Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2024 – 02:53 PM JST

PDB ID	:	8KAI
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

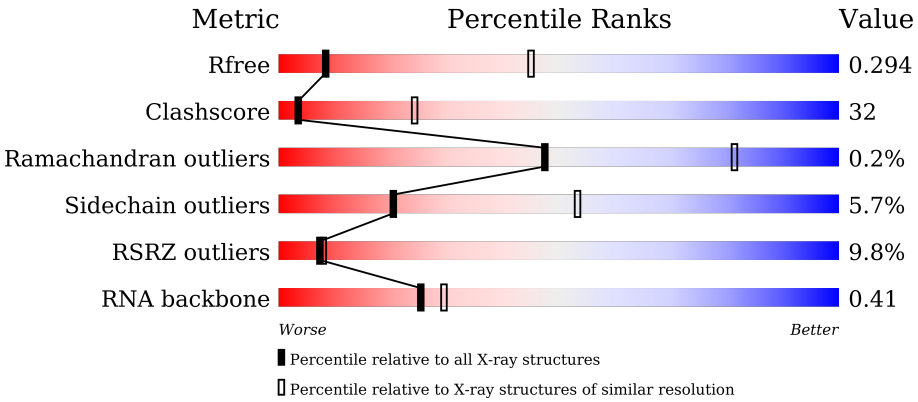
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (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 >=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 <=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	6% 9% 38% 32% 21%
1	E	34	9% 24% 26% 38% • 9%
2	B	1368	9% 45% 48% • •
2	F	1368	11% 44% 48% 5% •

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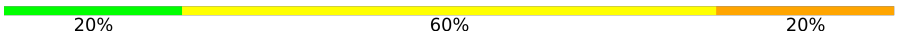
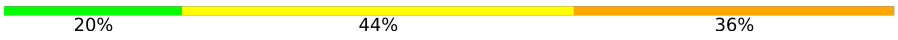
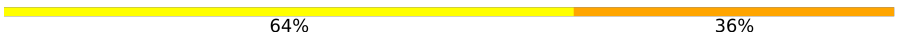
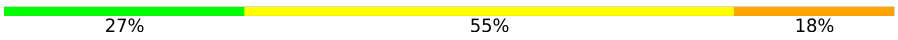
Mol	Chain	Length	Quality of chain
3	C	25	
3	G	25	
4	D	11	
4	H	11	
5	I	65	
5	J	65	

2 Entry composition (i)

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			

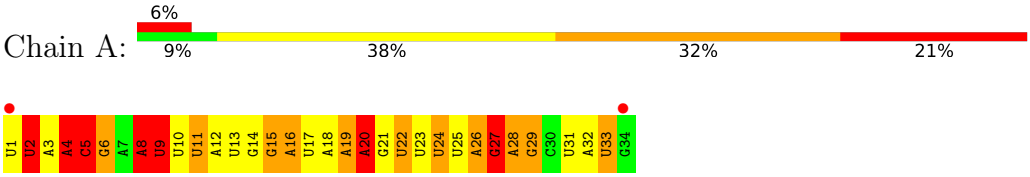
- Molecule 6 is water.

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

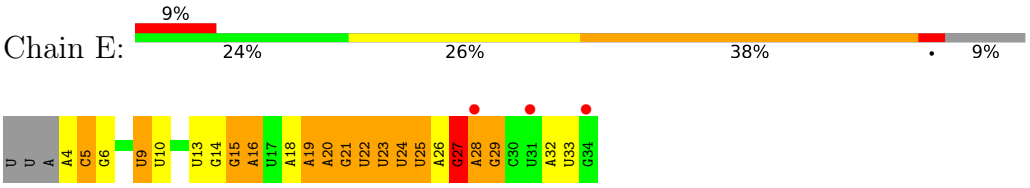
3 Residue-property plots (i)

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

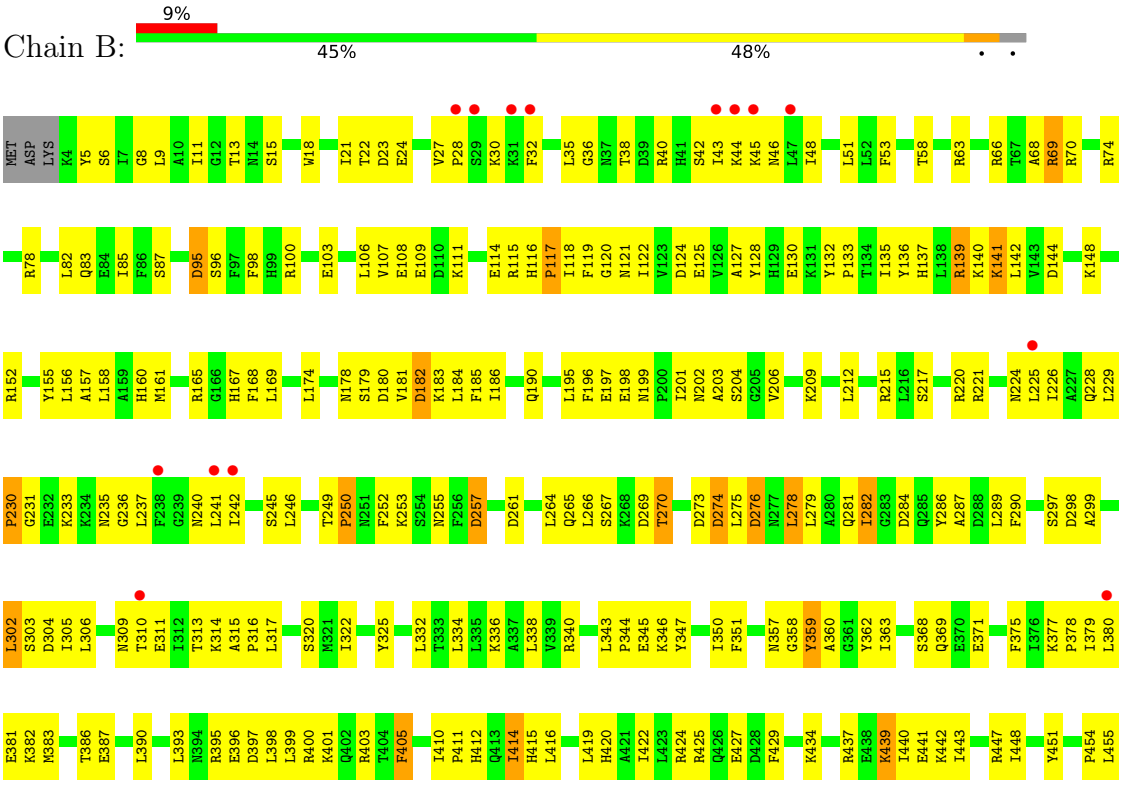
• Molecule 1: RNA (34-MER)

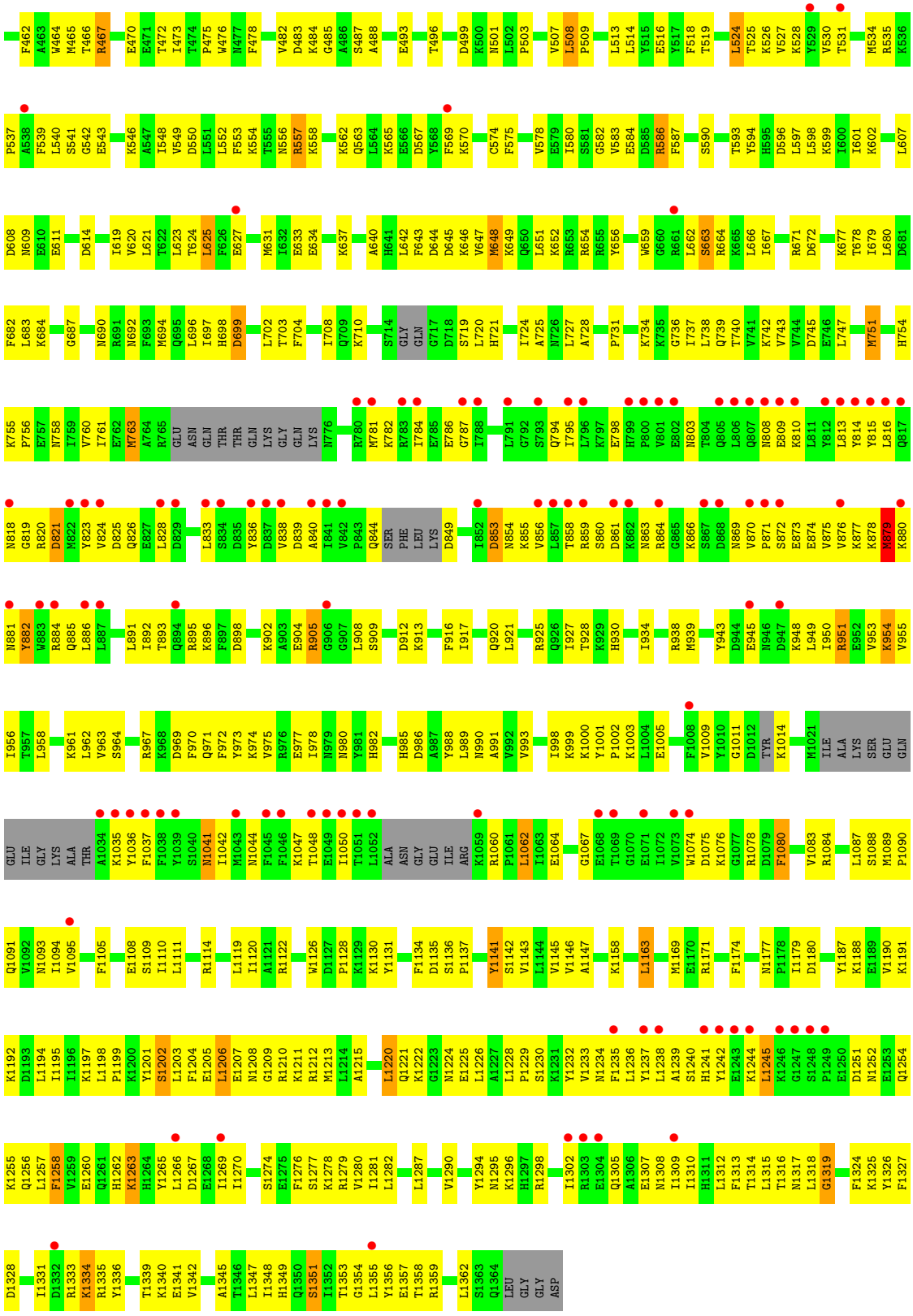


• Molecule 1: RNA (34-MER)



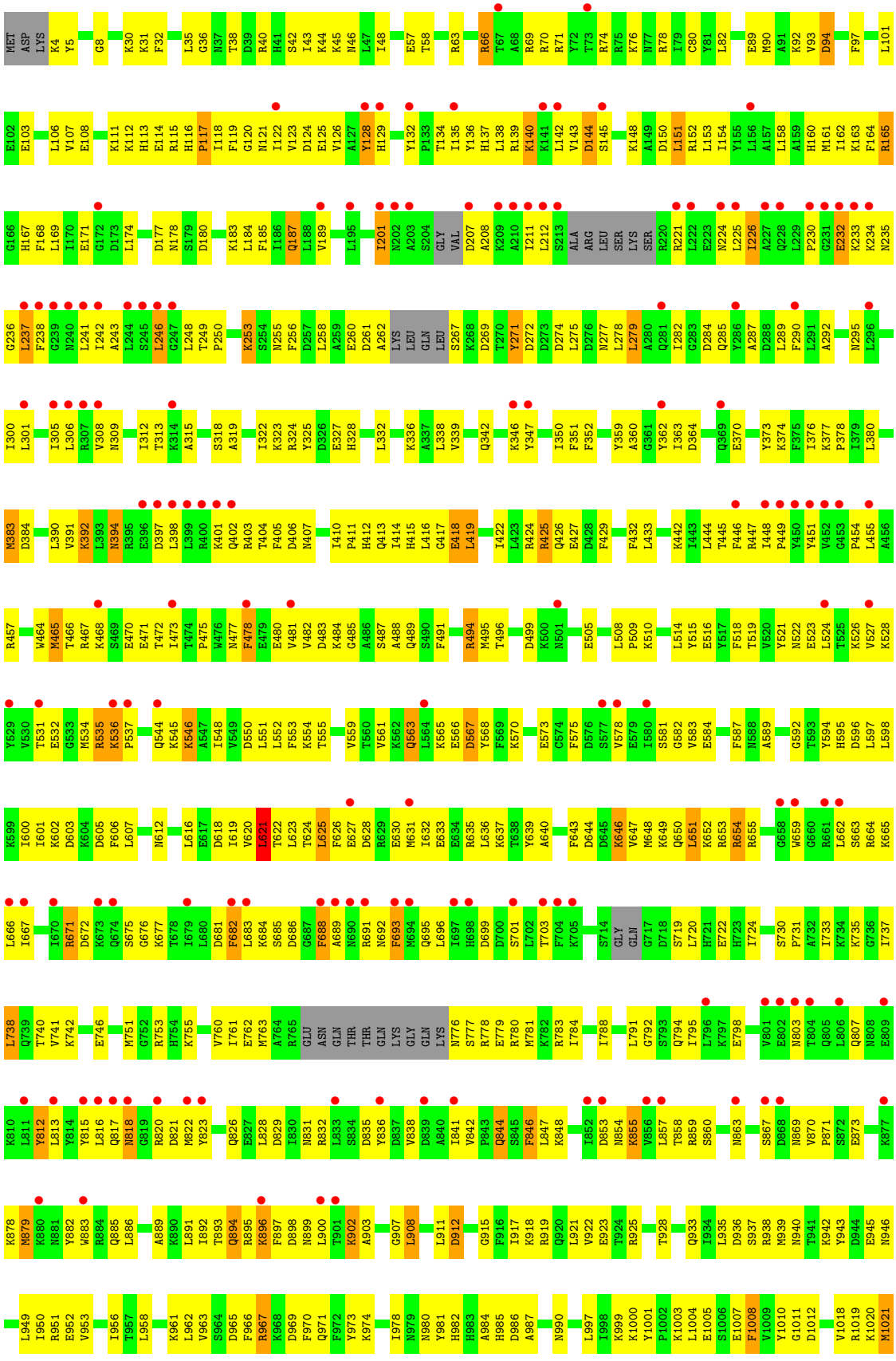
• Molecule 2: CRISPR-associated endonuclease Cas9/Csn1

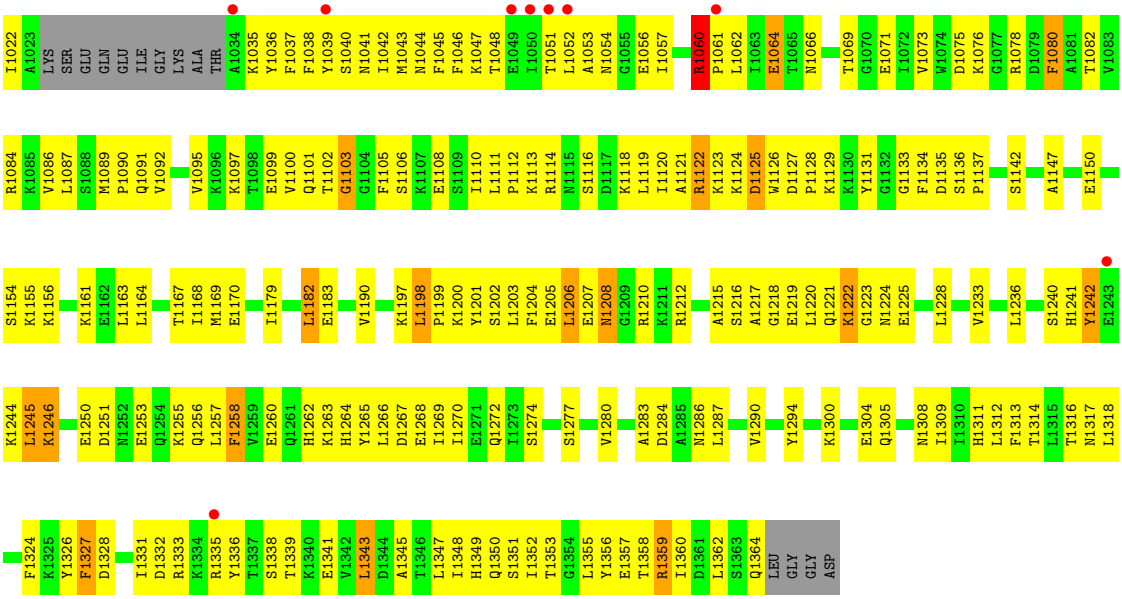




• Molecule 2: CRISPR-associated endonuclease Cas9/Csn1

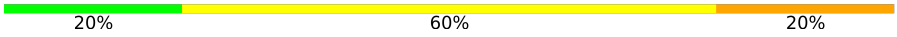
Chain F:





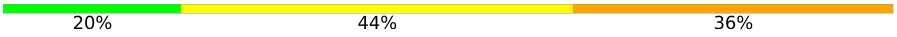
• Molecule 3: DNA (25-MER)

Chain C:



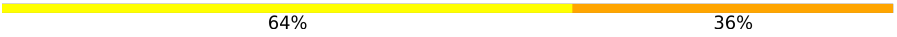
• Molecule 3: DNA (25-MER)

Chain G:



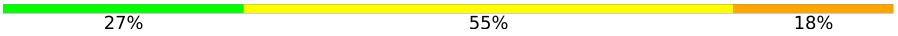
• Molecule 4: DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP*G)-3')

Chain D:



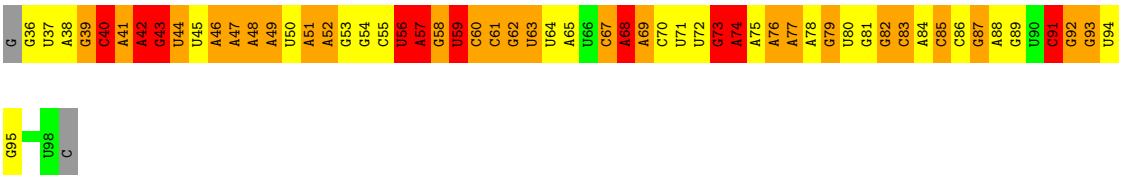
• Molecule 4: DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP*G)-3')

Chain H:



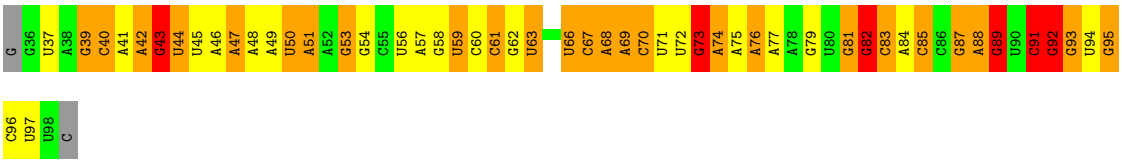
• Molecule 5: RNA (65-MER)

Chain I:



• Molecule 5: RNA (65-MER)

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	144.30Å 130.19Å 146.41Å 90.00° 104.02° 90.00°	Depositor
Resolution (Å)	48.57 – 3.49 48.57 – 3.45	Depositor EDS
% Data completeness (in resolution range)	79.0 (48.57-3.49) 76.2 (48.57-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.225 , 0.294 0.225 , 0.294	Depositor DCC
R_{free} test set	2620 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	62.1	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 40.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	725	0	362	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%)	41 75
2	F	1313/1368 (96%)	1266 (96%)	45 (3%)	2 (0%)	47 81
All	All	2625/2736 (96%)	2545 (97%)	74 (3%)	6 (0%)	47 81

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%)	24 58
2	F	1156/1225 (94%)	1083 (94%)	73 (6%)	18 51
All	All	2329/2450 (95%)	2197 (94%)	132 (6%)	20 53

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 (i)

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 monosaccharides 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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	34/34 (100%)	0.17	2 (5%) 22 20	19, 34, 129, 166	0
1	E	31/34 (91%)	0.32	3 (9%) 7 8	40, 71, 175, 230	0
2	B	1326/1368 (96%)	0.36	125 (9%) 8 9	13, 62, 175, 215	0
2	F	1327/1368 (97%)	0.46	157 (11%) 4 5	11, 88, 145, 197	0
3	C	25/25 (100%)	-0.31	0 100 100	25, 38, 81, 88	0
3	G	25/25 (100%)	-0.11	0 100 100	45, 59, 118, 139	0
4	D	11/11 (100%)	-0.11	0 100 100	30, 38, 122, 159	0
4	H	11/11 (100%)	-0.21	0 100 100	33, 60, 119, 189	0
5	I	63/65 (96%)	-0.26	0 100 100	17, 71, 122, 170	0
5	J	63/65 (96%)	-0.37	0 100 100	26, 58, 137, 191	0
All	All	2916/3006 (97%)	0.36	287 (9%) 7 8	11, 70, 162, 230	0

All (287) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	801	VAL	23.0
2	B	809	GLU	18.3
2	F	232	GLU	15.7
2	F	231	GLY	12.1
2	B	810	LYS	11.2
2	B	1034	ALA	10.8
2	B	784	ILE	9.6
2	B	812	TYR	9.4
2	B	857	LEU	9.1
2	F	228	GLN	8.7
2	B	838	VAL	8.4
2	B	813	LEU	8.3
2	B	858	THR	8.2

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Mol	Chain	Res	Type	RSRZ
2	F	230	PRO	8.1
2	B	796	LEU	8.1
2	B	1243	GLU	8.0
2	F	207	ASP	7.9
2	F	213	SER	7.7
2	F	306	LEU	7.6
2	B	817	GLN	7.5
2	B	1045	PHE	7.4
2	F	209	LYS	7.3
2	F	305	ILE	7.2
2	B	799	HIS	7.0
2	F	536	LYS	6.9
2	F	224	ASN	6.8
2	B	833	LEU	6.8
2	F	688	PHE	6.4
2	B	861	ASP	6.4
2	F	802	GLU	6.3
2	F	402	GLN	6.3
2	B	868	ASP	6.2
2	B	822	MET	6.1
2	B	1248	SER	6.1
2	F	202	ASN	6.1
2	B	1242	TYR	6.1
2	F	400	ARG	6.1
2	B	815	TYR	6.0
2	F	679	ILE	6.0
2	B	884	ARG	5.9
2	B	814	TYR	5.8
2	F	203	ALA	5.7
2	F	818	ASN	5.6
2	B	883	TRP	5.6
1	E	28	A	5.5
2	B	823	TYR	5.5
2	F	307	ARG	5.5
2	B	1048	THR	5.4
2	B	800	PRO	5.4
2	B	841	ILE	5.4
2	B	818	ASN	5.4
2	F	682	PHE	5.2
2	B	816	LEU	5.2
2	F	225	LEU	5.2
2	F	211	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
2	F	578	VAL	5.2
2	B	1046	PHE	5.1
2	F	796	LEU	5.0
2	F	238	PHE	5.0
2	F	531	THR	5.0
2	F	314	LYS	5.0
2	F	694	MET	5.0
2	F	691	ARG	5.0
2	B	783	ARG	4.9
2	F	227	ALA	4.9
2	F	815	TYR	4.9
2	F	804	THR	4.9
2	B	1052	LEU	4.9
2	F	544	GLN	4.8
2	B	791	LEU	4.8
2	F	308	VAL	4.8
1	A	1	U	4.7
2	F	301	LEU	4.6
2	B	1036	TYR	4.6
2	B	1037	PHE	4.6
2	F	693	PHE	4.6
2	B	871	PRO	4.6
2	F	697	ILE	4.6
2	B	806	LEU	4.5
1	E	34	G	4.5
2	B	856	VAL	4.4
2	F	369	GLN	4.3
2	B	808	ASN	4.3
2	B	802	GLU	4.2
2	F	683	LEU	4.2
2	F	806	LEU	4.2
2	B	872	SER	4.2
2	F	698	HIS	4.2
2	B	1238	LEU	4.2
2	B	837	ASP	4.2
2	B	795	ILE	4.1
2	B	807	GLN	4.1
2	F	857	LEU	4.1
2	F	537	PRO	4.0
2	B	44	LYS	4.0
2	B	1039	TYR	4.0
2	F	673	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
2	F	856	VAL	4.0
2	F	234	LYS	3.9
2	B	836	TYR	3.9
2	B	867	SER	3.9
2	F	580	ILE	3.9
2	F	240	ASN	3.9
2	B	834	SER	3.9
2	F	501	ASN	3.9
2	F	853	ASP	3.9
2	F	833	LEU	3.9
2	B	1038	PHE	3.8
2	B	1244	LYS	3.8
2	F	362	TYR	3.8
2	F	896	LYS	3.8
2	F	222	LEU	3.8
2	F	212	LEU	3.8
2	F	883	TRP	3.8
2	B	780	ARG	3.8
2	F	449	PRO	3.7
2	B	805	GLN	3.7
2	F	247	GLY	3.7
2	B	31	LYS	3.6
2	F	816	LEU	3.6
2	F	189	VAL	3.6
2	B	828	LEU	3.6
2	F	452	VAL	3.5
2	B	538	ALA	3.5
2	F	128	TYR	3.5
2	F	286	TYR	3.5
2	F	1052	LEU	3.5
2	F	801	VAL	3.5
2	B	852	ILE	3.5
2	F	627	GLU	3.4
2	F	701	SER	3.4
2	B	781	MET	3.4
2	F	210	ALA	3.4
2	F	399	LEU	3.4
2	B	47	LEU	3.4
2	F	244	LEU	3.4
2	F	398	LEU	3.4
2	F	662	LEU	3.3
2	F	201	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	241	LEU	3.3
2	B	824	VAL	3.3
2	F	73	THR	3.3
2	F	809	GLU	3.3
2	B	864	ARG	3.2
2	B	1355	LEU	3.2
2	F	245	SER	3.2
2	F	145	SER	3.2
2	F	135	ILE	3.2
2	F	822	MET	3.2
2	F	237	LEU	3.2
2	F	1051	THR	3.2
2	F	1243	GLU	3.2
2	B	1073	VAL	3.2
2	F	451	TYR	3.2
2	F	674	GLN	3.2
2	F	577	SER	3.1
2	F	803	ASN	3.1
2	F	296	LEU	3.1
2	F	246	LEU	3.1
2	F	817	GLN	3.1
2	F	1039	TYR	3.1
2	F	670	ILE	3.1
2	F	811	LEU	3.1
2	B	1269	ILE	3.1
2	F	281	GLN	3.0
2	F	524	LEU	3.0
2	F	877	LYS	3.0
2	F	473	ILE	3.0
2	F	661	ARG	3.0
2	B	32	PHE	3.0
2	B	793	SER	3.0
2	B	661	ARG	3.0
2	B	886	LEU	3.0
2	B	1303	ARG	3.0
2	F	705	LYS	3.0
2	B	881	ASN	3.0
2	F	690	ASN	2.9
2	F	703	THR	2.9
2	B	1050	ILE	2.9
2	B	238	PHE	2.9
2	B	788	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	1050	ILE	2.9
2	F	397	ASP	2.9
2	B	1035	LYS	2.9
2	B	880	LYS	2.8
2	B	1309	ILE	2.8
2	F	396	GLU	2.8
2	F	529	TYR	2.8
2	B	45	LYS	2.8
2	B	1049	GLU	2.8
2	B	1249	PRO	2.8
2	B	894	GLN	2.8
2	B	870	VAL	2.8
2	F	1034	ALA	2.8
2	F	478	PHE	2.8
2	B	945	GLU	2.8
1	A	34	G	2.7
2	F	401	LYS	2.7
2	F	239	GLY	2.7
2	B	1246	LYS	2.7
2	F	689	ALA	2.7
2	B	28	PRO	2.7
2	F	823	TYR	2.7
2	B	787	GLY	2.7
2	B	862	LYS	2.7
2	B	1069	THR	2.7
2	F	290	PHE	2.6
2	B	1068	GLU	2.6
2	F	455	LEU	2.6
2	B	1241	HIS	2.6
2	F	156	LEU	2.6
2	B	43	ILE	2.6
2	F	900	LEU	2.6
2	B	1332	ASP	2.6
2	F	1049	GLU	2.6
2	F	667	ILE	2.6
2	F	839	ASP	2.6
2	F	841	ILE	2.6
2	B	876	VAL	2.6
2	B	1247	GLY	2.6
2	F	527	VAL	2.6
2	B	947	ASP	2.5
2	B	1237	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	627	GLU	2.5
2	F	453	GLY	2.5
2	F	867	SER	2.5
2	F	132	TYR	2.5
2	F	666	LEU	2.5
2	B	1302	ILE	2.5
2	B	887	LEU	2.5
2	B	1235	PHE	2.4
2	B	1059	LYS	2.4
2	F	481	VAL	2.4
2	F	813	LEU	2.4
2	B	531	THR	2.4
2	B	1266	LEU	2.4
2	F	658	GLY	2.4
2	F	122	ILE	2.4
2	B	380	LEU	2.4
2	B	1071	GLU	2.4
2	F	852	ILE	2.4
2	B	1095	VAL	2.3
2	F	863	ASN	2.3
2	B	859	ARG	2.3
2	F	868	ASP	2.3
2	F	242	ILE	2.3
2	B	29	SER	2.3
2	F	631	MET	2.3
2	B	529	TYR	2.3
2	B	906	GLY	2.3
2	B	1304	GLU	2.3
2	F	142	LEU	2.2
2	F	880	LYS	2.2
2	F	1061	PRO	2.2
2	B	1074	TRP	2.2
2	F	141	LYS	2.2
2	B	1043	MET	2.2
2	F	347	TYR	2.2
2	B	225	LEU	2.2
2	B	569	PHE	2.2
2	F	659	TRP	2.2
2	F	901	THR	2.2
2	B	842	VAL	2.2
2	F	836	TYR	2.2
2	B	241	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	564	LEU	2.2
2	F	1335	ARG	2.2
2	B	829	ASP	2.2
2	B	1051	THR	2.2
2	B	310	THR	2.1
2	B	242	ILE	2.1
2	F	448	ILE	2.1
2	F	233	LYS	2.1
1	E	31	U	2.1
2	F	129	HIS	2.1
2	F	221	ARG	2.1
2	F	704	PHE	2.1
2	F	820	ARG	2.1
2	F	172	GLY	2.1
2	F	468	LYS	2.0
2	F	446	PHE	2.0
2	B	1008	PHE	2.0
2	F	67	THR	2.0
2	F	195	LEU	2.0
2	F	346	LYS	2.0
2	B	840	ALA	2.0
2	F	450	TYR	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.