



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Oct 28, 2019 – 03:14 PM EDT

PDB ID : 6A5O
EMDB ID: : EMD-6981
Title : RNA polymerase II elongation complex stalled at SHL(-6) of the nucleosome
Authors : Kujirai, T.; Ehara, H.; Fujino, Y.; Shirouzu, M.; Sekine, S.; Kurumizaka, H.
Deposited on : 2018-06-25
Resolution : 9.90 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

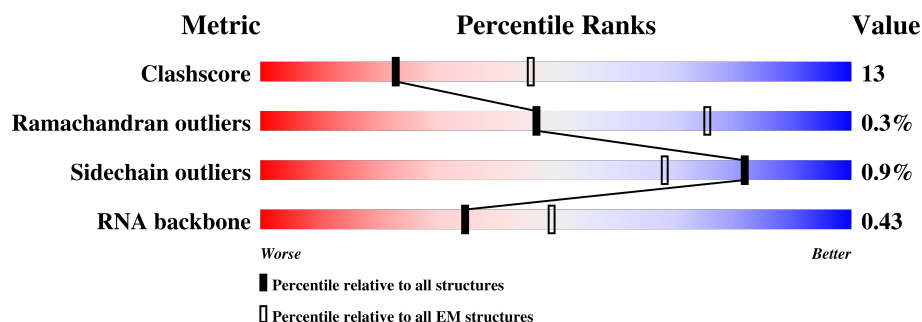
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.90 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1743	60% 20% . 19%
2	B	1227	67% 27% . 5%
3	C	304	69% 17% 13%
4	D	186	74% 9% .. 16%
5	E	214	76% 22% .
6	F	155	42% 12% 46%
7	G	171	81% 18% .
8	H	145	71% 21% 8%

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Mol	Chain	Length	Quality of chain
9	I	115	
10	J	72	
11	K	118	
12	L	72	
13	P	11	
14	T	198	
15	N	198	
16	a	139	
16	e	139	
17	b	106	
17	f	106	
18	c	133	
18	g	133	
19	d	129	
19	h	129	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 44485 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1408	Total	C	N	O	S	0	0
			11095	6997	1935	2093	70		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1161	Total	C	N	O	S	0	0
			9261	5835	1636	1732	58		

- Molecule 3 is a protein called RNA polymerase II third largest subunit B44, part of central core.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	263	Total	C	N	O	S	0	0
			2098	1319	354	413	12		

- Molecule 4 is a protein called RNA polymerase II subunit B32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	156	Total	C	N	O	S	0	0
			1210	753	210	245	2		

- Molecule 5 is a protein called RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1740	1094	312	324	10		

- Molecule 6 is a protein called RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	84	Total	C	N	O	S	0	0
			677	429	114	131	3		

- Molecule 7 is a protein called RNA polymerase II subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1324	858	214	247	5		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1052	671	169	208	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	111	Total	C	N	O	S	0	0
			917	565	161	180	11		

- Molecule 10 is a protein called RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			545	349	95	95	6		

- Molecule 11 is a protein called RNA polymerase II subunit B12.5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	113	Total	C	N	O	S	0	0
			932	599	160	169	4		

- Molecule 12 is a protein called RNA polymerase subunit ABC10-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			359	221	72	61	5		

- Molecule 13 is a RNA chain called RNA (5'-R(P*UP*GP*GP*GP*UP*GP*GP*UP*GP*GP*G P*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	11	Total	C	N	O	P	0	0
			232	103	34	84	11		

- Molecule 14 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	178	Total	C	N	O	P	0	0
			3631	1720	707	1027	177		

- Molecule 15 is a DNA chain called DNA (198-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	169	Total	C	N	O	P	0	0
			3476	1653	606	1048	169		

- Molecule 16 is a protein called Histone H3.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	a	97	Total	C	N	O	S	0	0
			797	503	155	137	2		
16	e	97	Total	C	N	O	S	0	0
			796	501	155	138	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-3	GLY	-	expression tag	UNP P84243
a	-2	SER	-	expression tag	UNP P84243
a	-1	HIS	-	expression tag	UNP P84243
e	-3	GLY	-	expression tag	UNP P84243
e	-2	SER	-	expression tag	UNP P84243
e	-1	HIS	-	expression tag	UNP P84243

- Molecule 17 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	80	Total	C	N	O	S	0	0
			638	401	125	111	1		
17	f	78	Total	C	N	O	S	0	0
			619	391	120	107	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	-3	GLY	-	expression tag	UNP P62805
b	-2	SER	-	expression tag	UNP P62805
b	-1	HIS	-	expression tag	UNP P62805
f	-3	GLY	-	expression tag	UNP P62805
f	-2	SER	-	expression tag	UNP P62805
f	-1	HIS	-	expression tag	UNP P62805

- Molecule 18 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	c	103	Total	C	N	O	0	0
			796	502	155	139		
18	g	105	Total	C	N	O	0	0
			810	511	158	141		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	-3	GLY	-	expression tag	UNP P04908
c	-2	SER	-	expression tag	UNP P04908
c	-1	HIS	-	expression tag	UNP P04908
g	-3	GLY	-	expression tag	UNP P04908
g	-2	SER	-	expression tag	UNP P04908
g	-1	HIS	-	expression tag	UNP P04908

- Molecule 19 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	d	95	Total	C	N	O	S	0
			746	468	136	140	2	0
19	h	93	Total	C	N	O	S	0
			725	456	130	137	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	-6	GLY	-	expression tag	UNP P06899
d	-5	SER	-	expression tag	UNP P06899
d	-4	HIS	-	expression tag	UNP P06899
h	-6	GLY	-	expression tag	UNP P06899
h	-5	SER	-	expression tag	UNP P06899
h	-4	HIS	-	expression tag	UNP P06899

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
20	J	1	Total 1	Zn 1	0
20	B	1	Total 1	Zn 1	0
20	I	2	Total 2	Zn 2	0
20	C	1	Total 1	Zn 1	0
20	A	2	Total 2	Zn 2	0
20	L	1	Total 1	Zn 1	0

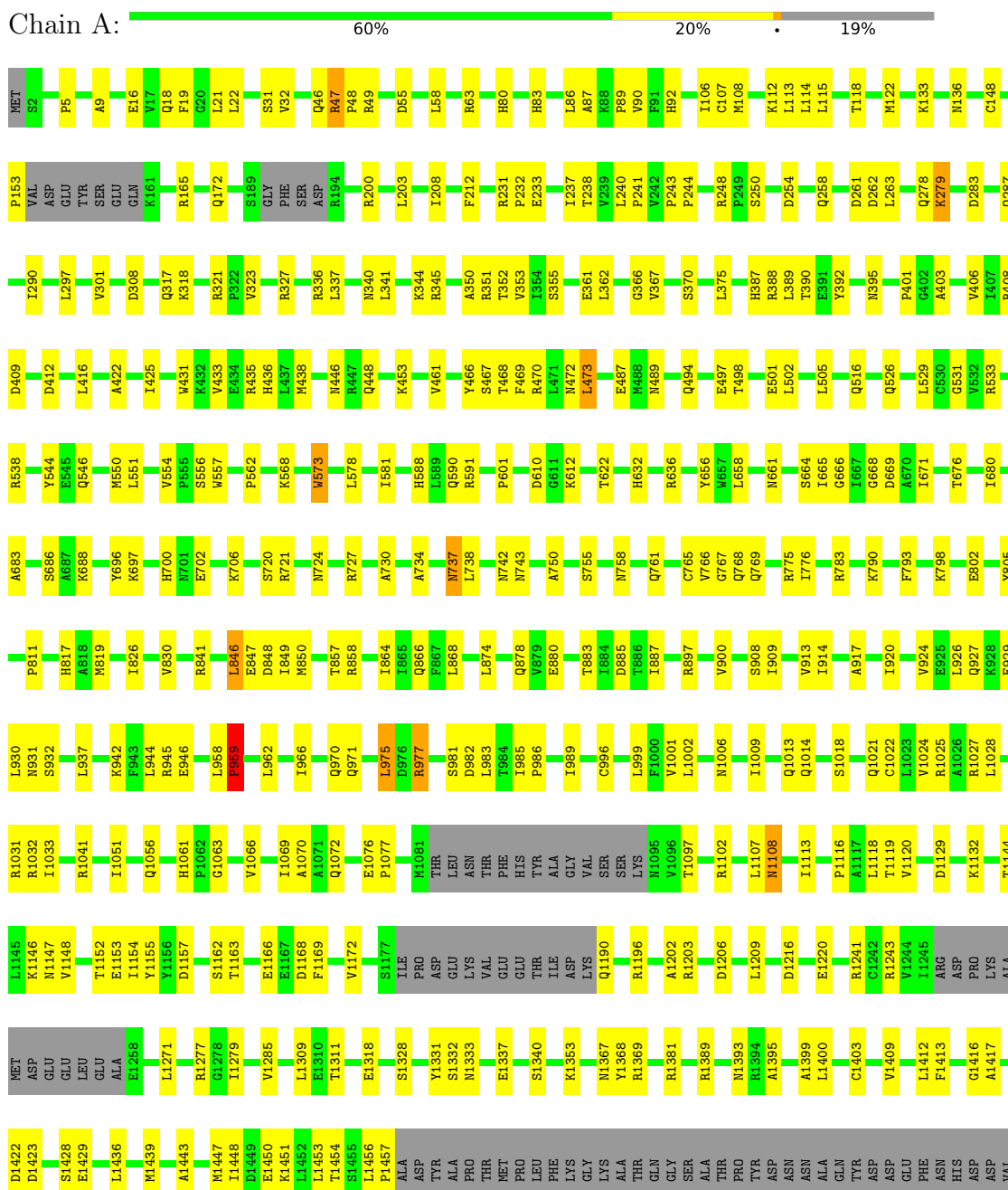
- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total 1	Mg 1	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

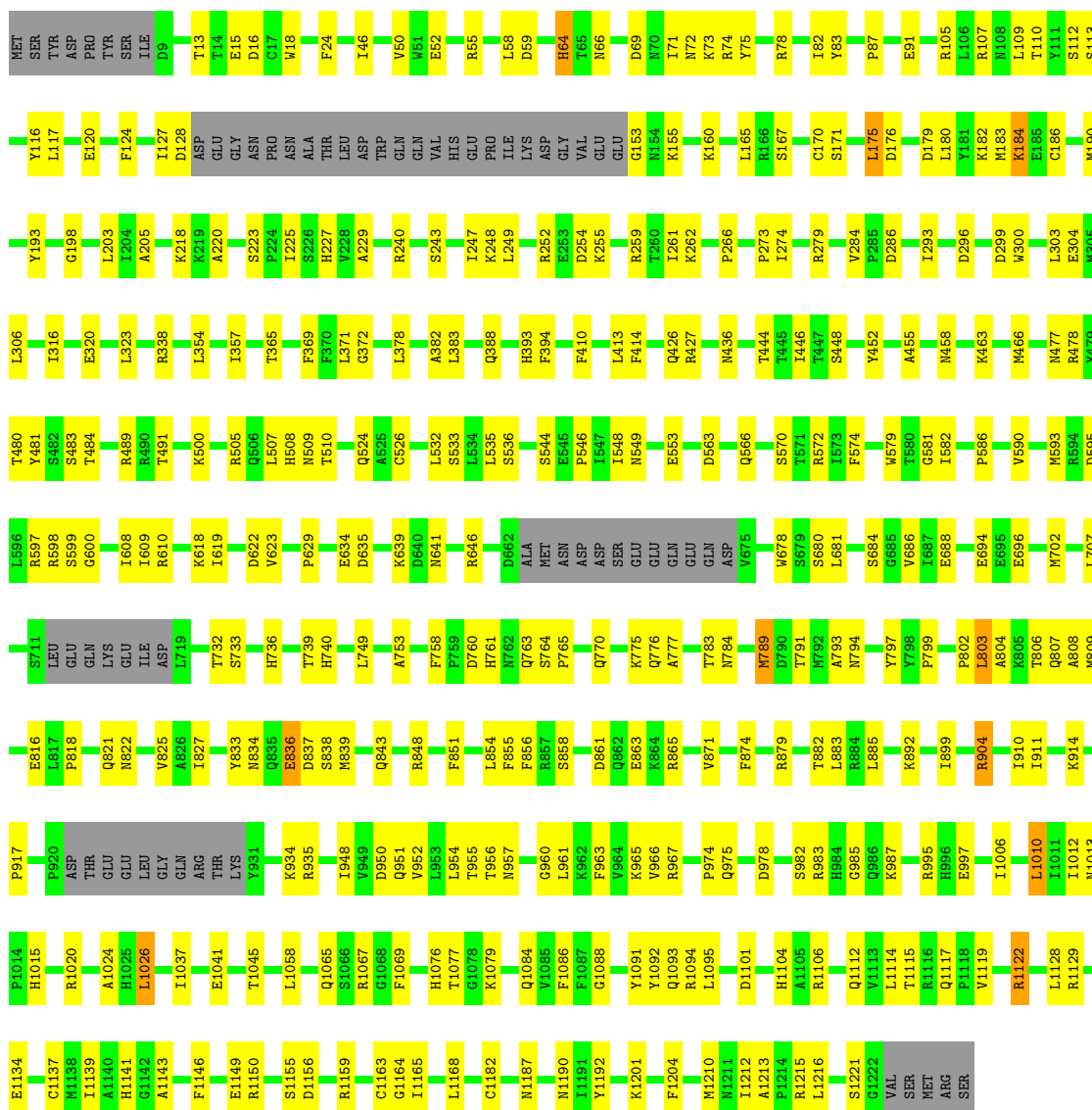
- Molecule 1: DNA-directed RNA polymerase subunit



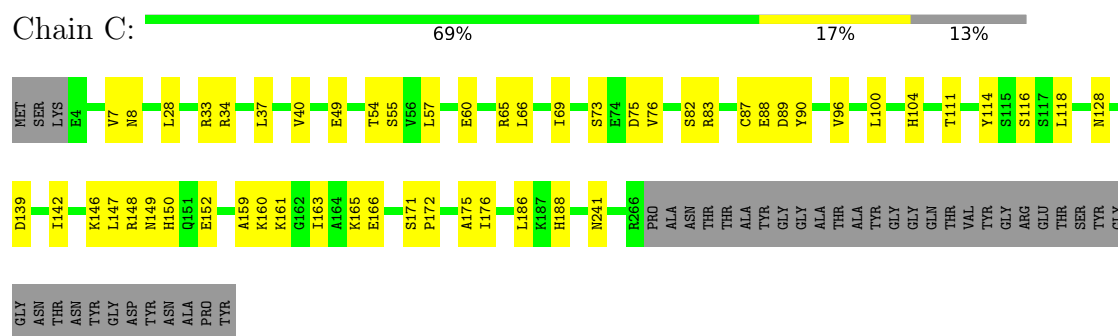
[illegible]

- Molecule 2: DNA-directed RNA polymerase subunit beta

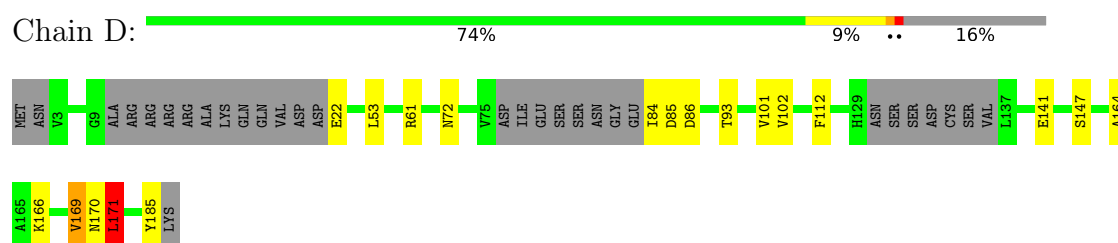
Chain B:  67% 27% 5%



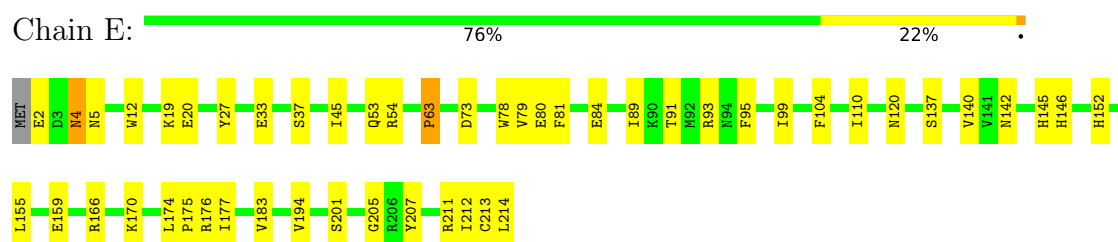
- Molecule 3: RNA polymerase II third largest subunit B44, part of central core



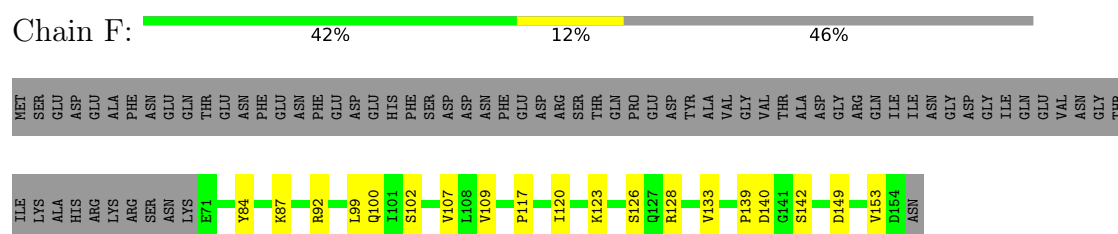
- Molecule 4: RNA polymerase II subunit B32



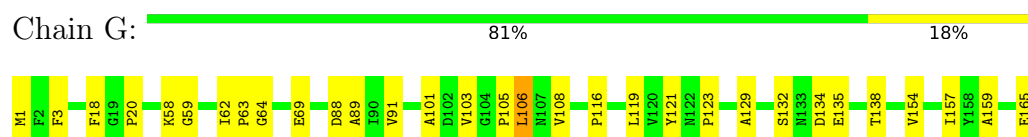
- Molecule 5: RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III



- Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III

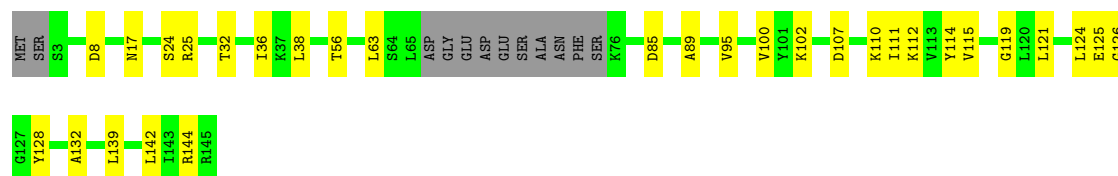


- Molecule 7: RNA polymerase II subunit



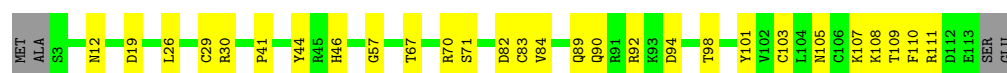
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 



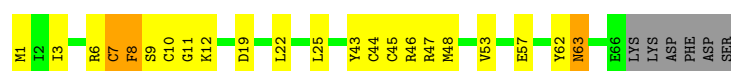
- Molecule 9: DNA-directed RNA polymerase subunit

Chain I: 



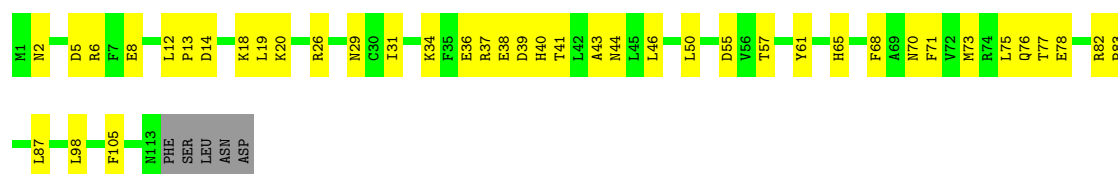
- Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III

Chain J: 



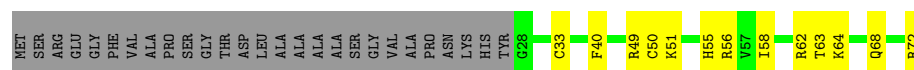
- Molecule 11: RNA polymerase II subunit B12.5

Chain K: 

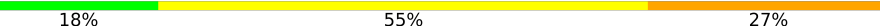


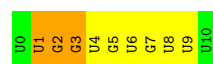
- Molecule 12: RNA polymerase subunit ABC10-alpha

Chain L: 



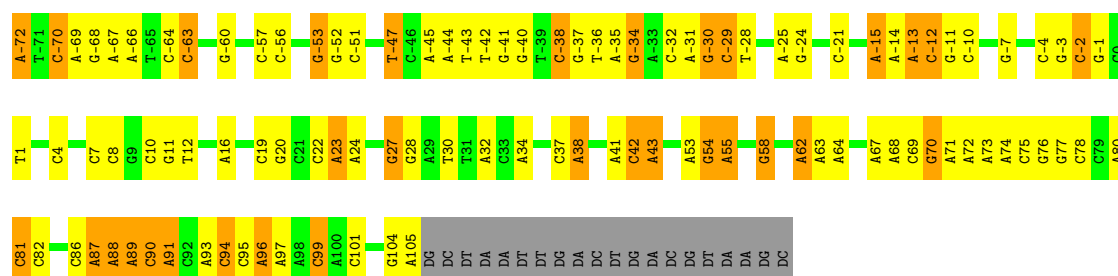
- Molecule 13: RNA (5'-R(P*UP*GP*GP*GP*UP*GP*GP*UP*GP*GP*C)-3')

Chain P: 



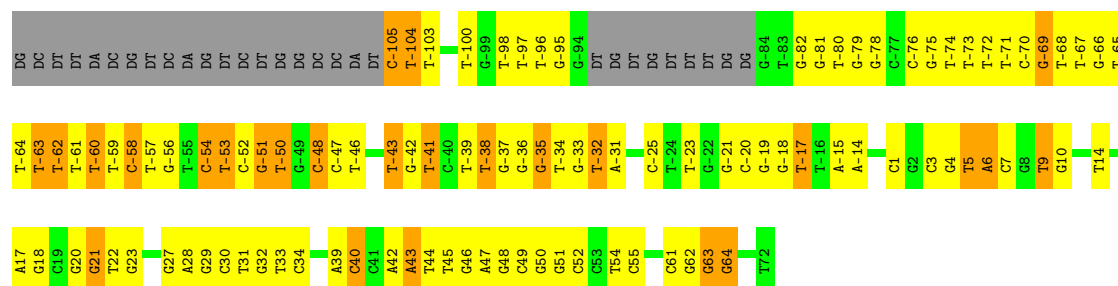
- Molecule 14: DNA (198-MER)

Chain T: 



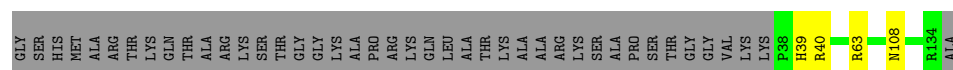
• Molecule 15: DNA (198-MER)

Chain N: 32% 40% 13% 15%



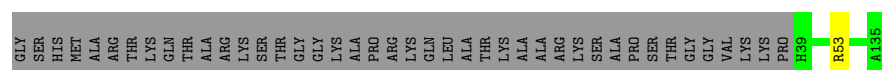
• Molecule 16: Histone H3.3

Chain a: 67% 30%



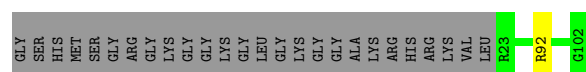
• Molecule 16: Histone H3.3

Chain e: 69% 30%



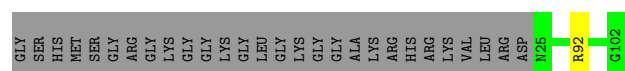
• Molecule 17: Histone H4

Chain b: 75% 25%



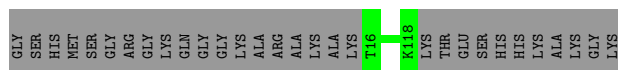
• Molecule 17: Histone H4

Chain f: 73% 26%



• Molecule 18: Histone H2A type 1-B/E

Chain c: 77% 23%



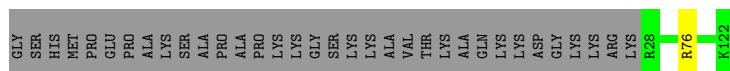
- Molecule 18: Histone H2A type 1-B/E

Chain g: 78% 21%



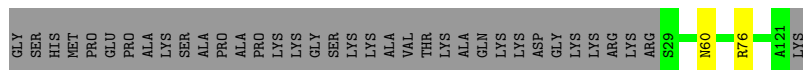
- Molecule 19: Histone H2B type 1-J

Chain d: 73% 26%



- Molecule 19: Histone H2B type 1-J

Chain h:  71% . 28%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12692	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.62	1/11299 (0.0%)	0.73	3/15266 (0.0%)
10	J	0.89	1/554 (0.2%)	0.82	0/742
11	K	0.56	0/953	0.66	0/1291
12	L	0.60	0/365	0.71	0/484
13	P	1.20	3/257 (1.2%)	1.40	2/398 (0.5%)
14	T	0.91	14/4083 (0.3%)	1.32	43/6289 (0.7%)
15	N	0.78	13/3889 (0.3%)	1.35	46/6007 (0.8%)
16	a	0.34	0/809	0.53	0/1085
16	e	0.38	0/807	0.52	0/1081
17	b	0.38	0/645	0.57	0/862
17	f	0.40	0/626	0.56	0/837
18	c	0.35	0/806	0.51	0/1089
18	g	0.35	0/820	0.52	0/1107
19	d	0.38	0/757	0.54	0/1015
19	h	0.38	0/736	0.55	0/990
2	B	0.65	1/9441 (0.0%)	0.76	2/12732 (0.0%)
3	C	0.66	0/2139	0.76	1/2895 (0.0%)
4	D	0.29	0/1221	0.52	0/1648
5	E	0.59	0/1772	0.66	0/2385
6	F	0.58	0/687	0.64	0/931
7	G	0.33	0/1353	0.61	0/1837
8	H	0.61	0/1069	0.67	0/1444
9	I	0.42	0/934	0.70	0/1257
All	All	0.64	33/46022 (0.1%)	0.86	97/63672 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
10	J	0	1
2	B	0	8
3	C	0	3
5	E	0	2
9	I	0	1
All	All	0	23

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	89	DA	C1'-N9	-12.43	1.29	1.47
14	T	88	DA	C1'-N9	-10.08	1.33	1.47
14	T	-72	DA	O5'-C5'	9.22	1.65	1.42
14	T	70	DG	C1'-N9	-7.41	1.36	1.47
15	N	-69	DG	C1'-N9	-6.89	1.37	1.47
14	T	93	DA	C1'-N9	-6.75	1.37	1.47
14	T	96	DA	C1'-N9	-6.40	1.38	1.47
14	T	97	DA	C1'-N9	-6.35	1.38	1.47
1	A	573	TRP	CB-CG	-6.04	1.39	1.50
13	P	1	U	C1'-N1	5.98	1.57	1.48
14	T	91	DA	C1'-N9	-5.93	1.39	1.47
14	T	81	DC	C1'-N1	5.87	1.56	1.49
2	B	789	MET	CA-CB	-5.83	1.41	1.53
15	N	-62	DT	C1'-N1	5.81	1.56	1.49
13	P	2	G	C1'-N9	-5.74	1.38	1.46
14	T	87	DA	C3'-O3'	-5.56	1.36	1.44
15	N	-41	DT	C1'-N1	5.50	1.56	1.49
10	J	7	CYS	CB-SG	-5.41	1.73	1.81
13	P	3	G	C1'-N9	-5.36	1.39	1.46
15	N	-97	DT	C1'-N1	5.30	1.56	1.49
15	N	-53	DT	C1'-N1	5.28	1.56	1.49
14	T	55	DA	C1'-N9	-5.27	1.39	1.47
15	N	-98	DT	C1'-N1	5.22	1.56	1.49
15	N	-96	DT	C1'-N1	5.19	1.56	1.49
15	N	-104	DT	C1'-N1	5.18	1.55	1.49
14	T	101	DC	C1'-N1	5.17	1.55	1.49
15	N	-103	DT	C1'-N1	5.17	1.55	1.49
15	N	-100	DT	C1'-N1	5.16	1.55	1.49
15	N	-60	DT	C1'-N1	5.11	1.55	1.49
15	N	-43	DT	C1'-N1	5.11	1.55	1.49
14	T	62	DA	C1'-N9	-5.10	1.40	1.47
15	N	-105	DC	C1'-N1	5.09	1.55	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	99	DC	C1'-N1	5.06	1.55	1.49

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	20	DG	O3'-P-O5'	-12.00	81.20	104.00
15	N	20	DG	OP2-P-O3'	-10.01	83.17	105.20
15	N	14	DT	O4'-C1'-N1	8.62	114.03	108.00
15	N	21	DG	O4'-C1'-N9	8.39	113.88	108.00
15	N	34	DC	P-O3'-C3'	7.98	129.28	119.70
15	N	64	DG	P-O3'-C3'	7.88	129.16	119.70
15	N	5	DT	O4'-C1'-N1	7.81	113.47	108.00
14	T	-53	DG	P-O3'-C3'	7.57	128.78	119.70
14	T	-47	DT	O4'-C1'-N1	7.55	113.29	108.00
14	T	-31	DA	O4'-C1'-N9	7.22	113.05	108.00
14	T	-21	DC	O4'-C1'-N1	7.21	113.05	108.00
15	N	-23	DT	O4'-C1'-N1	7.17	113.02	108.00
15	N	-35	DG	O4'-C1'-N9	-7.09	103.03	108.00
15	N	63	DG	P-O3'-C3'	7.03	128.14	119.70
15	N	-38	DT	P-O3'-C3'	6.95	128.03	119.70
15	N	23	DG	O4'-C1'-N9	6.90	112.83	108.00
15	N	54	DT	P-O3'-C3'	6.90	127.98	119.70
15	N	-63	DT	O4'-C1'-N1	6.88	112.81	108.00
14	T	43	DA	P-O3'-C3'	6.86	127.93	119.70
15	N	21	DG	P-O3'-C3'	6.85	127.92	119.70
14	T	42	DC	P-O3'-C3'	6.75	127.80	119.70
14	T	-51	DC	P-O3'-C3'	6.73	127.77	119.70
15	N	-33	DG	P-O3'-C3'	6.71	127.75	119.70
14	T	23	DA	P-O3'-C3'	6.69	127.73	119.70
13	P	2	G	C4-N9-C1'	6.68	135.18	126.50
2	B	1026	LEU	CA-CB-CG	-6.65	100.02	115.30
14	T	-12	DC	P-O3'-C3'	6.63	127.66	119.70
15	N	-21	DG	P-O3'-C3'	6.53	127.54	119.70
14	T	-13	DA	P-O3'-C3'	6.53	127.53	119.70
15	N	-54	DC	P-O3'-C3'	6.50	127.50	119.70
14	T	-63	DC	P-O3'-C3'	6.50	127.50	119.70
15	N	42	DA	P-O3'-C3'	6.44	127.43	119.70
14	T	16	DA	O4'-C1'-N9	6.40	112.48	108.00
15	N	30	DC	O4'-C1'-N1	6.39	112.48	108.00
15	N	-51	DG	P-O3'-C3'	6.37	127.35	119.70
14	T	58	DG	O4'-C1'-N9	-6.35	103.56	108.00
15	N	21	DG	O5'-P-OP2	6.28	118.23	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	20	DG	P-O3'-C3'	6.24	127.19	119.70
14	T	38	DA	P-O3'-C3'	6.18	127.12	119.70
14	T	22	DC	O4'-C1'-N1	6.16	112.31	108.00
15	N	20	DG	C3'-C2'-C1'	-6.13	95.14	102.50
14	T	12	DT	O4'-C1'-N1	6.04	112.23	108.00
14	T	-15	DA	O4'-C1'-N9	6.02	112.22	108.00
14	T	-29	DC	P-O3'-C3'	6.00	126.89	119.70
14	T	-30	DG	P-O3'-C3'	5.99	126.89	119.70
15	N	20	DG	OP1-P-O3'	-5.98	92.05	105.20
14	T	30	DT	P-O3'-C3'	5.90	126.78	119.70
15	N	9	DT	N3-C2-O2	-5.84	118.80	122.30
14	T	-70	DC	O4'-C1'-N1	5.83	112.08	108.00
1	A	279	LYS	CB-CA-C	5.77	121.94	110.40
14	T	90	DC	O4'-C4'-C3'	-5.76	102.19	104.50
14	T	94	DC	O4'-C1'-N1	5.74	112.02	108.00
15	N	-25	DC	O4'-C1'-N1	5.74	112.01	108.00
15	N	-63	DT	C1'-O4'-C4'	-5.73	104.37	110.10
14	T	-60	DG	O4'-C1'-N9	5.71	112.00	108.00
14	T	-43	DT	P-O3'-C3'	5.71	126.55	119.70
15	N	-58	DC	P-O3'-C3'	5.70	126.54	119.70
14	T	-38	DC	P-O3'-C3'	5.65	126.48	119.70
14	T	41	DA	O4'-C1'-N9	5.64	111.94	108.00
14	T	54	DG	P-O3'-C3'	5.63	126.45	119.70
1	A	977	ARG	CA-CB-CG	5.63	125.78	113.40
14	T	-2	DC	O4'-C1'-N1	5.55	111.89	108.00
13	P	2	G	C8-N9-C1'	-5.55	119.78	127.00
15	N	21	DG	C1'-O4'-C4'	-5.50	104.60	110.10
14	T	-34	DG	C3'-C2'-C1'	-5.47	95.94	102.50
14	T	-4	DC	P-O3'-C3'	5.46	126.26	119.70
14	T	32	DA	O4'-C1'-N9	5.45	111.81	108.00
14	T	1	DT	O4'-C1'-N1	5.41	111.79	108.00
15	N	-21	DG	C1'-O4'-C4'	-5.41	104.69	110.10
15	N	40	DC	P-O3'-C3'	5.41	126.19	119.70
15	N	-53	DT	O4'-C1'-N1	5.35	111.75	108.00
15	N	-53	DT	P-O3'-C3'	5.34	126.11	119.70
15	N	-48	DC	O4'-C1'-N1	5.34	111.74	108.00
15	N	27	DG	C1'-O4'-C4'	-5.34	104.76	110.10
15	N	29	DG	O4'-C1'-N9	5.30	111.71	108.00
15	N	43	DA	P-O3'-C3'	5.29	126.05	119.70
15	N	-17	DT	P-O3'-C3'	5.27	126.02	119.70
14	T	-47	DT	C1'-O4'-C4'	-5.26	104.84	110.10
15	N	-50	DT	O4'-C1'-N1	5.24	111.67	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	87	DA	O4'-C4'-C3'	-5.24	102.41	104.50
3	C	186	LEU	CA-CB-CG	-5.22	103.29	115.30
15	N	-36	DG	P-O3'-C3'	5.21	125.96	119.70
2	B	803	LEU	CA-CB-CG	-5.20	103.34	115.30
14	T	27	DG	O4'-C1'-N9	5.19	111.63	108.00
14	T	-40	DG	O4'-C1'-N9	5.18	111.62	108.00
14	T	70	DG	C4'-C3'-C2'	-5.17	98.44	103.10
15	N	21	DG	OP1-P-OP2	5.14	127.31	119.60
14	T	-2	DC	C1'-O4'-C4'	-5.09	105.01	110.10
15	N	6	DA	C3'-C2'-C1'	-5.07	96.41	102.50
15	N	-20	DC	O4'-C1'-N1	5.07	111.55	108.00
15	N	-32	DT	O4'-C1'-N1	5.06	111.54	108.00
15	N	1	DC	O4'-C1'-N1	5.06	111.54	108.00
14	T	4	DC	P-O3'-C3'	5.05	125.76	119.70
1	A	473	LEU	CA-CB-CG	-5.05	103.69	115.30
14	T	16	DA	C1'-O4'-C4'	-5.05	105.05	110.10
14	T	-1	DG	P-O3'-C3'	5.02	125.73	119.70
14	T	-32	DC	O4'-C1'-N1	5.02	111.52	108.00

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1108	ASN	Peptide
1	A	46	GLN	Peptide
1	A	466	TYR	Peptide
1	A	846	LEU	Peptide
1	A	920	ILE	Peptide
1	A	959	PRO	Peptide
1	A	975	LEU	Peptide
1	A	977	ARG	Peptide
2	B	1086	PHE	Peptide
2	B	175	LEU	Peptide
2	B	393	HIS	Peptide
2	B	458	ASN	Peptide
2	B	508	HIS	Peptide
2	B	64	HIS	Peptide
2	B	836	GLU	Peptide
2	B	910	ILE	Peptide
3	C	87	CYS	Peptide
3	C	88	GLU	Peptide
3	C	89	ASP	Peptide

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Mol	Chain	Res	Type	Group
5	E	170	LYS	Peptide
5	E	63	PRO	Peptide
9	I	94	ASP	Peptide
10	J	63	ASN	Peptide

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	11095	0	11132	298	0
2	B	9261	0	9265	256	0
3	C	2098	0	2060	34	0
4	D	1210	0	1205	15	0
5	E	1740	0	1754	28	0
6	F	677	0	693	15	0
7	G	1324	0	1342	27	0
8	H	1052	0	1050	19	0
9	I	917	0	870	18	0
10	J	545	0	561	24	0
11	K	932	0	944	35	0
12	L	359	0	359	8	0
13	P	232	0	114	14	0
14	T	3631	0	1981	161	0
15	N	3476	0	1916	126	0
16	a	797	0	835	0	0
16	e	796	0	832	0	0
17	b	638	0	676	0	0
17	f	619	0	659	0	0
18	c	796	0	848	0	0
18	g	810	0	866	0	0
19	d	746	0	771	0	0
19	h	725	0	745	0	0
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	A	1	0	0	0	0
All	All	44485	0	41478	898	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (898) 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)
15:N:-66:DG:H2''	15:N:-65:DT:C5'	1.29	1.61
14:T:-72:DA:O5'	14:T:-72:DA:C5'	1.65	1.44
15:N:-66:DG:C2'	15:N:-65:DT:H5'	1.49	1.43
1:A:63:ARG:HH22	14:T:-13:DA:C5'	112.64	1.39
1:A:118:THR:CB	14:T:-3:DG:H5''	49.05	1.33
1:A:318:LYS:HD2	14:T:96:DA:N6	1.44	1.30
14:T:62:DA:C6	14:T:63:DA:N6	2.02	1.26
1:A:63:ARG:NE	15:N:17:DA:H4'	115.16	1.23
2:B:452:TYR:CE1	14:T:95:DC:H5'	1.81	1.15
15:N:-66:DG:C2'	15:N:-65:DT:C5'	2.14	1.11
1:A:63:ARG:CD	15:N:17:DA:H4'	114.22	1.09
1:A:318:LYS:CD	14:T:96:DA:H61	1.64	1.08
14:T:69:DC:H2''	14:T:70:DG:OP1	1.45	1.08
1:A:118:THR:HB	14:T:-3:DG:C5'	48.01	1.07
15:N:-65:DT:C2'	15:N:-64:DT:H5''	1.85	1.07
15:N:-65:DT:H2''	15:N:-64:DT:H5''	1.11	1.06
1:A:63:ARG:HH22	14:T:-13:DA:H5'	113.00	1.06
14:T:62:DA:N1	14:T:63:DA:C6	2.24	1.05
1:A:497:GLU:OE1	7:G:64:GLY:HA2	1.57	1.05
1:A:63:ARG:NH2	14:T:-13:DA:H5'	112.26	1.05
2:B:452:TYR:HE1	14:T:95:DC:H5'	1.17	1.04
1:A:63:ARG:NH2	14:T:-13:DA:C5'	111.91	1.04
1:A:118:THR:CB	14:T:-3:DG:C5'	48.47	1.03
15:N:-65:DT:H2''	15:N:-64:DT:C5'	1.90	1.02
1:A:1202:ALA:O	1:A:1206:ASP:HB2	1.60	1.02
1:A:1448:ILE:HG22	7:G:59:GLY:H	1.24	1.01
14:T:71:DA:H2''	14:T:72:DA:OP1	1.60	1.00
14:T:62:DA:C2	14:T:63:DA:C6	2.51	0.98
1:A:63:ARG:HH22	14:T:-13:DA:H5''	113.40	0.98
1:A:318:LYS:HD2	14:T:96:DA:H61	0.84	0.98
14:T:62:DA:C2	14:T:63:DA:C5	2.53	0.97
14:T:34:DA:N6	15:N:-35:DG:C6	2.33	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:HE	15:N:17:DA:H4'	114.98	0.96
1:A:63:ARG:HD2	15:N:17:DA:O3'	115.70	0.96
14:T:34:DA:N6	15:N:-35:DG:O6	2.00	0.94
2:B:549:ASN:O	2:B:553:GLU:HB2	1.67	0.93
1:A:1450:GLU:OE1	7:G:58:LYS:HE2	1.67	0.93
14:T:77:DG:H2''	14:T:78:DC:OP1	1.68	0.93
1:A:118:THR:OG1	14:T:-3:DG:H5'	46.73	0.92
14:T:104:DG:H1	15:N:-104:DT:H3	1.18	0.92
14:T:62:DA:C6	14:T:63:DA:C6	2.58	0.91
15:N:-64:DT:H2''	15:N:-63:DT:O4'	1.70	0.90
1:A:118:THR:OG1	14:T:-3:DG:C5'	47.59	0.89
14:T:38:DA:C2	15:N:-37:DG:N2	2.42	0.88
14:T:69:DC:O2	15:N:-69:DG:N2	2.08	0.87
1:A:118:THR:HB	14:T:-3:DG:H5''	48.58	0.87
1:A:318:LYS:CD	14:T:96:DA:N6	2.30	0.86
14:T:-47:DT:O4	15:N:47:DA:N6	2.08	0.85
1:A:63:ARG:HE	15:N:17:DA:C4'	115.63	0.85
1:A:63:ARG:NH2	14:T:-13:DA:H5''	112.67	0.83
14:T:64:DA:N1	15:N:-64:DT:O4	2.11	0.83
1:A:318:LYS:HD2	14:T:96:DA:C6	2.16	0.81
14:T:80:DA:C2	15:N:-79:DG:C2	2.69	0.81
14:T:105:DA:H61	15:N:-105:DC:H42	1.25	0.80
14:T:77:DG:H2''	14:T:78:DC:H5'	1.63	0.79
14:T:95:DC:O5'	14:T:95:DC:H6	1.65	0.79
14:T:62:DA:N6	14:T:63:DA:N6	2.32	0.77
14:T:82:DC:O2	15:N:-82:DG:N2	2.14	0.77
2:B:463:LYS:NZ	15:N:-95:DG:H21	1.83	0.77
2:B:83:TYR:HB2	2:B:116:TYR:HB2	1.65	0.76
1:A:63:ARG:HD2	15:N:17:DA:H4'	114.02	0.76
2:B:1155:SER:HG	2:B:1156:ASP:H	1.33	0.76
14:T:62:DA:C4	14:T:63:DA:N7	2.54	0.76
2:B:46:ILE:O	15:N:7:DC:H3'	85.04	0.76
15:N:-76:DC:H2''	15:N:-75:DG:H8	1.52	0.75
1:A:63:ARG:HD2	15:N:17:DA:C3'	115.98	0.75
2:B:1187:ASN:HD21	2:B:1190:ASN:HB3	1.52	0.74
14:T:80:DA:N3	15:N:-79:DG:N2	2.35	0.74
14:T:-53:DG:H2''	14:T:-52:DG:OP2	1.87	0.73
7:G:106:LEU:HG	7:G:157:ILE:HD11	1.70	0.73
14:T:62:DA:N3	14:T:63:DA:C5	2.56	0.73
14:T:74:DA:H2'	14:T:75:DC:C6	2.24	0.72
15:N:-66:DG:H2''	15:N:-65:DT:C4'	2.17	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:7:G:C6	14:T:91:DA:C6	2.77	0.72
1:A:63:ARG:CD	15:N:17:DA:O3'	115.91	0.72
6:F:128:ARG:HH21	6:F:153:VAL:H	1.35	0.71
1:A:1448:ILE:HG22	7:G:59:GLY:N	2.01	0.71
1:A:819:MET:SD	2:B:509:ASN:ND2	2.61	0.71
10:J:10:CYS:SG	10:J:11:GLY:N	2.64	0.71
1:A:63:ARG:HH12	14:T:-13:DA:P	111.47	0.70
15:N:-66:DG:C2'	15:N:-65:DT:O5'	2.37	0.70
2:B:205:ALA:HB3	2:B:491:THR:HG22	1.73	0.70
12:L:49:ARG:HA	12:L:56:ARG:HA	1.73	0.70
7:G:132:SER:HB2	7:G:135:GLU:HB2	1.74	0.70
14:T:77:DG:C6	14:T:78:DC:C4	2.80	0.69
2:B:74:ARG:HB2	2:B:124:PHE:HB2	1.73	0.69
8:H:56:THR:HB	8:H:144:ARG:HB3	1.74	0.68
1:A:63:ARG:HD2	15:N:17:DA:C4'	114.68	0.68
1:A:63:ARG:CD	15:N:17:DA:C4'	114.88	0.68
2:B:78:ARG:HB3	15:N:28:DA:P	125.89	0.68
14:T:80:DA:C2	15:N:-79:DG:N2	2.61	0.68
9:I:29:CYS:SG	9:I:30:ARG:N	2.68	0.67
1:A:63:ARG:HE	15:N:17:DA:C5'	115.68	0.67
1:A:1448:ILE:CG2	7:G:59:GLY:H	2.04	0.67
9:I:70:ARG:HA	9:I:84:VAL:HA	1.75	0.67
1:A:588:HIS:HB3	1:A:590:GLN:HE22	1.59	0.67
2:B:770:GLN:HE22	2:B:1093:GLN:HE22	1.41	0.67
1:A:89:PRO:HB3	1:A:238:THR:HG22	1.75	0.67
1:A:1006:ASN:H	1:A:1009:ILE:HD12	1.58	0.67
13:P:2:G:C6	13:P:3:G:C6	2.83	0.67
3:C:49:GLU:HG2	12:L:68:GLN:HG2	1.75	0.67
14:T:62:DA:C5	14:T:63:DA:N6	2.62	0.67
1:A:352:THR:OG1	1:A:353:VAL:N	2.24	0.66
10:J:1:MET:N	10:J:53:VAL:O	2.28	0.66
3:C:28:LEU:HD21	11:K:98:LEU:HD21	1.77	0.66
14:T:77:DG:C2	14:T:78:DC:C2	2.83	0.66
2:B:66:ASN:HB3	2:B:69:ASP:H	1.59	0.65
14:T:75:DC:H2''	14:T:76:DG:H8	1.62	0.65
1:A:1413:PHE:O	1:A:1417:ALA:HB2	1.97	0.65
1:A:1436:LEU:HD22	7:G:63:PRO:HG2	1.79	0.65
1:A:883:THR:O	1:A:1027:ARG:NH2	2.28	0.65
1:A:113:LEU:O	1:A:165:ARG:NH2	2.30	0.65
1:A:588:HIS:NE2	1:A:971:GLN:OE1	2.29	0.65
1:A:883:THR:OG1	1:A:1027:ARG:NH2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:ARG:HH22	1:A:1108:ASN:HD21	1.43	0.64
4:D:169:VAL:HG12	4:D:170:ASN:N	2.11	0.64
15:N:48:DG:C4	15:N:49:DC:C5	2.85	0.64
7:G:89:ALA:HB2	7:G:103:VAL:HG22	1.79	0.64
2:B:524:GLN:HE22	14:T:86:DC:H41	1.46	0.64
9:I:70:ARG:HG2	9:I:84:VAL:HG12	1.79	0.64
1:A:351:ARG:NH2	1:A:487:GLU:OE1	2.27	0.64
2:B:574:PHE:HB2	2:B:618:LYS:HG2	1.80	0.64
1:A:996:CYS:SG	1:A:1025:ARG:NH1	2.71	0.64
2:B:455:ALA:HB1	14:T:94:DC:H5''	1.78	0.64
14:T:-45:DA:C2	15:N:46:DG:N2	2.66	0.64
1:A:562:PRO:HG2	1:A:573:TRP:HE1	1.61	0.64
2:B:995:ARG:NH2	11:K:39:ASP:OD2	2.31	0.63
1:A:203:LEU:HB3	1:A:208:ILE:HD11	1.79	0.63
4:D:169:VAL:C	4:D:171:LEU:H	2.02	0.63
2:B:105:ARG:O	2:B:965:LYS:NZ	2.31	0.63
15:N:-64:DT:H2'	15:N:-63:DT:C6	2.33	0.63
13:P:7:G:O6	14:T:91:DA:N6	2.31	0.63
2:B:193:TYR:OH	2:B:478:ARG:NH2	2.32	0.63
1:A:1457:PRO:O	7:G:20:PRO:HB3	1.99	0.63
2:B:688:GLU:OE2	2:B:740:HIS:NE2	2.32	0.62
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.82	0.62
2:B:1163:CYS:SG	2:B:1187:ASN:ND2	2.67	0.62
1:A:1119:THR:HB	1:A:1331:TYR:HB3	1.80	0.62
2:B:1065:GLN:OE1	2:B:1069:PHE:N	2.32	0.62
2:B:190:MET:SD	2:B:190:MET:N	2.72	0.62
2:B:833:TYR:O	2:B:838:SER:OG	2.18	0.62
9:I:98:THR:OG1	9:I:111:ARG:NH2	2.33	0.62
1:A:848:ASP:N	1:A:848:ASP:OD1	2.30	0.62
14:T:74:DA:H2''	14:T:75:DC:O5'	1.99	0.62
2:B:579:TRP:NE1	2:B:581:GLY:O	2.32	0.61
2:B:586:PRO:HG2	2:B:610:ARG:HH21	1.65	0.61
1:A:1448:ILE:N	7:G:59:GLY:O	2.33	0.61
1:A:874:LEU:HD13	1:A:959:PRO:HG3	1.81	0.61
1:A:366:GLY:HA3	1:A:470:ARG:HB2	1.82	0.61
1:A:944:LEU:HD11	1:A:1022:CYS:HB3	1.82	0.61
2:B:590:VAL:HG21	2:B:610:ARG:HD2	1.82	0.61
11:K:20:LYS:HB3	11:K:34:LYS:HB3	1.82	0.61
2:B:463:LYS:HZ2	15:N:-95:DG:H21	1.47	0.61
14:T:27:DG:H2''	14:T:28:DG:C8	2.35	0.61
1:A:664:SER:OG	1:A:665:ILE:N	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:807:GLN:N	2:B:1045:THR:OG1	2.28	0.61
14:T:34:DA:C6	15:N:-35:DG:C6	2.89	0.61
14:T:54:DG:H2''	14:T:55:DA:OP2	2.00	0.61
1:A:966:ILE:HD11	1:A:1028:LEU:HD21	1.83	0.61
2:B:761:HIS:HB2	2:B:1024:ALA:HB2	1.83	0.61
2:B:791:THR:HA	2:B:858:SER:H	1.65	0.60
1:A:327:ARG:HG3	1:A:1409:VAL:HG21	1.82	0.60
1:A:118:THR:N	14:T:-3:DG:OP1	50.77	0.60
14:T:80:DA:N6	15:N:-81:DG:N1	2.49	0.60
13:P:3:G:H2'	13:P:4:U:C6	2.36	0.60
14:T:62:DA:C4	14:T:63:DA:C5	2.89	0.60
1:A:1157:ASP:OD2	1:A:1241:ARG:NH2	2.35	0.60
2:B:109:LEU:O	2:B:198:GLY:N	2.34	0.60
2:B:821:GLN:HE22	2:B:851:PHE:H	1.50	0.60
3:C:65:ARG:NH2	10:J:3:ILE:O	2.33	0.60
11:K:50:LEU:HD11	11:K:87:LEU:HD13	1.84	0.60
9:I:70:ARG:NH2	9:I:82:ASP:OD1	2.35	0.60
14:T:62:DA:H2''	14:T:63:DA:OP2	2.01	0.60
15:N:-39:DT:H2''	15:N:-38:DT:C6	2.36	0.60
11:K:57:THR:H	11:K:77:THR:HA	1.67	0.59
1:A:308:ASP:OD2	1:A:327:ARG:NH1	2.36	0.59
2:B:680:SER:O	2:B:684:SER:HB3	2.02	0.59
15:N:50:DG:H2''	15:N:51:DG:OP2	2.01	0.59
1:A:336:ARG:O	1:A:340:ASN:HB2	2.01	0.59
15:N:48:DG:H2''	15:N:49:DC:OP2	2.01	0.59
14:T:70:DG:O6	15:N:-71:DT:O4	2.19	0.59
1:A:999:LEU:O	1:A:1013:GLN:NE2	2.35	0.59
1:A:279:LYS:O	1:A:283:ASP:OD1	2.19	0.59
4:D:84:ILE:HG23	4:D:85:ASP:H	1.68	0.59
15:N:-63:DT:N1	15:N:-62:DT:H72	2.17	0.59
2:B:635:ASP:OD1	2:B:635:ASP:N	2.31	0.59
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.36	0.59
2:B:843:GLN:HG2	11:K:6:ARG:HH22	1.68	0.59
15:N:63:DG:H2''	15:N:64:DG:OP2	2.01	0.59
14:T:-72:DA:C5'	14:T:-72:DA:HO5'	2.08	0.59
1:A:340:ASN:O	2:B:1117:GLN:NE2	2.34	0.59
13:P:5:G:H2'	13:P:6:U:C6	2.38	0.58
1:A:231:ARG:HD2	1:A:232:PRO:HD2	1.85	0.58
2:B:279:ARG:HG2	2:B:284:VAL:HA	1.85	0.58
14:T:62:DA:C2	14:T:63:DA:C4	2.91	0.58
1:A:467:SER:OG	11:K:2:ASN:ND2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLN:HB3	2:B:1215:ARG:HB2	1.85	0.58
2:B:635:ASP:HB3	2:B:739:THR:HA	1.84	0.58
2:B:807:GLN:H	2:B:1045:THR:HG1	1.49	0.58
2:B:822:ASN:O	10:J:47:ARG:NH1	2.36	0.58
3:C:33:ARG:HG3	3:C:176:ILE:HG21	1.85	0.58
1:A:16:GLU:OE2	2:B:1221:SER:N	2.35	0.58
1:A:351:ARG:NH1	1:A:489:ASN:OD1	2.36	0.58
1:A:345:ARG:NH2	14:T:89:DA:OP2	2.37	0.58
3:C:114:TYR:OH	10:J:19:ASP:OD2	2.20	0.58
3:C:166:GLU:OE2	12:L:72:ARG:NH2	2.37	0.58
1:A:1166:GLU:HA	1:A:1169:PHE:HB2	1.84	0.58
1:A:435:ARG:NH1	1:A:436:HIS:O	2.36	0.58
13:P:7:G:C6	14:T:91:DA:N1	2.71	0.57
2:B:1101:ASP:O	2:B:1122:ARG:NH1	2.37	0.57
2:B:153:GLY:N	2:B:436:ASN:O	2.37	0.57
4:D:169:VAL:HG13	4:D:171:LEU:CB	2.35	0.57
1:A:962:LEU:HD22	1:A:1051:ILE:HG12	1.85	0.57
1:A:1072:GLN:NE2	2:B:1137:CYS:SG	2.75	0.57
15:N:51:DG:H2"	15:N:52:DC:OP2	2.04	0.57
2:B:489:ARG:NH2	2:B:533:SER:O	2.38	0.57
2:B:505:ARG:NH1	2:B:526:CYS:O	2.37	0.57
2:B:793:ALA:HB3	2:B:856:PHE:HB2	1.85	0.57
3:C:76:VAL:O	3:C:161:LYS:NZ	2.33	0.57
14:T:-64:DC:H2"	14:T:-63:DC:OP2	2.05	0.57
2:B:279:ARG:NH2	2:B:286:ASP:OD1	2.38	0.57
2:B:794:ASN:HD21	2:B:855:PHE:HD1	1.51	0.57
2:B:955:THR:OG1	2:B:956:THR:N	2.38	0.57
1:A:996:CYS:O	1:A:1021:GLN:NE2	2.38	0.57
5:E:19:LYS:NZ	5:E:33:GLU:O	2.37	0.57
1:A:351:ARG:HB2	2:B:1128:LEU:HD11	1.86	0.57
2:B:279:ARG:NH1	2:B:316:ILE:O	2.38	0.57
1:A:453:LYS:O	2:B:1141:HIS:NE2	2.35	0.56
1:A:546:GLN:OE1	2:B:1079:LYS:NZ	2.38	0.56
2:B:167:SER:OG	2:B:170:CYS:N	2.38	0.56
3:C:104:HIS:ND1	3:C:111:THR:OG1	2.34	0.56
14:T:62:DA:N1	14:T:63:DA:N1	2.53	0.56
2:B:480:THR:OG1	2:B:481:TYR:N	2.38	0.56
11:K:5:ASP:HB2	11:K:8:GLU:HG2	1.87	0.56
1:A:406:VAL:HG22	1:A:433:VAL:HG22	1.87	0.56
1:A:738:LEU:HB3	1:A:742:ASN:HD22	1.70	0.56
4:D:61:ARG:NH1	4:D:86:ASP:OD1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:80:DA:H2'	14:T:81:DC:C6	2.39	0.56
1:A:1120:VAL:HB	1:A:1309:LEU:HB2	1.86	0.56
1:A:87:ALA:HB2	1:A:278:GLN:HE21	1.70	0.56
2:B:225:ILE:O	2:B:252:ARG:NH2	2.37	0.56
3:C:146:LYS:NZ	10:J:57:GLU:OE2	2.35	0.56
1:A:1144:THR:OG1	1:A:1147:ASN:N	2.37	0.56
5:E:174:LEU:HD12	5:E:212:ILE:HD12	1.86	0.56
10:J:7:CYS:SG	10:J:8:PHE:N	2.78	0.56
1:A:468:THR:OG1	1:A:470:ARG:NH1	2.38	0.56
2:B:303:LEU:HA	2:B:306:LEU:HD12	1.87	0.56
14:T:74:DA:C2'	14:T:75:DC:O5'	2.54	0.56
1:A:63:ARG:NH1	1:A:63:ARG:HG3	4.45	0.56
2:B:300:TRP:HA	2:B:303:LEU:HB2	1.86	0.56
1:A:601:PRO:HA	8:H:25:ARG:HH22	1.71	0.56
1:A:86:LEU:HD22	1:A:297:LEU:HD21	1.88	0.56
1:A:847:GLU:OE2	1:A:1428:SER:OG	2.22	0.56
1:A:243:PRO:O	1:A:248:ARG:NH1	2.37	0.56
7:G:121:TYR:CE2	7:G:123:PRO:HG3	2.41	0.56
14:T:38:DA:C2	15:N:-37:DG:C2	2.93	0.56
5:E:27:TYR:HA	5:E:63:PRO:HA	1.87	0.56
1:A:1367:ASN:HD21	1:A:1369:ARG:HE	1.53	0.55
1:A:761:GLN:HG2	1:A:766:VAL:HA	1.87	0.55
2:B:300:TRP:O	2:B:304:GLU:HB2	2.05	0.55
3:C:75:ASP:OD2	3:C:128:ASN:N	2.38	0.55
1:A:696:TYR:O	1:A:700:HIS:HB2	2.06	0.55
3:C:163:ILE:HG13	3:C:165:LYS:H	1.71	0.55
1:A:31:SER:OG	1:A:32:VAL:N	2.39	0.55
2:B:58:LEU:HB2	2:B:75:TYR:HB2	1.88	0.55
1:A:153:PRO:HD3	1:A:165:ARG:HD2	1.87	0.55
1:A:811:PRO:HG2	2:B:702:MET:HG2	1.89	0.55
2:B:243:SER:HB2	2:B:266:PRO:HG3	1.87	0.55
11:K:29:ASN:ND2	11:K:78:GLU:O	2.40	0.55
1:A:1154:ILE:HD12	9:I:44:TYR:HB3	1.88	0.55
1:A:557:TRP:O	11:K:26:ARG:NH1	2.39	0.55
13:P:5:G:H2'	13:P:6:U:H6	1.72	0.55
1:A:775:ARG:HH22	1:A:793:PHE:HB3	1.72	0.55
12:L:50:CYS:N	12:L:55:HIS:O	2.40	0.55
1:A:982:ASP:O	1:A:1041:ARG:NH2	2.40	0.55
15:N:31:DT:H2''	15:N:32:DG:C8	2.41	0.55
8:H:38:LEU:HD13	8:H:124:LEU:HD13	1.89	0.55
14:T:62:DA:N6	14:T:63:DA:H61	2.00	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1097:THR:HG22	1:A:1102:ARG:HB2	1.89	0.55
1:A:636:ARG:NH1	1:A:878:GLN:OE1	2.40	0.55
1:A:908:SER:OG	1:A:909:ILE:N	2.40	0.55
2:B:52:GLU:OE2	2:B:55:ARG:NH1	15.30	0.55
13:P:7:G:N1	14:T:91:DA:C6	2.75	0.55
13:P:7:G:C6	14:T:91:DA:N6	2.75	0.55
1:A:262:ASP:OD2	1:A:321:ARG:NH2	2.40	0.54
2:B:110:THR:HG22	2:B:112:SER:HB3	1.88	0.54
2:B:220:ALA:O	2:B:252:ARG:NH2	2.40	0.54
2:B:570:SER:HB3	2:B:582:ILE:HB	1.88	0.54
2:B:904:ARG:HA	2:B:948:ILE:HG13	1.89	0.54
1:A:755:SER:N	1:A:758:ASN:OD1	2.39	0.54
2:B:72:ASN:ND2	2:B:128:ASP:OD1	2.40	0.54
3:C:55:SER:OG	3:C:57:LEU:O	2.26	0.54
1:A:435:ARG:HH12	1:A:438:MET:H	1.56	0.54
1:A:448:GLN:NE2	2:B:1134:GLU:OE2	2.41	0.54
2:B:807:GLN:N	2:B:1045:THR:HG1	2.05	0.54
1:A:554:VAL:HG12	1:A:556:SER:H	1.72	0.54
1:A:768:GLN:NE2	1:A:769:GLN:O	2.36	0.54
2:B:369:PHE:HB3	2:B:579:TRP:HZ3	1.72	0.54
2:B:794:ASN:HD22	2:B:855:PHE:HA	1.73	0.54
1:A:63:ARG:NH1	14:T:-14:DA:O3'	111.39	0.54
1:A:362:LEU:HA	1:A:472:ASN:HD22	1.72	0.54
1:A:370:SER:H	11:K:2:ASN:HD21	1.54	0.54
2:B:833:TYR:HH	11:K:65:HIS:HE2	1.52	0.54
9:I:101:TYR:N	9:I:110:PHE:O	2.33	0.54
1:A:1413:PHE:O	1:A:1417:ALA:CB	2.55	0.54
2:B:1076:HIS:O	11:K:44:ASN:ND2	2.41	0.54
14:T:34:DA:N1	15:N:-35:DG:N1	2.56	0.54
2:B:249:LEU:HA	2:B:261:ILE:HG12	1.89	0.54
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.90	0.54
2:B:957:ASN:HD21	2:B:961:LEU:HB2	1.73	0.54
6:F:107:VAL:HG12	6:F:109:VAL:H	1.73	0.54
14:T:80:DA:H61	15:N:-80:DT:H3	1.55	0.54
5:E:54:ARG:HB3	5:E:81:PHE:HB2	1.89	0.53
11:K:55:ASP:OD1	11:K:55:ASP:N	2.40	0.53
1:A:1021:GLN:HB3	1:A:1025:ARG:HH12	1.72	0.53
2:B:218:LYS:HE2	2:B:388:GLN:HB3	1.91	0.53
2:B:444:THR:O	2:B:448:SER:CB	2.56	0.53
4:D:141:GLU:OE1	4:D:166:LYS:NZ	2.41	0.53
5:E:12:TRP:NE1	5:E:37:SER:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:LYS:HE3	1:A:721:ARG:HH12	1.73	0.53
2:B:825:VAL:N	2:B:1088:GLY:O	2.40	0.53
1:A:92:HIS:NE2	2:B:1210:MET:O	2.29	0.53
11:K:40:HIS:O	11:K:43:ALA:N	2.42	0.53
14:T:75:DC:H2''	14:T:76:DG:C8	2.41	0.53
1:A:1153:GLU:OE1	1:A:1196:ARG:NH1	2.37	0.53
3:C:82:SER:HB2	3:C:160:LYS:HB3	1.90	0.53
15:N:43:DA:H2''	15:N:44:DT:OP2	2.08	0.53
7:G:1:MET:HG3	7:G:3:PHE:CE2	2.43	0.53
14:T:-11:DG:H2''	14:T:-10:DC:OP2	2.09	0.53
1:A:113:LEU:HG	1:A:115:LEU:H	1.74	0.53
1:A:1439:MET:HE1	2:B:1139:ILE:HG12	1.90	0.53
7:G:116:PRO:HG2	7:G:119:LEU:HD12	1.90	0.53
14:T:-29:DC:H2''	14:T:-28:DT:OP2	2.08	0.53
1:A:924:VAL:HA	1:A:927:GLN:HB3	1.91	0.53
5:E:137:SER:HA	5:E:140:VAL:HG23	1.91	0.53
8:H:8:ASP:OD1	8:H:32:THR:OG1	2.25	0.53
15:N:-73:DT:H2''	15:N:-72:DT:H5'	1.89	0.53
2:B:71:ILE:HG13	2:B:127:ILE:HG22	1.89	0.53
2:B:879:ARG:HA	2:B:885:LEU:HD11	1.91	0.53
7:G:165:GLU:HB2	7:G:168:LEU:HD12	1.91	0.53
14:T:77:DG:C2'	14:T:78:DC:OP1	2.46	0.53
2:B:452:TYR:HE1	14:T:95:DC:C5'	2.06	0.52
3:C:40:VAL:HB	3:C:172:PRO:HG3	1.91	0.52
15:N:-76:DC:H2''	15:N:-75:DG:C8	2.40	0.52
4:D:93:THR:HG21	4:D:102:VAL:HG21	1.91	0.52
5:E:2:GLU:OE1	5:E:5:ASN:ND2	2.42	0.52
14:T:10:DC:H2''	14:T:11:DG:C8	2.45	0.52
1:A:526:GLN:HB3	2:B:1015:HIS:CG	2.45	0.52
1:A:1416:GLY:HA3	2:B:1212:ILE:HG23	1.91	0.52
2:B:354:LEU:HB3	2:B:357:ILE:HD12	1.91	0.52
1:A:318:LYS:CE	14:T:96:DA:N6	2.71	0.52
2:B:641:ASN:HD21	2:B:646:ARG:HA	1.75	0.52
10:J:7:CYS:HB3	10:J:11:GLY:H	1.75	0.52
14:T:74:DA:H2'	14:T:75:DC:C5	2.45	0.52
14:T:77:DG:H2''	14:T:78:DC:C5'	2.39	0.52
1:A:850:MET:HG3	1:A:1063:GLY:HA2	1.92	0.52
14:T:69:DC:N3	15:N:-69:DG:N1	2.42	0.52
2:B:427:ARG:HH22	14:T:99:DC:P	2.32	0.52
1:A:1190:GLN:OE1	1:A:1243:ARG:NH1	2.43	0.52
1:A:858:ARG:HG2	1:A:864:ILE:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:VAL:HG21	2:B:82:ILE:HD11	1.92	0.52
15:N:-66:DG:C2'	15:N:-65:DT:O4'	2.56	0.52
1:A:337:LEU:HA	1:A:341:LEU:HB2	1.92	0.52
14:T:95:DC:O5'	14:T:95:DC:C6	2.56	0.52
1:A:283:ASP:OD1	1:A:283:ASP:N	2.42	0.52
2:B:1156:ASP:OD1	2:B:1156:ASP:N	2.41	0.52
2:B:71:ILE:HG12	2:B:73:LYS:HG3	1.92	0.52
2:B:917:PRO:HA	2:B:934:LYS:HA	1.92	0.52
4:D:169:VAL:HG12	4:D:170:ASN:H	1.75	0.52
15:N:31:DT:H2''	15:N:32:DG:H8	1.74	0.52
15:N:-64:DT:C2'	15:N:-63:DT:O4'	2.51	0.52
14:T:-7:DG:C6	15:N:6:DA:N6	2.78	0.52
14:T:71:DA:N6	14:T:72:DA:C6	2.77	0.52
1:A:108:MET:H	1:A:172:GLN:HE22	1.58	0.51
2:B:463:LYS:NZ	15:N:-95:DG:N2	2.56	0.51
11:K:61:TYR:HA	11:K:73:MET:HA	1.92	0.51
11:K:36:GLU:OE1	11:K:37:ARG:NH1	2.43	0.51
14:T:67:DA:H2''	14:T:68:DA:C5	2.45	0.51
2:B:452:TYR:CD1	14:T:95:DC:H5'	2.39	0.51
2:B:78:ARG:HB3	2:B:120:GLU:HB3	1.93	0.51
2:B:865:ARG:HG3	2:B:871:VAL:HG12	1.93	0.51
15:N:-66:DG:H2'	15:N:-65:DT:C5'	2.30	0.51
3:C:66:LEU:HD23	3:C:69:ILE:HD12	1.91	0.51
4:D:169:VAL:HG13	4:D:171:LEU:HB3	1.92	0.51
1:A:914:ILE:HA	1:A:981:SER:H	1.74	0.51
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.92	0.51
2:B:229:ALA:HB3	2:B:247:ILE:HD12	1.93	0.51
2:B:463:LYS:HZ3	15:N:-95:DG:H21	1.55	0.51
1:A:1285:VAL:HG13	1:A:1311:THR:HG22	1.93	0.51
1:A:63:ARG:HH11	1:A:63:ARG:HG3	3.93	0.51
2:B:13:THR:N	2:B:16:ASP:OD2	2.35	0.51
2:B:609:ILE:HG12	2:B:694:GLU:HB2	1.93	0.51
14:T:10:DC:H2''	14:T:11:DG:H8	1.75	0.51
1:A:669:ASP:OD2	1:A:743:ASN:ND2	2.44	0.51
1:A:768:GLN:NE2	1:A:798:LYS:O	2.40	0.51
2:B:303:LEU:HD23	2:B:306:LEU:HD12	1.93	0.51
5:E:201:SER:HB2	5:E:207:TYR:HB2	1.92	0.51
15:N:-66:DG:H2''	15:N:-65:DT:H5'	0.54	0.51
1:A:317:GLN:HE21	1:A:323:VAL:HG22	1.76	0.51
2:B:572:ARG:HG2	2:B:582:ILE:HG22	1.92	0.51
2:B:595:ASP:HA	2:B:598:ARG:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:-53:DT:H2''	15:N:-52:DC:OP2	2.10	0.51
2:B:1155:SER:OG	2:B:1156:ASP:N	2.42	0.50
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.92	0.50
2:B:789:MET:HE1	2:B:965:LYS:HB3	1.93	0.50
5:E:2:GLU:HG2	5:E:4:ASN:H	1.75	0.50
1:A:1453:LEU:HD23	1:A:1456:LEU:HD12	1.92	0.50
1:A:367:VAL:HG21	1:A:461:VAL:HG13	1.92	0.50
5:E:175:PRO:HB2	5:E:211:ARG:HG2	1.93	0.50
10:J:22:LEU:HD23	10:J:25:LEU:HD12	1.92	0.50
14:T:81:DC:H2'	14:T:82:DC:C6	2.47	0.50
1:A:1014:GLN:O	1:A:1018:SER:OG	2.29	0.50
2:B:444:THR:O	2:B:448:SER:HB2	2.12	0.50
2:B:982:SER:OG	2:B:985:GLY:N	2.44	0.50
10:J:9:SER:HB2	10:J:44:CYS:HB2	1.93	0.50
11:K:31:ILE:HG13	11:K:75:LEU:HB3	1.94	0.50
15:N:3:DC:H2''	15:N:4:DG:C8	2.45	0.50
15:N:-61:DT:H2'	15:N:-60:DT:C6	2.46	0.50
15:N:-63:DT:C2'	15:N:-62:DT:H72	2.42	0.50
1:A:107:CYS:HB3	1:A:112:LYS:H	1.76	0.50
2:B:1112:GLN:HG3	2:B:1119:VAL:HG12	1.93	0.50
2:B:225:ILE:HD13	2:B:248:LYS:HD3	1.93	0.50
2:B:320:GLU:HA	2:B:323:LEU:HD12	1.94	0.50
15:N:17:DA:H2''	15:N:18:DG:C8	2.46	0.50
2:B:1114:LEU:HG	2:B:1115:THR:HG23	1.92	0.50
15:N:51:DG:OP2	15:N:51:DG:H2'	2.12	0.50
14:T:70:DG:H2''	14:T:71:DA:C8	2.47	0.50
1:A:250:SER:HB2	1:A:258:GLN:HB2	1.93	0.50
1:A:858:ARG:NH1	6:F:139:PRO:HB2	2.27	0.50
2:B:82:ILE:HD13	2:B:117:LEU:HD13	1.92	0.50
3:C:111:THR:HB	3:C:147:LEU:HB2	1.94	0.50
8:H:102:LYS:HB3	8:H:114:TYR:HB2	1.93	0.50
1:A:9:ALA:HB1	2:B:1192:TYR:HA	1.93	0.50
5:E:177:ILE:N	5:E:212:ILE:O	2.40	0.50
7:G:106:LEU:HG	7:G:157:ILE:CD1	2.42	0.50
14:T:-12:DC:H2''	14:T:-11:DG:C8	2.47	0.50
14:T:80:DA:H2'	14:T:81:DC:H6	1.77	0.50
1:A:344:LYS:NZ	2:B:1156:ASP:OD1	2.46	0.49
2:B:413:LEU:HB3	2:B:446:ILE:HG12	1.94	0.49
2:B:883:LEU:HG	2:B:935:ARG:HA	1.93	0.49
2:B:186:CYS:SG	2:B:783:THR:OG1	2.60	0.49
14:T:75:DC:C2	15:N:-75:DG:N2	2.79	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:149:ASP:N	6:F:149:ASP:OD1	2.45	0.49
8:H:63:LEU:HD21	8:H:142:LEU:HD11	1.93	0.49
2:B:91:GLU:OE1	12:L:56:ARG:NH1	2.46	0.49
1:A:498:THR:HB	2:B:1146:PHE:HD1	1.77	0.49
5:E:73:ASP:N	5:E:73:ASP:OD1	2.42	0.49
8:H:85:ASP:OD1	8:H:85:ASP:N	2.39	0.49
1:A:114:LEU:HD11	1:A:172:GLN:HG3	1.95	0.49
1:A:819:MET:HG2	2:B:507:LEU:HB3	1.94	0.49
2:B:1037:ILE:O	10:J:46:ARG:NH2	2.46	0.49
10:J:7:CYS:SG	10:J:9:SER:N	2.86	0.49
2:B:252:ARG:HB3	2:B:255:LYS:HB3	1.94	0.49
3:C:100:LEU:HD13	3:C:118:LEU:HD23	1.94	0.49
13:P:7:G:C2	14:T:91:DA:C2	3.00	0.49
14:T:80:DA:C5	14:T:81:DC:C4	3.01	0.49
2:B:320:GLU:OE1	2:B:338:ARG:NH1	2.45	0.49
2:B:563:ASP:OD2	2:B:566:GLN:N	2.44	0.49
2:B:634:GLU:HG2	2:B:641:ASN:HB3	1.94	0.49
1:A:1381:ARG:HH12	1:A:1395:ALA:HA	1.78	0.49
2:B:834:ASN:O	2:B:1013:ASN:ND2	2.45	0.49
14:T:77:DG:N1	14:T:78:DC:N3	2.60	0.49
1:A:776:ILE:O	1:A:798:LYS:NZ	2.32	0.49
3:C:149:ASN:OD1	3:C:150:HIS:ND1	2.46	0.49
1:A:1328:SER:HA	5:E:146:HIS:HA	1.95	0.49
5:E:213:CYS:SG	5:E:214:LEU:N	2.85	0.49
15:N:-66:DG:C5	15:N:-65:DT:C4	3.01	0.49
14:T:78:DC:H42	15:N:-78:DG:H1	1.61	0.49
2:B:466:MET:N	2:B:466:MET:SD	2.85	0.49
15:N:9:DT:H2''	15:N:10:DG:H8	1.77	0.49
14:T:19:DC:H42	15:N:-19:DG:H22	1.60	0.49
1:A:1152:THR:OG1	9:I:46:HIS:N	2.41	0.48
1:A:1148:VAL:HA	1:A:1203:ARG:HD3	1.95	0.48
11:K:14:ASP:OD1	11:K:14:ASP:N	2.44	0.48
1:A:370:SER:H	11:K:2:ASN:ND2	2.11	0.48
1:A:63:ARG:HH11	1:A:63:ARG:CG	3.42	0.48
1:A:55:ASP:HB3	1:A:58:LEU:HG	1.95	0.48
1:A:826:ILE:O	1:A:830:VAL:HB	2.14	0.48
1:A:538:ARG:NE	8:H:119:GLY:O	2.47	0.48
15:N:-65:DT:C6	15:N:-64:DT:H71	2.48	0.48
1:A:885:ASP:OD2	1:A:1027:ARG:NE	2.46	0.48
14:T:-12:DC:H2''	14:T:-11:DG:H8	1.79	0.48
1:A:448:GLN:HG2	14:T:88:DA:H4'	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:900:VAL:HG22	1:A:1031:ARG:HG3	1.96	0.48
2:B:1065:GLN:HE22	2:B:1067:ARG:HB2	1.78	0.48
2:B:477:ASN:O	2:B:484:THR:OG1	2.30	0.48
1:A:516:GLN:NE2	1:A:1076:GLU:OE1	2.46	0.48
2:B:410:PHE:O	2:B:414:PHE:HB2	2.13	0.48
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.78	0.48
2:B:892:LYS:HB3	2:B:899:ILE:HD12	1.96	0.48
5:E:84:GLU:OE1	5:E:91:THR:OG1	2.29	0.48
6:F:117:PRO:HA	6:F:120:ILE:HD12	1.94	0.48
14:T:-67:DA:H2''	14:T:-66:DA:O4'	2.13	0.48
1:A:389:LEU:HD23	1:A:392:TYR:HD2	1.77	0.48
8:H:107:ASP:HB2	8:H:110:LYS:HB2	1.96	0.48
15:N:-63:DT:C6	15:N:-62:DT:H72	2.49	0.48
1:A:408:ARG:HD3	1:A:412:ASP:HB2	1.95	0.48
1:A:550:MET:HG2	1:A:656:TYR:HD2	1.78	0.48
1:A:727:ARG:NH1	1:A:766:VAL:O	2.40	0.48
2:B:15:GLU:HA	2:B:18:TRP:HD1	1.77	0.48
2:B:950:ASP:OD2	2:B:967:ARG:NH2	2.39	0.48
15:N:39:DA:H1'	15:N:40:DC:H5'	1.96	0.48
1:A:118:THR:HG1	14:T:-3:DG:H5'	46.09	0.48
1:A:22:LEU:HG	2:B:1213:ALA:HB2	1.95	0.48
2:B:524:GLN:NE2	14:T:86:DC:H41	2.09	0.48
6:F:128:ARG:HE	6:F:153:VAL:HG23	1.79	0.48
14:T:-3:DG:C5	14:T:-2:DC:C4	3.01	0.48
9:I:108:LYS:NZ	9:I:109:THR:O	2.46	0.47
13:P:3:G:H2'	13:P:4:U:H6	1.77	0.47
1:A:1146:LYS:HB2	1:A:1271:LEU:HB3	1.95	0.47
1:A:387:HIS:O	1:A:390:THR:OG1	2.31	0.47
2:B:1165:ILE:HG13	2:B:1190:ASN:HD22	1.80	0.47
2:B:46:ILE:HG22	2:B:82:ILE:HG13	1.95	0.47
1:A:403:ALA:HA	1:A:435:ARG:HA	1.96	0.47
1:A:435:ARG:NH1	1:A:438:MET:H	2.11	0.47
2:B:452:TYR:CE1	14:T:95:DC:C5'	2.75	0.47
3:C:69:ILE:HG12	3:C:142:ILE:HD13	1.96	0.47
15:N:9:DT:H2''	15:N:10:DG:C8	2.48	0.47
15:N:-39:DT:H2''	15:N:-38:DT:C5	2.49	0.47
15:N:-63:DT:H2''	15:N:-62:DT:C7	2.44	0.47
14:T:73:DA:H2'	14:T:74:DA:C8	2.49	0.47
4:D:22:GLU:OE1	4:D:22:GLU:N	2.48	0.47
2:B:1149:GLU:OE2	2:B:1150:ARG:NH2	2.46	0.47
2:B:394:PHE:H	2:B:510:THR:HG21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:61:DC:H2''	15:N:62:DG:N7	2.29	0.47
13:P:2:G:C2	13:P:3:G:C4	3.03	0.47
2:B:1065:GLN:NE2	2:B:1067:ARG:H	2.12	0.47
2:B:483:SER:HA	2:B:775:LYS:HG2	1.96	0.47
5:E:194:VAL:HG22	5:E:212:ILE:HG13	1.97	0.47
10:J:43:TYR:HA	10:J:46:ARG:HD3	1.96	0.47
2:B:180:LEU:O	2:B:184:LYS:N	2.48	0.47
6:F:100:GLN:NE2	7:G:18:PHE:CE2	2.83	0.47
14:T:86:DC:H2'	14:T:87:DA:H8	1.80	0.47
1:A:90:VAL:O	1:A:237:ILE:N	2.48	0.47
2:B:863:GLU:HG3	2:B:874:PHE:CZ	2.50	0.47
2:B:957:ASN:OD1	2:B:960:GLY:N	2.48	0.47
11:K:65:HIS:HB3	11:K:68:PHE:HD2	1.80	0.47
15:N:-66:DG:H2'	15:N:-65:DT:O5'	2.14	0.47
1:A:841:ARG:NH1	1:A:1108:ASN:OD1	2.48	0.47
2:B:1204:PHE:HE2	2:B:1216:LEU:HD11	1.80	0.47
1:A:1102:ARG:HH12	1:A:1113:ILE:HD12	1.80	0.47
1:A:668:GLY:HA2	1:A:671:ILE:HD12	1.96	0.47
1:A:975:LEU:HA	1:A:975:LEU:HD23	1.77	0.47
1:A:929:GLU:HB3	1:A:989:ILE:HD13	1.97	0.47
14:T:-37:DG:H4'	14:T:-36:DT:OP1	2.14	0.47
1:A:361:GLU:O	1:A:472:ASN:ND2	2.48	0.46
2:B:533:SER:N	2:B:536:SER:OG	2.47	0.46
1:A:783:ARG:NH2	2:B:696:GLU:O	2.48	0.46
3:C:54:THR:OG1	3:C:152:GLU:N	2.48	0.46
2:B:480:THR:O	2:B:483:SER:OG	2.26	0.46
8:H:100:VAL:HA	8:H:115:VAL:HG22	1.97	0.46
15:N:4:DG:H2''	15:N:5:DT:OP2	2.15	0.46
1:A:632:HIS:HE1	1:A:880:GLU:HG2	1.81	0.46
2:B:802:PRO:HB3	2:B:1091:TYR:CG	2.50	0.46
2:B:254:ASP:OD1	2:B:259:ARG:NH2	2.48	0.46
2:B:975:GLN:N	2:B:978:ASP:OD2	2.41	0.46
7:G:91:VAL:HA	7:G:101:ALA:HA	1.98	0.46
15:N:-70:DC:H2''	15:N:-69:DG:H5''	1.96	0.46
14:T:-30:DG:H2''	14:T:-29:DC:OP2	2.15	0.46
1:A:472:ASN:OD1	1:A:473:LEU:N	2.49	0.46
1:A:983:LEU:HD22	1:A:1041:ARG:HA	1.97	0.46
1:A:501:GLU:OE1	2:B:1146:PHE:N	2.48	0.46
3:C:69:ILE:HG12	3:C:142:ILE:HG21	1.97	0.46
7:G:108:VAL:HG22	7:G:159:ALA:HB3	1.97	0.46
8:H:128:TYR:O	8:H:132:ALA:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:63:THR:OG1	12:L:64:LYS:N	2.48	0.46
15:N:47:DA:H2''	15:N:48:DG:C8	2.50	0.46
1:A:937:LEU:HD21	1:A:1025:ARG:HB3	1.97	0.46
1:A:970:GLN:HA	1:A:975:LEU:HD12	1.98	0.46
2:B:365:THR:O	2:B:369:PHE:HB2	2.16	0.46
2:B:1077:THR:HA	11:K:44:ASN:ND2	2.30	0.46
15:N:-66:DG:C2'	15:N:-65:DT:C4'	2.85	0.46
1:A:1001:VAL:H	1:A:1013:GLN:HE22	1.64	0.46
1:A:550:MET:HB3	1:A:550:MET:HE2	1.89	0.46
1:A:610:ASP:OD2	1:A:612:LYS:NZ	2.39	0.46
1:A:887:ILE:O	1:A:945:ARG:NH2	2.48	0.46
1:A:1400:LEU:HB2	1:A:1429:GLU:HG3	1.98	0.46
1:A:1456:LEU:HD23	1:A:1456:LEU:HA	1.79	0.46
2:B:760:ASP:OD1	2:B:760:ASP:N	2.35	0.46
2:B:821:GLN:NE2	2:B:851:PHE:H	2.14	0.46
1:A:1129:ASP:OD2	1:A:1132:LYS:N	2.43	0.46
14:T:80:DA:N6	15:N:-80:DT:H3	2.14	0.46
14:T:19:DC:H2''	14:T:20:DG:H8	1.80	0.46
14:T:94:DC:H2''	14:T:95:DC:C5	2.50	0.46
2:B:985:GLY:O	2:B:987:LYS:N	2.49	0.46
15:N:-48:DC:C2	15:N:-47:DC:C5	3.03	0.46
14:T:80:DA:N6	15:N:-81:DG:C6	2.84	0.46
14:T:62:DA:N3	14:T:63:DA:N7	2.63	0.46
3:C:241:ASN:OD1	3:C:241:ASN:N	2.47	0.46
1:A:106:ILE:HG22	1:A:113:LEU:HA	1.98	0.45
1:A:395:ASN:ND2	1:A:401:PRO:O	2.36	0.45
1:A:926:LEU:HD11	1:A:986:PRO:HD3	1.98	0.45
2:B:806:THR:OG1	2:B:808:ALA:N	2.49	0.45
6:F:99:LEU:O	6:F:102:SER:OG	2.27	0.45
9:I:90:GLN:HE21	9:I:92:ARG:HG3	1.80	0.45
1:A:240:LEU:HD22	1:A:301:VAL:HG13	1.99	0.45
1:A:846:LEU:HB3	1:A:849:ILE:HD12	1.98	0.45
2:B:995:ARG:NH2	2:B:997:GLU:OE2	2.49	0.45
4:D:53:LEU:HD13	4:D:147:SER:HB3	1.98	0.45
15:N:-60:DT:H2''	15:N:-59:DT:OP2	2.16	0.45
1:A:133:LYS:HA	1:A:136:ASN:HB2	1.97	0.45
1:A:254:ASP:OD1	1:A:254:ASP:N	2.48	0.45
1:A:817:HIS:CD2	2:B:764:SER:H	2.34	0.45
2:B:733:SER:HB3	2:B:736:HIS:CE1	2.51	0.45
10:J:7:CYS:HA	10:J:48:MET:HG3	1.97	0.45
1:A:1367:ASN:ND2	1:A:1369:ARG:HE	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:ARG:NH1	1:A:622:THR:OG1	2.37	0.45
1:A:340:ASN:ND2	2:B:1117:GLN:OE1	2.48	0.45
11:K:12:LEU:HD22	11:K:18:LYS:HB2	1.97	0.45
12:L:33:CYS:HB2	12:L:40:PHE:HE1	1.80	0.45
15:N:45:DT:H2''	15:N:46:DG:C8	2.51	0.45
14:T:71:DA:C6	14:T:72:DA:C6	3.04	0.45
1:A:526:GLN:HG3	2:B:836:GLU:HG2	1.98	0.45
15:N:55:DC:H2'	15:N:55:DC:OP2	2.17	0.45
1:A:90:VAL:HG21	1:A:301:VAL:HG11	1.99	0.45
13:P:8:U:H2'	13:P:9:U:C6	2.52	0.45
1:A:1331:TYR:CZ	1:A:1353:LYS:HD3	2.51	0.45
1:A:1412:LEU:HA	1:A:1412:LEU:HD23	1.79	0.45
1:A:1399:ALA:N	1:A:1422:ASP:OD2	2.43	0.45
2:B:707:LEU:HA	2:B:707:LEU:HD23	1.80	0.45
2:B:861:ASP:OD1	2:B:914:LYS:NZ	2.42	0.45
1:A:680:ILE:HG23	1:A:730:ALA:HB1	1.99	0.45
2:B:1155:SER:HG	2:B:1156:ASP:N	2.07	0.45
2:B:354:LEU:HD11	2:B:371:LEU:HD11	1.98	0.45
2:B:599:SER:OG	2:B:600:GLY:N	2.50	0.45
5:E:79:VAL:HG13	5:E:110:ILE:HD13	1.98	0.45
15:N:-32:DT:H2''	15:N:-31:DA:C8	2.51	0.45
14:T:69:DC:C2'	14:T:70:DG:OP1	2.37	0.45
14:T:80:DA:C2	15:N:-79:DG:N1	2.85	0.45
1:A:1423:ASP:OD1	1:A:1423:ASP:N	2.49	0.45
1:A:63:ARG:HE	15:N:17:DA:H5''	115.48	0.45
1:A:846:LEU:O	1:A:848:ASP:N	2.49	0.45
1:A:914:ILE:HG13	1:A:917:ALA:HB2	1.99	0.45
2:B:776:GLN:HB2	2:B:1095:LEU:HD22	1.99	0.45
2:B:262:LYS:HA	2:B:273:PRO:HA	1.99	0.45
2:B:227:HIS:HB3	2:B:378:LEU:HD11	1.99	0.45
2:B:804:ALA:HB3	2:B:983:ARG:HH22	1.82	0.45
2:B:1006:ILE:HD13	10:J:43:TYR:CZ	2.51	0.45
15:N:-68:DT:H1'	15:N:-67:DT:C2	2.52	0.45
14:T:70:DG:N2	14:T:71:DA:C2	2.85	0.45
1:A:930:LEU:HD11	1:A:985:ILE:HG21	1.98	0.45
2:B:444:THR:O	2:B:448:SER:OG	2.27	0.45
5:E:99:ILE:HG23	5:E:104:PHE:HD2	1.82	0.45
14:T:-38:DC:H2''	14:T:-37:DG:OP2	2.17	0.45
1:A:1451:LYS:O	1:A:1454:THR:OG1	2.30	0.44
3:C:116:SER:OG	3:C:139:ASP:O	2.35	0.44
14:T:23:DA:H2''	14:T:24:DA:OP2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ARG:HB3	1:A:392:TYR:CZ	2.52	0.44
1:A:544:TYR:OH	11:K:57:THR:O	2.35	0.44
1:A:720:SER:O	1:A:724:ASN:ND2	2.50	0.44
1:A:929:GLU:O	1:A:932:SER:OG	2.31	0.44
2:B:1104:HIS:HE1	2:B:1106:ARG:HB2	1.82	0.44
9:I:71:SER:N	9:I:83:CYS:O	2.40	0.44
10:J:8:PHE:H	10:J:48:MET:HG3	1.81	0.44
14:T:37:DC:N3	14:T:38:DA:C6	2.85	0.44
14:T:58:DG:H1	15:N:-58:DC:H42	1.64	0.44
14:T:7:DC:H2''	14:T:8:DC:C6	2.53	0.44
1:A:21:LEU:HA	1:A:21:LEU:HD23	1.75	0.44
1:A:680:ILE:HD11	1:A:734:ALA:HB2	1.99	0.44
2:B:369:PHE:HB3	2:B:579:TRP:CZ3	2.51	0.44
9:I:57:GLY:H	9:I:89:GLN:HG3	1.82	0.44
15:N:-67:DT:O5'	15:N:-67:DT:C6	2.70	0.44
1:A:212:PHE:HB3	1:A:233:GLU:HB3	1.99	0.44
1:A:697:LYS:HB3	1:A:702:GLU:HB2	1.99	0.44
1:A:1155:TYR:HD1	9:I:41:PRO:HB2	1.83	0.44
1:A:1066:VAL:O	1:A:1070:ALA:HB2	2.17	0.44
1:A:237:ILE:HD13	1:A:240:LEU:HD13	2.00	0.44
2:B:58:LEU:HD21	2:B:426:GLN:HE21	1.81	0.44
3:C:83:ARG:NH2	3:C:166:GLU:OE2	2.47	0.44
5:E:152:HIS:NE2	5:E:183:VAL:HG11	2.33	0.44
14:T:-25:DA:H1'	14:T:-24:DG:C8	2.53	0.44
1:A:107:CYS:SG	1:A:108:MET:N	2.90	0.44
1:A:1107:LEU:HA	1:A:1107:LEU:HD23	1.75	0.44
2:B:803:LEU:HD23	2:B:1041:GLU:HG2	1.99	0.44
2:B:974:PRO:HG3	2:B:1094:ARG:HH12	1.82	0.44
3:C:34:ARG:CZ	11:K:40:HIS:HB2	2.48	0.44
14:T:62:DA:C2'	14:T:63:DA:OP2	2.64	0.44
14:T:-69:DA:H1'	14:T:-68:DG:H5'	2.00	0.44
14:T:77:DG:C6	14:T:78:DC:N3	2.86	0.44
1:A:1447:MET:HB2	6:F:133:VAL:HB	1.98	0.44
9:I:103:CYS:HB3	9:I:107:LYS:H	1.83	0.44
14:T:-57:DC:H2''	14:T:-56:DC:C5	2.53	0.44
1:A:897:ARG:HD3	1:A:1032:ARG:HD2	2.00	0.44
1:A:115:LEU:HB3	1:A:122:MET:HG2	2.00	0.44
1:A:133:LYS:HA	1:A:136:ASN:HD22	1.82	0.44
2:B:532:LEU:HA	2:B:532:LEU:HD23	1.78	0.44
2:B:546:PRO:HA	2:B:549:ASN:HD22	1.83	0.44
14:T:-69:DA:H2''	14:T:-68:DG:OP2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ARG:HB3	1:A:263:LEU:HD12	1.98	0.43
2:B:681:LEU:HD22	2:B:686:VAL:HG21	2.00	0.43
2:B:732:THR:OG1	2:B:733:SER:N	2.51	0.43
8:H:112:LYS:HG2	8:H:125:GLU:HG2	2.00	0.43
11:K:57:THR:OG1	11:K:76:GLN:O	2.33	0.43
1:A:1448:ILE:O	7:G:58:LYS:HD3	2.18	0.43
1:A:350:ALA:HB2	1:A:375:LEU:HD11	1.99	0.43
3:C:37:LEU:HD23	3:C:37:LEU:HA	1.82	0.43
1:A:80:HIS:H	1:A:244:PRO:HB3	1.83	0.43
1:A:529:LEU:HA	1:A:529:LEU:HD12	1.80	0.43
11:K:38:GLU:HB2	11:K:71:PHE:HE1	1.83	0.43
11:K:70:ASN:N	11:K:70:ASN:OD1	2.51	0.43
15:N:-65:DT:C5	15:N:-64:DT:H71	2.54	0.43
2:B:1069:PHE:HB3	2:B:1084:GLN:HB3	2.00	0.43
2:B:1128:LEU:HD23	2:B:1128:LEU:HA	1.80	0.43
2:B:794:ASN:ND2	2:B:855:PHE:HA	2.33	0.43
1:A:1279:ILE:HD12	1:A:1318:GLU:HB3	2.00	0.43
1:A:551:LEU:HD21	1:A:578:LEU:HG	2.01	0.43
1:A:5:PRO:HG2	2:B:1159:ARG:HH22	1.83	0.43
1:A:958:LEU:HD23	1:A:958:LEU:HA	1.78	0.43
2:B:608:ILE:HG12	2:B:619:ILE:HG12	2.01	0.43
2:B:78:ARG:HB3	15:N:28:DA:OP2	126.73	0.43
4:D:112:PHE:CE1	7:G:88:ASP:HB3	2.53	0.43
5:E:155:LEU:HD22	5:E:159:GLU:HB3	2.00	0.43
1:A:1116:PRO:HA	1:A:1333:ASN:HD21	1.84	0.43
15:N:17:DA:H2''	15:N:18:DG:H8	1.83	0.43
15:N:-43:DT:H2''	15:N:-42:DG:H8	1.83	0.43
14:T:-14:DA:C2	14:T:-13:DA:C4	3.06	0.43
1:A:1028:LEU:HB3	1:A:1033:ILE:HD11	2.01	0.43
1:A:1439:MET:HA	1:A:1443:ALA:HB2	2.01	0.43
1:A:287:GLN:HA	1:A:290:ILE:HD12	2.00	0.43
1:A:49:ARG:HD2	15:N:-66:DG:O3'	86.93	0.43
1:A:868:LEU:HD13	1:A:1002:LEU:HD11	1.99	0.43
1:A:494:GLN:N	2:B:1149:GLU:OE2	2.51	0.43
2:B:784:ASN:HB3	10:J:62:TYR:OH	2.17	0.43
3:C:34:ARG:NE	11:K:41:THR:OG1	2.39	0.43
14:T:34:DA:C6	15:N:-35:DG:O6	2.68	0.43
14:T:-42:DT:H2''	14:T:-41:DG:C8	2.54	0.43
1:A:1367:ASN:OD1	1:A:1368:TYR:N	2.52	0.43
3:C:96:VAL:HB	3:C:159:ALA:HB3	2.01	0.43
11:K:46:LEU:HA	11:K:46:LEU:HD23	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:-35:DA:H1'	14:T:-34:DG:H5'	2.01	0.43
14:T:73:DA:H61	15:N:-73:DT:H3	1.66	0.43
1:A:502:LEU:HD23	1:A:502:LEU:HA	1.82	0.43
2:B:955:THR:O	2:B:963:PHE:N	2.50	0.43
1:A:318:LYS:HB3	14:T:96:DA:C6	2.54	0.43
1:A:1216:ASP:O	1:A:1220:GLU:HG2	2.19	0.43
2:B:179:ASP:O	2:B:183:MET:N	2.52	0.43
5:E:20:GLU:OE1	5:E:142:ASN:ND2	2.45	0.43
6:F:123:LYS:O	6:F:126:SER:OG	2.37	0.43
10:J:12:LYS:HB3	10:J:45:CYS:SG	2.59	0.43
1:A:857:THR:HB	1:A:866:GLN:H	1.84	0.42
1:A:92:HIS:CD2	1:A:237:ILE:HD11	2.53	0.42
2:B:105:ARG:NH2	2:B:165:LEU:HD21	2.34	0.42
2:B:535:LEU:HA	2:B:535:LEU:HD23	1.85	0.42
2:B:797:TYR:HE1	2:B:854:LEU:HG	1.84	0.42
2:B:951:GLN:OE1	2:B:967:ARG:NH2	2.52	0.42
4:D:169:VAL:HG13	4:D:171:LEU:HB2	2.01	0.42
5:E:201:SER:O	5:E:205:GLY:N	2.47	0.42
15:N:-35:DG:H2''	15:N:-34:DT:C6	2.53	0.42
2:B:749:LEU:HB3	2:B:753:ALA:HB3	2.00	0.42
5:E:176:ARG:HD3	5:E:214:LEU:HD21	2.01	0.42
2:B:1026:LEU:HA	2:B:1026:LEU:HD23	1.85	0.42
2:B:223:SER:HB3	2:B:252:ARG:HH21	1.84	0.42
1:A:868:LEU:HD12	1:A:868:LEU:HA	1.78	0.42
2:B:274:ILE:HA	2:B:274:ILE:HD13	1.90	0.42
2:B:839:MET:SD	2:B:1010:LEU:HD21	2.59	0.42
2:B:848:ARG:HD3	10:J:7:CYS:O	2.19	0.42
2:B:816:GLU:HA	10:J:53:VAL:HG11	2.01	0.42
15:N:-42:DG:H2'	15:N:-41:DT:H71	2.02	0.42
1:A:409:ASP:N	1:A:409:ASP:OD1	2.52	0.42
1:A:531:GLY:HA3	1:A:658:LEU:HD22	2.02	0.42
2:B:803:LEU:HA	2:B:803:LEU:HD23	1.76	0.42
1:A:19:PHE:HB3	1:A:1416:GLY:HA2	2.02	0.42
1:A:676:THR:OG1	1:A:737:ASN:OD1	2.23	0.42
2:B:1182:CYS:HB3	2:B:1187:ASN:HB3	2.02	0.42
5:E:95:PHE:O	5:E:99:ILE:HG12	2.18	0.42
6:F:140:ASP:OD1	6:F:142:SER:N	2.45	0.42
1:A:610:ASP:HA	1:A:971:GLN:HE22	1.85	0.42
4:D:169:VAL:CG1	4:D:170:ASN:N	2.78	0.42
1:A:568:LYS:NZ	8:H:89:ALA:O	2.51	0.42
1:A:1168:ASP:HB3	1:A:1172:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:927:GLN:HE21	1:A:931:ASN:HD21	1.67	0.42
5:E:89:ILE:O	5:E:93:ARG:HB2	2.19	0.42
3:C:7:VAL:HG11	11:K:105:PHE:HD1	1.84	0.42
11:K:82:ARG:HA	11:K:83:PRO:HD3	1.84	0.42
14:T:72:DA:H2'	14:T:73:DA:C8	2.53	0.42
1:A:1028:LEU:HA	1:A:1028:LEU:HD23	1.83	0.42
8:H:139:LEU:HD23	8:H:139:LEU:HA	1.83	0.42
15:N:-65:DT:C5	15:N:-64:DT:C7	3.02	0.42
1:A:1162:SER:OG	1:A:1163:THR:N	2.53	0.42
1:A:697:LYS:O	1:A:702:GLU:N	2.41	0.42
2:B:107:ARG:HB2	2:B:109:LEU:HG	2.01	0.42
2:B:55:ARG:HD3	2:B:78:ARG:HD2	2.01	0.42
2:B:59:ASP:N	2:B:59:ASP:OD1	2.53	0.42
3:C:148:ARG:HB3	3:C:149:ASN:H	1.73	0.42
3:C:60:GLU:N	3:C:60:GLU:OE1	2.39	0.42
6:F:92:ARG:NH2	7:G:63:PRO:HG3	2.35	0.42
1:A:114:LEU:HD22	1:A:148:CYS:HA	2.02	0.41
2:B:227:HIS:CE1	2:B:382:ALA:HA	2.55	0.41
2:B:544:SER:O	2:B:548:ILE:HG12	2.20	0.41
5:E:20:GLU:OE1	5:E:145:HIS:NE2	2.53	0.41
14:T:73:DA:C6	14:T:74:DA:C6	3.08	0.41
1:A:551:LEU:HD22	1:A:581:ILE:HG21	2.02	0.41
1:A:765:CYS:SG	1:A:767:GLY:N	2.92	0.41
2:B:112:SER:HB2	2:B:160:LYS:HB3	2.02	0.41
2:B:806:THR:HG1	2:B:809:MET:H	1.66	0.41
3:C:73:SER:HB3	3:C:76:VAL:HB	2.02	0.41
7:G:129:ALA:HB2	7:G:138:THR:HB	2.02	0.41
14:T:82:DC:H6	14:T:82:DC:O5'	2.03	0.41
1:A:355:SER:N	1:A:469:PHE:O	2.44	0.41
1:A:505:LEU:HD12	2:B:1143:ALA:HB2	2.03	0.41
1:A:790:LYS:N	9:I:67:THR:O	2.53	0.41
3:C:171:SER:HB3	10:J:6:ARG:HH12	1.85	0.41
14:T:90:DC:H2'	14:T:91:DA:C8	2.55	0.41
1:A:516:GLN:HE21	1:A:1077:PRO:HG3	1.84	0.41
1:A:1118:LEU:HD23	1:A:1332:SER:HB2	2.03	0.41
1:A:1389:ARG:O	1:A:1393:ASN:HB2	2.21	0.41
1:A:900:VAL:HG11	1:A:930:LEU:HD13	2.03	0.41
2:B:1168:LEU:HA	2:B:1168:LEU:HD23	1.88	0.41
7:G:62:ILE:HD11	7:G:69:GLU:HB2	2.01	0.41
15:N:-47:DC:H2''	15:N:-46:DT:H71	2.01	0.41
1:A:83:HIS:HA	1:A:241:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:PRO:HA	2:B:113:SER:HA	2.01	0.41
15:N:61:DC:H2''	15:N:62:DG:C8	2.55	0.41
15:N:-64:DT:H2'	15:N:-63:DT:H6	1.80	0.41
14:T:-68:DG:H2''	14:T:-67:DA:H5''	2.02	0.41
1:A:408:ARG:HG3	1:A:431:TRP:CZ2	2.56	0.41
2:B:1092:TYR:HD1	2:B:1092:TYR:HA	1.56	0.41
2:B:24:PHE:HD1	2:B:678:TRP:CE2	2.38	0.41
2:B:535:LEU:HB3	2:B:629:PRO:HD2	2.03	0.41
5:E:45:ILE:HG22	5:E:53:GLN:H	1.86	0.41
8:H:111:ILE:HD13	8:H:128:TYR:HD1	1.84	0.41
8:H:89:ALA:HB1	8:H:95:VAL:HG21	2.01	0.41
15:N:-73:DT:H2''	15:N:-72:DT:C6	2.56	0.41
15:N:-75:DG:C2	15:N:-74:DT:C2	3.09	0.41
14:T:67:DA:N6	15:N:-68:DT:O4	2.53	0.41
14:T:-70:DC:H2'	14:T:-69:DA:C8	2.55	0.41
14:T:70:DG:C2	14:T:71:DA:C2	3.08	0.41
14:T:81:DC:C4	14:T:82:DC:N4	2.89	0.41
1:A:533:ARG:HD3	1:A:750:ALA:HA	2.01	0.41
2:B:1058:LEU:HD23	2:B:1058:LEU:HA	1.87	0.41
2:B:78:ARG:N	2:B:120:GLU:O	2.43	0.41
2:B:293:ILE:HG12	2:B:372:GLY:HA2	2.03	0.41
2:B:911:ILE:HD12	2:B:966:VAL:HG21	2.03	0.41
9:I:19:ASP:HB2	9:I:26:LEU:HD11	2.01	0.41
15:N:21:DG:H2''	15:N:22:DT:OP2	2.21	0.41
14:T:53:DA:N6	15:N:-54:DC:N4	2.68	0.41
1:A:63:ARG:NH1	14:T:-13:DA:OP1	111.80	0.41
14:T:62:DA:C2	14:T:63:DA:N1	2.87	0.41
2:B:480:THR:HG21	2:B:777:ALA:HB3	2.02	0.41
2:B:593:MET:HB3	2:B:608:ILE:HD13	2.01	0.41
2:B:182:LYS:HG3	10:J:63:ASN:HD22	1.86	0.41
1:A:453:LYS:HD3	1:A:1069:ILE:HG12	2.03	0.41
2:B:176:ASP:O	2:B:179:ASP:N	2.53	0.41
1:A:1061:HIS:CE1	6:F:87:LYS:HE3	2.56	0.41
11:K:12:LEU:HD12	11:K:13:PRO:HD2	2.02	0.41
1:A:448:GLN:OE1	1:A:489:ASN:ND2	2.54	0.41
1:A:913:VAL:O	1:A:981:SER:N	2.52	0.41
8:H:121:LEU:HD23	8:H:121:LEU:HA	1.89	0.41
11:K:31:ILE:HD11	11:K:83:PRO:HB2	2.02	0.41
2:B:203:LEU:HA	2:B:203:LEU:HD23	1.72	0.41
2:B:549:ASN:O	2:B:553:GLU:CB	2.55	0.41
2:B:597:ARG:NH1	2:B:608:ILE:H	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:639:LYS:HB3	2:B:639:LYS:HE3	1.93	0.41
4:D:101:VAL:HG13	7:G:105:PRO:HB3	2.03	0.41
8:H:36:ILE:HG12	8:H:126:GLY:HA3	2.02	0.41
15:N:-65:DT:C3'	15:N:-64:DT:H5''	2.40	0.41
15:N:-71:DT:H2''	15:N:-70:DC:C6	2.56	0.41
14:T:-15:DA:C6	14:T:-14:DA:C6	3.09	0.41
1:A:248:ARG:HB2	1:A:261:ASP:HB3	2.02	0.40
1:A:962:LEU:HD11	1:A:1024:VAL:HG22	2.03	0.40
2:B:827:ILE:HG23	2:B:1012:ILE:HG13	2.03	0.40
2:B:622:ASP:OD1	2:B:623:VAL:N	2.54	0.40
7:G:106:LEU:H	7:G:106:LEU:CD1	2.35	0.40
8:H:17:ASN:OD1	8:H:24:SER:OG	2.25	0.40
2:B:733:SER:HA	9:I:70:ARG:HB2	2.03	0.40
2:B:954:LEU:HD23	12:L:58:ILE:HD11	2.02	0.40
13:P:6:U:H2'	13:P:7:G:C8	2.56	0.40
14:T:42:DC:H2''	14:T:43:DA:OP2	2.21	0.40
1:A:1056:GLN:HB3	6:F:84:TYR:HE2	1.85	0.40
1:A:422:ALA:HA	1:A:425:ILE:HD12	2.04	0.40
2:B:170:CYS:SG	2:B:171:SER:N	2.94	0.40
2:B:286:ASP:OD2	9:I:12:ASN:ND2	2.35	0.40
2:B:383:LEU:HA	2:B:383:LEU:HD23	1.87	0.40
2:B:882:THR:HG22	2:B:934:LYS:HB2	2.03	0.40
15:N:32:DG:H2''	15:N:33:DT:H71	2.03	0.40
15:N:-51:DG:H2''	15:N:-50:DT:OP2	2.21	0.40
15:N:-57:DT:H2''	15:N:-56:DG:C8	2.56	0.40
1:A:1209:LEU:HD23	1:A:1277:ARG:HH21	1.86	0.40
1:A:47:ARG:HA	1:A:48:PRO:HD2	1.87	0.40
1:A:683:ALA:O	1:A:686:SER:OG	2.30	0.40
1:A:942:LYS:NZ	1:A:946:GLU:OE1	2.36	0.40
2:B:296:ASP:HB3	2:B:299:ASP:HB2	2.03	0.40
11:K:39:ASP:HB3	11:K:40:HIS:H	1.70	0.40
14:T:-45:DA:C6	14:T:-44:DA:C6	3.10	0.40
2:B:1164:GLY:N	2:B:1190:ASN:O	2.37	0.40
2:B:64:HIS:H	2:B:66:ASN:ND2	2.20	0.40
2:B:797:TYR:O	2:B:799:PRO:HD3	2.20	0.40
5:E:78:TRP:NE1	5:E:80:GLU:OE1	2.43	0.40
10:J:22:LEU:HA	10:J:22:LEU:HD23	1.82	0.40
15:N:17:DA:C6	15:N:18:DG:C6	3.10	0.40
15:N:-18:DG:H2''	15:N:-17:DT:OP2	2.21	0.40
1:A:1337:GLU:O	1:A:1340:SER:OG	2.29	0.40
1:A:416:LEU:HD23	1:A:416:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:GLY:HA3	2:B:1069:PHE:CZ	2.57	0.40
1:A:688:LYS:NZ	1:A:802:GLU:OE1	2.53	0.40
2:B:1129:ARG:HD3	14:T:88:DA:H5"	2.04	0.40
6:F:100:GLN:NE2	7:G:18:PHE:HE2	2.20	0.40
15:N:-15:DA:H2"	15:N:-14:DA:H8	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1396/1743 (80%)	1252 (90%)	142 (10%)	2 (0%)	53	88
2	B	1151/1227 (94%)	1018 (88%)	131 (11%)	2 (0%)	49	85
3	C	261/304 (86%)	231 (88%)	29 (11%)	1 (0%)	36	77
4	D	148/186 (80%)	136 (92%)	9 (6%)	3 (2%)	8	45
5	E	211/214 (99%)	195 (92%)	16 (8%)	0	100	100
6	F	82/155 (53%)	73 (89%)	9 (11%)	0	100	100
7	G	169/171 (99%)	159 (94%)	8 (5%)	2 (1%)	14	56
8	H	129/145 (89%)	113 (88%)	16 (12%)	0	100	100
9	I	109/115 (95%)	94 (86%)	15 (14%)	0	100	100
10	J	64/72 (89%)	57 (89%)	7 (11%)	0	100	100
11	K	111/118 (94%)	100 (90%)	11 (10%)	0	100	100
12	L	43/72 (60%)	40 (93%)	3 (7%)	0	100	100
16	a	95/139 (68%)	89 (94%)	3 (3%)	3 (3%)	4	34
16	e	95/139 (68%)	90 (95%)	5 (5%)	0	100	100
17	b	78/106 (74%)	75 (96%)	3 (4%)	0	100	100
17	f	76/106 (72%)	72 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	c	101/133 (76%)	95 (94%)	6 (6%)	0	100	100
18	g	103/133 (77%)	97 (94%)	6 (6%)	0	100	100
19	d	93/129 (72%)	89 (96%)	4 (4%)	0	100	100
19	h	91/129 (70%)	88 (97%)	3 (3%)	0	100	100
All	All	4606/5536 (83%)	4163 (90%)	430 (9%)	13 (0%)	47	81

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	171	LEU
7	G	134	ASP
4	D	169	VAL
7	G	154	VAL
16	a	63	ARG
4	D	164	ALA
16	a	39	HIS
2	B	155	LYS
16	a	40	ARG
2	B	175	LEU
3	C	90	TYR
1	A	47	ARG
1	A	959	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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1223/1528 (80%)	1217 (100%)	6 (0%)	90	95
2	B	1016/1077 (94%)	1009 (99%)	7 (1%)	85	93
3	C	236/264 (89%)	234 (99%)	2 (1%)	83	92
4	D	133/160 (83%)	130 (98%)	3 (2%)	53	76
5	E	196/197 (100%)	193 (98%)	3 (2%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	148/148 (100%)	147 (99%)	1 (1%)	85	93
8	H	120/130 (92%)	120 (100%)	0	100	100
9	I	106/109 (97%)	105 (99%)	1 (1%)	81	90
10	J	60/66 (91%)	59 (98%)	1 (2%)	63	83
11	K	104/109 (95%)	103 (99%)	1 (1%)	78	89
12	L	38/56 (68%)	36 (95%)	2 (5%)	25	56
16	a	83/112 (74%)	82 (99%)	1 (1%)	74	87
16	e	82/112 (73%)	81 (99%)	1 (1%)	74	87
17	b	65/81 (80%)	64 (98%)	1 (2%)	67	85
17	f	63/81 (78%)	62 (98%)	1 (2%)	65	84
18	c	82/102 (80%)	82 (100%)	0	100	100
18	g	83/102 (81%)	82 (99%)	1 (1%)	74	87
19	d	81/107 (76%)	80 (99%)	1 (1%)	74	87
19	h	79/107 (74%)	77 (98%)	2 (2%)	50	74
All	All	4073/4785 (85%)	4038 (99%)	35 (1%)	82	90

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	200	ARG
1	A	446	ASN
1	A	661	ASN
1	A	737	ASN
1	A	805	TYR
1	A	1403	CYS
2	B	184	LYS
2	B	240	ARG
2	B	500	LYS
2	B	904	ARG
2	B	1010	LEU
2	B	1122	ARG
2	B	1201	LYS
3	C	8	ASN
3	C	188	HIS
4	D	72	ASN
4	D	171	LEU

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Mol	Chain	Res	Type
4	D	185	TYR
5	E	4	ASN
5	E	120	ASN
5	E	166	ARG
7	G	106	LEU
9	I	105	ASN
10	J	8	PHE
11	K	19	LEU
12	L	51	LYS
12	L	62	ARG
16	a	108	ASN
17	b	92	ARG
19	d	76	ARG
16	e	53	ARG
17	f	92	ARG
18	g	71	ARG
19	h	60	ASN
19	h	76	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	278	GLN
1	A	291	ASN
1	A	298	GLN
1	A	317	GLN
1	A	446	ASN
1	A	516	GLN
1	A	590	GLN
1	A	632	HIS
1	A	651	GLN
1	A	661	ASN
1	A	743	ASN
1	A	787	HIS
1	A	927	GLN
1	A	931	ASN
1	A	968	ASN
1	A	1013	GLN
1	A	1072	GLN
2	B	72	ASN
2	B	426	GLN

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Mol	Chain	Res	Type
2	B	524	GLN
2	B	549	ASN
2	B	641	ASN
2	B	761	HIS
2	B	794	ASN
2	B	996	HIS
2	B	1025	HIS
2	B	1093	GLN
3	C	8	ASN
5	E	4	ASN
5	E	112	GLN
5	E	120	ASN
9	I	105	ASN
10	J	63	ASN
11	K	2	ASN
11	K	44	ASN
11	K	110	ASN
16	a	68	GLN
19	d	81	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	P	10/11 (90%)	1 (10%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	P	1	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.