HB3	2:F:676:GLY:HA2	1.79	0.65
2:F:966:PHE:O	2:F:970:PHE:HD2	1.80	0.65
2:B:378:PRO:O	2:B:382:LYS:HG2	1.96	0.64
2:B:633:GLU:OE1	2:B:652:LYS:HE3	1.96	0.64
1:E:14:G:OP2	2:F:63:ARG:HD3	1.98	0.64
2:F:143:VAL:O	2:F:425:ARG:NH1	2.30	0.64
2:F:274:ASP:O	2:F:278:LEU:HD12	1.95	0.64
2:F:943:TYR:CE2	2:F:949:LEU:HD13	2.32	0.64
2:B:619:ILE:O	2:B:623:LEU:HB2	1.98	0.64
2:B:1308:ASN:ND2	2:B:1327:PHE:CB	2.59	0.64
2:F:142:LEU:HB3	2:F:422:ILE:HD12	1.79	0.64
2:F:180:ASP:HB3	2:F:183:LYS:HD3	1.80	0.64
2:F:208:ALA:O	2:F:212:LEU:HG	1.96	0.64
2:F:622:THR:HG21	2:F:635:ARG:HG3	1.79	0.64
2:B:317:LEU:HD11	2:B:410:ILE:CD1	2.27	0.64
2:F:623:LEU:HD11	2:F:654:ARG:O	1.96	0.64
2:B:970:PHE:CD1	2:B:1080:PHE:CZ	2.86	0.64
2:F:791:LEU:HD22	2:F:891:LEU:HD22	1.79	0.64
2:F:828:LEU:HD22	2:F:836:TYR:CE2	2.32	0.64
2:F:328:HIS:NE2	2:F:359:TYR:OH	2.29	0.64
2:F:762:GLU:OE1	2:F:990:ASN:ND2	2.30	0.64
2:B:1003:LYS:CG	2:B:1036:TYR:HE2	2.10	0.64
3:C:18:DA:H2'	3:C:19:DA:C8	2.32	0.64
2:F:478:PHE:CE2	2:F:482:VAL:HB	2.28	0.64
2:B:892:ILE:HB	2:B:896:LYS:HD3	1.80	0.64
2:F:103:GLU:OE2	2:F:113:HIS:N	2.31	0.64
2:F:545:LYS:NZ	2:F:683:LEU:O	2.31	0.64
1:E:25:U:H5'	2:F:107:VAL:HG12	1.80	0.64
2:F:143:VAL:CG2	2:F:422:ILE:CD1	2.75	0.63
2:F:891:LEU:HD12	2:F:892:ILE:HG23	1.80	0.63
2:B:893:THR:HG23	2:B:896:LYS:H	1.64	0.63
2:F:900:LEU:H	2:F:900:LEU:HD12	1.63	0.63
2:F:921:LEU:CG	2:F:1008:PHE:HE2	2.10	0.63
5:I:36:G:H2'	5:I:37:U:C6	2.34	0.63
2:F:1347:LEU:N	2:F:1360:ILE:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:432:PHE:CE1	2:F:433:LEU:HG	2.34	0.63
2:F:691:ARG:HG2	2:F:695:GLN:HE21	1.63	0.63
2:F:821:ASP:HB2	2:F:828:LEU:HD21	1.80	0.63
2:B:282:ILE:HG22	2:B:286:TYR:CD1	2.33	0.63
2:F:158:LEU:HA	2:F:161:MET:SD	2.39	0.63
2:F:817:GLN:NE2	2:F:857:LEU:O	2.29	0.63
2:B:278:LEU:O	2:B:282:ILE:HG13	1.98	0.63
2:B:548:ILE:HG23	2:B:552:LEU:CD1	2.29	0.63
2:B:139:ARG:CZ	2:B:161:MET:HG2	2.29	0.62
2:F:649:LYS:HB3	2:F:653:ARG:HH21	1.64	0.62
2:F:933:GLN:HE22	2:F:937:SER:HB3	1.64	0.62
2:F:1123:LYS:HG3	5:J:53:G:OP1	1.99	0.62
2:F:1326:TYR:HE2	2:F:1327:PHE:CD2	2.16	0.62
2:B:275:LEU:O	2:B:279:LEU:HB2	1.99	0.62
2:B:782:LYS:O	2:B:786:GLU:HG3	1.99	0.62
2:F:5:TYR:CZ	2:F:751:MET:HG3	2.34	0.62
2:F:359:TYR:CE2	2:F:363:ILE:HG13	2.34	0.62
2:F:1311:HIS:O	2:F:1314:THR:HG22	1.98	0.62
2:B:824:VAL:HG22	2:B:863:ASN:HD22	1.65	0.62
2:B:985:HIS:ND1	2:B:1087:LEU:HD13	2.14	0.62
2:B:1290:VAL:HG22	2:B:1331:ILE:HD13	1.81	0.62
2:F:1206:LEU:HD11	2:F:1210:ARG:NH2	2.14	0.62
2:B:1207:GLU:HG3	2:B:1208:ASN:H	1.62	0.62
2:B:5:TYR:OH	2:B:754:HIS:O	2.18	0.62
2:B:121:ASN:OD1	2:B:124:ASP:HB2	1.99	0.62
2:B:864:ARG:O	2:B:872:SER:N	2.32	0.62
2:F:143:VAL:HG22	2:F:422:ILE:CD1	2.30	0.62
2:F:171:GLU:HG2	2:F:269:ASP:CB	2.30	0.62
2:F:553:PHE:CE2	2:F:559:VAL:HG21	2.35	0.62
2:B:720:LEU:HD13	2:B:938:ARG:NH1	2.14	0.62
2:B:493:GLU:O	2:B:496:THR:OG1	2.14	0.62
2:F:1253:GLU:O	2:F:1257:LEU:HD12	2.00	0.62
2:F:289:LEU:O	2:F:292:ALA:HB3	2.00	0.62
5:I:94:U:H2'	5:I:95:G:C8	2.35	0.62
2:B:45:LYS:NZ	2:B:1354:GLY:O	2.32	0.62
2:B:245:SER:HA	2:B:297:SER:HB2	1.82	0.62
2:B:970:PHE:HD1	2:B:1080:PHE:CZ	2.17	0.62
2:B:44:LYS:HE2	5:I:92:G:O6	1.99	0.61
2:F:1042:ILE:HG23	2:F:1043:MET:HE2	1.81	0.61
2:F:1167:THR:CG2	2:F:1170:GLU:HG3	2.30	0.61
2:F:410:ILE:HG21	2:F:415:HIS:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:42:A:H8	5:I:42:A:H5''	1.65	0.61
2:B:955:VAL:O	2:B:1009:VAL:HG13	1.99	0.61
2:F:485:GLY:HA3	2:F:631:MET:HG3	1.82	0.61
2:F:777:SER:HA	2:F:807:GLN:HE21	1.66	0.61
2:F:842:VAL:HG12	2:F:854:ASN:HD21	1.65	0.61
2:B:640:ALA:HA	2:B:648:MET:CE	2.29	0.61
2:B:1245:LEU:HB2	2:B:1252:ASN:HD21	1.64	0.61
5:I:94:U:H2'	5:I:95:G:H8	1.66	0.61
2:F:471:GLU:OE1	2:F:477:ASN:ND2	2.33	0.61
2:F:978:ILE:HD13	2:F:1228:LEU:HD23	1.81	0.61
2:F:1051:THR:HG22	2:F:1053:ALA:H	1.65	0.61
2:B:1002:PRO:HD2	2:B:1036:TYR:OH	2.00	0.61
2:F:933:GLN:NE2	2:F:937:SER:HB3	2.16	0.61
2:B:634:GLU:HA	2:B:637:LYS:HZ3	1.64	0.61
2:B:1228:LEU:HD12	2:B:1229:PRO:CD	2.29	0.61
2:B:1349:HIS:CE1	5:I:69:A:H4'	2.36	0.61
2:F:776:ASN:O	2:F:780:ARG:HG2	1.99	0.61
2:B:844:GLN:C	2:B:1041:ASN:HB3	2.22	0.61
2:F:788:ILE:O	2:F:792:GLY:N	2.29	0.60
2:F:961:LYS:HG2	2:F:965:ASP:OD2	2.00	0.60
2:B:40:ARG:NE	2:B:43:ILE:HD11	2.15	0.60
2:B:158:LEU:HD22	2:B:419:LEU:HG	1.81	0.60
2:B:1105:PHE:CG	2:B:1169:MET:HG3	2.36	0.60
2:F:174:LEU:CG	2:F:413:GLN:HB2	2.31	0.60
2:B:644:ASP:HB3	2:B:647:VAL:HG23	1.83	0.60
2:B:1205:GLU:HG3	2:B:1209:GLY:HA2	1.82	0.60
2:F:730:SER:HB2	2:F:733:ILE:HG22	1.84	0.60
2:F:1000:LYS:HG3	2:F:1001:TYR:CD2	2.36	0.60
2:B:542:GLY:O	2:B:546:LYS:HG3	2.01	0.60
2:B:809:GLU:OE1	2:B:855:LYS:HE2	2.00	0.60
2:F:32:PHE:CE1	2:F:1355:LEU:HB3	2.37	0.60
2:F:328:HIS:CG	5:J:44:U:C2	2.90	0.60
2:F:528:LYS:O	2:F:581:SER:N	2.25	0.60
2:F:82:LEU:HD11	2:F:162:ILE:HD13	1.83	0.60
2:B:96:SER:O	2:B:100:ARG:HG3	2.01	0.60
2:B:310:THR:OG1	2:B:316:PRO:HB3	2.00	0.60
3:C:19:DA:H2'	3:C:20:DA:C8	2.36	0.60
3:G:3:DA:N6	4:H:9:DA:H61	2.00	0.60
2:B:6:SER:HB3	2:B:758:ASN:HB2	1.83	0.60
2:B:148:LYS:HB2	2:B:429:PHE:CD1	2.36	0.60
2:B:645:ASP:O	2:B:649:LYS:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:692:ASN:O	2:B:696:LEU:HD23	2.02	0.60
2:B:973:TYR:HB3	2:B:1237:TYR:CD1	2.37	0.60
2:B:1251:ASP:O	2:B:1255:LYS:HG3	2.02	0.60
2:F:226:ILE:HG13	2:F:232:GLU:HB3	1.84	0.60
2:F:279:LEU:HD21	2:F:287:ALA:HB2	1.84	0.60
2:F:598:LEU:HG	2:F:607:LEU:HD12	1.83	0.60
2:F:794:GLN:O	2:F:798:GLU:HG3	2.02	0.60
2:B:455:LEU:HD23	2:B:473:ILE:HD12	1.84	0.60
2:B:1091:GLN:HG3	5:I:91:C:H5''	1.83	0.60
2:F:38:THR:HG22	2:F:40:ARG:H	1.66	0.60
2:F:921:LEU:CD2	2:F:1042:ILE:CD1	2.79	0.60
2:B:140:LYS:HD3	2:B:322:ILE:HD12	1.84	0.60
2:B:549:VAL:HA	2:B:553:PHE:CD2	2.36	0.60
2:B:1213:MET:HE1	2:B:1318:LEU:HD21	1.82	0.60
2:F:780:ARG:HD2	2:F:812:TYR:CE2	2.37	0.60
2:B:35:LEU:HB2	2:B:1358:THR:HG22	1.84	0.59
2:F:619:ILE:HD11	2:F:651:LEU:HD11	1.84	0.59
2:F:1095:VAL:HG13	2:F:1350:GLN:OE1	2.01	0.59
2:B:180:ASP:HB3	2:B:183:LYS:HB2	1.83	0.59
3:C:22:DT:H2''	3:C:23:DC:O5'	2.02	0.59
2:F:44:LYS:HD3	5:J:92:G:N7	2.17	0.59
2:B:823:TYR:HA	2:B:875:VAL:CG1	2.33	0.59
2:F:791:LEU:HD11	2:F:885:GLN:HB3	1.84	0.59
2:B:1215:ALA:HB2	2:B:1221:GLN:HB2	1.84	0.59
1:A:8:A:H2'	1:A:9:U:C6	2.37	0.59
2:B:550:ASP:HA	2:B:554:LYS:HD3	1.84	0.59
2:F:720:LEU:HD13	2:F:938:ARG:HD2	1.84	0.59
2:F:921:LEU:HG	2:F:1008:PHE:CE2	2.37	0.59
2:F:942:LYS:HE3	2:F:952:GLU:OE2	2.03	0.59
2:F:1001:TYR:CE2	2:F:1045:PHE:CE1	2.87	0.59
2:F:1272:GLN:HE22	5:J:89:G:H1	1.51	0.59
3:G:3:DA:H61	4:H:9:DA:H61	1.51	0.59
5:I:37:U:H2'	5:I:38:A:H8	1.68	0.59
2:B:1236:LEU:HA	2:B:1239:ALA:HB3	1.84	0.59
2:F:1060:ARG:HE	2:F:1061:PRO:CD	1.96	0.59
2:F:1266:LEU:HD12	2:F:1309:ILE:HD12	1.85	0.59
2:B:917:ILE:HD11	2:B:1042:ILE:HG22	1.84	0.59
2:F:818:ASN:O	2:F:818:ASN:ND2	2.36	0.59
2:B:332:LEU:HD13	2:B:359:TYR:CE1	2.38	0.59
2:B:720:LEU:HD13	2:B:938:ARG:HH11	1.67	0.59
2:F:134:THR:HG22	5:J:45:U:H4'	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:784:ILE:HG21	2:F:815:TYR:HD1	1.68	0.59
2:F:1270:ILE:HG13	2:F:1294:TYR:CD2	2.38	0.59
2:B:516:GLU:O	2:B:519:THR:HG22	2.02	0.59
2:B:1235:PHE:CE1	2:B:1239:ALA:HB2	2.37	0.59
2:F:531:THR:HG1	2:F:575:PHE:HD1	1.49	0.59
2:B:345:GLU:OE1	2:B:345:GLU:N	2.36	0.59
2:F:1270:ILE:HG13	2:F:1294:TYR:CE2	2.38	0.59
2:B:527:VAL:HA	2:B:582:GLY:HA3	1.84	0.58
2:B:594:TYR:O	2:B:598:LEU:N	2.31	0.58
2:F:359:TYR:HE2	2:F:363:ILE:HG13	1.67	0.58
2:F:841:ILE:HD13	2:F:896:LYS:HG3	1.85	0.58
2:F:923:GLU:HG3	2:F:925:ARG:H	1.67	0.58
2:F:1250:GLU:HG3	2:F:1251:ASP:N	2.17	0.58
5:J:42:A:O2'	5:J:43:G:OP1	2.19	0.58
2:B:977:GLU:N	2:B:977:GLU:OE1	2.35	0.58
1:E:27:G:H1'	2:F:129:HIS:CD2	2.37	0.58
2:F:515:TYR:O	2:F:519:THR:HG22	2.03	0.58
2:F:1218:GLY:HA2	2:F:1339:THR:CG2	2.33	0.58
2:B:1263:LYS:HG3	2:B:1302:ILE:HD13	1.85	0.58
2:B:1315:LEU:HB2	2:B:1324:PHE:CE1	2.38	0.58
2:F:1047:LYS:O	2:F:1076:LYS:NZ	2.37	0.58
3:G:19:DA:H2'	3:G:20:DA:C8	2.38	0.58
2:B:640:ALA:HA	2:B:648:MET:HE2	1.86	0.58
2:F:475:PRO:HG3	5:J:59:U:O4	2.03	0.58
2:B:1000:LYS:O	2:B:1000:LYS:HD3	2.04	0.58
2:F:836:TYR:HB2	2:F:857:LEU:HD11	1.85	0.58
2:B:48:ILE:O	2:B:1093:ASN:ND2	2.36	0.58
1:A:15:G:H2'	1:A:16:A:C8	2.38	0.58
2:F:226:ILE:CG1	2:F:232:GLU:HB3	2.33	0.58
2:B:825:ASP:HA	2:B:879:MET:HE3	1.85	0.58
2:B:1207:GLU:CG	2:B:1208:ASN:H	2.15	0.58
2:F:971:GLN:HG2	2:F:973:TYR:CE2	2.39	0.58
2:F:1038:PHE:CD2	2:F:1039:TYR:HE1	2.21	0.58
2:F:922:VAL:CG1	2:F:1007:GLU:HB3	2.25	0.58
2:B:70:ARG:HH21	5:I:61:C:P	2.24	0.57
2:B:121:ASN:H	2:B:121:ASN:ND2	2.01	0.57
2:B:978:ILE:HG22	2:B:1313:PHE:CE2	2.39	0.57
2:F:630:GLU:HG3	2:F:631:MET:N	2.19	0.57
2:F:1312:LEU:HD21	2:F:1326:TYR:HD1	1.68	0.57
5:I:88:A:N6	5:I:91:C:H42	2.02	0.57
2:B:83:GLN:HG2	2:B:98:PHE:CZ	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1210:ARG:NH2	2:B:1341:GLU:OE1	2.36	0.57
2:F:339:VAL:HG12	2:F:347:TYR:HB2	1.86	0.57
2:F:535:ARG:HH11	2:F:535:ARG:HG3	1.69	0.57
2:B:1041:ASN:ND2	2:B:1044:ASN:HD21	2.03	0.57
2:F:967:ARG:NH1	2:F:986:ASP:OD1	2.37	0.57
5:J:40:C:H2'	5:J:41:A:H8	1.66	0.57
2:B:168:PHE:CD2	2:B:447:ARG:HD3	2.39	0.57
1:E:23:U:O2	2:F:1122:ARG:NH2	2.37	0.57
2:F:144:ASP:OD1	2:F:144:ASP:N	2.36	0.57
2:B:279:LEU:CD1	2:B:284:ASP:HA	2.31	0.57
2:B:1111:LEU:HD12	2:B:1135:ASP:CB	2.35	0.57
2:F:174:LEU:CD2	2:F:174:LEU:N	2.67	0.57
2:B:853:ASP:OD2	2:B:893:THR:HG21	2.04	0.57
2:B:866:LYS:HB3	2:B:869:ASN:HB2	1.87	0.57
2:B:1266:LEU:O	2:B:1270:ILE:HG12	2.03	0.57
2:F:174:LEU:CD2	2:F:413:GLN:CB	2.83	0.57
2:F:618:ASP:OD2	2:F:639:TYR:OH	2.22	0.57
2:F:969:ASP:HB2	2:F:970:PHE:CD2	2.40	0.57
2:B:278:LEU:HG	2:B:282:ILE:HD11	1.87	0.57
2:B:727:LEU:HD21	2:B:934:ILE:HD11	1.87	0.57
2:B:781:MET:HG3	2:B:803:ASN:ND2	2.19	0.57
2:F:63:ARG:HA	2:F:66:ARG:HD3	1.86	0.57
2:F:221:ARG:HA	2:F:224:ASN:HB2	1.87	0.57
2:F:550:ASP:HA	2:F:554:LYS:HG3	1.85	0.57
1:A:10:U:H2'	1:A:11:U:C6	2.39	0.57
3:C:2:DA:H2'	3:C:3:DA:C8	2.40	0.57
2:F:112:LYS:O	2:F:113:HIS:ND1	2.34	0.57
2:B:340:ARG:HH21	5:I:41:A:P	2.28	0.57
2:B:620:VAL:HG13	2:B:656:TYR:HD2	1.70	0.57
2:B:1208:ASN:OD1	2:B:1279:ARG:HG3	2.04	0.57
2:F:662:LEU:HB3	2:F:666:LEU:HD23	1.87	0.57
2:F:1108:GLU:N	3:G:9:DT:OP1	2.33	0.57
2:B:109:GLU:OE1	2:B:1130:LYS:HD3	2.04	0.56
2:B:1000:LYS:HG3	2:B:1001:TYR:CZ	2.37	0.56
2:B:1236:LEU:O	2:B:1240:SER:OG	2.16	0.56
2:F:523:GLU:OE1	2:F:589:ALA:N	2.37	0.56
2:F:870:VAL:HB	2:F:903:ALA:HB2	1.85	0.56
5:J:44:U:O2'	5:J:45:U:H5'	2.04	0.56
2:B:241:LEU:CD1	2:B:289:LEU:HD21	2.32	0.56
2:B:948:LYS:H	2:B:948:LYS:HD2	1.70	0.56
2:F:241:LEU:HD23	2:F:241:LEU:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:936:ASP:CB	2:F:1010:TYR:CD2	2.88	0.56
2:F:981:TYR:CZ	2:F:1092:VAL:HB	2.40	0.56
2:B:378:PRO:HG2	2:B:379:ILE:HD12	1.86	0.56
2:B:410:ILE:CG2	2:B:414:ILE:CD1	2.64	0.56
2:F:117:PRO:HD2	2:F:118:ILE:HD12	1.88	0.56
2:F:563:GLN:O	2:F:567:ASP:HB2	2.04	0.56
2:F:841:ILE:HD12	2:F:854:ASN:HA	1.88	0.56
2:F:1011:GLY:O	2:F:1012:ASP:HB2	2.05	0.56
2:F:1215:ALA:HB2	2:F:1221:GLN:HG3	1.86	0.56
2:B:74:ARG:O	2:B:78:ARG:HG3	2.05	0.56
2:B:824:VAL:HG22	2:B:863:ASN:ND2	2.21	0.56
2:B:1048:THR:HG22	2:B:1076:LYS:CB	2.35	0.56
2:F:76:LYS:O	2:F:80:CYS:HB2	2.06	0.56
2:F:362:TYR:OH	2:F:401:LYS:HG3	2.04	0.56
2:F:373:TYR:HE1	2:F:398:LEU:HB3	1.71	0.56
2:F:620:VAL:O	2:F:624:THR:N	2.28	0.56
2:F:622:THR:HG21	2:F:635:ARG:CG	2.35	0.56
2:F:893:THR:HG23	2:F:896:LYS:HB3	1.88	0.56
2:F:1267:ASP:OD1	2:F:1294:TYR:OH	2.22	0.56
2:B:970:PHE:HD1	2:B:1080:PHE:CE1	2.24	0.56
2:B:198:GLU:HG2	2:B:199:ASN:N	2.19	0.56
2:B:351:PHE:C	2:B:360:ALA:HB2	2.26	0.56
2:B:679:ILE:O	2:B:683:LEU:HD13	2.05	0.56
2:B:814:TYR:HD1	2:B:815:TYR:CD1	2.23	0.56
2:B:1075:ASP:OD1	2:B:1078:ARG:N	2.27	0.56
2:F:40:ARG:HD3	2:F:43:ILE:HD11	1.88	0.56
2:F:595:HIS:HD1	2:F:595:HIS:H	1.53	0.56
2:B:451:TYR:CD1	2:B:488:ALA:HB2	2.40	0.56
2:B:662:LEU:HD23	2:B:666:LEU:HD22	1.86	0.56
2:B:821:ASP:OD2	2:B:828:LEU:HG	2.06	0.56
2:B:609:ASN:ND2	2:B:611:GLU:OE1	2.39	0.56
2:B:1041:ASN:ND2	2:B:1044:ASN:ND2	2.54	0.56
2:B:1295:ASN:HA	2:B:1298:ARG:NH1	2.20	0.56
2:F:623:LEU:HD11	2:F:655:ARG:HA	1.88	0.56
2:F:781:MET:HG3	2:F:803:ASN:ND2	2.21	0.56
2:B:784:ILE:HD13	2:B:815:TYR:HB3	1.87	0.56
2:F:1326:TYR:CE2	2:F:1327:PHE:CD2	2.94	0.56
3:G:3:DA:H61	4:H:9:DA:N6	2.04	0.56
2:B:727:LEU:O	2:B:734:LYS:NZ	2.34	0.56
2:F:221:ARG:O	2:F:225:LEU:N	2.33	0.56
2:F:895:ARG:O	2:F:899:ASN:ND2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1106:SER:HA	2:F:1137:PRO:HA	1.88	0.56
2:B:816:LEU:HD12	2:B:891:LEU:O	2.04	0.55
2:B:1345:ALA:O	2:B:1362:LEU:HG	2.07	0.55
2:F:32:PHE:O	2:F:42:SER:HA	2.06	0.55
2:F:180:ASP:CB	2:F:183:LYS:HB2	2.29	0.55
5:J:92:G:H2'	5:J:93:G:C8	2.42	0.55
2:B:118:ILE:HG22	2:B:119:PHE:CE1	2.41	0.55
2:B:379:ILE:HD12	2:B:379:ILE:H	1.71	0.55
2:F:936:ASP:HB3	2:F:1010:TYR:CD2	2.41	0.55
2:F:1207:GLU:OE2	2:F:1210:ARG:NH1	2.40	0.55
2:F:1218:GLY:C	2:F:1339:THR:HG23	2.27	0.55
2:F:1313:PHE:O	2:F:1316:THR:N	2.39	0.55
2:B:317:LEU:CD1	2:B:410:ILE:HD13	2.37	0.55
2:F:48:ILE:CG1	2:F:984:ALA:HB1	2.37	0.55
2:F:724:ILE:HD13	2:F:738:LEU:HG	1.88	0.55
2:B:531:THR:HG23	2:B:534:MET:HG3	1.88	0.55
2:B:1197:LYS:O	2:B:1199:PRO:HD3	2.06	0.55
2:F:391:VAL:HA	2:F:394:ASN:OD1	2.07	0.55
5:I:37:U:H2'	5:I:38:A:C8	2.42	0.55
2:B:383:MET:O	2:B:386:THR:CG2	2.53	0.55
2:B:905:ARG:HG2	2:B:905:ARG:HH11	1.71	0.55
2:B:920:GLN:HG3	2:B:921:LEU:HD23	1.89	0.55
2:F:551:LEU:O	2:F:555:THR:OG1	2.17	0.55
2:F:699:ASP:OD1	2:F:701:SER:OG	2.23	0.55
2:B:183:LYS:NZ	2:B:311:GLU:OE2	2.39	0.55
2:B:823:TYR:CD1	2:B:875:VAL:HG11	2.41	0.55
2:F:97:PHE:O	2:F:101:LEU:HD13	2.07	0.55
2:F:621:LEU:O	2:F:625:LEU:HB2	2.07	0.55
2:F:742:LYS:HE2	2:F:1352:ILE:HD13	1.89	0.55
2:F:1000:LYS:HG3	2:F:1001:TYR:CE2	2.42	0.55
2:F:1102:THR:OG1	2:F:1103:GLY:N	2.39	0.55
2:B:1062:LEU:HD23	2:B:1062:LEU:H	1.71	0.55
2:B:1318:LEU:HD23	2:B:1319:GLY:N	2.21	0.55
2:F:455:LEU:O	5:J:60:C:H5'	2.07	0.55
2:F:813:LEU:O	2:F:817:GLN:HG3	2.06	0.55
2:F:949:LEU:HD23	2:F:951:ARG:HH22	1.71	0.55
2:B:114:GLU:HG3	2:B:115:ARG:N	2.22	0.55
2:F:869:ASN:HD21	2:F:907:GLY:HA3	1.71	0.55
2:B:1074:TRP:CZ2	2:B:1080:PHE:HE2	2.20	0.55
2:F:606:PHE:CE1	2:F:612:ASN:HB3	2.42	0.55
2:F:886:LEU:HB3	2:F:892:ILE:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:925:ARG:HG3	3:C:21:DT:OP1	2.07	0.55
2:B:1351:SER:HG	5:I:68:A:H62	1.39	0.55
2:B:1207:GLU:HG3	2:B:1208:ASN:N	2.22	0.54
2:F:351:PHE:HB3	5:J:43:G:O6	2.06	0.54
2:F:870:VAL:CG1	2:F:871:PRO:HD2	2.37	0.54
2:B:252:PHE:CE1	2:B:290:PHE:HE2	2.25	0.54
2:B:601:ILE:HD11	2:B:607:LEU:HD21	1.88	0.54
2:B:823:TYR:HA	2:B:875:VAL:HG11	1.89	0.54
2:B:943:TYR:CZ	2:B:949:LEU:HD13	2.42	0.54
1:E:22:U:O2	2:F:1110:ILE:HD12	2.07	0.54
2:B:118:ILE:HG22	2:B:119:PHE:CD1	2.43	0.54
2:B:165:ARG:O	2:B:412:HIS:HA	2.08	0.54
2:F:36:GLY:HA3	2:F:1359:ARG:O	2.08	0.54
2:F:90:MET:HA	2:F:151:LEU:CD2	2.32	0.54
2:F:467:ARG:HD3	2:F:470:GLU:HA	1.88	0.54
2:F:1314:THR:HA	2:F:1317:ASN:CG	2.27	0.54
2:B:699:ASP:HB3	2:B:702:LEU:HB2	1.90	0.54
2:B:949:LEU:HD12	2:B:950:ILE:H	1.72	0.54
2:B:1251:ASP:O	2:B:1254:GLN:HG2	2.07	0.54
2:F:535:ARG:H	2:F:535:ARG:HD2	1.73	0.54
2:F:677:LYS:NZ	2:F:685:SER:O	2.40	0.54
2:F:1147:ALA:HB2	2:F:1190:VAL:HA	1.90	0.54
2:B:332:LEU:HD21	2:B:336:LYS:HE3	1.88	0.54
2:B:682:PHE:HB3	2:B:696:LEU:HD11	1.90	0.54
2:B:963:VAL:HG21	2:B:990:ASN:OD1	2.07	0.54
1:E:20:A:OP1	2:F:404:THR:N	2.40	0.54
2:F:925:ARG:HB3	2:F:928:THR:HG22	1.88	0.54
2:B:32:PHE:N	2:B:43:ILE:O	2.29	0.54
2:F:70:ARG:HH21	5:J:61:C:P	2.31	0.54
2:F:410:ILE:HG21	2:F:415:HIS:NE2	2.22	0.54
2:F:1075:ASP:OD2	2:F:1078:ARG:NH2	2.40	0.54
2:B:253:LYS:HD3	2:B:261:ASP:HA	1.90	0.54
2:B:621:LEU:O	2:B:625:LEU:HB2	2.08	0.54
2:F:233:LYS:HG2	2:F:235:ASN:HB2	1.89	0.54
2:F:363:ILE:HD12	5:J:44:U:H5'	1.90	0.54
2:B:1263:LYS:HG3	2:B:1302:ILE:CD1	2.38	0.54
2:F:467:ARG:HE	2:F:473:ILE:HD11	1.72	0.54
2:F:536:LYS:HD2	2:F:537:PRO:HD2	1.89	0.54
2:F:573:GLU:OE1	2:F:573:GLU:HA	2.07	0.54
2:F:643:PHE:CD1	2:F:647:VAL:HG11	2.38	0.54
2:B:1110:ILE:CD1	2:B:1122:ARG:HD2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1143:VAL:HG13	2:B:1195:ILE:HG23	1.90	0.54
2:F:963:VAL:HG21	2:F:990:ASN:OD1	2.08	0.54
3:G:23:DC:H2'	3:G:24:DG:O4'	2.06	0.54
2:B:972:PHE:HE1	2:B:1084:ARG:HB2	1.73	0.53
5:J:91:C:O2'	5:J:92:G:P	2.67	0.53
2:F:238:PHE:O	2:F:242:ILE:HG12	2.08	0.53
2:F:688:PHE:CD2	2:F:689:ALA:N	2.76	0.53
2:F:817:GLN:HB3	2:F:820:ARG:O	2.09	0.53
2:F:1343:LEU:O	2:F:1362:LEU:HB2	2.08	0.53
2:B:642:LEU:HB2	2:B:643:PHE:CE2	2.43	0.53
2:F:468:LYS:HE3	2:F:483:ASP:HB3	1.90	0.53
2:F:632:ILE:HG22	2:F:636:LEU:HD13	1.91	0.53
2:F:795:ILE:HG13	2:F:795:ILE:O	2.07	0.53
2:F:896:LYS:O	2:F:900:LEU:HD12	2.09	0.53
5:J:45:U:C2	5:J:46:A:C8	2.96	0.53
2:B:787:GLY:HA3	2:B:891:LEU:HD21	1.89	0.53
2:B:876:VAL:O	2:B:880:LYS:N	2.41	0.53
2:F:253:LYS:HG3	2:F:261:ASP:HA	1.89	0.53
2:B:225:LEU:HD13	2:B:242:ILE:HG21	1.91	0.53
2:B:824:VAL:HG11	2:B:859:ARG:NH1	2.20	0.53
2:B:1314:THR:CG2	2:B:1324:PHE:HB3	2.38	0.53
2:F:644:ASP:HB3	2:F:647:VAL:HG23	1.90	0.53
2:F:949:LEU:HD12	2:F:950:ILE:H	1.73	0.53
2:F:1161:LYS:NZ	2:F:1364:GLN:HG2	2.23	0.53
2:B:751:MET:O	2:B:754:HIS:HB2	2.08	0.53
2:B:951:ARG:CZ	2:B:1011:GLY:HA2	2.38	0.53
2:B:1211:LYS:HB2	2:B:1224:ASN:ND2	2.24	0.53
2:F:424:ARG:O	2:F:427:GLU:HG2	2.09	0.53
2:B:30:LYS:HD3	5:I:83:C:P	2.49	0.53
2:B:839:ASP:O	2:B:856:VAL:N	2.42	0.53
2:B:985:HIS:O	2:B:989:LEU:HG	2.08	0.53
2:F:551:LEU:HG	2:F:552:LEU:HD23	1.91	0.53
2:F:616:LEU:HA	2:F:619:ILE:HG22	1.89	0.53
2:F:829:ASP:OD1	2:F:831:ASN:N	2.42	0.53
5:J:95:G:C6	5:J:96:C:N4	2.77	0.53
2:B:818:ASN:ND2	2:B:818:ASN:O	2.42	0.53
2:F:442:LYS:HA	2:F:445:THR:HG22	1.91	0.53
2:F:1204:PHE:CE1	2:F:1347:LEU:HG	2.44	0.53
2:F:1241:HIS:HE1	2:F:1244:LYS:HA	1.68	0.53
2:B:22:THR:HG22	2:B:23:ASP:H	1.74	0.53
2:B:302:LEU:HA	2:B:305:ILE:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:340:ARG:NH2	5:I:41:A:P	2.82	0.53
2:F:309:ASN:OD1	2:F:312:ILE:HG23	2.09	0.53
2:F:1351:SER:OG	2:F:1356:TYR:HB2	2.09	0.53
2:F:136:TYR:CE2	2:F:160:HIS:NE2	2.77	0.52
2:F:616:LEU:O	2:F:620:VAL:HG23	2.09	0.52
2:F:1066:ASN:OD1	2:F:1069:THR:OG1	2.22	0.52
2:F:1263:LYS:O	2:F:1266:LEU:HD22	2.09	0.52
2:F:1264:HIS:O	2:F:1268:GLU:HG3	2.09	0.52
5:I:57:A:N6	5:J:74:A:H1'	2.24	0.52
2:B:144:ASP:OD1	2:B:313:THR:OG1	2.27	0.52
1:A:20:A:P	2:B:403:ARG:NH1	2.83	0.52
2:B:106:LEU:O	2:B:111:LYS:HE3	2.09	0.52
2:B:527:VAL:HG12	2:B:540:LEU:CD1	2.39	0.52
2:F:189:VAL:HG13	2:F:201:ILE:HG22	1.92	0.52
2:F:363:ILE:HD12	5:J:44:U:C5'	2.40	0.52
2:F:939:MET:HG3	2:F:953:VAL:HG11	1.91	0.52
2:F:1108:GLU:HB2	3:G:9:DT:C5'	2.29	0.52
2:B:677:LYS:HD3	2:B:682:PHE:CZ	2.44	0.52
2:F:735:LYS:HE3	5:J:66:U:OP2	2.09	0.52
2:B:135:ILE:HG21	2:B:160:HIS:NE2	2.25	0.52
2:F:446:PHE:CZ	2:F:478:PHE:HD1	2.24	0.52
2:F:921:LEU:CD2	2:F:1008:PHE:HE2	2.22	0.52
5:I:64:U:C2	5:I:65:A:C8	2.97	0.52
2:B:462:PHE:N	2:B:462:PHE:CD1	2.76	0.52
2:B:864:ARG:NH2	2:B:871:PRO:HD3	2.24	0.52
2:B:939:MET:HG3	2:B:953:VAL:HG11	1.92	0.52
2:B:1312:LEU:O	2:B:1315:LEU:HB3	2.10	0.52
2:B:1357:GLU:O	5:I:81:G:N2	2.43	0.52
1:E:27:G:H5'	1:E:28:A:O5'	2.08	0.52
2:F:360:ALA:O	2:F:364:ASP:N	2.43	0.52
2:F:666:LEU:HD11	2:F:693:PHE:HE1	1.75	0.52
2:F:882:TYR:CD2	2:F:883:TRP:CD1	2.98	0.52
2:F:1090:PRO:HD2	5:J:88:A:C2	2.43	0.52
2:F:1312:LEU:HD21	2:F:1326:TYR:CD1	2.44	0.52
2:B:279:LEU:HD13	2:B:279:LEU:O	2.10	0.52
2:B:1235:PHE:O	2:B:1239:ALA:N	2.28	0.52
4:D:11:DT:H2''	4:D:12:DG:C8	2.45	0.52
2:F:174:LEU:CD2	2:F:413:GLN:HB2	2.40	0.52
2:F:346:LYS:O	2:F:350:ILE:HG13	2.09	0.52
2:F:516:GLU:OE1	2:F:592:GLY:N	2.43	0.52
2:F:982:HIS:HA	2:F:985:HIS:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:35:LEU:HB2	2:F:1358:THR:HB	1.91	0.52
2:F:1304:GLU:O	2:F:1308:ASN:ND2	2.42	0.52
2:B:237:LEU:CA	2:B:255:ASN:HD21	2.23	0.52
2:B:507:VAL:HG12	2:B:508:LEU:O	2.09	0.52
2:B:1315:LEU:HD13	2:B:1324:PHE:HZ	1.75	0.52
2:F:226:ILE:HD12	2:F:232:GLU:HB3	1.90	0.52
2:F:496:THR:HG21	2:F:659:TRP:CZ2	2.45	0.52
2:F:633:GLU:O	2:F:637:LYS:N	2.42	0.52
2:F:1212:ARG:HD2	2:F:1336:TYR:HD2	1.74	0.52
2:B:30:LYS:HD3	5:I:83:C:OP2	2.10	0.51
2:B:945:GLU:N	2:B:945:GLU:OE1	2.42	0.51
2:B:975:VAL:CG1	2:B:1310:ILE:HD11	2.40	0.51
2:B:1000:LYS:HG3	2:B:1001:TYR:CD1	2.44	0.51
1:E:16:A:H5"	2:F:74:ARG:HH12	1.75	0.51
2:F:138:LEU:HD21	2:F:153:LEU:CD2	2.31	0.51
2:F:846:PHE:O	2:F:1040:SER:OG	2.16	0.51
2:F:967:ARG:CZ	2:F:974:LYS:HB2	2.40	0.51
2:B:252:PHE:CE1	2:B:264:LEU:HD13	2.44	0.51
2:B:317:LEU:O	2:B:320:SER:HB3	2.11	0.51
2:B:332:LEU:HD21	2:B:336:LYS:CE	2.40	0.51
2:F:406:ASP:N	2:F:406:ASP:OD1	2.41	0.51
2:F:544:GLN:O	2:F:548:ILE:HG13	2.10	0.51
2:B:548:ILE:HG23	2:B:552:LEU:HD12	1.91	0.51
2:B:763:MET:SD	2:B:928:THR:HG22	2.50	0.51
2:B:828:LEU:HD21	2:B:859:ARG:HG2	1.92	0.51
2:B:1146:VAL:HG13	2:B:1191:LYS:HG3	1.92	0.51
2:F:514:LEU:HD21	2:F:664:ARG:HH21	1.76	0.51
2:F:1114:ARG:NH1	4:H:9:DA:OP1	2.44	0.51
2:B:736:GLY:O	2:B:740:THR:N	2.39	0.51
2:B:823:TYR:HD2	2:B:858:THR:HG21	1.76	0.51
2:B:913:LYS:O	2:B:916:PHE:HB2	2.11	0.51
2:B:1270:ILE:HG13	2:B:1294:TYR:CE2	2.46	0.51
2:F:165:ARG:O	2:F:412:HIS:HA	2.11	0.51
2:F:893:THR:HG23	2:F:896:LYS:H	1.75	0.51
2:F:1269:ILE:O	2:F:1272:GLN:HB2	2.11	0.51
1:E:4:A:C2	1:E:5:C:C4	2.99	0.51
2:F:122:ILE:O	2:F:126:VAL:HG23	2.10	0.51
2:F:730:SER:O	2:F:733:ILE:HG22	2.10	0.51
2:F:1097:LYS:HE2	2:F:1099:GLU:OE2	2.10	0.51
5:J:94:U:H2'	5:J:95:G:C8	2.45	0.51
2:B:66:ARG:CD	2:B:462:PHE:HE2	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:874:GLU:O	2:B:878:LYS:HE3	2.10	0.51
2:B:980:ASN:HB2	2:B:1225:GLU:CD	2.31	0.51
2:B:1263:LYS:O	2:B:1263:LYS:HG2	2.11	0.51
5:I:92:G:H2'	5:I:93:G:H8	1.76	0.51
2:B:620:VAL:HG13	2:B:656:TYR:CD2	2.45	0.51
2:B:1199:PRO:O	2:B:1202:SER:HB2	2.11	0.51
5:I:45:U:H2'	5:I:46:A:O4'	2.11	0.51
2:B:11:ILE:O	2:B:763:MET:HA	2.09	0.51
2:B:554:LYS:HG3	2:B:594:TYR:CE2	2.46	0.51
2:B:943:TYR:CE2	2:B:949:LEU:HA	2.46	0.51
2:B:1226:LEU:HB2	2:B:1276:PHE:CZ	2.46	0.51
2:F:1125:ASP:OD2	2:F:1125:ASP:N	2.44	0.51
2:F:1127:ASP:OD1	2:F:1129:LYS:N	2.43	0.51
2:F:1218:GLY:HA2	2:F:1339:THR:HG23	1.93	0.51
2:B:181:VAL:CG2	2:B:209:LYS:HA	2.41	0.51
2:B:967:ARG:NE	2:B:974:LYS:HB2	2.23	0.51
2:F:140:LYS:HB3	2:F:322:ILE:CD1	2.41	0.51
2:F:140:LYS:HZ3	2:F:313:THR:HB	1.71	0.51
2:F:233:LYS:HG2	2:F:236:GLY:N	2.26	0.51
2:F:1000:LYS:HB2	2:F:1073:VAL:HG21	1.93	0.51
5:J:91:C:O2'	5:J:92:G:O5'	2.25	0.51
5:J:91:C:HO2'	5:J:92:G:P	2.34	0.51
2:B:201:ILE:HG22	2:B:202:ASN:H	1.76	0.50
2:B:879:MET:HG2	2:B:882:TYR:HB2	1.92	0.50
2:B:1270:ILE:HG13	2:B:1294:TYR:CD2	2.46	0.50
2:B:1326:TYR:HD2	2:B:1327:PHE:N	2.07	0.50
2:F:688:PHE:HD2	2:F:689:ALA:N	2.08	0.50
2:B:334:LEU:O	2:B:338:LEU:HG	2.11	0.50
2:B:973:TYR:CD1	2:B:1237:TYR:CD1	2.99	0.50
2:B:1349:HIS:ND1	5:I:69:A:H4'	2.26	0.50
1:E:25:U:O5'	1:E:25:U:H6	1.93	0.50
2:F:40:ARG:NE	2:F:43:ILE:HD11	2.26	0.50
2:F:412:HIS:CD2	2:F:413:GLN:NE2	2.80	0.50
2:F:597:LEU:O	2:F:601:ILE:HG12	2.11	0.50
2:F:936:ASP:CB	2:F:1010:TYR:HD2	2.24	0.50
2:B:136:TYR:HE2	2:B:403:ARG:HD3	1.75	0.50
2:B:1111:LEU:HD12	2:B:1135:ASP:HB2	1.93	0.50
1:E:19:A:O3'	2:F:407:ASN:HB2	2.11	0.50
2:F:138:LEU:HD11	2:F:153:LEU:HD21	1.92	0.50
2:F:165:ARG:O	2:F:415:HIS:HD2	1.93	0.50
2:F:921:LEU:CD1	2:F:1042:ILE:HD13	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:939:MET:CE	2:F:953:VAL:HG21	2.41	0.50
2:B:358:GLY:O	2:B:362:TYR:N	2.40	0.50
2:B:386:THR:OG1	2:B:387:GLU:OE1	2.21	0.50
2:B:737:ILE:O	2:B:740:THR:HG22	2.11	0.50
2:B:866:LYS:HB3	2:B:869:ASN:CB	2.41	0.50
3:C:20:DA:C8	3:C:21:DT:H72	2.46	0.50
2:F:561:VAL:O	2:F:565:LYS:HG3	2.12	0.50
2:B:499:ASP:OD2	2:B:663:SER:HB3	2.12	0.50
5:I:71:U:O2'	5:I:72:U:H5'	2.12	0.50
2:F:622:THR:HG23	2:F:626:PHE:CD1	2.47	0.50
1:A:24:U:O2	1:A:25:U:C2	2.65	0.50
2:B:902:LYS:HE3	2:B:908:LEU:HA	1.93	0.50
2:B:1258:PHE:CE1	2:B:1262:HIS:HD2	2.17	0.50
2:F:69:ARG:NH2	5:J:63:U:OP2	2.45	0.50
2:F:140:LYS:HB3	2:F:322:ILE:HD11	1.94	0.50
2:F:390:LEU:O	2:F:394:ASN:ND2	2.45	0.50
2:F:882:TYR:HD2	2:F:883:TRP:CD1	2.29	0.50
2:F:1283:ALA:HB1	2:F:1286:ASN:HB2	1.93	0.50
2:B:317:LEU:CD1	2:B:410:ILE:CD1	2.90	0.50
2:B:927:ILE:HG23	2:B:928:THR:N	2.26	0.50
2:F:1082:THR:O	2:F:1086:VAL:HG23	2.12	0.50
2:B:1145:VAL:HG11	2:B:1187:TYR:CD2	2.46	0.50
2:B:1314:THR:HG21	2:B:1324:PHE:HB3	1.93	0.50
2:F:570:LYS:HA	2:F:575:PHE:O	2.11	0.50
2:F:583:VAL:HG22	2:F:584:GLU:N	2.27	0.50
2:F:999:LYS:HB3	2:F:1073:VAL:HG12	1.94	0.50
5:J:95:G:H2'	5:J:96:C:H6	1.75	0.50
2:B:36:GLY:HA3	2:B:1359:ARG:O	2.11	0.49
2:B:954:LYS:HG3	2:B:1009:VAL:HG11	1.94	0.49
2:B:989:LEU:HD21	2:B:1087:LEU:HD21	1.94	0.49
2:B:1296:LYS:HD3	2:B:1296:LYS:N	2.26	0.49
2:F:936:ASP:CG	2:F:1010:TYR:HD2	2.15	0.49
5:I:85:C:H2'	5:I:86:C:C6	2.47	0.49
2:F:1216:SER:OG	2:F:1217:ALA:N	2.45	0.49
2:B:5:TYR:CE2	2:B:756:PRO:HB3	2.47	0.49
2:B:108:GLU:HG3	2:B:115:ARG:HG2	1.93	0.49
2:B:340:ARG:HA	2:B:344:PRO:HB3	1.94	0.49
2:B:410:ILE:HG23	2:B:414:ILE:HD13	1.86	0.49
2:B:467:ARG:HD3	2:B:470:GLU:HA	1.95	0.49
2:B:913:LYS:HA	2:B:916:PHE:HD2	1.77	0.49
2:B:1041:ASN:ND2	2:B:1044:ASN:OD1	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1110:ILE:CD1	2:B:1122:ARG:NH1	2.75	0.49
2:B:548:ILE:HG23	2:B:552:LEU:HD13	1.94	0.49
2:B:882:TYR:O	2:B:886:LEU:HG	2.12	0.49
2:B:951:ARG:NH2	2:B:1011:GLY:HA2	2.27	0.49
2:F:1105:PHE:CD1	2:F:1169:MET:HG3	2.47	0.49
3:G:2:DA:H2''	3:G:3:DA:OP1	2.10	0.49
2:B:1308:ASN:HD22	2:B:1327:PHE:CA	2.24	0.49
2:F:402:GLN:OE1	5:J:44:U:O2'	2.26	0.49
5:I:56:U:O2'	5:I:57:A:H5''	2.13	0.49
2:B:95:ASP:OD1	2:B:95:ASP:N	2.45	0.49
2:B:167:HIS:CE1	2:B:411:PRO:HA	2.47	0.49
2:B:369:GLN:OE1	2:B:400:ARG:NH1	2.46	0.49
2:B:704:PHE:O	2:B:708:ILE:HG12	2.13	0.49
2:B:988:TYR:HE2	2:B:1083:VAL:HG13	1.77	0.49
2:B:1094:ILE:HG21	2:B:1225:GLU:OE2	2.12	0.49
2:F:554:LYS:HB3	2:F:594:TYR:CE2	2.47	0.49
2:F:621:LEU:HD23	2:F:622:THR:H	1.76	0.49
2:F:737:ILE:O	2:F:741:VAL:HG23	2.13	0.49
2:B:448:ILE:HD13	2:B:455:LEU:CD1	2.41	0.49
4:D:5:DA:H1'	4:D:6:DG:C8	2.47	0.49
2:F:167:HIS:CD2	2:F:169:LEU:HB2	2.47	0.49
2:F:1147:ALA:HB2	2:F:1190:VAL:HG22	1.95	0.49
5:J:49:A:H2'	5:J:50:U:O4'	2.13	0.49
2:B:270:THR:O	2:B:270:THR:OG1	2.31	0.49
1:E:25:U:O2'	2:F:111:LYS:NZ	2.45	0.49
2:F:143:VAL:HG22	2:F:422:ILE:HD13	1.95	0.49
2:F:691:ARG:HG2	2:F:695:GLN:NE2	2.27	0.49
2:F:746:GLU:OE2	2:F:1353:THR:OG1	2.24	0.49
2:B:956:ILE:HG12	2:B:1009:VAL:HG22	1.94	0.49
2:B:1005:GLU:O	2:B:1009:VAL:HB	2.12	0.49
2:B:1147:ALA:HB2	2:B:1190:VAL:CA	2.39	0.49
2:B:1308:ASN:ND2	2:B:1327:PHE:CA	2.75	0.49
2:B:1326:TYR:CD2	2:B:1327:PHE:N	2.73	0.49
2:F:491:PHE:O	2:F:494:ARG:HG2	2.13	0.49
2:F:902:LYS:NZ	2:F:912:ASP:OD1	2.46	0.49
2:F:1333:ARG:CZ	2:F:1335:ARG:HD2	2.43	0.49
2:B:369:GLN:HE22	2:B:400:ARG:NH1	2.10	0.49
2:B:909:SER:H	2:B:912:ASP:CB	2.26	0.49
2:B:1236:LEU:HD11	2:B:1269:ILE:HD13	1.95	0.49
2:F:90:MET:SD	2:F:151:LEU:CD2	3.01	0.49
2:F:140:LYS:NZ	2:F:144:ASP:OD2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:258:LEU:CD2	2:F:260:GLU:H	2.25	0.49
2:B:1041:ASN:O	2:B:1044:ASN:ND2	2.46	0.48
2:F:114:GLU:HG2	2:F:120:GLY:HA2	1.95	0.48
2:F:135:ILE:HG21	5:J:46:A:H5'	1.94	0.48
2:F:915:GLY:O	2:F:919:ARG:HB2	2.13	0.48
2:B:814:TYR:HD1	2:B:815:TYR:HD1	1.60	0.48
2:F:32:PHE:HD1	2:F:45:LYS:HD3	1.77	0.48
2:F:596:ASP:CG	2:F:654:ARG:HH21	2.16	0.48
2:F:816:LEU:HD22	2:F:891:LEU:O	2.14	0.48
2:F:1126:TRP:HB3	2:F:1131:TYR:CD2	2.48	0.48
2:B:309:ASN:OD1	2:B:311:GLU:HB2	2.13	0.48
2:B:925:ARG:HG2	2:B:927:ILE:HG22	1.96	0.48
2:B:1110:ILE:HD11	2:B:1122:ARG:NH1	2.28	0.48
2:B:1256:GLN:NE2	2:B:1256:GLN:O	2.46	0.48
2:B:1277:SER:HA	2:B:1281:ILE:CG1	2.35	0.48
2:F:143:VAL:HG23	2:F:422:ILE:CD1	2.37	0.48
2:F:601:ILE:HD11	2:F:607:LEU:HD11	1.95	0.48
2:F:867:SER:HB2	2:F:1053:ALA:C	2.32	0.48
2:B:1211:LYS:HB2	2:B:1224:ASN:HD21	1.77	0.48
2:F:870:VAL:HG12	2:F:871:PRO:HD2	1.95	0.48
5:J:82:G:N7	5:J:97:U:O2	2.46	0.48
5:J:96:C:H2'	5:J:97:U:O4'	2.14	0.48
2:B:237:LEU:HA	2:B:255:ASN:ND2	2.27	0.48
2:B:381:GLU:O	2:B:382:LYS:HD3	2.14	0.48
2:B:427:GLU:OE1	2:B:437:ARG:NH1	2.46	0.48
2:B:925:ARG:HB3	2:B:928:THR:CG2	2.43	0.48
4:D:6:DG:H2''	4:D:7:DG:H5''	1.95	0.48
2:F:58:THR:HG22	2:F:731:PRO:CG	2.43	0.48
2:F:836:TYR:CB	2:F:857:LEU:HD11	2.44	0.48
2:F:1056:GLU:O	2:F:1057:ILE:HD12	2.14	0.48
5:J:76:A:C5	5:J:77:A:H1'	2.49	0.48
2:B:565:LYS:HA	2:B:569:PHE:HB2	1.95	0.48
2:F:738:LEU:HA	2:F:738:LEU:HD23	1.54	0.48
2:F:1224:ASN:HB2	2:F:1280:VAL:HG11	1.94	0.48
2:B:640:ALA:HA	2:B:648:MET:HE3	1.96	0.48
2:B:934:ILE:O	2:B:938:ARG:HG3	2.14	0.48
2:F:108:GLU:CD	2:F:115:ARG:HD3	2.34	0.48
2:F:163:LYS:HG2	2:F:164:PHE:CD1	2.49	0.48
2:F:671:ARG:HG2	2:F:676:GLY:O	2.14	0.48
2:F:853:ASP:HB3	2:F:895:ARG:HH11	1.78	0.48
2:B:18:TRP:HZ2	2:B:1353:THR:O	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:527:VAL:HG12	2:B:540:LEU:HD11	1.95	0.48
2:B:625:LEU:CD1	2:B:659:TRP:HZ2	2.27	0.48
2:B:1105:PHE:CD2	2:B:1169:MET:HG3	2.48	0.48
2:F:594:TYR:O	2:F:598:LEU:HB2	2.14	0.48
2:F:848:LYS:HE2	2:F:965:ASP:HB3	1.96	0.48
2:B:276:ASP:HA	2:B:279:LEU:HB3	1.95	0.48
2:B:1111:LEU:HD23	2:B:1111:LEU:HA	1.50	0.48
2:B:1240:SER:HB2	2:B:1242:TYR:CD1	2.48	0.48
2:F:163:LYS:HG2	2:F:164:PHE:HE1	1.75	0.48
2:F:1287:LEU:HD12	2:F:1287:LEU:O	2.13	0.48
2:B:289:LEU:C	2:B:289:LEU:HD23	2.34	0.48
2:B:325:TYR:CD1	5:I:44:U:C2	3.02	0.48
2:B:362:TYR:OH	2:B:401:LYS:HG3	2.14	0.48
2:F:583:VAL:HG22	2:F:584:GLU:H	1.79	0.48
2:F:1251:ASP:O	2:F:1255:LYS:HG2	2.13	0.48
5:I:47:A:C6	5:I:48:A:C6	3.02	0.48
2:B:42:SER:O	2:B:43:ILE:HG13	2.13	0.47
2:B:167:HIS:HB2	2:B:169:LEU:HG	1.96	0.47
2:B:273:ASP:OD1	2:B:273:ASP:N	2.35	0.47
2:B:485:GLY:HA3	2:B:631:MET:SD	2.54	0.47
2:B:570:LYS:O	2:B:574:CYS:HA	2.13	0.47
2:F:640:ALA:HA	2:F:648:MET:CE	2.44	0.47
2:F:921:LEU:HD21	2:F:1008:PHE:CE2	2.48	0.47
2:F:1207:GLU:HG3	2:F:1208:ASN:N	2.29	0.47
2:B:40:ARG:HH21	2:B:43:ILE:HG12	1.79	0.47
2:B:63:ARG:O	2:B:66:ARG:HB3	2.14	0.47
2:B:119:PHE:CD1	2:B:152:ARG:NH1	2.82	0.47
2:F:1111:LEU:N	2:F:1133:GLY:O	2.40	0.47
1:A:31:U:C2	1:A:32:A:C8	3.02	0.47
2:B:270:THR:O	2:B:274:ASP:HB2	2.14	0.47
2:B:958:LEU:HD22	2:B:962:LEU:HD12	1.97	0.47
2:B:973:TYR:CE1	2:B:1238:LEU:HD21	2.49	0.47
2:F:246:LEU:CD2	2:F:248:LEU:HD12	2.44	0.47
2:F:325:TYR:O	2:F:328:HIS:HB3	2.13	0.47
2:B:325:TYR:HD1	5:I:44:U:C2	2.32	0.47
4:D:3:DT:H1'	4:D:4:DT:H5'	1.97	0.47
2:F:253:LYS:HA	2:F:256:PHE:CD2	2.49	0.47
2:F:279:LEU:CD2	2:F:287:ALA:HB2	2.43	0.47
2:F:531:THR:HG22	2:F:534:MET:HG2	1.97	0.47
2:F:821:ASP:OD1	2:F:858:THR:OG1	2.30	0.47
5:I:92:G:H2'	5:I:93:G:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:A:H4'	2:B:448:ILE:O	2.14	0.47
2:B:1158:LYS:HB2	2:B:1158:LYS:HE3	1.47	0.47
2:B:1204:PHE:CG	2:B:1342:VAL:HG13	2.49	0.47
2:F:143:VAL:HG21	2:F:315:ALA:CB	2.43	0.47
2:F:527:VAL:HA	2:F:582:GLY:CA	2.35	0.47
2:F:730:SER:HB2	2:F:733:ILE:H	1.80	0.47
2:F:1101:GLN:O	2:F:1168:ILE:HD11	2.15	0.47
2:F:1312:LEU:O	2:F:1314:THR:N	2.47	0.47
1:A:11:U:C2	1:A:12:A:C8	3.02	0.47
2:B:212:LEU:O	2:B:221:ARG:HD2	2.14	0.47
2:B:338:LEU:O	2:B:383:MET:CE	2.62	0.47
2:B:1041:ASN:HD22	2:B:1044:ASN:CG	2.16	0.47
2:F:32:PHE:CZ	2:F:1355:LEU:HB3	2.50	0.47
2:F:97:PHE:CE2	2:F:152:ARG:HA	2.50	0.47
2:F:499:ASP:CB	2:F:663:SER:HB3	2.43	0.47
2:F:1150:GLU:HB3	2:F:1155:LYS:HA	1.97	0.47
4:H:11:DT:H2''	4:H:12:DG:H8	1.78	0.47
2:B:197:GLU:N	2:B:197:GLU:OE1	2.47	0.47
2:B:242:ILE:O	2:B:246:LEU:HG	2.14	0.47
2:B:252:PHE:CE1	2:B:290:PHE:CE2	3.02	0.47
2:B:451:TYR:HE1	2:B:484:LYS:HG2	1.80	0.47
2:B:466:THR:OG1	2:B:483:ASP:HB3	2.14	0.47
2:B:870:VAL:HG21	2:B:908:LEU:H	1.80	0.47
2:B:1000:LYS:HZ3	2:B:1067:GLY:H	1.63	0.47
2:B:1213:MET:CE	2:B:1318:LEU:HD21	2.44	0.47
2:B:1295:ASN:HA	2:B:1298:ARG:HH11	1.80	0.47
1:E:27:G:H5'	1:E:28:A:C5'	2.45	0.47
2:F:150:ASP:O	2:F:154:ILE:HD12	2.15	0.47
2:F:351:PHE:CD1	5:J:43:G:O6	2.68	0.47
2:F:404:THR:HG22	2:F:405:PHE:H	1.79	0.47
2:F:622:THR:HG21	2:F:635:ARG:CB	2.44	0.47
2:F:737:ILE:HA	2:F:740:THR:HG22	1.97	0.47
2:F:921:LEU:CD2	2:F:1042:ILE:HD11	2.44	0.47
2:F:1216:SER:HB3	2:F:1219:GLU:H	1.78	0.47
2:F:1345:ALA:O	2:F:1362:LEU:HD12	2.14	0.47
5:J:43:G:H3'	5:J:44:U:H6	1.80	0.47
1:A:31:U:N3	1:A:32:A:N7	2.62	0.47
2:B:530:VAL:CG2	2:B:537:PRO:HB3	2.45	0.47
2:B:625:LEU:HD12	2:B:625:LEU:HA	1.60	0.47
2:B:840:ALA:HA	2:B:854:ASN:O	2.14	0.47
2:B:1226:LEU:HD13	2:B:1276:PHE:CG	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:908:LEU:HA	2:F:908:LEU:HD23	1.61	0.47
2:B:869:ASN:OD1	2:B:870:VAL:N	2.48	0.47
1:E:15:G:P	2:F:66:ARG:HH12	2.38	0.47
2:F:135:ILE:CG2	5:J:46:A:H5'	2.45	0.47
2:F:509:PRO:HB3	2:F:624:THR:HG21	1.97	0.47
2:F:526:LYS:HD3	2:F:526:LYS:HA	1.38	0.47
2:F:1222:LYS:NZ	2:F:1314:THR:O	2.48	0.47
1:A:26:A:C6	5:I:46:A:C2	3.04	0.47
2:B:22:THR:HG22	2:B:23:ASP:N	2.30	0.47
2:B:133:PRO:HD2	2:B:137:HIS:CG	2.50	0.47
2:B:334:LEU:HD12	2:B:338:LEU:HG	1.96	0.47
2:B:380:LEU:O	2:B:386:THR:CB	2.54	0.47
2:B:1000:LYS:NZ	2:B:1067:GLY:H	2.13	0.47
2:B:1241:HIS:HE1	2:B:1244:LYS:HA	1.76	0.47
2:B:1256:GLN:HE22	2:B:1260:GLU:HG2	1.79	0.47
1:E:4:A:N1	3:G:25:DT:O4	2.48	0.47
1:E:19:A:H4'	2:F:407:ASN:C	2.35	0.47
2:F:58:THR:HG22	2:F:731:PRO:HG3	1.96	0.47
2:F:413:GLN:CD	2:F:413:GLN:H	2.18	0.47
2:F:422:ILE:O	2:F:425:ARG:HG2	2.16	0.47
2:F:780:ARG:HD2	2:F:812:TYR:HE2	1.77	0.47
2:F:1001:TYR:CE2	2:F:1045:PHE:CD1	2.99	0.47
2:F:1001:TYR:HB3	2:F:1004:LEU:HD12	1.97	0.47
2:F:1294:TYR:HE1	2:F:1305:GLN:HE21	1.61	0.47
1:A:19:A:H61	3:C:10:DT:H3	1.63	0.46
2:B:114:GLU:CG	2:B:120:GLY:O	2.63	0.46
2:B:472:THR:HG23	5:I:59:U:OP2	2.15	0.46
2:B:864:ARG:HB2	2:B:871:PRO:HA	1.97	0.46
2:B:51:LEU:HA	2:B:1095:VAL:HG23	1.97	0.46
2:B:909:SER:O	2:B:913:LYS:N	2.29	0.46
2:B:1241:HIS:ND1	2:B:1244:LYS:HA	2.30	0.46
2:F:253:LYS:HE3	2:F:261:ASP:HB3	1.97	0.46
2:F:531:THR:HB	2:F:578:VAL:HG23	1.98	0.46
2:B:32:PHE:CE1	2:B:1355:LEU:HD22	2.51	0.46
2:B:398:LEU:HG	2:B:399:LEU:HG	1.97	0.46
2:B:558:LYS:HE2	2:B:587:PHE:O	2.15	0.46
2:B:694:MET:HG3	2:B:698:HIS:CD2	2.50	0.46
2:B:739:GLN:NE2	5:I:67:C:OP1	2.49	0.46
2:F:40:ARG:CD	2:F:43:ILE:HD11	2.45	0.46
2:F:628:ASP:O	2:F:632:ILE:HG13	2.16	0.46
2:F:719:SER:HB3	2:F:722:GLU:OE2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1089:MET:HA	2:F:1090:PRO:HD3	1.76	0.46
2:F:1198:LEU:HA	2:F:1198:LEU:HD23	1.63	0.46
2:F:1258:PHE:O	2:F:1258:PHE:HD1	1.98	0.46
2:B:139:ARG:NH2	2:B:161:MET:HG2	2.30	0.46
2:B:217:SER:O	2:B:221:ARG:HG3	2.15	0.46
2:B:478:PHE:CZ	2:B:482:VAL:HG11	2.49	0.46
2:B:1204:PHE:HE1	2:B:1347:LEU:HB2	1.81	0.46
2:B:1226:LEU:HB2	2:B:1276:PHE:CD2	2.49	0.46
2:F:8:GLY:O	2:F:987:ALA:HB1	2.15	0.46
2:F:623:LEU:HD12	2:F:623:LEU:O	2.14	0.46
2:F:791:LEU:HD12	2:F:791:LEU:HA	1.71	0.46
2:F:1100:VAL:N	5:J:67:C:H42	2.13	0.46
2:F:1351:SER:OG	2:F:1356:TYR:O	2.24	0.46
2:B:395:ARG:O	2:B:396:GLU:HB2	2.16	0.46
2:B:866:LYS:HE2	2:B:866:LYS:HB2	1.56	0.46
2:B:1135:ASP:OD1	2:B:1136:SER:N	2.48	0.46
2:B:1260:GLU:HA	2:B:1260:GLU:OE2	2.16	0.46
1:E:18:A:OP2	2:F:71:ARG:HD2	2.16	0.46
2:F:237:LEU:HD12	2:F:238:PHE:N	2.30	0.46
2:F:324:ARG:O	2:F:327:GLU:HB2	2.15	0.46
2:F:632:ILE:O	2:F:636:LEU:HD13	2.15	0.46
2:F:653:ARG:H	2:F:653:ARG:HG2	1.48	0.46
2:F:967:ARG:NH2	2:F:974:LYS:HB2	2.31	0.46
2:B:127:ALA:O	2:B:130:GLU:HB2	2.16	0.46
2:B:269:ASP:OD1	2:B:270:THR:N	2.49	0.46
2:B:623:LEU:HG	2:B:654:ARG:O	2.15	0.46
2:B:646:LYS:HA	2:B:649:LYS:HG3	1.96	0.46
2:B:1204:PHE:CE2	2:B:1342:VAL:HG11	2.50	0.46
2:B:1206:LEU:HG	2:B:1207:GLU:HG2	1.97	0.46
3:C:19:DA:H2''	3:C:20:DA:O4'	2.15	0.46
1:E:23:U:C5'	2:F:1112:PRO:HG3	2.32	0.46
2:F:1019:ARG:O	2:F:1021:MET:N	2.48	0.46
2:F:1203:LEU:HD23	2:F:1348:ILE:HB	1.98	0.46
2:B:27:VAL:HG21	2:B:48:ILE:HB	1.96	0.46
2:B:74:ARG:HH21	5:I:60:C:P	2.38	0.46
2:B:336:LYS:HG2	2:B:347:TYR:HE2	1.81	0.46
2:B:410:ILE:HG21	2:B:414:ILE:HD11	1.89	0.46
2:B:838:VAL:HG11	2:B:855:LYS:HE3	1.96	0.46
2:B:978:ILE:CD1	2:B:1233:VAL:HG22	2.38	0.46
2:F:174:LEU:HD23	2:F:413:GLN:CB	2.46	0.46
2:F:465:MET:SD	2:F:482:VAL:HG11	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:733:ILE:HD11	2:F:763:MET:CE	2.41	0.46
2:F:1042:ILE:O	2:F:1045:PHE:CE1	2.68	0.46
2:F:1272:GLN:NE2	5:J:89:G:H1	2.14	0.46
2:B:111:LYS:HD3	2:B:115:ARG:HA	1.98	0.46
2:B:161:MET:HE1	2:B:422:ILE:HD12	1.97	0.46
2:B:808:ASN:HD22	2:B:1244:LYS:HE3	1.81	0.46
3:C:12:DA:OP1	3:C:12:DA:H4'	2.16	0.46
2:F:272:ASP:HA	2:F:275:LEU:CB	2.44	0.46
2:F:380:LEU:CD1	2:F:390:LEU:HG	2.38	0.46
2:F:755:LYS:HD3	2:F:939:MET:HE3	1.97	0.46
2:F:918:LYS:HD3	2:F:918:LYS:HA	1.74	0.46
2:F:967:ARG:HH12	2:F:974:LYS:HE3	1.80	0.46
2:B:83:GLN:O	2:B:87:SER:N	2.49	0.46
2:B:282:ILE:HG22	2:B:286:TYR:CE1	2.50	0.46
2:B:340:ARG:NH2	5:I:41:A:OP2	2.48	0.46
2:B:880:LYS:HE2	2:B:904:GLU:OE2	2.16	0.46
2:B:954:LYS:HB2	2:B:954:LYS:HE3	1.53	0.46
2:B:1202:SER:O	2:B:1213:MET:HA	2.16	0.46
2:F:212:LEU:HD13	2:F:300:ILE:HD11	1.98	0.46
2:F:352:PHE:CE1	5:J:42:A:N6	2.84	0.46
2:F:601:ILE:CD1	2:F:607:LEU:HD21	2.46	0.46
2:F:813:LEU:HB3	2:F:857:LEU:HB3	1.96	0.46
2:F:892:ILE:HB	2:F:896:LYS:NZ	2.30	0.46
2:F:1120:ILE:CD1	2:F:1134:PHE:HB2	2.45	0.46
2:F:1212:ARG:CZ	2:F:1336:TYR:HE2	2.29	0.46
2:B:142:LEU:HD12	2:B:157:ALA:HB2	1.98	0.46
2:B:279:LEU:HD21	2:B:287:ALA:HB2	1.96	0.46
2:B:281:GLN:OE1	2:B:281:GLN:N	2.31	0.46
2:B:455:LEU:HD12	2:B:455:LEU:N	2.31	0.46
2:B:1062:LEU:O	2:B:1075:ASP:HA	2.15	0.46
2:B:1211:LYS:CB	2:B:1224:ASN:HD21	2.28	0.46
2:B:1245:LEU:CB	2:B:1252:ASN:ND2	2.71	0.46
2:F:74:ARG:NE	5:J:60:C:OP2	2.39	0.46
2:F:93:VAL:CG2	2:F:151:LEU:HD22	2.46	0.46
2:F:134:THR:O	2:F:137:HIS:HB2	2.16	0.46
2:F:1084:ARG:CZ	2:F:1084:ARG:CB	2.94	0.46
2:F:1167:THR:OG1	2:F:1168:ILE:N	2.49	0.46
2:B:203:ALA:O	2:B:206:VAL:HG22	2.17	0.45
2:F:97:PHE:CE1	2:F:101:LEU:HD11	2.51	0.45
2:F:161:MET:HE1	2:F:419:LEU:HD12	1.97	0.45
2:F:246:LEU:HD22	2:F:248:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:253:LYS:HB2	2:F:262:ALA:N	2.27	0.45
2:F:554:LYS:HD3	2:F:594:TYR:CZ	2.52	0.45
2:F:632:ILE:HG22	2:F:636:LEU:CD1	2.46	0.45
2:F:682:PHE:O	2:F:686:ASP:OD2	2.34	0.45
2:F:886:LEU:HD22	2:F:891:LEU:HD11	1.97	0.45
4:H:12:DG:H2'	4:H:12:DG:OP2	2.15	0.45
2:B:114:GLU:HG3	2:B:116:HIS:N	2.27	0.45
2:B:1313:PHE:O	2:B:1317:ASN:N	2.48	0.45
2:B:1333:ARG:NH2	2:B:1335:ARG:HH11	2.14	0.45
2:F:527:VAL:HG22	2:F:582:GLY:HA3	1.98	0.45
2:F:1044:ASN:O	2:F:1047:LYS:N	2.43	0.45
2:F:1111:LEU:HD23	2:F:1111:LEU:HA	1.63	0.45
2:F:1236:LEU:HD11	2:F:1269:ILE:HD13	1.98	0.45
5:J:91:C:H6	5:J:91:C:H2'	1.34	0.45
2:B:743:VAL:O	2:B:747:LEU:HD23	2.16	0.45
2:B:820:ARG:HA	2:B:826:GLN:O	2.15	0.45
2:B:839:ASP:N	2:B:856:VAL:O	2.28	0.45
2:F:148:LYS:HA	2:F:429:PHE:CD2	2.51	0.45
2:F:737:ILE:O	2:F:740:THR:HG22	2.16	0.45
2:F:933:GLN:CG	2:F:1010:TYR:OH	2.57	0.45
2:F:1300:LYS:NZ	2:F:1304:GLU:OE1	2.49	0.45
2:B:265:GLN:HG2	2:B:267:SER:H	1.81	0.45
2:B:359:TYR:CE2	2:B:363:ILE:HG13	2.52	0.45
2:B:1145:VAL:HG11	2:B:1187:TYR:CE2	2.51	0.45
2:F:600:ILE:HG23	2:F:650:GLN:HB2	1.99	0.45
2:B:24:GLU:OE1	2:B:24:GLU:HA	2.16	0.45
2:B:137:HIS:HE1	2:B:325:TYR:CD2	2.33	0.45
2:F:377:LYS:N	2:F:378:PRO:HD2	2.32	0.45
2:F:495:MET:O	3:G:17:DT:H2'	2.17	0.45
2:F:760:VAL:HG13	2:F:956:ILE:HB	1.98	0.45
5:J:46:A:C2	5:J:47:A:C5	3.05	0.45
2:B:642:LEU:HB2	2:B:643:PHE:CD2	2.51	0.45
2:B:930:HIS:O	2:B:934:ILE:HG13	2.16	0.45
2:B:1163:LEU:HD23	2:B:1163:LEU:HA	1.69	0.45
2:F:43:ILE:HD12	2:F:43:ILE:HG23	1.64	0.45
2:F:211:ILE:HG13	2:F:224:ASN:HB3	1.97	0.45
3:G:24:DG:C3'	3:G:25:DT:H4'	2.47	0.45
2:B:128:TYR:CD1	2:B:132:TYR:HD2	2.35	0.45
2:B:178:ASN:HD22	2:B:298:ASP:HB2	1.82	0.45
2:B:390:LEU:HD23	2:B:393:LEU:HB3	1.98	0.45
2:F:118:ILE:HD13	2:F:125:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:332:LEU:HD13	2:F:359:TYR:CE1	2.52	0.45
2:F:844:GLN:OE1	2:F:848:LYS:HD2	2.16	0.45
2:B:513:LEU:HD23	2:B:513:LEU:HA	1.77	0.45
2:B:518:PHE:CD2	2:B:518:PHE:C	2.90	0.45
2:B:794:GLN:HG2	2:B:798:GLU:HG3	1.99	0.45
2:B:1280:VAL:HG12	2:B:1281:ILE:HD13	1.98	0.45
2:F:401:LYS:HB3	5:J:45:U:OP1	2.17	0.45
2:F:684:LYS:HB2	2:F:684:LYS:HE3	1.32	0.45
2:F:971:GLN:HG2	2:F:973:TYR:HE2	1.82	0.45
2:F:1105:PHE:CG	2:F:1169:MET:HG3	2.51	0.45
2:F:1126:TRP:N	2:F:1126:TRP:CD1	2.85	0.45
5:I:48:A:H2'	5:I:49:A:C8	2.51	0.45
2:B:32:PHE:CZ	2:B:1355:LEU:HD13	2.52	0.45
2:B:233:LYS:O	2:B:236:GLY:N	2.47	0.45
2:B:357:ASN:O	2:B:375:PHE:CD2	2.70	0.45
2:B:509:PRO:HG3	2:B:621:LEU:HD12	1.99	0.45
2:B:760:VAL:HG11	2:B:958:LEU:HD12	1.98	0.45
2:F:119:PHE:HE1	2:F:150:ASP:OD2	2.00	0.45
2:F:128:TYR:CD1	2:F:132:TYR:HD2	2.34	0.45
2:F:821:ASP:OD1	2:F:822:MET:N	2.50	0.45
2:F:842:VAL:CG1	2:F:854:ASN:HD21	2.29	0.45
2:F:911:LEU:H	2:F:911:LEU:HD12	1.82	0.45
2:F:939:MET:HE2	2:F:953:VAL:HG21	1.98	0.45
2:F:949:LEU:HD23	2:F:951:ARG:NH2	2.31	0.45
2:F:1135:ASP:OD1	4:H:8:DT:H5''	2.17	0.45
2:F:1347:LEU:HD22	2:F:1349:HIS:CD2	2.51	0.45
3:G:19:DA:C2'	3:G:20:DA:C8	2.99	0.45
1:A:15:G:OP1	2:B:70:ARG:NH1	2.44	0.45
1:A:29:G:N3	5:I:41:A:C2	2.84	0.45
2:B:1274:SER:O	2:B:1278:LYS:HG3	2.17	0.45
2:F:306:LEU:HD21	2:F:414:ILE:HD12	1.98	0.45
2:B:215:ARG:NE	2:B:215:ARG:O	2.50	0.44
2:B:597:LEU:O	2:B:601:ILE:HG12	2.17	0.44
2:B:651:LEU:HA	2:B:651:LEU:HD23	1.73	0.44
2:B:724:ILE:O	2:B:727:LEU:HB2	2.17	0.44
2:B:970:PHE:CE2	2:B:1047:LYS:HD3	2.51	0.44
2:F:390:LEU:HD23	2:F:390:LEU:HA	1.83	0.44
2:F:592:GLY:O	2:F:596:ASP:OD1	2.35	0.44
2:B:229:LEU:O	2:B:231:GLY:N	2.51	0.44
2:B:1315:LEU:HD13	2:B:1324:PHE:CZ	2.51	0.44
2:F:139:ARG:NH1	2:F:418:GLU:CD	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:693:PHE:HA	2:F:696:LEU:HD12	1.98	0.44
2:F:742:LYS:HE2	2:F:742:LYS:HB3	1.63	0.44
2:B:721:HIS:O	2:B:725:ALA:N	2.32	0.44
2:F:138:LEU:CD2	2:F:153:LEU:HD21	2.34	0.44
2:F:917:ILE:HA	2:F:917:ILE:HD13	1.70	0.44
2:B:377:LYS:N	2:B:378:PRO:HD2	2.33	0.44
2:B:1207:GLU:HG2	2:B:1210:ARG:NH1	2.32	0.44
2:F:616:LEU:O	2:F:619:ILE:HG22	2.18	0.44
2:F:893:THR:HG23	2:F:896:LYS:CB	2.46	0.44
2:F:1219:GLU:OE2	2:F:1335:ARG:HB3	2.18	0.44
1:A:27:G:N2	5:I:44:U:OP2	2.51	0.44
2:B:161:MET:SD	2:B:419:LEU:HB2	2.57	0.44
2:B:528:LYS:HD2	2:B:539:PHE:CE1	2.53	0.44
2:B:973:TYR:HD1	2:B:1237:TYR:CE1	2.35	0.44
2:F:677:LYS:HE2	2:F:681:ASP:HB3	2.00	0.44
2:F:791:LEU:HD23	2:F:818:ASN:OD1	2.18	0.44
2:F:883:TRP:HB3	2:F:897:PHE:HD1	1.82	0.44
2:F:1228:LEU:HD12	2:F:1228:LEU:HA	1.82	0.44
5:I:58:G:C2	5:I:60:C:O2	2.71	0.44
2:B:155:TYR:HD2	2:B:156:LEU:HD23	1.83	0.44
2:B:1110:ILE:HD13	2:B:1134:PHE:CE1	2.53	0.44
2:F:153:LEU:HD23	2:F:153:LEU:C	2.38	0.44
2:F:177:ASP:OD1	2:F:177:ASP:N	2.50	0.44
2:F:1215:ALA:O	4:H:6:DG:H5'	2.18	0.44
2:F:1218:GLY:CA	2:F:1339:THR:HG23	2.48	0.44
5:I:76:A:H2'	5:I:77:A:O4'	2.17	0.44
2:B:1201:TYR:N	2:B:1201:TYR:CD1	2.86	0.44
2:F:546:LYS:HE3	2:F:546:LYS:HB3	1.81	0.44
2:F:760:VAL:CG2	2:F:956:ILE:HD12	2.35	0.44
2:F:1123:LYS:HG3	2:F:1124:LYS:H	1.82	0.44
2:B:528:LYS:HG2	2:B:539:PHE:CD1	2.53	0.44
2:B:530:VAL:HG22	2:B:537:PRO:HB3	1.98	0.44
2:B:989:LEU:O	2:B:993:VAL:HG23	2.18	0.44
4:D:2:DT:H6	4:D:2:DT:H2'	1.56	0.44
2:F:794:GLN:CD	2:F:794:GLN:H	2.21	0.44
2:F:835:ASP:OD1	2:F:835:ASP:N	2.51	0.44
2:F:1163:LEU:HD12	2:F:1339:THR:HB	1.99	0.44
2:F:1210:ARG:HG3	2:F:1280:VAL:HA	2.00	0.44
2:F:1218:GLY:HA2	2:F:1339:THR:HG21	2.00	0.44
5:I:37:U:C2	5:I:38:A:C8	3.05	0.44
2:B:13:THR:O	2:B:53:PHE:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:PHE:HE1	2:B:242:ILE:HD11	1.82	0.44
2:B:784:ILE:HD13	2:B:815:TYR:CB	2.47	0.44
2:B:810:LYS:O	2:B:833:LEU:HD13	2.18	0.44
5:I:40:C:H2'	5:I:41:A:C8	2.52	0.44
1:A:26:A:O3'	2:B:116:HIS:CD2	2.71	0.43
2:B:265:GLN:HG2	2:B:266:LEU:N	2.32	0.43
2:B:472:THR:HG23	5:I:59:U:P	2.58	0.43
2:B:601:ILE:HA	2:B:647:VAL:HG13	2.00	0.43
2:B:607:LEU:HD23	2:B:607:LEU:HA	1.72	0.43
2:B:1336:TYR:N	2:B:1336:TYR:CD1	2.84	0.43
2:F:514:LEU:H	2:F:514:LEU:HD12	1.82	0.43
5:J:46:A:C2	5:J:47:A:C6	3.06	0.43
2:B:346:LYS:O	2:B:350:ILE:HG13	2.18	0.43
2:B:478:PHE:CE2	2:B:482:VAL:HG11	2.53	0.43
2:B:1089:MET:HA	2:B:1090:PRO:HD3	1.70	0.43
2:F:285:GLN:OE1	2:F:285:GLN:N	2.51	0.43
5:J:84:A:C2	5:J:85:C:C2	3.06	0.43
2:B:195:LEU:HB3	2:B:196:PHE:HD1	1.82	0.43
2:B:524:LEU:CD1	2:B:587:PHE:CE2	2.99	0.43
2:B:980:ASN:HB2	2:B:1225:GLU:OE2	2.18	0.43
1:E:16:A:OP1	2:F:454:PRO:HG3	2.18	0.43
2:F:82:LEU:HD23	2:F:82:LEU:HA	1.79	0.43
2:F:119:PHE:CD2	2:F:124:ASP:HB3	2.53	0.43
2:F:332:LEU:HD11	2:F:336:LYS:HE3	2.01	0.43
2:F:425:ARG:HG3	2:F:426:GLN:N	2.33	0.43
2:F:779:GLU:O	2:F:783:ARG:HD3	2.18	0.43
2:F:918:LYS:HE3	2:F:1018:VAL:HG11	1.99	0.43
2:F:1039:TYR:CD1	2:F:1039:TYR:N	2.87	0.43
2:F:1120:ILE:HD11	2:F:1135:ASP:N	2.32	0.43
2:F:1124:LYS:N	5:J:53:G:OP1	2.41	0.43
2:F:1147:ALA:CB	2:F:1190:VAL:HG22	2.48	0.43
2:F:1245:LEU:HD23	2:F:1245:LEU:HA	1.81	0.43
5:I:75:A:C2	5:I:76:A:C4	3.06	0.43
2:B:142:LEU:HD23	2:B:142:LEU:HA	1.74	0.43
2:B:201:ILE:HG22	2:B:202:ASN:N	2.33	0.43
2:B:565:LYS:HE2	2:B:580:ILE:HG12	2.00	0.43
2:B:813:LEU:HD11	2:B:855:LYS:HB3	1.99	0.43
2:B:1229:PRO:HB2	2:B:1232:TYR:CD2	2.52	0.43
2:F:121:ASN:HB2	2:F:123:VAL:HG12	2.00	0.43
2:F:351:PHE:HD1	5:J:43:G:O6	2.00	0.43
2:F:1255:LYS:N	2:F:1255:LYS:HE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:ARG:HD3	5:I:62:G:C5	2.53	0.43
2:B:119:PHE:CD2	2:B:124:ASP:HB3	2.54	0.43
2:B:141:LYS:HD3	2:B:141:LYS:C	2.39	0.43
2:B:682:PHE:CB	2:B:696:LEU:HD11	2.48	0.43
2:B:1035:LYS:HD3	2:B:1035:LYS:HA	1.60	0.43
2:F:4:LYS:HE2	2:F:4:LYS:HB2	1.71	0.43
2:F:31:LYS:HD2	5:J:83:C:H41	1.83	0.43
2:F:137:HIS:CD2	2:F:322:ILE:CG1	2.79	0.43
2:F:243:ALA:HB3	2:F:250:PRO:HG3	2.01	0.43
2:F:473:ILE:HG13	5:J:59:U:OP1	2.18	0.43
2:F:508:LEU:HD11	2:F:664:ARG:HA	2.00	0.43
2:F:848:LYS:CE	2:F:965:ASP:HB3	2.48	0.43
2:F:1060:ARG:HH22	2:F:1064:GLU:HB2	1.83	0.43
2:B:369:GLN:NE2	2:B:405:PHE:CZ	2.79	0.43
2:F:137:HIS:HA	2:F:322:ILE:HG12	2.01	0.43
2:F:601:ILE:HD11	2:F:607:LEU:HD21	2.01	0.43
2:F:1113:LYS:HB2	2:F:1129:LYS:O	2.19	0.43
2:F:1197:LYS:O	2:F:1199:PRO:HD3	2.19	0.43
1:A:2:U:H3	1:A:4:A:H3'	1.83	0.43
2:B:967:ARG:HH11	2:B:989:LEU:HD12	1.83	0.43
2:B:1294:TYR:HE1	2:B:1305:GLN:HE21	1.65	0.43
2:F:174:LEU:HA	2:F:174:LEU:HD13	1.79	0.43
2:F:643:PHE:HB2	2:F:648:MET:HE3	2.01	0.43
2:F:795:ILE:HA	2:F:798:GLU:OE1	2.19	0.43
5:I:47:A:H2'	5:I:48:A:C8	2.54	0.43
5:I:87:G:N2	5:I:92:G:C5	2.86	0.43
2:B:226:ILE:HA	2:B:229:LEU:HG	2.01	0.43
2:B:1114:ARG:NH1	4:D:9:DA:OP1	2.51	0.43
2:F:233:LYS:HG2	2:F:236:GLY:H	1.84	0.43
2:F:464:TRP:CD1	2:F:464:TRP:C	2.92	0.43
2:F:531:THR:HG21	2:F:575:PHE:HE1	1.75	0.43
2:F:553:PHE:CD2	2:F:559:VAL:HG21	2.53	0.43
2:F:662:LEU:HD22	2:F:666:LEU:HD21	2.01	0.43
2:F:970:PHE:CD1	2:F:1080:PHE:CZ	3.07	0.43
5:J:70:C:H2'	5:J:71:U:H6	1.84	0.43
2:B:253:LYS:O	2:B:257:ASP:N	2.51	0.43
2:B:710:LYS:HZ1	2:F:480:GLU:HB3	1.83	0.43
2:B:917:ILE:HG12	2:B:1042:ILE:HB	2.00	0.43
2:B:986:ASP:O	2:B:990:ASN:N	2.45	0.43
2:B:1003:LYS:CG	2:B:1036:TYR:CE2	2.95	0.43
2:B:1110:ILE:HD12	2:B:1122:ARG:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1169:MET:HE1	5:I:52:A:H1'	2.01	0.43
2:B:1191:LYS:HD2	2:B:1194:LEU:HD12	2.00	0.43
2:F:621:LEU:HD23	2:F:622:THR:N	2.33	0.43
2:F:844:GLN:HG2	2:F:848:LYS:HA	2.00	0.43
2:F:847:LEU:N	2:F:847:LEU:HD23	2.33	0.43
3:G:4:DT:H2''	3:G:5:DA:H5'	2.01	0.43
1:A:4:A:H2'	1:A:5:C:C6	2.54	0.43
2:B:501:ASN:HB2	2:B:666:LEU:CD1	2.49	0.43
2:B:870:VAL:HG13	2:B:871:PRO:HD2	2.01	0.43
2:B:1041:ASN:HD22	2:B:1044:ASN:ND2	2.17	0.43
1:E:21:G:H2'	1:E:22:U:O4'	2.18	0.43
2:F:226:ILE:HA	2:F:226:ILE:HD13	1.55	0.43
2:F:465:MET:SD	2:F:482:VAL:HG21	2.59	0.43
2:F:619:ILE:HD13	2:F:619:ILE:HG21	1.79	0.43
2:F:675:SER:HB3	2:F:682:PHE:CZ	2.54	0.43
2:F:902:LYS:NZ	2:F:912:ASP:CG	2.72	0.43
2:F:1182:LEU:HD12	2:F:1183:GLU:N	2.34	0.43
2:B:103:GLU:OE2	2:B:111:LYS:HG2	2.19	0.42
2:B:332:LEU:HD11	2:B:336:LYS:HE2	2.01	0.42
2:B:369:GLN:HE22	2:B:400:ARG:HH12	1.65	0.42
2:B:1333:ARG:CZ	2:B:1335:ARG:HD2	2.48	0.42
2:F:134:THR:HG22	5:J:45:U:C4'	2.48	0.42
2:F:401:LYS:HD3	5:J:45:U:OP2	2.19	0.42
2:F:404:THR:HG22	2:F:405:PHE:N	2.33	0.42
2:F:1062:LEU:HD12	2:F:1076:LYS:HB2	2.00	0.42
2:B:27:VAL:HA	2:B:28:PRO:HD3	1.89	0.42
2:B:1207:GLU:CD	2:B:1210:ARG:HH11	2.22	0.42
2:F:136:TYR:CZ	2:F:160:HIS:NE2	2.83	0.42
2:F:332:LEU:HD11	2:F:336:LYS:CE	2.49	0.42
2:F:535:ARG:HG3	2:F:535:ARG:NH1	2.34	0.42
2:F:1207:GLU:HG3	2:F:1208:ASN:H	1.85	0.42
5:I:42:A:C8	5:I:42:A:H3'	2.54	0.42
1:A:16:A:OP1	2:B:454:PRO:HG3	2.19	0.42
2:B:168:PHE:HA	2:B:412:HIS:HD2	1.84	0.42
2:B:383:MET:HB3	2:B:383:MET:HE2	1.73	0.42
2:B:475:PRO:HG3	5:I:59:U:O4	2.19	0.42
2:B:516:GLU:HA	2:B:519:THR:HG22	2.01	0.42
2:B:814:TYR:CE2	2:B:819:GLY:HA2	2.54	0.42
2:F:373:TYR:CE1	2:F:398:LEU:HB3	2.53	0.42
2:B:35:LEU:HD12	2:B:1358:THR:HG22	2.02	0.42
2:B:439:LYS:O	2:B:476:TRP:NE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:518:PHE:CG	2:B:667:ILE:HD13	2.54	0.42
2:B:734:LYS:O	2:B:737:ILE:HB	2.20	0.42
2:F:226:ILE:O	2:F:230:PRO:HA	2.19	0.42
2:F:359:TYR:CE2	2:F:363:ILE:CG1	3.02	0.42
2:F:370:GLU:OE2	2:F:374:LYS:NZ	2.50	0.42
2:F:551:LEU:HG	2:F:552:LEU:CD2	2.49	0.42
2:F:1207:GLU:CG	2:F:1208:ASN:H	2.32	0.42
2:B:728:ALA:O	2:B:927:ILE:HD13	2.20	0.42
2:B:1110:ILE:HD12	2:B:1122:ARG:CZ	2.49	0.42
2:B:1279:ARG:HG2	2:B:1280:VAL:HG23	2.02	0.42
2:B:1351:SER:O	2:B:1354:GLY:N	2.53	0.42
2:F:89:GLU:HG3	2:F:432:PHE:CD2	2.55	0.42
2:F:256:PHE:CD1	2:F:282:ILE:HD11	2.55	0.42
2:F:274:ASP:O	2:F:277:ASN:OD1	2.37	0.42
2:F:451:TYR:HB2	2:F:488:ALA:HA	2.01	0.42
2:F:842:VAL:HG23	2:F:908:LEU:HD11	2.00	0.42
2:F:902:LYS:NZ	2:F:912:ASP:OD2	2.52	0.42
2:F:936:ASP:OD1	2:F:940:ASN:ND2	2.53	0.42
2:F:1038:PHE:CD2	2:F:1039:TYR:CE1	3.03	0.42
5:I:73:G:H5'	5:I:74:A:OP2	2.20	0.42
2:B:864:ARG:HH21	2:B:871:PRO:HD3	1.84	0.42
2:B:1119:LEU:HD12	2:B:1119:LEU:HA	1.84	0.42
2:F:1069:THR:HB	2:F:1071:GLU:H	1.85	0.42
2:F:1265:TYR:O	2:F:1268:GLU:N	2.53	0.42
1:A:11:U:N3	1:A:12:A:N7	2.67	0.42
2:B:828:LEU:HD13	2:B:836:TYR:CD2	2.55	0.42
2:B:998:ILE:HG13	2:B:999:LYS:N	2.34	0.42
2:B:1208:ASN:O	2:B:1208:ASN:CG	2.57	0.42
1:E:25:U:H2'	1:E:26:A:H8	1.84	0.42
2:F:1090:PRO:HD2	5:J:88:A:N3	2.35	0.42
3:G:24:DG:O3'	3:G:25:DT:H4'	2.20	0.42
2:B:760:VAL:HG11	2:B:990:ASN:O	2.20	0.42
2:B:1110:ILE:HD13	2:B:1134:PHE:HE1	1.85	0.42
2:F:90:MET:SD	2:F:97:PHE:HD2	2.42	0.42
2:F:167:HIS:HD2	2:F:169:LEU:HD12	1.85	0.42
2:F:226:ILE:HD11	2:F:232:GLU:HB3	1.98	0.42
2:F:262:ALA:C	2:F:278:LEU:HD21	2.40	0.42
2:F:308:VAL:HG21	2:F:319:ALA:HB1	2.02	0.42
2:F:518:PHE:CD1	2:F:667:ILE:HD13	2.54	0.42
2:F:1045:PHE:CA	2:F:1060:ARG:HH11	2.30	0.42
2:F:1142:SER:HA	2:F:1164:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1179:ILE:O	2:F:1183:GLU:HG3	2.19	0.42
2:F:1277:SER:CB	2:F:1287:LEU:HD22	2.49	0.42
2:F:1343:LEU:H	2:F:1343:LEU:HG	1.41	0.42
5:I:42:A:H5''	5:I:42:A:C8	2.49	0.42
5:J:73:G:C5'	5:J:73:G:H8	2.33	0.42
2:B:338:LEU:C	2:B:383:MET:HE1	2.40	0.42
2:B:478:PHE:CE1	2:B:482:VAL:HG21	2.55	0.42
2:B:558:LYS:HD2	2:B:586:ARG:HD2	2.01	0.42
2:B:795:ILE:O	2:B:795:ILE:HG13	2.20	0.42
2:B:973:TYR:HD2	2:B:1234:ASN:OD1	2.03	0.42
2:F:106:LEU:HD23	2:F:106:LEU:HA	1.65	0.42
2:F:1110:ILE:HD13	2:F:1110:ILE:HG21	1.87	0.42
2:F:1336:TYR:N	2:F:1336:TYR:CD1	2.85	0.42
3:G:1:DC:H2'	3:G:2:DA:C8	2.55	0.42
5:I:69:A:H2'	5:I:70:C:C6	2.55	0.42
5:J:58:G:C4	5:J:60:C:H1'	2.55	0.42
2:B:38:THR:HG22	2:B:40:ARG:N	2.28	0.42
2:B:305:ILE:HG13	2:B:306:LEU:N	2.34	0.42
2:B:602:LYS:HB2	2:B:602:LYS:HE3	1.83	0.42
2:B:738:LEU:HD23	2:B:742:LYS:HG3	2.02	0.42
2:B:1334:LYS:NZ	3:C:3:DA:OP2	2.53	0.42
1:E:4:A:C2	1:E:5:C:C5	3.08	0.42
2:F:70:ARG:NH2	5:J:61:C:OP1	2.50	0.42
2:F:189:VAL:CG1	2:F:201:ILE:HG22	2.50	0.42
2:F:561:VAL:HG22	2:F:583:VAL:HG21	2.01	0.42
2:F:595:HIS:ND1	2:F:595:HIS:N	2.67	0.42
2:F:821:ASP:HA	2:F:828:LEU:HD11	2.01	0.42
2:F:867:SER:HB2	2:F:1054:ASN:N	2.34	0.42
1:A:11:U:O5'	1:A:11:U:H6	2.03	0.41
2:B:85:ILE:HD12	2:B:440:ILE:HG12	2.02	0.41
2:B:114:GLU:HG2	2:B:120:GLY:HA2	2.01	0.41
1:E:15:G:P	2:F:66:ARG:HH22	2.41	0.41
2:F:444:LEU:HD23	2:F:444:LEU:O	2.19	0.41
2:F:448:ILE:HA	2:F:449:PRO:HD3	1.91	0.41
2:F:487:SER:O	2:F:491:PHE:N	2.48	0.41
1:A:29:G:C4	5:I:41:A:C2	3.07	0.41
2:B:40:ARG:HE	2:B:43:ILE:HD11	1.84	0.41
2:B:442:LYS:HE3	2:B:476:TRP:HA	2.02	0.41
2:B:873:GLU:O	2:B:877:LYS:HG2	2.20	0.41
2:B:988:TYR:CE2	2:B:1083:VAL:HG13	2.55	0.41
2:F:1111:LEU:HD12	2:F:1135:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:ASP:HA	2:B:279:LEU:CB	2.51	0.41
2:B:1002:PRO:O	2:B:1005:GLU:HB2	2.19	0.41
2:B:1222:LYS:HD2	2:B:1317:ASN:O	2.20	0.41
2:F:524:LEU:HD23	2:F:587:PHE:HE2	1.85	0.41
2:F:566:GLU:O	2:F:570:LYS:HB3	2.20	0.41
2:F:894:GLN:HE22	2:F:898:ASP:CG	2.24	0.41
2:F:1022:ILE:HG23	2:F:1038:PHE:HA	2.01	0.41
2:F:1284:ASP:OD1	2:F:1284:ASP:N	2.41	0.41
2:B:184:LEU:HD23	2:B:184:LEU:HA	1.42	0.41
2:B:275:LEU:O	2:B:275:LEU:HD12	2.20	0.41
2:B:440:ILE:O	2:B:443:ILE:N	2.50	0.41
2:B:1088:SER:HA	2:B:1230:SER:OG	2.21	0.41
2:B:1141:TYR:C	2:B:1141:TYR:CD1	2.94	0.41
2:B:1147:ALA:HB2	2:B:1190:VAL:HG22	2.02	0.41
2:F:761:ILE:HD13	2:F:761:ILE:HG21	1.76	0.41
2:F:1046:PHE:C	2:F:1076:LYS:HZ2	2.24	0.41
2:F:1355:LEU:HA	2:F:1355:LEU:HD23	1.81	0.41
2:B:106:LEU:HA	2:B:106:LEU:HD12	1.81	0.41
2:B:114:GLU:OE2	2:B:120:GLY:O	2.38	0.41
2:B:823:TYR:HD1	2:B:875:VAL:HG11	1.83	0.41
2:B:982:HIS:HA	2:B:985:HIS:HB2	2.03	0.41
2:B:1203:LEU:HD23	2:B:1348:ILE:HB	2.02	0.41
2:F:342:GLN:HB2	2:F:383:MET:SD	2.60	0.41
2:F:935:LEU:O	2:F:939:MET:HG2	2.20	0.41
3:G:16:DA:H2'	3:G:17:DT:C6	2.56	0.41
2:B:180:ASP:OD2	2:B:183:LYS:HE3	2.20	0.41
2:B:1060:ARG:HD3	2:B:1064:GLU:OE2	2.19	0.41
2:B:1143:VAL:HG21	2:B:1174:PHE:CZ	2.55	0.41
2:F:781:MET:HB2	2:F:803:ASN:HD22	1.85	0.41
2:F:1019:ARG:C	2:F:1021:MET:H	2.24	0.41
2:F:1045:PHE:O	2:F:1076:LYS:NZ	2.38	0.41
2:F:1048:THR:HG22	2:F:1076:LYS:HD2	2.02	0.41
2:F:1121:ALA:HB2	2:F:1128:PRO:HD3	2.03	0.41
4:H:11:DT:H2''	4:H:12:DG:C8	2.56	0.41
2:B:756:PRO:HD2	2:B:939:MET:HE2	2.02	0.41
2:B:1258:PHE:HE1	2:B:1262:HIS:NE2	2.09	0.41
2:B:1258:PHE:CZ	2:B:1262:HIS:CD2	3.03	0.41
1:E:15:G:H4'	2:F:454:PRO:HD3	2.03	0.41
2:F:121:ASN:ND2	2:F:121:ASN:H	2.19	0.41
2:F:373:TYR:O	2:F:376:ILE:HG22	2.19	0.41
5:J:72:U:H2'	5:J:73:G:H5''	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:ALA:O	2:B:69:ARG:C	2.57	0.41
2:B:970:PHE:CZ	2:B:1047:LYS:HD3	2.56	0.41
2:B:1224:ASN:N	2:B:1224:ASN:HD22	2.19	0.41
2:F:1087:LEU:HD23	2:F:1087:LEU:HA	1.83	0.41
2:F:1154:SER:OG	2:F:1156:LYS:HB3	2.20	0.41
2:B:21:ILE:O	2:B:21:ILE:HG13	2.20	0.41
2:B:127:ALA:HA	2:B:130:GLU:HB2	2.03	0.41
2:B:186:ILE:O	2:B:190:GLN:HG3	2.20	0.41
2:B:1136:SER:N	2:B:1137:PRO:HD3	2.36	0.41
2:B:1279:ARG:HH11	2:B:1279:ARG:HD2	1.77	0.41
1:E:27:G:H5'	1:E:28:A:H5''	2.02	0.41
2:F:43:ILE:HD13	2:F:43:ILE:HA	1.87	0.41
2:F:677:LYS:HG2	2:F:681:ASP:HB2	2.02	0.41
2:F:846:PHE:O	2:F:1040:SER:C	2.59	0.41
2:F:997:LEU:HD23	2:F:997:LEU:HA	1.89	0.41
2:F:1045:PHE:HB2	2:F:1064:GLU:CG	2.38	0.41
5:I:79:G:O2'	5:I:80:U:H5'	2.21	0.41
1:A:31:U:H1'	5:I:39:G:N2	2.36	0.41
2:B:478:PHE:O	2:B:482:VAL:HB	2.21	0.41
2:B:737:ILE:O	2:B:738:LEU:C	2.59	0.41
2:B:1003:LYS:H	2:B:1003:LYS:HG2	1.51	0.41
2:B:1142:SER:O	2:B:1198:LEU:N	2.34	0.41
2:B:1146:VAL:CG1	2:B:1191:LYS:HB2	2.51	0.41
2:B:1203:LEU:HA	2:B:1203:LEU:HD12	1.79	0.41
2:F:301:LEU:O	2:F:305:ILE:HG12	2.21	0.41
2:F:619:ILE:HD11	2:F:651:LEU:CD1	2.50	0.41
2:F:784:ILE:HD13	2:F:815:TYR:HB3	2.03	0.41
2:F:1242:TYR:H	2:F:1242:TYR:HD1	1.69	0.41
5:I:47:A:N6	5:I:48:A:C6	2.89	0.41
1:A:1:U:O5'	1:A:1:U:H6	2.04	0.40
2:B:601:ILE:HG22	2:B:647:VAL:HG11	2.03	0.40
2:F:565:LYS:HE2	2:F:565:LYS:HB3	1.84	0.40
2:F:1161:LYS:HZ3	2:F:1364:GLN:HG2	1.86	0.40
2:B:35:LEU:HB2	2:B:1358:THR:CG2	2.51	0.40
2:B:118:ILE:HG12	2:B:156:LEU:HD11	2.03	0.40
2:B:861:ASP:O	2:B:864:ARG:HG2	2.20	0.40
2:B:1229:PRO:HB2	2:B:1232:TYR:HD2	1.87	0.40
2:F:553:PHE:HZ	2:F:587:PHE:CD2	2.38	0.40
2:F:781:MET:CB	2:F:803:ASN:HD22	2.34	0.40
2:F:956:ILE:H	2:F:956:ILE:HG13	1.69	0.40
2:F:1035:LYS:HD3	2:F:1035:LYS:HA	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1052:LEU:HD12	2:F:1052:LEU:HA	1.96	0.40
2:F:1110:ILE:HD13	2:F:1122:ARG:CZ	2.52	0.40
2:F:1216:SER:OG	4:H:7:DG:OP1	2.32	0.40
2:B:583:VAL:HG22	2:B:584:GLU:N	2.37	0.40
2:B:697:ILE:HG22	2:B:698:HIS:ND1	2.37	0.40
2:B:836:TYR:CD1	2:B:836:TYR:N	2.87	0.40
2:B:836:TYR:CD1	2:B:859:ARG:HA	2.57	0.40
2:B:961:LYS:HA	2:B:964:SER:HB3	2.03	0.40
2:B:1212:ARG:HD3	2:B:1212:ARG:HA	1.89	0.40
2:B:1287:LEU:HD12	2:B:1287:LEU:HA	1.82	0.40
1:E:27:G:H1	5:J:44:U:P	2.44	0.40
2:F:477:ASN:O	2:F:481:VAL:HG23	2.21	0.40
2:F:873:GLU:OE1	2:F:873:GLU:N	2.46	0.40
2:F:1223:GLY:HA2	2:F:1318:LEU:HG	2.02	0.40
5:I:88:A:N1	5:I:91:C:N3	2.70	0.40
2:B:593:THR:O	2:B:594:TYR:C	2.59	0.40
2:B:680:LEU:HD12	2:B:680:LEU:HA	1.84	0.40
2:B:973:TYR:CD1	2:B:1237:TYR:HD1	2.39	0.40
2:B:1205:GLU:CG	2:B:1209:GLY:HA2	2.49	0.40
2:B:1251:ASP:OD1	2:B:1254:GLN:NE2	2.54	0.40
2:F:546:LYS:HZ2	2:F:546:LYS:C	2.24	0.40
2:F:1200:LYS:HG2	2:F:1201:TYR:CD1	2.56	0.40
2:F:1219:GLU:O	2:F:1220:LEU:HD23	2.22	0.40
2:F:1263:LYS:O	2:F:1266:LEU:CD2	2.70	0.40
2:F:1349:HIS:CE1	5:J:69:A:H5'	2.56	0.40
5:J:50:U:O3'	5:J:51:A:H4'	2.21	0.40
2:B:58:THR:HG22	2:B:731:PRO:HG3	2.04	0.40
2:B:165:ARG:O	2:B:415:HIS:HD2	2.04	0.40
2:B:317:LEU:HD13	2:B:410:ILE:HD13	2.03	0.40
2:F:44:LYS:O	5:J:91:C:H2'	2.22	0.40
2:F:336:LYS:HG2	2:F:351:PHE:CE1	2.57	0.40
2:F:842:VAL:HG12	2:F:854:ASN:ND2	2.35	0.40
2:F:945:GLU:HG2	2:F:946:ASN:N	2.36	0.40
2:F:1120:ILE:H	2:F:1120:ILE:HG12	1.63	0.40

All (2) 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
2:B:228:GLN:NE2	2:B:543:GLU:OE2[2_545]	2.18	0.02

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1312/1368 (96%)	1279 (98%)	29 (2%)	4 (0%)	37	68
2	F	1313/1368 (96%)	1266 (96%)	45 (3%)	2 (0%)	44	75
All	All	2625/2736 (96%)	2545 (97%)	74 (3%)	6 (0%)	44	75

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	270	THR
2	F	1020	LYS
2	F	117	PRO
2	B	117	PRO
2	B	250	PRO
2	B	230	PRO

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	1173/1225 (96%)	1114 (95%)	59 (5%)	20	49
2	F	1156/1225 (94%)	1083 (94%)	73 (6%)	15	42
All	All	2329/2450 (95%)	2197 (94%)	132 (6%)	17	45

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	15	SER
2	B	95	ASP
2	B	141	LYS
2	B	179	SER
2	B	182	ASP
2	B	257	ASP
2	B	274	ASP
2	B	276	ASP
2	B	302	LEU
2	B	304	ASP
2	B	314	LYS
2	B	359	TYR
2	B	405	PHE
2	B	425	ARG
2	B	434	LYS
2	B	465	MET
2	B	467	ARG
2	B	487	SER
2	B	503	PRO
2	B	535	ARG
2	B	556	ASN
2	B	557	ARG
2	B	562	LYS
2	B	586	ARG
2	B	599	LYS
2	B	614	ASP
2	B	648	MET
2	B	663	SER
2	B	684	LYS
2	B	699	ASP
2	B	719	SER
2	B	751	MET
2	B	763	MET
2	B	853	ASP
2	B	879	MET
2	B	882	TYR
2	B	884	ARG
2	B	898	ASP
2	B	905	ARG
2	B	951	ARG
2	B	954	LYS
2	B	969	ASP
2	B	1037	PHE

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Mol	Chain	Res	Type
2	B	1041	ASN
2	B	1062	LEU
2	B	1080	PHE
2	B	1141	TYR
2	B	1171	ARG
2	B	1202	SER
2	B	1206	LEU
2	B	1220	LEU
2	B	1258	PHE
2	B	1263	LYS
2	B	1267	ASP
2	B	1325	LYS
2	B	1328	ASP
2	B	1334	LYS
2	B	1340	LYS
2	B	1351	SER
2	F	94	ASP
2	F	128	TYR
2	F	140	LYS
2	F	144	ASP
2	F	145	SER
2	F	165	ARG
2	F	187	GLN
2	F	237	LEU
2	F	253	LYS
2	F	255	ASN
2	F	271	TYR
2	F	279	LEU
2	F	284	ASP
2	F	290	PHE
2	F	384	ASP
2	F	392	LYS
2	F	394	ASN
2	F	403	ARG
2	F	419	LEU
2	F	457	ARG
2	F	465	MET
2	F	478	PHE
2	F	484	LYS
2	F	494	ARG
2	F	510	LYS
2	F	532	GLU

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Mol	Chain	Res	Type
2	F	535	ARG
2	F	536	LYS
2	F	546	LYS
2	F	563	GLN
2	F	567	ASP
2	F	602	LYS
2	F	605	ASP
2	F	621	LEU
2	F	646	LYS
2	F	654	ARG
2	F	671	ARG
2	F	682	PHE
2	F	688	PHE
2	F	693	PHE
2	F	738	LEU
2	F	753	ARG
2	F	778	ARG
2	F	812	TYR
2	F	818	ASN
2	F	844	GLN
2	F	846	PHE
2	F	855	LYS
2	F	879	MET
2	F	894	GLN
2	F	912	ASP
2	F	1003	LYS
2	F	1008	PHE
2	F	1021	MET
2	F	1037	PHE
2	F	1060	ARG
2	F	1080	PHE
2	F	1118	LYS
2	F	1122	ARG
2	F	1125	ASP
2	F	1202	SER
2	F	1206	LEU
2	F	1208	ASN
2	F	1222	LYS
2	F	1242	TYR
2	F	1246	LYS
2	F	1258	PHE
2	F	1274	SER

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Mol	Chain	Res	Type
2	F	1324	PHE
2	F	1327	PHE
2	F	1328	ASP
2	F	1338	SER
2	F	1359	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	137	HIS
2	B	178	ASN
2	B	224	ASN
2	B	255	ASN
2	B	415	HIS
2	B	1041	ASN
2	B	1221	GLN
2	B	1224	ASN
2	B	1252	ASN
2	B	1254	GLN
2	B	1256	GLN
2	B	1262	HIS
2	B	1308	ASN
2	B	1317	ASN
2	B	1364	GLN
2	F	178	ASN
2	F	187	GLN
2	F	329	HIS
2	F	415	HIS
2	F	650	GLN
2	F	690	ASN
2	F	803	ASN
2	F	894	GLN
2	F	933	GLN
2	F	1256	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	33/34 (97%)	9 (27%)	3 (9%)
1	E	30/34 (88%)	9 (30%)	1 (3%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	I	62/65 (95%)	20 (32%)	2 (3%)
5	J	62/65 (95%)	19 (30%)	1 (1%)
All	All	187/198 (94%)	57 (30%)	7 (3%)

All (57) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	4	A
1	A	5	C
1	A	6	G
1	A	9	U
1	A	20	A
1	A	28	A
1	A	29	G
1	A	33	U
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	32	A
1	E	33	U
5	I	39	G
5	I	40	C
5	I	42	A
5	I	43	G
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	69	A
5	I	73	G
5	I	74	A
5	I	77	A
5	I	82	G
5	I	87	G

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Mol	Chain	Res	Type
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	73	G
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 (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	27	G
1	A	28	A
1	E	27	G
5	I	42	A
5	I	68	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

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	34/34 (100%)	-0.41	1 (2%) 54 36	19, 34, 129, 166	0
1	E	31/34 (91%)	0.12	1 (3%) 50 34	40, 71, 175, 230	0
2	B	1326/1368 (96%)	0.20	79 (5%) 29 22	13, 62, 175, 215	0
2	F	1327/1368 (97%)	0.58	147 (11%) 12 9	11, 88, 145, 197	0
3	C	25/25 (100%)	-0.60	0 100 100	25, 38, 81, 88	0
3	G	25/25 (100%)	0.04	0 100 100	45, 59, 118, 139	0
4	D	11/11 (100%)	0.00	1 (9%) 16 13	30, 38, 122, 159	0
4	H	11/11 (100%)	0.00	1 (9%) 16 13	33, 60, 119, 189	0
5	I	63/65 (96%)	-0.46	0 100 100	17, 71, 122, 170	0
5	J	63/65 (96%)	-0.36	1 (1%) 70 51	26, 58, 137, 191	0
All	All	2916/3006 (97%)	0.33	231 (7%) 20 16	11, 70, 162, 230	0

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	305	ILE	7.7
2	B	801	VAL	7.0
2	F	73	THR	6.9
2	B	809	GLU	6.9
2	B	1243	GLU	6.6
2	F	362	TYR	6.5
2	F	402	GLN	6.2
2	B	1242	TYR	6.1
2	F	815	TYR	6.0
2	F	82	LEU	5.8
2	F	679	ILE	5.7
2	F	369	GLN	5.3
2	B	900	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
2	F	232	GLU	4.9
2	F	1049	GLU	4.9
2	F	400	ARG	4.9
2	F	224	ASN	4.8
2	B	47	LEU	4.6
2	F	301	LEU	4.6
2	B	883	TRP	4.5
2	F	230	PRO	4.5
2	B	44	LYS	4.5
2	B	813	LEU	4.3
2	F	802	GLU	4.3
2	F	811	LEU	4.2
2	F	693	PHE	4.1
2	B	810	LYS	4.0
2	F	451	TYR	4.0
2	B	627	GLU	4.0
2	B	1045	PHE	3.9
2	F	449	PRO	3.9
2	F	714	SER	3.9
2	F	688	PHE	3.8
2	F	244	LEU	3.8
4	H	2	DT	3.8
2	F	128	TYR	3.8
2	F	419	LEU	3.7
2	B	1248	SER	3.7
2	F	627	GLU	3.6
2	F	682	PHE	3.6
2	B	661	ARG	3.6
2	B	812	TYR	3.6
2	F	213	SER	3.6
2	F	580	ILE	3.6
2	B	1052	LEU	3.5
2	F	818	ASN	3.5
2	B	1002	PRO	3.5
2	F	661	ARG	3.5
2	F	444	LEU	3.4
2	F	777	SER	3.4
2	F	544	GLN	3.4
2	B	796	LEU	3.4
2	F	227	ALA	3.4
2	B	242	ILE	3.4
2	F	335	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	430	TYR	3.4
2	F	501	ASN	3.3
2	F	72	TYR	3.3
2	B	858	THR	3.3
2	F	225	LEU	3.3
2	F	74	ARG	3.3
2	B	784	ILE	3.3
2	F	1050	ILE	3.3
2	F	441	GLU	3.3
2	B	1235	PHE	3.2
2	F	711	ALA	3.2
2	F	697	ILE	3.2
2	F	247	GLY	3.2
2	B	822	MET	3.2
2	F	856	VAL	3.2
2	B	1238	LEU	3.2
2	F	68	ALA	3.2
2	B	31	LYS	3.1
2	F	210	ALA	3.1
2	F	241	LEU	3.1
2	F	367	ALA	3.1
2	F	297	SER	3.0
2	F	79	ILE	3.0
2	B	814	TYR	3.0
2	B	872	SER	3.0
2	F	452	VAL	3.0
2	F	796	LEU	3.0
2	B	867	SER	3.0
2	F	473	ILE	2.9
2	B	1355	LEU	2.9
2	B	1042	ILE	2.9
2	B	823	TYR	2.9
2	B	1050	ILE	2.9
2	B	777	SER	2.8
2	F	149	ALA	2.8
2	F	423	LEU	2.8
2	F	683	LEU	2.8
2	F	478	PHE	2.8
2	F	804	THR	2.8
2	F	231	GLY	2.8
4	D	12	DG	2.8
2	F	1168	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	1048	THR	2.8
1	E	28	A	2.8
2	F	207	ASP	2.8
2	F	338	LEU	2.7
2	F	211	ILE	2.7
2	F	1039	TYR	2.7
2	F	690	ASN	2.7
2	F	40	ARG	2.7
2	B	538	ALA	2.7
2	F	1111	LEU	2.7
2	B	32	PHE	2.7
2	F	238	PHE	2.7
2	F	246	LEU	2.7
2	F	389	LEU	2.7
2	F	1060	ARG	2.7
2	F	853	ASP	2.7
2	F	445	THR	2.7
2	B	1237	TYR	2.7
2	F	1243	GLU	2.6
2	F	306	LEU	2.6
2	B	1051	THR	2.6
2	F	129	HIS	2.6
2	B	45	LYS	2.6
2	F	813	LEU	2.6
2	B	1073	VAL	2.6
2	F	245	SER	2.6
2	F	308	VAL	2.6
2	F	481	VAL	2.6
2	F	142	LEU	2.5
2	F	181	VAL	2.5
2	F	443	ILE	2.5
2	B	1036	TYR	2.5
2	F	477	ASN	2.5
2	F	1051	THR	2.5
2	F	658	GLY	2.5
2	F	240	ASN	2.5
2	F	713	VAL	2.5
2	F	503	PRO	2.5
2	B	385	GLY	2.4
2	B	844	GLN	2.4
2	F	257	ASP	2.4
2	B	502	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	237	LEU	2.4
2	B	238	PHE	2.4
2	B	1350	GLN	2.4
2	B	1249	PRO	2.4
2	B	1269	ILE	2.4
2	B	1309	ILE	2.4
2	F	220	ARG	2.4
2	F	531	THR	2.4
2	B	28	PRO	2.4
2	B	685	SER	2.4
2	F	156	LEU	2.4
2	F	702	LEU	2.4
2	F	162	ILE	2.3
2	B	910	GLU	2.3
2	B	984	ALA	2.3
2	B	1241	HIS	2.3
2	F	717	GLY	2.3
2	F	1048	THR	2.3
2	B	43	ILE	2.3
2	B	1156	LYS	2.3
2	F	1061	PRO	2.3
2	B	1332	ASP	2.3
2	F	322	ILE	2.3
2	F	795	ILE	2.3
2	B	484	LYS	2.3
2	B	799	HIS	2.3
2	F	296	LEU	2.3
2	F	312	ILE	2.3
2	B	817	GLN	2.3
2	B	1034	ALA	2.3
2	F	348	LYS	2.3
2	F	480	GLU	2.3
2	B	700	ASP	2.3
2	F	1337	THR	2.3
2	F	228	GLN	2.3
2	F	1356	TYR	2.3
2	F	203	ALA	2.3
2	F	262	ALA	2.3
2	B	628	ASP	2.2
2	B	29	SER	2.2
2	B	834	SER	2.2
2	F	376	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	843	PRO	2.2
2	F	401	LYS	2.2
2	F	568	TYR	2.2
2	F	877	LYS	2.2
2	B	876	VAL	2.2
5	J	36	G	2.2
2	B	1095	VAL	2.2
2	F	132	TYR	2.2
2	F	662	LEU	2.2
2	F	290	PHE	2.2
2	F	484	LYS	2.2
2	B	849	ASP	2.2
2	B	906	GLY	2.1
2	B	1046	PHE	2.1
2	F	117	PRO	2.1
2	F	107	VAL	2.1
2	F	578	VAL	2.1
2	B	1331	ILE	2.1
2	F	742	LYS	2.1
2	B	225	LEU	2.1
2	F	67	THR	2.1
2	B	808	ASN	2.1
2	B	852	ILE	2.1
2	F	317	LEU	2.1
2	F	145	SER	2.1
2	F	303	SER	2.1
2	F	440	ILE	2.1
2	F	803	ASN	2.1
2	B	380	LEU	2.1
2	B	857	LEU	2.1
2	F	778	ARG	2.1
2	F	788	ILE	2.1
2	F	386	THR	2.1
2	F	42	SER	2.1
2	F	357	ASN	2.1
2	F	433	LEU	2.1
2	F	196	PHE	2.0
2	F	334	LEU	2.0
2	F	455	LEU	2.0
1	A	1	U	2.0
2	F	201	ILE	2.0
2	F	286	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	98	PHE	2.0
2	F	229	LEU	2.0
2	F	868	ASP	2.0
2	F	536	LYS	2.0
2	F	1335	ARG	2.0
2	B	1304	GLU	2.0
2	F	315	ALA	2.0
2	F	172	GLY	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.