



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:18 PM BST

PDB ID : 5FUR  
EMDB ID: : EMD-3305  
Title : Structure of human TFIID-IIA bound to core promoter DNA  
Authors : Louder, R.K.; He, Y.; Lopez-Blanco, J.R.; Fang, J.; Chacon, P.; Nogales, E.  
Deposited on : 2016-01-29  
Resolution : 8.50 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

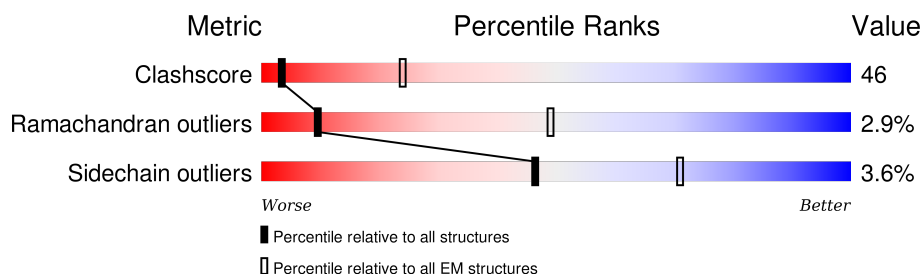
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.50 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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  $\geq 3$ , 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	339	
2	B	43	
3	C	47	
4	D	97	
5	E	89	
6	F	93	
7	G	1893	
8	H	349	
9	I	1199	

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Mol	Chain	Length	Quality of chain
10	J	677	<div><div></div><div>22%8%..68%</div></div>
10	K	677	<div><div></div><div>18%8%..71%</div></div>
11	L	310	<div><div></div><div>• 5%91%</div></div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21485 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 TATA-BOX-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	180	Total	C	N	O	S	0	0
			1429	927	252	243	7		

- Molecule 2 is a protein called TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	43	Total	C	N	O	S	0	0
			356	228	56	70	2		

- Molecule 3 is a protein called TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	47	Total	C	N	O	S	0	0
			393	250	70	71	2		

- Molecule 4 is a protein called TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	97	Total	C	N	O	S	0	0
			793	502	140	149	2		

- Molecule 5 is a DNA chain called SUPER CORE PROMOTER.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	80	Total	C	N	O	P	0	0
			1654	778	320	476	80		

- Molecule 6 is a DNA chain called SUPER CORE PROMOTER.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	80	Total	C	N	O	P	0	0
			1626	770	292	484	80		

- Molecule 7 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	406	Total	C	N	O	P	S	
			3290	2090	580	596	2	22	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	178	VAL	-	INSERTION	UNP P21675
G	179	SER	-	INSERTION	UNP P21675
G	180	GLU	-	INSERTION	UNP P21675
G	181	ASN	-	INSERTION	UNP P21675
G	182	GLY	-	INSERTION	UNP P21675
G	183	GLU	-	INSERTION	UNP P21675
G	184	GLY	-	INSERTION	UNP P21675
G	185	ILE	-	INSERTION	UNP P21675
G	186	ILE	-	INSERTION	UNP P21675
G	187	LEU	-	INSERTION	UNP P21675
G	188	PRO	-	INSERTION	UNP P21675
G	189	SER	-	INSERTION	UNP P21675
G	190	ILE	-	INSERTION	UNP P21675
G	191	ILE	-	INSERTION	UNP P21675
G	192	ALA	-	INSERTION	UNP P21675
G	193	PRO	-	INSERTION	UNP P21675
G	194	SER	-	INSERTION	UNP P21675
G	195	SER	-	INSERTION	UNP P21675
G	196	LEU	-	INSERTION	UNP P21675
G	197	ALA	-	INSERTION	UNP P21675
G	198	SER	-	INSERTION	UNP P21675

- Molecule 8 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	123	Total	C	N	O	S		
			998	638	184	172	4	0	0

- Molecule 9 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	914	Total	C	N	O	S		
			7404	4761	1251	1336	56	0	2

- Molecule 10 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	220	Total	C	N	O	S	0	0
			1741	1106	306	318	11		
10	K	198	Total	C	N	O	S	0	0
			1582	1006	276	290	10		

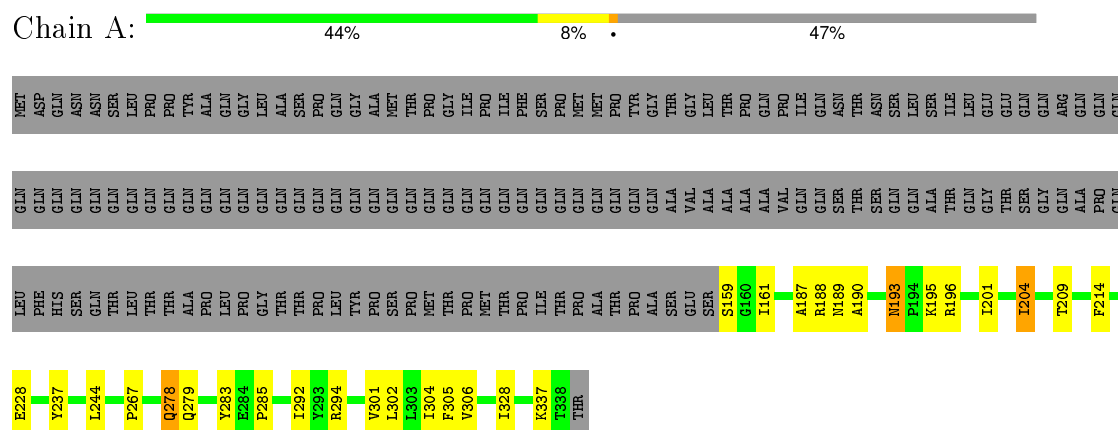
- Molecule 11 is a protein called TRANSCRIPTION INITIATION FACTOR TFIID SUBUNIT 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	27	Total	C	N	O	S	0	1
			219	134	46	38	1		

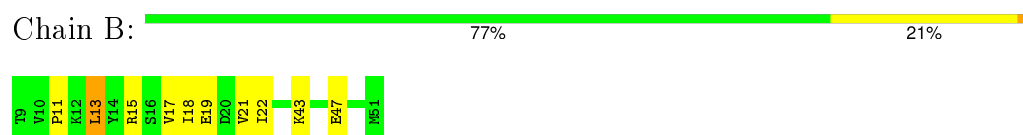
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

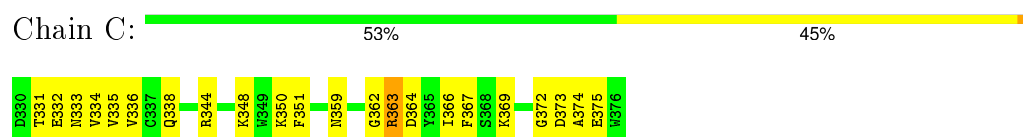
#### • Molecule 1: TATA-BOX-BINDING PROTEIN



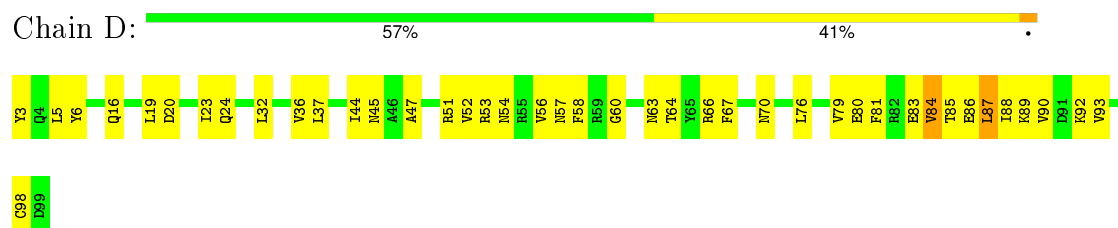
#### • Molecule 2: TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 1



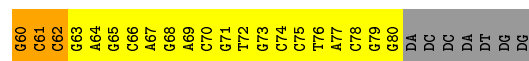
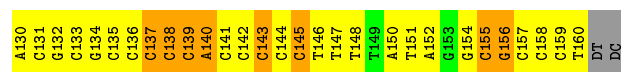
#### • Molecule 3: TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 1



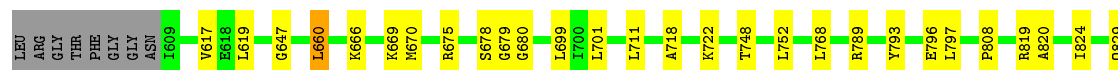
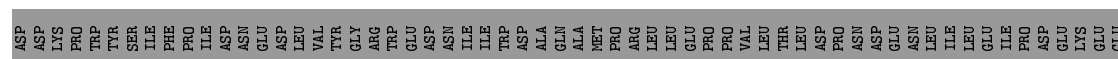
#### • Molecule 4: TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT 2



#### • Molecule 5: SUPER CORE PROMOTER

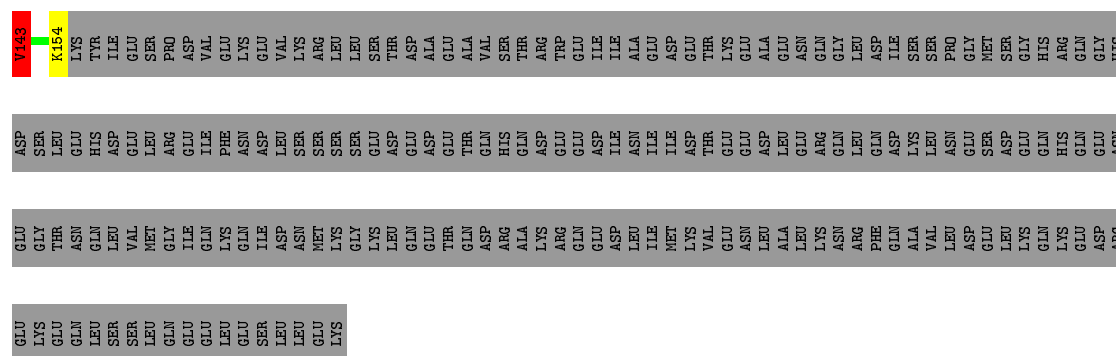
[illegible]

MET	GLY	PRO	GLY	CYS	ASP	LEU	LEU	ARG	THR	ALA	ALA	ILE	THR	THR	THR	ASP	ASP	ASP	ASP	SER	SER	GLU	GLY	GLY	GLY	PHE	SER	SER	LEU	GLY	PHE	LEU	PHE	GLY	ASN	ASN	ALA	ALA	GLN	LEU	GLY	VAL	SER	LEU	ASP
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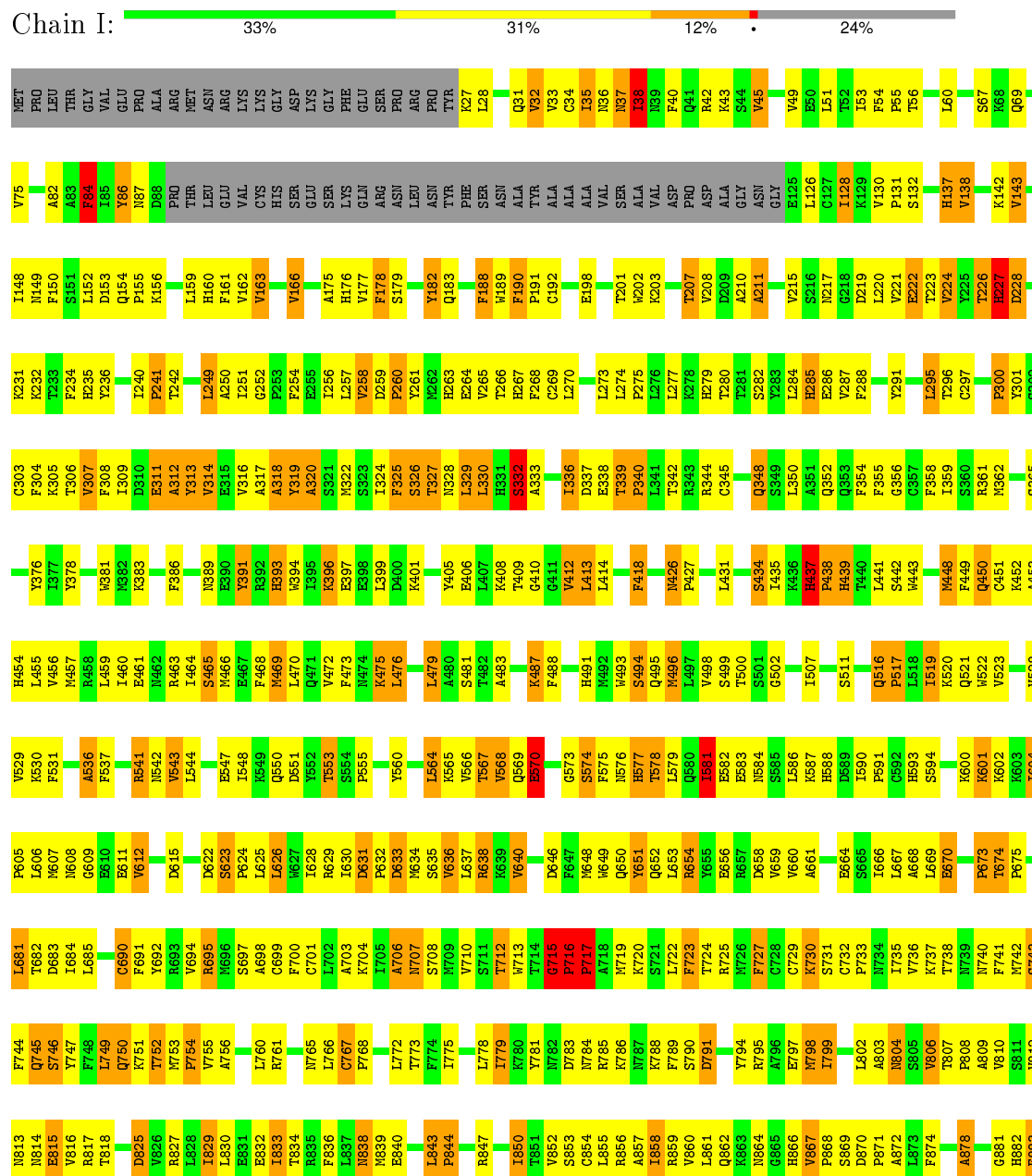








## • Molecule 9: TRANSCRIPTION INITIATION FACTOR TFIIID SUBUNIT 2







## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE, Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.52	0/1455	0.69	0/1958
10	J	0.74	0/1773	1.42	26/2408 (1.1%)
10	K	0.75	0/1612	1.38	21/2188 (1.0%)
11	L	0.61	1/220 (0.5%)	1.10	0/292
2	B	0.34	0/360	0.53	0/487
3	C	0.40	0/402	0.83	1/539 (0.2%)
4	D	0.35	0/803	0.73	2/1088 (0.2%)
5	E	3.85	16/1806 (0.9%)	1.89	49/2658 (1.8%)
6	F	3.55	15/1764 (0.9%)	2.11	46/2582 (1.8%)
7	G	0.41	0/3349	0.55	0/4506
8	H	0.42	0/1017	0.59	1/1370 (0.1%)
9	I	0.84	8/7587 (0.1%)	0.82	5/10278 (0.0%)
All	All	1.61	40/22148 (0.2%)	1.16	151/30354 (0.5%)

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
10	J	2	16
10	K	1	12
5	E	0	2
7	G	0	1
9	I	0	235
All	All	3	266

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	43	DC	O3'-P	49.26	2.20	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	44	DG	O3'-P	48.90	2.19	1.61
5	E	62	DC	O3'-P	48.41	2.19	1.61
5	E	59	DA	O3'-P	46.14	2.16	1.61
6	F	105	DA	O3'-P	46.09	2.16	1.61
5	E	42	DT	O3'-P	45.29	2.15	1.61
5	E	24	DG	O3'-P	45.02	2.15	1.61
5	E	61	DC	O3'-P	44.21	2.14	1.61
6	F	120	DC	O3'-P	43.85	2.13	1.61
5	E	41	DG	O3'-P	43.48	2.13	1.61
6	F	103	DC	O3'-P	42.62	2.12	1.61
5	E	60	DG	O3'-P	41.70	2.11	1.61
6	F	145	DC	P-O5'	41.60	2.01	1.59
5	E	18	DG	O3'-P	41.56	2.11	1.61
6	F	102	DT	O3'-P	41.30	2.10	1.61
5	E	7	DC	C1'-N1	40.11	2.03	1.47
6	F	140	DA	O3'-P	39.88	2.08	1.61
6	F	137	DC	O3'-P	39.76	2.08	1.61
6	F	156	DG	P-O5'	39.57	1.99	1.59
6	F	104	DG	O3'-P	39.09	2.08	1.61
5	E	17	DG	P-O5'	38.03	1.97	1.59
5	E	26	DG	O3'-P	37.88	2.06	1.61
6	F	122	DG	O3'-P	36.50	2.04	1.61
6	F	139	DC	O3'-P	35.21	2.03	1.61
6	F	121	DT	O3'-P	35.12	2.03	1.61
5	E	25	DG	O3'-P	34.91	2.03	1.61
6	F	138	DC	O3'-P	33.55	2.01	1.61
6	F	156	DG	O3'-P	27.84	1.94	1.61
6	F	143	DC	O3'-P	-25.92	1.30	1.61
9	I	716	PRO	N-CD	-14.30	1.27	1.47
5	E	4	DG	O3'-P	-8.33	1.51	1.61
5	E	5	DC	O3'-P	6.54	1.69	1.61
9	I	87	ASN	C-N	-5.92	1.20	1.34
9	I	975	TYR	C-N	-5.89	1.20	1.34
9	I	717	PRO	N-CD	-5.84	1.39	1.47
9	I	555	PRO	N-CD	-5.72	1.39	1.47
9	I	241	PRO	N-CD	-5.71	1.39	1.47
9	I	754	PRO	N-CD	-5.52	1.40	1.47
11	L	197	THR	C-N	-5.41	1.23	1.33
9	I	673	PRO	N-CD	-5.39	1.40	1.47

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	145	DC	O5'-P-OP2	-41.73	60.62	110.70
9	I	437	HIS	C-N-CD	-27.62	59.83	120.60
5	E	17	DG	P-O3'-C3'	-27.17	87.10	119.70
6	F	145	DC	P-O5'-C5'	-24.28	82.05	120.90
6	F	156	DG	O5'-P-OP1	-23.00	83.11	110.70
5	E	17	DG	O3'-P-O5'	-18.75	68.37	104.00
6	F	103	DC	P-O3'-C3'	-18.46	97.55	119.70
5	E	62	DC	P-O3'-C3'	-18.17	97.89	119.70
6	F	156	DG	P-O3'-C3'	18.06	141.38	119.70
5	E	43	DC	P-O3'-C3'	-17.88	98.24	119.70
6	F	145	DC	O5'-P-OP1	17.60	131.81	110.70
6	F	121	DT	P-O3'-C3'	-17.53	98.67	119.70
6	F	120	DC	P-O3'-C3'	-17.49	98.71	119.70
5	E	59	DA	P-O3'-C3'	-16.50	99.90	119.70
6	F	139	DC	P-O3'-C3'	-16.21	100.24	119.70
6	F	105	DA	P-O3'-C3'	-16.19	100.27	119.70
5	E	17	DG	OP1-P-O3'	14.76	137.66	105.20
5	E	61	DC	P-O3'-C3'	-14.55	102.24	119.70
5	E	18	DG	P-O3'-C3'	-14.54	102.25	119.70
6	F	138	DC	P-O3'-C3'	-13.99	102.92	119.70
6	F	143	DC	P-O3'-C3'	-13.70	103.26	119.70
5	E	24	DG	P-O3'-C3'	-13.62	103.36	119.70
5	E	25	DG	P-O3'-C3'	-13.57	103.41	119.70
6	F	137	DC	P-O3'-C3'	-13.41	103.60	119.70
5	E	17	DG	P-O5'-C5'	-13.32	99.58	120.90
6	F	122	DG	P-O3'-C3'	-13.13	103.94	119.70
6	F	140	DA	P-O3'-C3'	-13.11	103.96	119.70
6	F	104	DG	P-O3'-C3'	-12.96	104.15	119.70
5	E	7	DC	C2-N1-C1'	-12.95	104.55	118.80
5	E	41	DG	P-O3'-C3'	-12.84	104.29	119.70
6	F	102	DT	P-O3'-C3'	-12.40	104.82	119.70
5	E	42	DT	P-O3'-C3'	-12.14	105.13	119.70
9	I	716	PRO	N-CA-C	11.95	143.16	112.10
6	F	143	DC	O3'-P-O5'	-11.58	82.00	104.00
5	E	7	DC	C6-N1-C1'	11.25	134.30	120.80
5	E	5	DC	OP1-P-O3'	11.09	129.59	105.20
6	F	143	DC	OP1-P-O3'	10.83	129.03	105.20
5	E	60	DG	P-O3'-C3'	-10.78	106.76	119.70
5	E	44	DG	P-O3'-C3'	-10.55	107.04	119.70
5	E	7	DC	O4'-C1'-N1	-10.19	100.87	108.00
10	J	239	ARG	NE-CZ-NH1	9.97	125.29	120.30
10	J	370	TRP	CD1-CG-CD2	-9.62	98.60	106.30
10	K	239	ARG	NE-CZ-NH1	9.55	125.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	370	TRP	CD1-CG-CD2	-9.54	98.67	106.30
5	E	26	DG	P-O3'-C3'	-9.52	108.27	119.70
9	I	716	PRO	CA-N-CD	9.52	125.03	111.70
6	F	103	DC	O3'-P-O5'	-9.08	86.76	104.00
5	E	5	DC	P-O3'-C3'	9.02	130.53	119.70
5	E	17	DG	O5'-P-OP2	-8.99	97.61	105.70
10	J	284	ARG	NE-CZ-NH2	8.92	124.76	120.30
6	F	137	DC	O3'-P-O5'	-8.91	87.07	104.00
5	E	43	DC	O3'-P-O5'	-8.75	87.37	104.00
5	E	62	DC	O3'-P-O5'	-8.72	87.42	104.00
10	K	284	ARG	NE-CZ-NH2	8.71	124.66	120.30
6	F	154	DG	O4'-C1'-N9	-8.67	101.93	108.00
6	F	138	DC	O3'-P-O5'	-8.54	87.77	104.00
5	E	25	DG	O3'-P-O5'	-8.45	87.94	104.00
6	F	155	DC	O3'-P-O5'	8.44	120.04	104.00
5	E	59	DA	O3'-P-O5'	-8.34	88.16	104.00
5	E	24	DG	O3'-P-O5'	-8.32	88.18	104.00
5	E	43	DC	OP2-P-O3'	8.31	123.49	105.20
5	E	59	DA	OP2-P-O3'	8.25	123.35	105.20
6	F	103	DC	OP2-P-O3'	8.25	123.34	105.20
5	E	62	DC	OP2-P-O3'	8.24	123.33	105.20
9	I	716	PRO	N-CA-CB	-8.21	93.45	103.30
6	F	120	DC	O3'-P-O5'	-8.06	88.69	104.00
6	F	105	DA	OP2-P-O3'	8.05	122.92	105.20
10	J	330	ARG	NE-CZ-NH1	7.97	124.29	120.30
6	F	120	DC	OP2-P-O3'	7.92	122.62	105.20
6	F	156	DG	O3'-P-O5'	7.88	118.97	104.00
6	F	139	DC	O3'-P-O5'	-7.86	89.07	104.00
6	F	121	DT	O3'-P-O5'	-7.79	89.20	104.00
6	F	105	DA	O3'-P-O5'	-7.75	89.27	104.00
5	E	24	DG	OP2-P-O3'	7.69	122.11	105.20
6	F	156	DG	OP2-P-O3'	-7.66	88.35	105.20
10	K	330	ARG	NE-CZ-NH1	7.62	124.11	120.30
10	J	402	ARG	NE-CZ-NH1	7.62	124.11	120.30
5	E	41	DG	OP2-P-O3'	7.57	121.86	105.20
5	E	16	DG	O3'-P-O5'	7.55	118.34	104.00
5	E	4	DG	OP1-P-O3'	7.51	121.73	105.20
5	E	61	DC	O3'-P-O5'	-7.49	89.76	104.00
10	J	412	LEU	CA-CB-CG	7.45	132.44	115.30
6	F	121	DT	OP2-P-O3'	7.39	121.47	105.20
10	J	326	HIS	CA-CB-CG	7.29	125.99	113.60
10	K	326	HIS	CA-CB-CG	7.28	125.97	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	320	ARG	NE-CZ-NH1	7.22	123.91	120.30
4	D	87	LEU	N-CA-C	7.03	129.98	111.00
5	E	18	DG	O3'-P-O5'	-6.91	90.87	104.00
5	E	42	DT	OP2-P-O3'	6.90	120.38	105.20
10	K	370	TRP	CB-CG-CD2	6.89	135.56	126.60
10	K	402	ARG	NE-CZ-NH1	6.89	123.74	120.30
10	J	370	TRP	NE1-CE2-CD2	-6.87	100.43	107.30
10	J	370	TRP	CB-CG-CD2	6.86	135.51	126.60
10	K	370	TRP	NE1-CE2-CD2	-6.82	100.48	107.30
5	E	26	DG	O3'-P-O5'	-6.81	91.05	104.00
10	J	407	LEU	CB-CA-C	6.80	123.13	110.20
5	E	18	DG	OP2-P-O3'	6.80	120.15	105.20
10	K	407	LEU	CB-CA-C	6.74	123.00	110.20
6	F	137	DC	OP2-P-O3'	6.70	119.93	105.20
10	J	239	ARG	NE-CZ-NH2	-6.65	116.97	120.30
10	K	320	ARG	NE-CZ-NH1	6.64	123.62	120.30
5	E	42	DT	O3'-P-O5'	-6.63	91.40	104.00
5	E	41	DG	O3'-P-O5'	-6.63	91.41	104.00
5	E	61	DC	OP2-P-O3'	6.62	119.76	105.20
6	F	122	DG	OP2-P-O3'	6.60	119.72	105.20
5	E	25	DG	OP2-P-O3'	6.58	119.67	105.20
10	J	373	ARG	NE-CZ-NH1	6.54	123.57	120.30
6	F	102	DT	OP2-P-O3'	6.54	119.59	105.20
6	F	102	DT	O3'-P-O5'	-6.53	91.59	104.00
10	J	354	ARG	NE-CZ-NH1	6.51	123.56	120.30
10	K	239	ARG	NE-CZ-NH2	-6.51	117.05	120.30
10	J	395	ARG	NE-CZ-NH1	6.49	123.54	120.30
10	K	373	ARG	NE-CZ-NH1	6.47	123.54	120.30
10	J	284	ARG	NH1-CZ-NH2	-6.38	112.38	119.40
6	F	139	DC	OP2-P-O3'	6.37	119.22	105.20
10	K	284	ARG	NH1-CZ-NH2	-6.37	112.39	119.40
10	K	395	ARG	NE-CZ-NH1	6.32	123.46	120.30
6	F	104	DG	OP2-P-O3'	6.30	119.05	105.20
10	J	417	ARG	NE-CZ-NH1	6.28	123.44	120.30
10	K	354	ARG	NE-CZ-NH1	6.17	123.39	120.30
6	F	140	DA	O3'-P-O5'	-6.13	92.36	104.00
5	E	44	DG	OP2-P-O3'	6.05	118.51	105.20
6	F	138	DC	OP2-P-O3'	6.04	118.48	105.20
6	F	104	DG	O3'-P-O5'	-5.95	92.70	104.00
9	I	715	GLY	C-N-CD	-5.92	107.57	120.60
10	K	281	TYR	CB-CG-CD2	-5.86	117.48	121.00
6	F	122	DG	O3'-P-O5'	-5.84	92.89	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	140	DA	OP2-P-O3'	5.79	117.93	105.20
5	E	60	DG	O3'-P-O5'	-5.75	93.07	104.00
10	K	257	PRO	N-CA-C	5.71	126.95	112.10
5	E	60	DG	OP2-P-O3'	5.67	117.68	105.20
6	F	156	DG	O5'-P-OP2	5.67	117.50	110.70
10	K	315	ARG	NE-CZ-NH1	5.65	123.13	120.30
10	J	257	PRO	N-CA-C	5.65	126.79	112.10
10	J	315	ARG	NE-CZ-NH1	5.55	123.07	120.30
10	J	404	ARG	NE-CZ-NH1	5.41	123.00	120.30
5	E	44	DG	O3'-P-O5'	-5.32	93.89	104.00
10	J	415	ILE	CB-CA-C	5.29	122.19	111.60
10	K	284	ARG	NE-CZ-NH1	5.27	122.93	120.30
5	E	5	DC	O3'-P-O5'	-5.26	94.00	104.00
10	J	386	ASP	CB-CA-C	5.24	120.87	110.40
5	E	26	DG	OP2-P-O3'	5.23	116.70	105.20
10	K	386	ASP	CB-CA-C	5.23	120.85	110.40
8	H	143	VAL	CB-CA-C	-5.22	101.49	111.40
10	J	281	TYR	CB-CG-CD2	-5.21	117.87	121.00
3	C	363	ARG	CG-CD-NE	-5.20	100.88	111.80
10	J	411	VAL	N-CA-C	-5.15	97.11	111.00
4	D	86	GLU	N-CA-C	5.14	124.87	111.00
10	J	284	ARG	NE-CZ-NH1	5.09	122.85	120.30
10	J	406	VAL	CB-CA-C	5.04	120.98	111.40
10	K	406	VAL	CB-CA-C	5.02	120.93	111.40

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	J	326	HIS	CA
10	J	411	VAL	CA
10	K	326	HIS	CA

All (266) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	10	DA	Sidechain
5	E	7	DC	Sidechain
7	G	1104	LEU	Peptide
9	I	128	ILE	Mainchain
9	I	132	SER	Mainchain
9	I	137	HIS	Mainchain,Peptide
9	I	138	VAL	Mainchain

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Mol	Chain	Res	Type	Group
9	I	142	LYS	Mainchain
9	I	143	VAL	Mainchain
9	I	149	ASN	Mainchain
9	I	150	PHE	Mainchain
9	I	160	HIS	Mainchain
9	I	163	VAL	Mainchain
9	I	166	VAL	Mainchain
9	I	175	ALA	Mainchain
9	I	178	PHE	Mainchain
9	I	182	TYR	Mainchain,Peptide
9	I	188	PHE	Mainchain
9	I	190	PHE	Mainchain
9	I	201	THR	Mainchain
9	I	202	TRP	Mainchain
9	I	207	THR	Mainchain
9	I	208	VAL	Mainchain
9	I	211	ALA	Mainchain
9	I	217	ASN	Mainchain
9	I	224	VAL	Mainchain
9	I	226	THR	Mainchain
9	I	227	HIS	Mainchain
9	I	228	ASP	Mainchain,Peptide
9	I	242	THR	Mainchain
9	I	249	LEU	Mainchain
9	I	258	VAL	Mainchain
9	I	263	HIS	Mainchain
9	I	264	GLU	Mainchain
9	I	279	HIS	Mainchain
9	I	285	HIS	Mainchain
9	I	286	GLU	Mainchain
9	I	295	LEU	Mainchain
9	I	300	PRO	Mainchain
9	I	303	CYS	Mainchain
9	I	307	VAL	Mainchain
9	I	311	GLU	Mainchain
9	I	312	ALA	Mainchain
9	I	313	TYR	Mainchain
9	I	316	VAL	Mainchain,Peptide
9	I	318	ALA	Mainchain,Peptide
9	I	32	VAL	Mainchain
9	I	320	ALA	Mainchain
9	I	325	PHE	Mainchain

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Mol	Chain	Res	Type	Group
9	I	326	SER	Mainchain
9	I	327	THR	Mainchain
9	I	329	LEU	Mainchain
9	I	33	VAL	Mainchain
9	I	330	LEU	Mainchain
9	I	332	SER	Mainchain
9	I	34	CYS	Mainchain
9	I	348	GLN	Mainchain
9	I	35	ILE	Mainchain
9	I	350	LEU	Mainchain
9	I	352	GLN	Mainchain
9	I	356	GLY	Mainchain
9	I	362	MET	Mainchain
9	I	365	SER	Mainchain
9	I	376	TYR	Mainchain
9	I	38	ILE	Mainchain
9	I	386	PHE	Mainchain
9	I	391	TYR	Mainchain
9	I	393	HIS	Mainchain
9	I	396	LYS	Mainchain
9	I	40	PHE	Mainchain
9	I	409	THR	Mainchain
9	I	410	GLY	Mainchain
9	I	412	VAL	Mainchain,Peptide
9	I	418	PHE	Mainchain
9	I	42	ARG	Mainchain
9	I	426	ASN	Mainchain
9	I	431	LEU	Mainchain
9	I	434	SER	Peptide
9	I	437	HIS	Peptide
9	I	439	HIS	Mainchain
9	I	441	LEU	Mainchain
9	I	448	MET	Mainchain
9	I	449	PHE	Mainchain
9	I	45	VAL	Mainchain
9	I	450	GLN	Mainchain
9	I	453	ALA	Mainchain
9	I	456	VAL	Mainchain
9	I	457	MET	Mainchain
9	I	459	LEU	Mainchain
9	I	463	ARG	Mainchain
9	I	466	MET	Mainchain

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Mol	Chain	Res	Type	Group
9	I	468	PHE	Mainchain
9	I	469	MET	Mainchain
9	I	475	LYS	Mainchain
9	I	476	LEU	Mainchain
9	I	479	LEU	Mainchain
9	I	481	SER	Mainchain
9	I	487	LYS	Mainchain
9	I	493	TRP	Mainchain
9	I	494	SER	Peptide
9	I	499	SER	Mainchain
9	I	502	GLY	Mainchain
9	I	516	GLN	Mainchain
9	I	517	PRO	Mainchain
9	I	519	ILE	Mainchain
9	I	520	LYS	Mainchain
9	I	521	GLN	Mainchain
9	I	529	VAL	Mainchain
9	I	530	LYS	Mainchain
9	I	536	ALA	Mainchain
9	I	541	ARG	Mainchain
9	I	543	VAL	Mainchain
9	I	547	GLU	Mainchain
9	I	551	ASP	Mainchain
9	I	553	THR	Mainchain
9	I	56	THR	Mainchain
9	I	560	TYR	Mainchain
9	I	564	LEU	Mainchain
9	I	565	LYS	Mainchain
9	I	567	THR	Mainchain
9	I	568	VAL	Mainchain
9	I	570	GLU	Mainchain
9	I	574	SER	Mainchain
9	I	581	ILE	Mainchain
9	I	582	GLU	Mainchain
9	I	583	GLU	Mainchain
9	I	587	LYS	Mainchain
9	I	588	HIS	Mainchain
9	I	590	ILE	Mainchain
9	I	60	LEU	Mainchain
9	I	600	LYS	Mainchain
9	I	601	LYS	Mainchain,Peptide
9	I	604	ILE	Peptide

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Mol	Chain	Res	Type	Group
9	I	607	MET	Mainchain
9	I	611	GLU	Mainchain
9	I	612	VAL	Mainchain
9	I	615	ASP	Mainchain
9	I	623	SER	Mainchain
9	I	626	LEU	Mainchain
9	I	631	ASP	Mainchain
9	I	632	PRO	Mainchain
9	I	636	VAL	Mainchain
9	I	637	LEU	Mainchain
9	I	640	VAL	Mainchain
9	I	650	GLN	Mainchain
9	I	651	TYR	Mainchain
9	I	654	ARG	Mainchain
9	I	658	ASP	Mainchain
9	I	667	LEU	Mainchain
9	I	670	GLU	Mainchain
9	I	673	PRO	Mainchain
9	I	674	THR	Mainchain
9	I	681	LEU	Mainchain
9	I	684	ILE	Mainchain
9	I	690	CYS	Mainchain
9	I	695	ARG	Mainchain
9	I	697	SER	Mainchain
9	I	698	ALA	Mainchain
9	I	704	LYS	Mainchain
9	I	706	ALA	Mainchain
9	I	710	VAL	Mainchain
9	I	712	THR	Mainchain
9	I	716	PRO	Mainchain
9	I	717	PRO	Mainchain
9	I	723	PHE	Mainchain
9	I	724	THR	Mainchain
9	I	727	PHE	Mainchain
9	I	730	LYS	Mainchain
9	I	736	VAL	Mainchain
9	I	738	THR	Mainchain
9	I	740	ASN	Mainchain
9	I	743	SER	Mainchain
9	I	745	GLN	Mainchain
9	I	749	LEU	Mainchain
9	I	750	GLN	Mainchain

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Mol	Chain	Res	Type	Group
9	I	752	THR	Mainchain
9	I	765	ASN	Mainchain
9	I	766	LEU	Mainchain
9	I	767	CYS	Mainchain,Peptide
9	I	772	LEU	Mainchain
9	I	773	THR	Mainchain
9	I	775	ILE	Mainchain
9	I	779	ILE	Mainchain
9	I	791	ASP	Mainchain
9	I	798	MET	Mainchain
9	I	799	ILE	Mainchain
9	I	803	ALA	Mainchain
9	I	804	ASN	Mainchain
9	I	806	VAL	Mainchain
9	I	812	VAL	Mainchain
9	I	815	GLU	Mainchain
9	I	818	THR	Mainchain
9	I	82	ALA	Mainchain
9	I	825	ASP	Mainchain
9	I	829	ILE	Mainchain
9	I	833	ILE	Mainchain
9	I	834	THR	Mainchain
9	I	836	PHE	Mainchain
9	I	838	ASN	Mainchain
9	I	839	MET	Mainchain
9	I	84	PHE	Mainchain
9	I	840	GLU	Mainchain
9	I	843	LEU	Mainchain
9	I	844	PRO	Mainchain
9	I	850	ILE	Mainchain
9	I	857	ALA	Mainchain
9	I	858	ILE	Mainchain
9	I	86	TYR	Mainchain
9	I	861	LEU	Mainchain
9	I	872	ALA	Mainchain
9	I	878	ALA	Mainchain
9	I	881	GLY	Mainchain
9	I	888	ILE	Mainchain
9	I	894	VAL	Mainchain
9	I	895	VAL	Mainchain
9	I	896	ASP	Mainchain
9	I	897	TYR	Mainchain

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Mol	Chain	Res	Type	Group
9	I	898	THR	Mainchain
9	I	901	ASP	Mainchain
9	I	916	ASN	Mainchain
9	I	917	ASP	Peptide
9	I	922	VAL	Mainchain
9	I	925	LYS	Mainchain
9	I	931	THR	Mainchain
9	I	947	GLU	Mainchain
9	I	954	TRP	Mainchain
9	I	957	MET	Mainchain
9	I	963	HIS	Mainchain
9	I	968	ARG	Mainchain
9	I	972	VAL	Mainchain
10	J	255	MET	Peptide
10	J	256	LEU	Peptide
10	J	258	ARG	Peptide
10	J	321	PRO	Peptide
10	J	326	HIS	Peptide
10	J	365	ASP	Peptide
10	J	403	ILE	Peptide
10	J	405	SER	Mainchain,Peptide
10	J	407	LEU	Peptide
10	J	408	ASP	Peptide
10	J	409	GLY	Peptide
10	J	410	PRO	Peptide
10	J	412	LEU	Peptide
10	J	415	ILE	Peptide
10	J	420	ALA	Peptide
10	K	255	MET	Peptide
10	K	256	LEU	Peptide
10	K	258	ARG	Peptide
10	K	321	PRO	Peptide
10	K	326	HIS	Peptide
10	K	365	ASP	Peptide
10	K	403	ILE	Peptide
10	K	405	SER	Mainchain,Peptide
10	K	407	LEU	Peptide
10	K	408	ASP	Peptide
10	K	409	GLY	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1429	0	1521	49	0
2	B	356	0	360	7	0
3	C	393	0	380	26	0
4	D	793	0	801	39	0
5	E	1654	0	958	423	0
6	F	1626	0	962	396	0
7	G	3290	0	3276	61	0
8	H	998	0	1055	6	0
9	I	7404	0	7381	897	0
10	J	1741	0	1782	103	0
10	K	1582	0	1612	40	0
11	L	219	0	222	130	0
All	All	21485	0	20310	1916	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 46.

All (1916) 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)
9:I:84:PHE:HZ	9:I:126:LEU:CG	1.10	1.64
5:E:70:DC:C5'	7:G:875:ARG:NH1	1.68	1.53
9:I:566:VAL:HB	9:I:579:LEU:CD1	1.36	1.51
9:I:309:ILE:CG2	9:I:312:ALA:HB2	1.42	1.48
9:I:84:PHE:CZ	9:I:126:LEU:CG	1.96	1.47
9:I:838:ASN:CG	11:L:178:LYS:HD2	1.12	1.47
9:I:730:LYS:NZ	11:L:195:ALA:CB	1.75	1.44
9:I:577:HIS:NE2	9:I:579:LEU:HG	1.28	1.44
9:I:783:ASP:HB3	11:L:188:ARG:NH1	1.32	1.42
9:I:730:LYS:HZ1	11:L:195:ALA:CB	1.28	1.42
9:I:786:LYS:NZ	10:J:218:VAL:HG23	1.12	1.42
9:I:159:LEU:HD13	9:I:161:PHE:CZ	1.56	1.41
9:I:730:LYS:NZ	11:L:195:ALA:HB1	1.18	1.40
9:I:405:TYR:O	9:I:414:LEU:CD2	1.67	1.40
9:I:566:VAL:CB	9:I:579:LEU:HD12	1.51	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:84:PHE:CZ	9:I:126:LEU:HG	1.58	1.37
5:E:17:DG:H2"	5:E:18:DG:C8	1.56	1.36
9:I:84:PHE:CE2	9:I:126:LEU:HD23	1.61	1.35
5:E:70:DC:H5'	7:G:875:ARG:NH1	1.04	1.35
9:I:838:ASN:HD22	11:L:178:LYS:CE	1.38	1.34
10:J:222:LEU:HB3	11:L:178:LYS:NZ	1.39	1.32
9:I:314:VAL:CG2	9:I:317:ALA:C	1.97	1.32
9:I:867:VAL:HG13	9:I:897:TYR:OH	1.22	1.31
9:I:314:VAL:HG23	9:I:317:ALA:O	1.26	1.30
10:J:223:TYR:CE2	11:L:178:LYS:C	1.94	1.30
9:I:159:LEU:HD13	9:I:161:PHE:CE1	1.63	1.30
9:I:838:ASN:ND2	11:L:178:LYS:CG	1.94	1.29
9:I:309:ILE:CG2	9:I:312:ALA:CB	2.09	1.29
9:I:786:LYS:NZ	10:J:218:VAL:CG2	1.94	1.29
9:I:54:PHE:CE2	9:I:143:VAL:HG22	1.66	1.29
9:I:267:HIS:CD2	9:I:277:LEU:HD23	1.65	1.29
9:I:84:PHE:CE2	9:I:126:LEU:HB3	1.69	1.26
9:I:241:PRO:CD	9:I:496:MET:SD	2.23	1.26
9:I:838:ASN:ND2	11:L:178:LYS:CE	1.97	1.25
9:I:733:PRO:HD2	11:L:192:ARG:NH1	1.51	1.25
9:I:723:PHE:CZ	9:I:778:LEU:HB2	1.72	1.24
9:I:159:LEU:CD1	9:I:161:PHE:CE1	2.19	1.23
9:I:84:PHE:CZ	9:I:126:LEU:CB	2.22	1.22
10:J:223:TYR:HE2	11:L:178:LYS:O	1.18	1.22
9:I:314:VAL:HG12	9:I:921:TYR:CZ	1.74	1.22
10:J:250:PRO:O	11:L:183:ARG:NE	1.73	1.21
5:E:7:DC:C1'	5:E:7:DC:N1	2.03	1.21
5:E:17:DG:O5'	5:E:17:DG:P	1.97	1.21
10:J:223:TYR:CE2	11:L:178:LYS:O	1.91	1.21
6:F:156:DG:O5'	6:F:156:DG:P	1.99	1.20
9:I:883:PHE:CE2	9:I:886:ILE:N	2.10	1.20
6:F:145:DC:P	6:F:145:DC:C5'	2.30	1.20
9:I:405:TYR:O	9:I:414:LEU:HD21	1.19	1.20
5:E:70:DC:C4'	7:G:875:ARG:NH1	2.06	1.19
6:F:159:DC:H2"	6:F:160:DT:C7	1.73	1.19
9:I:443:TRP:CE2	9:I:969:CYS:HB2	1.76	1.19
6:F:138:DC:O3'	6:F:139:DC:P	2.01	1.19
10:J:226:GLU:OE2	11:L:178:LYS:NZ	1.75	1.19
9:I:827:ARG:NE	11:L:184:ARG:NH2	1.90	1.19
6:F:145:DC:O5'	6:F:145:DC:P	2.01	1.18
10:J:250:PRO:O	11:L:183:ARG:CD	1.91	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:54:PHE:CE2	9:I:143:VAL:CG2	2.26	1.18
9:I:867:VAL:CG1	9:I:897:TYR:OH	1.90	1.18
9:I:159:LEU:CB	9:I:161:PHE:HE1	1.57	1.17
6:F:139:DC:O3'	6:F:140:DA:P	2.03	1.17
5:E:25:DG:O3'	5:E:26:DG:P	2.03	1.16
6:F:121:DT:O3'	6:F:122:DG:P	2.03	1.15
9:I:309:ILE:HG23	9:I:312:ALA:CB	1.73	1.15
6:F:122:DG:O3'	6:F:123:DA:P	2.04	1.14
9:I:438:PRO:HB3	9:I:965:TRP:CH2	1.82	1.14
5:E:26:DG:O3'	5:E:27:DC:P	2.06	1.14
9:I:84:PHE:CZ	9:I:126:LEU:CD2	2.31	1.13
10:J:238:LYS:NZ	11:L:175:LEU:HD22	1.63	1.13
1:A:302:LEU:HD22	1:A:328:ILE:HD12	1.31	1.12
5:E:70:DC:H5"	7:G:875:ARG:HG3	1.19	1.12
9:I:567:THR:HA	9:I:577:HIS:CB	1.80	1.12
9:I:827:ARG:NE	11:L:184:ARG:HH22	1.44	1.12
9:I:412:VAL:CG1	9:I:413:LEU:HB2	1.80	1.12
6:F:104:DG:O3'	6:F:105:DA:P	2.08	1.11
6:F:140:DA:O3'	6:F:141:DC:P	2.09	1.11
9:I:566:VAL:O	9:I:577:HIS:CG	2.03	1.11
9:I:84:PHE:CZ	9:I:126:LEU:HB3	1.83	1.11
9:I:161:PHE:CE2	9:I:177:VAL:HG21	1.86	1.11
9:I:438:PRO:HB3	9:I:965:TRP:CZ3	1.86	1.10
5:E:30:DG:N2	6:F:132:DG:C2	2.19	1.10
5:E:70:DC:O4'	7:G:875:ARG:NH1	1.85	1.10
6:F:137:DC:O3'	6:F:138:DC:P	2.08	1.09
9:I:314:VAL:HG21	9:I:317:ALA:C	1.64	1.09
10:J:222:LEU:CB	11:L:178:LYS:HZ1	1.65	1.09
10:J:250:PRO:CG	11:L:183:ARG:HD3	1.83	1.09
10:J:250:PRO:HG2	11:L:183:ARG:HD3	1.29	1.09
6:F:159:DC:H2"	6:F:160:DT:C5	1.88	1.09
5:E:60:DG:O3'	5:E:61:DC:P	2.11	1.08
5:E:18:DG:O3'	5:E:19:DG:P	2.11	1.08
5:E:69:DA:O3'	7:G:875:ARG:NH1	1.86	1.08
9:I:847:ARG:HB3	9:I:883:PHE:CZ	1.86	1.08
6:F:102:DT:O3'	6:F:103:DC:P	2.10	1.08
5:E:41:DG:O3'	5:E:42:DT:P	2.13	1.07
9:I:783:ASP:CB	11:L:188:ARG:NH1	2.16	1.07
5:E:1:DA:N6	6:F:160:DT:H3	1.53	1.07
6:F:103:DC:O3'	6:F:104:DG:P	2.12	1.07
9:I:577:HIS:CE1	9:I:579:LEU:HG	1.90	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:145:DC:H5'	6:F:145:DC:P	1.92	1.06
9:I:577:HIS:NE2	9:I:579:LEU:CG	2.17	1.06
5:E:70:DC:H5'	7:G:875:ARG:CZ	1.83	1.06
5:E:71:DG:H5''	7:G:877:GLY:HA2	1.36	1.06
9:I:412:VAL:HG13	9:I:413:LEU:HB2	1.34	1.06
9:I:84:PHE:CZ	9:I:126:LEU:HD23	1.90	1.06
5:E:17:DG:C2'	5:E:18:DG:C8	2.38	1.06
9:I:568:VAL:O	9:I:575:PHE:HB3	1.54	1.05
5:E:61:DC:O3'	5:E:62:DC:P	2.14	1.05
9:I:84:PHE:CE2	9:I:126:LEU:CD2	2.38	1.05
10:J:223:TYR:HB2	11:L:182:GLN:OE1	1.53	1.05
9:I:241:PRO:HD3	9:I:496:MET:SD	1.90	1.05
6:F:120:DC:O3'	6:F:121:DT:P	2.13	1.05
5:E:42:DT:O3'	5:E:43:DC:P	2.15	1.04
5:E:24:DG:O3'	5:E:25:DG:P	2.15	1.04
9:I:730:LYS:HZ2	11:L:195:ALA:HB3	1.21	1.04
5:E:59:DA:O3'	5:E:60:DG:P	2.16	1.03
9:I:159:LEU:CB	9:I:161:PHE:CE1	2.41	1.03
9:I:159:LEU:HB3	9:I:161:PHE:CE1	1.93	1.03
9:I:867:VAL:HB	9:I:868:PRO:HD3	1.34	1.03
6:F:105:DA:O3'	6:F:106:DG:P	2.16	1.02
5:E:30:DG:C2	6:F:132:DG:N2	2.28	1.02
1:A:204:ILE:HD11	1:A:209:THR:OG1	1.60	1.02
5:E:29:DC:O3'	5:E:30:DG:H5'	1.60	1.01
9:I:577:HIS:O	9:I:578:THR:OG1	1.76	1.01
9:I:567:THR:HA	9:I:577:HIS:HB3	1.40	1.01
9:I:786:LYS:HZ3	10:J:218:VAL:CG2	1.57	1.01
6:F:131:DC:O3'	6:F:132:DG:H5'	1.60	1.01
10:J:250:PRO:O	11:L:183:ARG:CG	2.07	1.01
5:E:71:DG:C5'	7:G:877:GLY:HA2	1.89	1.00
9:I:318:ALA:HA	9:I:319:TYR:HB3	1.40	1.00
5:E:62:DC:O3'	5:E:63:DG:P	2.19	1.00
9:I:566:VAL:CB	9:I:579:LEU:CD1	2.21	1.00
10:J:250:PRO:O	11:L:183:ARG:HG2	1.62	1.00
9:I:267:HIS:CE1	9:I:277:LEU:HG	1.97	0.99
5:E:44:DG:O3'	5:E:45:DC:P	2.19	0.99
6:F:92:DT:O3'	6:F:93:DC:P	2.21	0.99
6:F:133:DC:O3'	6:F:134:DG:P	2.21	0.99
5:E:43:DC:O3'	5:E:44:DG:P	2.20	0.99
10:J:241:GLU:HG3	11:L:172:TYR:HD1	1.21	0.99
9:I:695:ARG:HB3	9:I:749:LEU:HD22	1.43	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:827:ARG:CZ	11:L:184:ARG:HH21	1.76	0.99
6:F:94:DT:OP2	7:G:860:GLU:OE2	1.79	0.99
9:I:309:ILE:HG21	9:I:312:ALA:HB2	1.01	0.99
9:I:267:HIS:CG	9:I:277:LEU:HD23	1.98	0.99
6:F:123:DA:O3'	6:F:124:DG:P	2.20	0.99
6:F:91:DG:O3'	6:F:92:DT:P	2.21	0.99
5:E:40:DA:O3'	5:E:41:DG:P	2.20	0.98
5:E:1:DA:N1	6:F:160:DT:O2	1.94	0.98
9:I:783:ASP:CB	11:L:188:ARG:HH12	1.73	0.98
9:I:566:VAL:HB	9:I:579:LEU:HD11	1.45	0.98
5:E:68:DG:O3'	5:E:69:DA:P	2.21	0.98
6:F:106:DG:O3'	6:F:107:DT:P	2.22	0.98
5:E:38:DT:O3'	5:E:39:DC:P	2.20	0.98
9:I:838:ASN:HD22	11:L:178:LYS:CG	1.68	0.98
5:E:67:DA:O3'	5:E:68:DG:P	2.22	0.98
9:I:438:PRO:CB	9:I:965:TRP:CZ3	2.47	0.97
5:E:58:DG:O3'	5:E:59:DA:P	2.23	0.97
9:I:827:ARG:HE	11:L:184:ARG:HH22	0.98	0.97
9:I:314:VAL:CG2	9:I:317:ALA:O	2.08	0.97
9:I:54:PHE:CD2	9:I:143:VAL:HG22	1.99	0.97
9:I:568:VAL:HB	9:I:575:PHE:CE2	1.99	0.96
9:I:548:ILE:HG13	9:I:581:ILE:HD13	1.47	0.96
6:F:133:DC:O3'	6:F:134:DG:H5'	1.64	0.96
6:F:145:DC:O5'	6:F:145:DC:OP2	1.82	0.96
9:I:314:VAL:HG12	9:I:921:TYR:CE2	2.00	0.96
6:F:119:DA:O3'	6:F:120:DC:P	2.23	0.96
5:E:31:DT:O3'	5:E:32:DT:P	2.23	0.96
5:E:33:DC:O3'	5:E:34:DG:H5'	1.65	0.96
6:F:103:DC:O3'	6:F:104:DG:H5'	1.66	0.96
6:F:124:DG:O3'	6:F:125:DG:P	2.24	0.96
6:F:90:DC:O3'	6:F:91:DG:P	2.24	0.96
5:E:27:DC:O3'	5:E:28:DG:H5'	1.65	0.95
5:E:39:DC:O3'	5:E:40:DA:P	2.22	0.95
9:I:314:VAL:HG23	9:I:317:ALA:C	1.70	0.95
9:I:723:PHE:HZ	9:I:778:LEU:HB2	1.07	0.95
6:F:89:DA:O3'	6:F:90:DC:P	2.25	0.95
6:F:88:DC:O3'	6:F:89:DA:P	2.24	0.95
9:I:314:VAL:CG2	9:I:318:ALA:N	2.30	0.95
9:I:737:LYS:HD3	9:I:786:LYS:HG3	1.47	0.95
9:I:443:TRP:CD1	9:I:969:CYS:SG	2.59	0.95
5:E:69:DA:O3'	5:E:70:DC:P	2.24	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:827:ARG:HE	11:L:184:ARG:NH2	1.56	0.95
9:I:159:LEU:CD1	9:I:161:PHE:CZ	2.42	0.95
9:I:883:PHE:CE2	9:I:886:ILE:CA	2.38	0.95
5:E:53:DC:O3'	5:E:54:DA:P	2.25	0.94
6:F:101:DC:O3'	6:F:102:DT:P	2.25	0.94
5:E:57:DC:O3'	5:E:58:DG:H5'	1.67	0.94
5:E:71:DG:O3'	5:E:72:DT:P	2.25	0.94
9:I:483:ALA:HB3	9:I:491:HIS:HB2	1.47	0.94
5:E:66:DC:O3'	5:E:67:DA:P	2.25	0.94
9:I:629:ARG:HD3	9:I:651:TYR:CB	1.97	0.94
9:I:786:LYS:HZ2	10:J:218:VAL:CG2	1.65	0.94
9:I:730:LYS:HZ2	11:L:195:ALA:CB	1.61	0.94
5:E:52:DA:O3'	5:E:53:DC:P	2.24	0.94
5:E:70:DC:O3'	5:E:71:DG:P	2.26	0.94
9:I:783:ASP:HB3	11:L:188:ARG:HH12	1.22	0.94
9:I:161:PHE:CZ	9:I:177:VAL:HG21	2.00	0.94
5:E:3:DG:H2''	5:E:4:DG:C8	2.02	0.94
5:E:1:DA:N1	6:F:160:DT:C2	2.36	0.94
5:E:62:DC:O3'	5:E:63:DG:H5'	1.68	0.94
6:F:114:DT:O3'	6:F:115:DC:P	2.25	0.94
9:I:241:PRO:HD2	9:I:496:MET:SD	2.06	0.93
9:I:707:ASN:OD1	9:I:760:LEU:HD11	1.68	0.93
6:F:97:DT:O3'	6:F:98:DC:P	2.27	0.93
6:F:106:DG:H5''	9:I:542:ASN:HD22	1.33	0.93
5:E:43:DC:O3'	5:E:44:DG:H5'	1.68	0.93
9:I:314:VAL:HG21	9:I:317:ALA:CA	1.99	0.93
6:F:100:DG:O3'	6:F:101:DC:P	2.26	0.93
5:E:37:DC:O3'	5:E:38:DT:P	2.26	0.93
9:I:566:VAL:HG11	9:I:628:ILE:CG2	1.98	0.93
6:F:99:DG:O3'	6:F:100:DG:P	2.26	0.93
9:I:309:ILE:HG21	9:I:312:ALA:CB	1.86	0.92
9:I:314:VAL:HG12	9:I:921:TYR:OH	1.70	0.92
9:I:159:LEU:HD13	9:I:161:PHE:HZ	1.27	0.92
9:I:267:HIS:CE1	9:I:277:LEU:CG	2.51	0.92
9:I:159:LEU:CD1	9:I:161:PHE:HE1	1.70	0.92
5:E:30:DG:C2	6:F:132:DG:C2	2.56	0.92
5:E:28:DG:N2	6:F:134:DG:C2	2.36	0.92
9:I:622:ASP:O	9:I:625:LEU:HD23	1.69	0.92
9:I:783:ASP:HB3	11:L:188:ARG:HH11	1.12	0.92
9:I:159:LEU:HB3	9:I:161:PHE:HE1	1.27	0.92
9:I:267:HIS:CD2	9:I:277:LEU:CD2	2.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:32:DT:O3'	5:E:33:DC:P	2.28	0.92
10:K:276:LEU:HD22	10:K:325:ASN:HB3	1.51	0.92
5:E:72:DT:O3'	5:E:73:DG:P	2.27	0.92
6:F:127:DC:O3'	6:F:128:DG:H5'	1.70	0.92
9:I:178:PHE:CD2	9:I:309:ILE:HD11	2.04	0.92
9:I:847:ARG:CB	9:I:883:PHE:CZ	2.53	0.92
5:E:1:DA:H61	6:F:160:DT:H3	1.08	0.91
5:E:63:DG:O3'	5:E:64:DA:P	2.28	0.91
9:I:883:PHE:CE1	9:I:885:ASP:HB2	2.06	0.91
5:E:51:DA:O3'	5:E:52:DA:P	2.28	0.91
6:F:113:DA:O3'	6:F:114:DT:P	2.27	0.91
10:J:250:PRO:HG2	11:L:183:ARG:CD	1.99	0.91
9:I:838:ASN:HD21	11:L:178:LYS:HD3	0.83	0.91
9:I:84:PHE:CE2	9:I:126:LEU:CB	2.46	0.91
6:F:115:DC:O3'	6:F:116:DG:P	2.29	0.91
6:F:93:DC:O3'	6:F:94:DT:P	2.28	0.91
5:E:45:DC:O3'	5:E:46:DG:H5'	1.69	0.91
9:I:567:THR:HA	9:I:577:HIS:HB2	1.52	0.91
9:I:577:HIS:CE1	9:I:579:LEU:CG	2.53	0.91
5:E:49:DC:O3'	5:E:50:DG:H5'	1.71	0.91
6:F:111:DC:O3'	6:F:112:DG:H5'	1.70	0.91
6:F:94:DT:O3'	6:F:95:DG:P	2.29	0.91
9:I:882:HIS:O	9:I:883:PHE:HB3	1.71	0.91
4:D:87:LEU:HD11	4:D:89:LYS:HE3	1.53	0.91
5:E:56:DT:O3'	5:E:57:DC:P	2.29	0.91
5:E:59:DA:O3'	5:E:60:DG:H5'	1.70	0.91
6:F:132:DG:O3'	6:F:133:DC:P	2.29	0.91
6:F:87:DG:O3'	6:F:88:DC:P	2.29	0.91
9:I:548:ILE:HG13	9:I:581:ILE:CD1	2.00	0.91
9:I:883:PHE:CZ	9:I:885:ASP:HB2	2.05	0.91
6:F:118:DG:O3'	6:F:119:DA:P	2.28	0.90
5:E:40:DA:O3'	5:E:41:DG:H5'	1.72	0.90
6:F:115:DC:O3'	6:F:116:DG:H5'	1.71	0.90
6:F:117:DC:O3'	6:F:118:DG:H5'	1.70	0.90
5:E:30:DG:O3'	5:E:31:DT:P	2.29	0.90
6:F:136:DC:O3'	6:F:137:DC:H5'	1.72	0.90
10:K:374:TYR:HB2	10:K:407:LEU:HD21	1.54	0.90
10:J:241:GLU:HG3	11:L:172:TYR:CD1	2.07	0.90
9:I:309:ILE:HG23	9:I:312:ALA:HB3	1.49	0.90
9:I:338:GLU:OE1	9:I:342:THR:OG1	1.89	0.90
6:F:82:DC:O3'	6:F:83:DG:H5'	1.69	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:577:HIS:CE1	9:I:579:LEU:CD1	2.54	0.90
9:I:838:ASN:ND2	11:L:178:LYS:CD	0.75	0.90
10:K:310:THR:O	10:K:314:SER:CB	2.19	0.90
9:I:788:LYS:HB3	9:I:791:ASP:OD2	1.72	0.90
5:E:54:DA:O3'	5:E:55:DC:P	2.29	0.89
6:F:86:DG:O3'	6:F:87:DG:P	2.30	0.89
9:I:744:PHE:HB2	9:I:747:TYR:CZ	2.07	0.89
9:I:344:ARG:HB2	9:I:378:TYR:OH	1.71	0.89
6:F:101:DC:O3'	6:F:102:DT:H5'	1.72	0.89
5:E:47:DA:O3'	5:E:48:DT:H5'	1.73	0.89
9:I:629:ARG:HD3	9:I:651:TYR:HB2	1.53	0.89
5:E:65:DG:O3'	5:E:66:DC:P	2.30	0.89
6:F:107:DT:O3'	6:F:108:DG:H5'	1.72	0.89
9:I:827:ARG:CZ	11:L:184:ARG:NH2	2.34	0.89
9:I:833:ILE:HG12	9:I:856:ARG:HG2	1.55	0.89
6:F:136:DC:O3'	6:F:137:DC:P	2.31	0.89
9:I:838:ASN:ND2	11:L:178:LYS:HD3	1.32	0.89
7:G:679:GLY:HA3	9:I:479:LEU:HD13	1.52	0.89
5:E:19:DG:O3'	5:E:20:DG:P	2.30	0.89
6:F:98:DC:O3'	6:F:99:DG:H5'	1.73	0.89
9:I:568:VAL:HB	9:I:575:PHE:CD2	2.07	0.89
10:K:310:THR:O	10:K:314:SER:HB3	1.71	0.89
5:E:25:DG:O3'	5:E:26:DG:H5'	1.73	0.89
6:F:120:DC:O3'	6:F:121:DT:H5'	1.72	0.89
5:E:57:DC:O3'	5:E:58:DG:P	2.31	0.89
6:F:125:DG:O3'	6:F:126:DA:P	2.31	0.89
6:F:137:DC:O3'	6:F:138:DC:H5'	1.71	0.89
6:F:98:DC:O3'	6:F:99:DG:P	2.31	0.89
5:E:64:DA:O3'	5:E:65:DG:P	2.31	0.88
6:F:95:DG:O3'	6:F:96:DC:P	2.30	0.88
9:I:49:VAL:HG22	9:I:51:LEU:CD1	2.03	0.88
6:F:123:DA:O3'	6:F:124:DG:H5'	1.73	0.88
9:I:727:PHE:CE2	9:I:729:CYS:HB3	2.08	0.88
6:F:96:DC:O3'	6:F:97:DT:P	2.32	0.88
5:E:34:DG:C2	6:F:128:DG:N2	2.41	0.88
5:E:24:DG:O3'	5:E:25:DG:H5'	1.72	0.88
5:E:45:DC:O3'	5:E:46:DG:P	2.31	0.88
5:E:34:DG:N2	6:F:128:DG:C2	2.41	0.88
9:I:314:VAL:HG21	9:I:317:ALA:CB	2.04	0.88
9:I:911:LEU:HD11	9:I:930:LEU:CD2	2.04	0.88
5:E:55:DC:O3'	5:E:56:DT:P	2.31	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:107:DT:O3'	6:F:108:DG:P	2.32	0.88
5:E:78:DC:O3'	5:E:79:DG:H5'	1.73	0.87
6:F:121:DT:O3'	6:F:122:DG:H5'	1.75	0.87
5:E:70:DC:C5'	7:G:875:ARG:HG3	2.04	0.87
9:I:867:VAL:HG13	9:I:897:TYR:HH	1.08	0.87
9:I:761:ARG:NE	9:I:768:PRO:HB3	1.89	0.87
9:I:531:PHE:CD1	9:I:638:ARG:HG2	2.10	0.87
5:E:33:DC:O3'	5:E:34:DG:P	2.33	0.87
5:E:70:DC:O3'	5:E:71:DG:H5'	1.75	0.87
9:I:725:ARG:HB3	9:I:744:PHE:CZ	2.10	0.87
6:F:138:DC:O3'	6:F:139:DC:H5'	1.74	0.87
9:I:75:VAL:HG11	9:I:128:ILE:CD1	2.04	0.87
6:F:159:DC:H2''	6:F:160:DT:H73	1.57	0.87
9:I:741:PHE:CE1	9:I:791:ASP:HB3	2.09	0.87
9:I:741:PHE:HB3	9:I:747:TYR:OH	1.73	0.87
6:F:116:DG:O3'	6:F:117:DC:P	2.32	0.87
5:E:71:DG:H5''	7:G:877:GLY:CA	2.04	0.87
9:I:730:LYS:NZ	11:L:195:ALA:HB3	1.80	0.87
9:I:751:LYS:HG3	9:I:797:GLU:HB3	1.55	0.87
9:I:84:PHE:HZ	9:I:126:LEU:HG	0.71	0.87
9:I:75:VAL:HG11	9:I:128:ILE:HD12	1.57	0.86
6:F:141:DC:O3'	6:F:142:DC:P	2.33	0.86
5:E:17:DG:H2''	5:E:18:DG:H8	0.91	0.86
9:I:35:ILE:CG2	9:I:45:VAL:CG1	2.54	0.86
9:I:847:ARG:HB3	9:I:883:PHE:HZ	1.35	0.86
9:I:883:PHE:CD2	9:I:886:ILE:N	2.26	0.86
9:I:439:HIS:HA	9:I:965:TRP:HB3	1.58	0.86
5:E:23:DG:O3'	5:E:24:DG:H5'	1.76	0.86
6:F:105:DA:O3'	6:F:106:DG:H5'	1.74	0.86
5:E:50:DG:N2	6:F:112:DG:C2	2.43	0.86
9:I:537:PHE:CB	9:I:625:LEU:HD13	2.05	0.86
9:I:566:VAL:O	9:I:577:HIS:HB3	1.76	0.86
9:I:314:VAL:CG1	9:I:921:TYR:CZ	2.58	0.86
9:I:786:LYS:HZ3	10:J:218:VAL:HG21	1.39	0.86
9:I:537:PHE:HB3	9:I:625:LEU:HD13	1.57	0.86
5:E:53:DC:O3'	5:E:54:DA:H5'	1.75	0.85
5:E:39:DC:O3'	5:E:40:DA:H5'	1.76	0.85
6:F:129:DA:O3'	6:F:130:DA:H5'	1.76	0.85
9:I:159:LEU:CG	9:I:161:PHE:HE1	1.89	0.85
5:E:17:DG:C5'	5:E:17:DG:P	2.63	0.85
5:E:31:DT:O3'	5:E:32:DT:H5'	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:139:DC:O3'	6:F:140:DA:H5'	1.77	0.85
6:F:90:DC:O3'	6:F:91:DG:H5'	1.77	0.85
9:I:804:ASN:HA	9:I:807:THR:HB	1.59	0.85
9:I:38:ILE:HD13	9:I:45:VAL:HG13	1.59	0.85
6:F:117:DC:O3'	6:F:118:DG:P	2.35	0.85
9:I:241:PRO:CG	9:I:496:MET:SD	2.64	0.85
9:I:737:LYS:HD3	9:I:786:LYS:CG	2.06	0.84
9:I:75:VAL:CG1	9:I:128:ILE:CD1	2.54	0.84
9:I:646:ASP:CG	9:I:675:PRO:HD2	1.97	0.84
1:A:305:PHE:CZ	6:F:151:DT:H1'	2.12	0.84
9:I:548:ILE:CG1	9:I:581:ILE:HD13	2.07	0.84
9:I:67:SER:HB2	9:I:126:LEU:HD11	1.59	0.84
5:E:30:DG:O3'	5:E:31:DT:H5'	1.78	0.84
6:F:124:DG:O3'	6:F:125:DG:H5'	1.78	0.84
10:J:223:TYR:CZ	11:L:179:ALA:N	2.33	0.84
9:I:741:PHE:HD2	9:I:747:TYR:HH	1.19	0.84
5:E:75:DC:O3'	5:E:76:DT:H5'	1.76	0.84
9:I:715:GLY:N	9:I:716:PRO:HD2	1.92	0.84
5:E:28:DG:C2	6:F:134:DG:N2	2.45	0.84
5:E:55:DC:O3'	5:E:56:DT:H5'	1.78	0.84
9:I:731:SER:HB2	9:I:735:ILE:HG12	1.60	0.84
9:I:566:VAL:CG1	9:I:628:ILE:CG2	2.56	0.84
9:I:241:PRO:HG3	9:I:496:MET:CE	2.07	0.84
5:E:34:DG:O3'	5:E:35:DT:P	2.35	0.83
9:I:577:HIS:CE1	9:I:579:LEU:HD11	2.12	0.83
5:E:37:DC:O3'	5:E:38:DT:H5'	1.78	0.83
10:J:223:TYR:CE2	11:L:179:ALA:N	2.46	0.83
6:F:121:DT:C3'	6:F:122:DG:P	2.65	0.83
6:F:131:DC:O3'	6:F:132:DG:P	2.36	0.83
10:J:219:GLU:CB	11:L:182:GLN:HG2	2.08	0.83
5:E:70:DC:H5"	7:G:875:ARG:CG	2.04	0.83
9:I:49:VAL:HG22	9:I:51:LEU:HD12	1.59	0.83
9:I:75:VAL:CG1	9:I:128:ILE:HD12	2.08	0.83
9:I:838:ASN:HD22	11:L:178:LYS:CD	0.75	0.83
6:F:135:DC:O3'	6:F:136:DC:H5'	1.76	0.83
9:I:221:VAL:O	9:I:222:GLU:HB2	1.77	0.83
9:I:267:HIS:NE2	9:I:277:LEU:HD23	1.94	0.83
5:E:64:DA:O3'	5:E:65:DG:H5'	1.78	0.83
6:F:113:DA:O3'	6:F:114:DT:H5'	1.79	0.83
5:E:3:DG:O3'	5:E:4:DG:H5'	1.79	0.83
5:E:79:DG:O3'	5:E:80:DG:P	2.37	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:250:PRO:C	11:L:183:ARG:CD	2.47	0.82
9:I:566:VAL:O	9:I:577:HIS:CB	2.26	0.82
9:I:267:HIS:ND1	9:I:277:LEU:HB3	1.93	0.82
9:I:669:LEU:HD13	9:I:681:LEU:HD11	1.61	0.82
5:E:47:DA:O3'	5:E:48:DT:P	2.37	0.82
5:E:73:DG:O3'	5:E:74:DC:P	2.37	0.82
10:J:250:PRO:CG	11:L:183:ARG:CD	2.57	0.82
5:E:22:DG:O3'	5:E:23:DG:H5'	1.79	0.82
5:E:21:DT:O3'	5:E:22:DG:H5'	1.80	0.82
5:E:36:DC:O3'	5:E:37:DC:P	2.38	0.82
6:F:109:DT:O3'	6:F:110:DT:P	2.38	0.82
9:I:723:PHE:HZ	9:I:778:LEU:CB	1.90	0.82
9:I:761:ARG:CZ	9:I:808:PRO:HB2	2.09	0.82
5:E:51:DA:O3'	5:E:52:DA:H5'	1.79	0.81
6:F:85:DA:O3'	6:F:86:DG:H5'	1.77	0.81
6:F:94:DT:O3'	6:F:95:DG:H5'	1.80	0.81
9:I:725:ARG:HH22	9:I:749:LEU:HG	1.43	0.81
5:E:61:DC:O3'	5:E:62:DC:H5'	1.79	0.81
5:E:76:DT:O3'	5:E:77:DA:H5'	1.80	0.81
6:F:99:DG:O3'	6:F:100:DG:H5'	1.80	0.81
6:F:110:DT:O3'	6:F:111:DC:P	2.38	0.81
6:F:93:DC:O3'	6:F:94:DT:H5'	1.80	0.81
9:I:443:TRP:CZ2	9:I:969:CYS:HB2	2.16	0.81
6:F:139:DC:C3'	6:F:140:DA:P	2.68	0.81
6:F:96:DC:O3'	6:F:97:DT:H5'	1.80	0.81
9:I:314:VAL:HG21	9:I:317:ALA:HB3	1.61	0.81
1:A:204:ILE:HD12	1:A:237:TYR:OH	1.81	0.81
9:I:786:LYS:HZ3	10:J:218:VAL:HG23	1.18	0.81
9:I:494:SER:N	9:I:496:MET:HB3	1.48	0.81
9:I:744:PHE:CB	9:I:747:TYR:CE1	2.64	0.81
9:I:531:PHE:CD1	9:I:638:ARG:CG	2.64	0.81
5:E:72:DT:O3'	5:E:73:DG:H5'	1.80	0.81
9:I:827:ARG:NH2	11:L:184:ARG:HH21	1.79	0.81
9:I:84:PHE:HE2	9:I:126:LEU:HD23	1.43	0.81
5:E:69:DA:HO3'	5:E:70:DC:P	2.02	0.80
6:F:84:DT:O3'	6:F:85:DA:H5'	1.80	0.80
9:I:240:ILE:HG23	9:I:496:MET:HA	1.61	0.80
9:I:969:CYS:HA	9:I:972:VAL:HB	1.62	0.80
6:F:88:DC:O3'	6:F:89:DA:H5'	1.82	0.80
5:E:1:DA:C2	6:F:160:DT:O2	2.35	0.80
10:J:250:PRO:CD	11:L:183:ARG:CD	2.56	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:695:ARG:C	9:I:749:LEU:HD13	2.01	0.80
5:E:18:DG:O3'	5:E:19:DG:H5'	1.82	0.80
5:E:78:DC:O3'	5:E:79:DG:P	2.40	0.80
6:F:143:DC:H2''	6:F:144:DC:C6	2.17	0.80
5:E:23:DG:O3'	5:E:24:DG:P	2.40	0.80
9:I:566:VAL:CG2	9:I:579:LEU:CD1	2.60	0.80
9:I:750:GLN:O	9:I:754:PRO:HD2	1.82	0.80
9:I:537:PHE:HB3	9:I:625:LEU:HD22	1.64	0.80
6:F:85:DA:O3'	6:F:86:DG:P	2.40	0.80
10:J:223:TYR:H	11:L:182:GLN:HE22	1.30	0.80
5:E:74:DC:O3'	5:E:75:DC:H5'	1.81	0.80
9:I:566:VAL:CG2	9:I:579:LEU:HD12	2.12	0.80
9:I:707:ASN:CG	9:I:760:LEU:HD11	2.00	0.80
5:E:41:DG:O3'	5:E:42:DT:H5'	1.82	0.79
5:E:50:DG:O3'	5:E:51:DA:P	2.40	0.79
6:F:130:DA:O3'	6:F:131:DC:H5'	1.80	0.79
9:I:54:PHE:CE2	9:I:143:VAL:HG21	2.15	0.79
6:F:103:DC:C3'	6:F:104:DG:P	2.70	0.79
9:I:566:VAL:HB	9:I:579:LEU:HD12	0.79	0.79
9:I:531:PHE:CE1	9:I:638:ARG:HB3	2.16	0.79
9:I:221:VAL:O	9:I:222:GLU:CB	2.29	0.79
6:F:141:DC:O3'	6:F:142:DC:H5'	1.83	0.79
6:F:81:DC:O3'	6:F:82:DC:H5'	1.82	0.79
10:J:250:PRO:C	11:L:183:ARG:HD3	2.03	0.79
1:A:283:TYR:CZ	1:A:285:PRO:HG3	2.17	0.79
9:I:408:LYS:O	9:I:414:LEU:HG	1.83	0.79
6:F:110:DT:O3'	6:F:111:DC:H5'	1.83	0.79
9:I:267:HIS:NE2	9:I:277:LEU:CD2	2.46	0.79
9:I:968:ARG:O	9:I:972:VAL:HG23	1.83	0.79
10:J:222:LEU:HB3	11:L:178:LYS:CE	2.13	0.79
10:J:241:GLU:CG	11:L:172:TYR:HD1	1.95	0.78
9:I:799:ILE:CG2	9:I:856:ARG:HB2	2.12	0.78
5:E:67:DA:O3'	5:E:68:DG:H5'	1.83	0.78
5:E:66:DC:O3'	5:E:67:DA:H5'	1.83	0.78
5:E:50:DG:C2	6:F:112:DG:N2	2.51	0.78
6:F:108:DG:O3'	6:F:109:DT:P	2.40	0.78
6:F:94:DT:H5''	7:G:873:PHE:CZ	2.18	0.78
9:I:443:TRP:NE1	9:I:969:CYS:HB2	1.98	0.78
6:F:138:DC:C3'	6:F:139:DC:P	2.71	0.78
9:I:531:PHE:CD1	9:I:638:ARG:CB	2.66	0.78
5:E:36:DC:O3'	5:E:37:DC:H5'	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:109:DT:O3'	6:F:110:DT:H5'	1.84	0.78
5:E:34:DG:C2	6:F:128:DG:C2	2.72	0.78
10:J:238:LYS:HZ1	11:L:175:LEU:HD22	1.47	0.78
9:I:867:VAL:CB	9:I:868:PRO:HD3	2.13	0.78
9:I:784:ASN:HB3	11:L:192:ARG:HH12	1.47	0.78
9:I:309:ILE:HG12	9:I:311:GLU:H	1.49	0.77
5:E:6:DG:H2''	5:E:7:DC:O5'	1.82	0.77
2:B:43:LYS:O	2:B:47:GLU:HG3	1.84	0.77
9:I:178:PHE:CD2	9:I:309:ILE:CD1	2.66	0.77
9:I:408:LYS:O	9:I:414:LEU:CD1	2.32	0.77
5:E:35:DT:O3'	5:E:36:DC:P	2.43	0.77
6:F:102:DT:O3'	6:F:103:DC:H5'	1.85	0.77
9:I:318:ALA:HA	9:I:319:TYR:CB	2.14	0.77
9:I:744:PHE:HB2	9:I:747:TYR:CE1	2.19	0.77
9:I:707:ASN:OD1	9:I:712:THR:HB	1.85	0.77
9:I:629:ARG:HD3	9:I:651:TYR:HB3	1.67	0.77
5:E:29:DC:O3'	5:E:30:DG:P	2.42	0.77
5:E:42:DT:O3'	5:E:43:DC:H5'	1.84	0.77
6:F:135:DC:O3'	6:F:136:DC:P	2.43	0.77
10:J:223:TYR:N	11:L:182:GLN:HE22	1.81	0.77
5:E:4:DG:H2''	5:E:5:DC:C6	2.19	0.77
6:F:126:DA:O3'	6:F:127:DC:P	2.42	0.77
9:I:577:HIS:HE1	9:I:579:LEU:HD11	1.47	0.77
5:E:30:DG:N2	6:F:132:DG:N3	2.33	0.77
10:J:219:GLU:CG	11:L:182:GLN:HA	2.15	0.77
5:E:46:DG:O3'	5:E:47:DA:P	2.42	0.77
6:F:106:DG:O3'	6:F:107:DT:H5'	1.85	0.77
6:F:86:DG:O3'	6:F:87:DG:H5'	1.85	0.77
9:I:494:SER:N	9:I:496:MET:CB	2.39	0.77
9:I:361:ARG:HB2	9:I:500:THR:CG2	2.14	0.77
3:C:366:ILE:HG21	4:D:52:VAL:HG21	1.66	0.76
9:I:882:HIS:O	9:I:883:PHE:CB	2.33	0.76
5:E:25:DG:C3'	5:E:26:DG:P	2.73	0.76
5:E:34:DG:O3'	5:E:35:DT:H5'	1.85	0.76
9:I:867:VAL:HB	9:I:868:PRO:CD	2.13	0.76
9:I:733:PRO:HD2	11:L:192:ARG:CZ	2.15	0.76
6:F:119:DA:O3'	6:F:120:DC:H5'	1.85	0.76
10:J:219:GLU:HG2	11:L:182:GLN:HA	1.67	0.76
9:I:396:LYS:HG2	9:I:660:VAL:CG1	2.16	0.76
1:A:193:ASN:ND2	1:A:195:LYS:HG2	2.00	0.76
9:I:917:ASP:H	9:I:918:PRO:HA	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:30:DG:N3	6:F:132:DG:N2	2.33	0.76
6:F:126:DA:O3'	6:F:127:DC:H5'	1.86	0.76
6:F:83:DG:O3'	6:F:84:DT:H5'	1.85	0.76
9:I:753:MET:HB3	9:I:754:PRO:HD3	1.66	0.76
5:E:20:DG:O3'	5:E:21:DT:P	2.44	0.76
10:J:222:LEU:CB	11:L:178:LYS:NZ	2.35	0.76
5:E:32:DT:O3'	5:E:33:DC:H5'	1.85	0.76
5:E:79:DG:O3'	5:E:80:DG:H5'	1.86	0.76
10:J:238:LYS:HZ2	11:L:175:LEU:HD22	1.50	0.76
9:I:729:CYS:HG	9:I:781:TYR:HE1	1.33	0.76
6:F:120:DC:C3'	6:F:121:DT:P	2.74	0.76
6:F:125:DG:O3'	6:F:126:DA:H5'	1.84	0.76
5:E:27:DC:O3'	5:E:28:DG:P	2.44	0.75
9:I:630:ILE:HB	9:I:648:MET:SD	2.26	0.75
9:I:309:ILE:HG23	9:I:312:ALA:HB2	1.35	0.75
9:I:737:LYS:CD	9:I:786:LYS:HG3	2.16	0.75
6:F:112:DG:O3'	6:F:113:DA:P	2.44	0.75
1:A:204:ILE:HD13	1:A:204:ILE:O	1.86	0.75
6:F:118:DG:O3'	6:F:119:DA:H5'	1.86	0.75
6:F:144:DC:O3'	6:F:145:DC:P	2.44	0.75
6:F:114:DT:O3'	6:F:115:DC:H5'	1.86	0.75
9:I:159:LEU:HD12	9:I:161:PHE:CE1	2.19	0.75
9:I:412:VAL:HG12	9:I:413:LEU:HB2	1.66	0.75
5:E:26:DG:O3'	5:E:27:DC:H5'	1.86	0.75
5:E:58:DG:O3'	5:E:59:DA:H5'	1.86	0.75
6:F:132:DG:O3'	6:F:133:DC:H5'	1.87	0.75
9:I:568:VAL:O	9:I:575:PHE:HD2	1.69	0.75
5:E:28:DG:O3'	5:E:29:DC:H5'	1.86	0.75
9:I:575:PHE:CD2	9:I:576:ASN:O	2.39	0.75
9:I:838:ASN:HD21	11:L:178:LYS:CG	1.80	0.75
9:I:855:LEU:HA	9:I:858:ILE:HG22	1.69	0.75
9:I:495:GLN:O	9:I:496:MET:HB2	1.86	0.74
1:A:193:ASN:HD21	1:A:195:LYS:HG2	1.51	0.74
1:A:302:LEU:HD22	1:A:328:ILE:CD1	2.15	0.74
9:I:344:ARG:HA	9:I:378:TYR:CE1	2.22	0.74
9:I:38:ILE:HA	9:I:45:VAL:HG22	1.69	0.74
3:C:331:THR:OG1	3:C:362:GLY:HA2	1.87	0.74
6:F:128:DG:O3'	6:F:129:DA:H5'	1.88	0.74
5:E:50:DG:C2	6:F:112:DG:C2	2.75	0.74
6:F:112:DG:O3'	6:F:113:DA:H5'	1.87	0.74
9:I:784:ASN:CB	11:L:192:ARG:HH12	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:46:DG:O3'	5:E:47:DA:H5'	1.87	0.74
5:E:54:DA:O3'	5:E:55:DC:H5'	1.88	0.74
9:I:319:TYR:CG	9:I:320:ALA:N	2.56	0.74
5:E:52:DA:O3'	5:E:53:DC:H5'	1.87	0.74
5:E:77:DA:O3'	5:E:78:DC:H5'	1.88	0.74
6:F:122:DG:C3'	6:F:123:DA:P	2.76	0.74
6:F:81:DC:O3'	6:F:82:DC:P	2.45	0.74
9:I:359:ILE:HG13	9:I:359:ILE:O	1.86	0.74
5:E:35:DT:O3'	5:E:36:DC:H5'	1.88	0.74
6:F:159:DC:C2'	6:F:160:DT:C7	2.61	0.74
6:F:127:DC:O3'	6:F:128:DG:P	2.46	0.74
9:I:733:PRO:CD	11:L:192:ARG:NH1	2.43	0.74
9:I:911:LEU:HD11	9:I:930:LEU:HD21	1.68	0.74
6:F:108:DG:O3'	6:F:109:DT:H5'	1.87	0.73
4:D:47:ALA:O	4:D:51:ARG:HB2	1.87	0.73
1:A:267:PRO:HB2	1:A:337:LYS:HB2	1.70	0.73
5:E:28:DG:O3'	5:E:29:DC:P	2.47	0.73
9:I:43:LYS:HD3	9:I:163:VAL:HG13	1.69	0.73
5:E:49:DC:O3'	5:E:50:DG:P	2.46	0.73
6:F:122:DG:O3'	6:F:123:DA:H5'	1.87	0.73
9:I:49:VAL:CG2	9:I:51:LEU:HD11	2.17	0.73
9:I:443:TRP:NE1	9:I:969:CYS:SG	2.62	0.73
6:F:128:DG:O3'	6:F:129:DA:P	2.46	0.73
9:I:190:PHE:CE2	9:I:192:CYS:HB3	2.23	0.73
6:F:140:DA:O3'	6:F:141:DC:H5'	1.89	0.73
9:I:314:VAL:CG1	9:I:921:TYR:OH	2.37	0.73
5:E:22:DG:O3'	5:E:23:DG:P	2.47	0.73
5:E:28:DG:C2	6:F:134:DG:C2	2.76	0.72
9:I:725:ARG:HH12	9:I:749:LEU:HD23	1.53	0.72
9:I:866:HIS:CE1	9:I:869:SER:HB2	2.24	0.72
6:F:134:DG:O3'	6:F:135:DC:P	2.48	0.72
6:F:94:DT:H5''	7:G:873:PHE:CE1	2.24	0.72
5:E:38:DT:O3'	5:E:39:DC:H5'	1.89	0.72
6:F:111:DC:O3'	6:F:112:DG:P	2.47	0.72
9:I:786:LYS:HZ1	10:J:218:VAL:HG23	1.52	0.72
9:I:274:LEU:N	9:I:275:PRO:CD	2.51	0.72
5:E:70:DC:H5'	7:G:875:ARG:CD	2.20	0.72
5:E:62:DC:C3'	5:E:63:DG:P	2.77	0.72
6:F:104:DG:O3'	6:F:105:DA:H5'	1.88	0.72
6:F:130:DA:O3'	6:F:131:DC:P	2.48	0.72
6:F:129:DA:O3'	6:F:130:DA:P	2.47	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:568:VAL:O	9:I:575:PHE:CD2	2.43	0.72
9:I:838:ASN:HD21	11:L:178:LYS:CD	0.91	0.72
9:I:723:PHE:CE1	9:I:778:LEU:HB2	2.25	0.72
5:E:19:DG:O3'	5:E:20:DG:H5'	1.90	0.72
6:F:133:DC:HO3'	6:F:134:DG:H5'	1.54	0.72
5:E:59:DA:C3'	5:E:60:DG:P	2.78	0.71
9:I:629:ARG:HA	9:I:648:MET:HG3	1.72	0.71
10:J:219:GLU:HB2	11:L:182:GLN:HG2	1.72	0.71
5:E:18:DG:C3'	5:E:19:DG:P	2.78	0.71
5:E:74:DC:O3'	5:E:75:DC:P	2.47	0.71
5:E:50:DG:O3'	5:E:51:DA:H5'	1.90	0.71
5:E:77:DA:O3'	5:E:78:DC:P	2.48	0.71
9:I:883:PHE:CZ	9:I:885:ASP:CB	2.73	0.71
9:I:355:PHE:CD2	9:I:359:ILE:HD11	2.25	0.71
5:E:43:DC:C3'	5:E:44:DG:P	2.79	0.71
6:F:142:DC:O3'	6:F:143:DC:H5'	1.89	0.71
9:I:569:GLN:HB3	9:I:573:GLY:HA2	1.73	0.71
10:K:276:LEU:CD2	10:K:325:ASN:HB3	2.21	0.71
9:I:566:VAL:CG1	9:I:628:ILE:HG23	2.21	0.71
6:F:104:DG:C3'	6:F:105:DA:P	2.79	0.71
6:F:106:DG:H5''	9:I:542:ASN:ND2	2.05	0.71
5:E:30:DG:N2	6:F:132:DG:N2	2.35	0.71
9:I:566:VAL:HG12	9:I:577:HIS:HD1	1.56	0.71
9:I:816:VAL:HA	9:I:864:ASN:HB3	1.71	0.71
6:F:100:DG:O3'	6:F:101:DC:H5'	1.91	0.71
10:J:219:GLU:C	11:L:182:GLN:HG2	2.12	0.71
9:I:438:PRO:HB2	9:I:965:TRP:CZ3	2.25	0.71
9:I:747:TYR:CD1	9:I:794:TYR:CD1	2.79	0.71
9:I:631:ASP:HB2	9:I:638:ARG:HH22	1.55	0.71
9:I:361:ARG:HB2	9:I:500:THR:HG23	1.70	0.71
9:I:267:HIS:CE1	9:I:277:LEU:CB	2.74	0.70
9:I:274:LEU:H	9:I:275:PRO:CD	2.04	0.70
5:E:56:DT:O3'	5:E:57:DC:H5'	1.91	0.70
6:F:137:DC:C3'	6:F:138:DC:P	2.79	0.70
9:I:786:LYS:HZ2	10:J:218:VAL:HG23	0.84	0.70
9:I:602:LYS:C	9:I:605:PRO:HD2	2.10	0.70
5:E:48:DT:O3'	5:E:49:DC:P	2.49	0.70
9:I:161:PHE:CZ	9:I:177:VAL:CG2	2.73	0.70
5:E:1:DA:O3'	5:E:2:DG:H5'	1.91	0.70
9:I:443:TRP:CE2	9:I:969:CYS:CB	2.68	0.70
5:E:60:DG:O3'	5:E:61:DC:H5'	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:84:DT:O3'	6:F:85:DA:P	2.49	0.70
9:I:729:CYS:HA	9:I:732:CYS:HB2	1.73	0.70
6:F:140:DA:C3'	6:F:141:DC:P	2.79	0.70
9:I:575:PHE:CG	9:I:576:ASN:N	2.59	0.70
9:I:807:THR:HB	9:I:808:PRO:HD3	1.71	0.70
9:I:713:TRP:HA	9:I:716:PRO:HG2	1.72	0.70
6:F:105:DA:C3'	6:F:106:DG:P	2.79	0.70
5:E:7:DC:C2	5:E:7:DC:C1'	2.74	0.70
9:I:548:ILE:CB	9:I:581:ILE:HD13	2.22	0.70
6:F:91:DG:O3'	6:F:92:DT:H5'	1.92	0.70
9:I:838:ASN:CB	11:L:178:LYS:HD2	2.17	0.70
9:I:666:ILE:HD12	9:I:669:LEU:HB2	1.72	0.70
9:I:666:ILE:HD11	9:I:701:CYS:HB2	1.72	0.70
3:C:332:GLU:HG2	3:C:334:VAL:HG23	1.72	0.70
9:I:767:CYS:N	9:I:768:PRO:HD3	2.07	0.69
5:E:46:DG:C2	6:F:116:DG:N2	2.60	0.69
5:E:48:DT:O3'	5:E:49:DC:H5'	1.90	0.69
9:I:568:VAL:C	9:I:575:PHE:CD2	2.66	0.69
6:F:82:DC:O3'	6:F:83:DG:P	2.50	0.69
6:F:97:DT:O3'	6:F:98:DC:H5'	1.92	0.69
9:I:577:HIS:CD2	9:I:579:LEU:HG	2.23	0.69
9:I:568:VAL:C	9:I:575:PHE:HD2	1.96	0.69
9:I:309:ILE:CG2	9:I:312:ALA:HB3	2.09	0.69
1:A:196:ARG:O	6:F:145:DC:H2''	1.93	0.69
6:F:90:DC:C3'	6:F:91:DG:P	2.80	0.69
10:J:251:GLY:HA3	11:L:183:ARG:HG2	1.73	0.69
7:G:819:ARG:HH11	7:G:819:ARG:HG3	1.56	0.69
9:I:215:VAL:CG2	9:I:250:ALA:HB3	2.22	0.69
9:I:405:TYR:O	9:I:414:LEU:HD22	1.84	0.69
6:F:134:DG:O3'	6:F:135:DC:H5'	1.93	0.69
5:E:61:DC:C3'	5:E:62:DC:P	2.81	0.69
9:I:741:PHE:CD2	9:I:747:TYR:OH	2.45	0.69
9:I:761:ARG:HG2	9:I:808:PRO:HG2	1.74	0.69
9:I:182:TYR:CD2	9:I:182:TYR:O	2.46	0.69
9:I:690:CYS:HB3	9:I:694:VAL:CG1	2.23	0.69
5:E:71:DG:O3'	5:E:72:DT:H5'	1.92	0.69
9:I:566:VAL:O	9:I:577:HIS:ND1	2.25	0.69
9:I:767:CYS:H	9:I:768:PRO:HD3	1.58	0.69
5:E:75:DC:O3'	5:E:76:DT:P	2.51	0.69
6:F:131:DC:HO3'	6:F:132:DG:H5'	1.58	0.69
10:K:327:TRP:CD1	10:K:374:TYR:HE2	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:767:CYS:N	9:I:768:PRO:CD	2.56	0.69
9:I:707:ASN:CG	9:I:712:THR:HA	2.14	0.68
9:I:396:LYS:HG2	9:I:660:VAL:HG13	1.75	0.68
5:E:25:DG:HO3'	5:E:26:DG:P	2.16	0.68
6:F:83:DG:O3'	6:F:84:DT:P	2.51	0.68
9:I:699:CYS:SG	9:I:753:MET:HA	2.33	0.68
10:K:310:THR:O	10:K:314:SER:HB2	1.93	0.68
3:C:336:VAL:HG12	4:D:5:LEU:HG	1.76	0.68
6:F:133:DC:C3'	6:F:134:DG:P	2.82	0.68
9:I:84:PHE:C	9:I:84:PHE:CD1	2.65	0.68
5:E:44:DG:C2	6:F:118:DG:N2	2.62	0.68
7:G:680:GLY:N	9:I:475:LYS:CD	2.56	0.68
6:F:103:DC:O3'	6:F:104:DG:C5'	2.42	0.68
9:I:226:THR:O	9:I:227:HIS:C	2.31	0.68
9:I:605:PRO:HA	9:I:608:ASN:HB2	1.75	0.68
9:I:814:ASN:O	9:I:815:GLU:HB2	1.94	0.68
5:E:69:DA:O3'	5:E:70:DC:H5'	1.94	0.68
5:E:44:DG:O3'	5:E:45:DC:H5'	1.94	0.68
6:F:103:DC:HO3'	6:F:104:DG:H5'	1.56	0.68
9:I:622:ASP:O	9:I:625:LEU:CD2	2.42	0.68
9:I:75:VAL:CG1	9:I:128:ILE:HD11	2.23	0.68
9:I:649:TRP:HB3	9:I:669:LEU:HG	1.76	0.68
9:I:537:PHE:HB3	9:I:625:LEU:CD1	2.24	0.68
7:G:680:GLY:H	9:I:475:LYS:HD2	1.59	0.68
10:K:311:CYS:O	10:K:317:LEU:HD23	1.94	0.68
10:K:373:ARG:HH11	10:K:408:ASP:HB2	1.57	0.68
9:I:783:ASP:OD2	11:L:185:ASP:OD1	2.10	0.67
9:I:707:ASN:OD1	9:I:712:THR:CB	2.41	0.67
9:I:761:ARG:NE	9:I:768:PRO:CB	2.55	0.67
5:E:71:DG:C5'	7:G:877:GLY:CA	2.66	0.67
9:I:729:CYS:SG	9:I:781:TYR:CE1	2.88	0.67
9:I:883:PHE:HE2	9:I:886:ILE:CA	2.07	0.67
9:I:295:LEU:CD1	9:I:354:PHE:CE1	2.76	0.67
5:E:70:DC:C3'	5:E:71:DG:P	2.82	0.67
9:I:744:PHE:HB3	9:I:747:TYR:CE1	2.29	0.67
9:I:338:GLU:CB	9:I:342:THR:OG1	2.42	0.67
9:I:49:VAL:CG1	9:I:51:LEU:HD11	2.25	0.67
5:E:21:DT:O3'	5:E:22:DG:P	2.52	0.67
5:E:63:DG:O3'	5:E:64:DA:H5'	1.94	0.67
6:F:92:DT:O3'	6:F:93:DC:H5'	1.95	0.67
9:I:576:ASN:O	9:I:577:HIS:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:40:DA:C3'	5:E:41:DG:P	2.82	0.67
9:I:161:PHE:CD1	9:I:177:VAL:HG23	2.29	0.67
9:I:866:HIS:NE2	9:I:869:SER:HB2	2.08	0.67
9:I:295:LEU:HD12	9:I:354:PHE:CZ	2.29	0.67
5:E:26:DG:HO3'	5:E:27:DC:P	2.14	0.67
6:F:122:DG:HO3'	6:F:123:DA:P	2.17	0.67
6:F:89:DA:O3'	6:F:90:DC:H5'	1.94	0.67
9:I:741:PHE:CE1	9:I:791:ASP:CB	2.78	0.67
9:I:649:TRP:CZ2	9:I:668:ALA:HB1	2.29	0.67
6:F:102:DT:C3'	6:F:103:DC:P	2.82	0.67
4:D:53:ARG:HG2	4:D:53:ARG:O	1.94	0.67
9:I:566:VAL:HB	9:I:577:HIS:CE1	2.30	0.67
9:I:211:ALA:O	9:I:254:PHE:CD2	2.47	0.67
6:F:123:DA:C3'	6:F:124:DG:P	2.83	0.66
9:I:161:PHE:CD2	9:I:177:VAL:HG21	2.31	0.66
5:E:39:DC:C3'	5:E:40:DA:P	2.83	0.66
9:I:178:PHE:CG	9:I:309:ILE:HD12	2.30	0.66
9:I:35:ILE:HD13	9:I:189:TRP:HE1	1.60	0.66
10:J:250:PRO:HD2	11:L:183:ARG:CD	2.16	0.66
9:I:516:GLN:HB2	9:I:517:PRO:HD3	1.77	0.66
9:I:652:GLN:HA	9:I:656:GLU:HG2	1.78	0.66
5:E:76:DT:O3'	5:E:77:DA:P	2.53	0.66
6:F:116:DG:O3'	6:F:117:DC:H5'	1.96	0.66
6:F:95:DG:O3'	6:F:96:DC:H5'	1.95	0.66
9:I:838:ASN:ND2	11:L:178:LYS:CB	2.59	0.66
9:I:405:TYR:O	9:I:414:LEU:HD23	1.88	0.66
9:I:536:ALA:O	9:I:544:LEU:HD12	1.95	0.66
5:E:73:DG:O3'	5:E:74:DC:H5'	1.96	0.66
10:K:309:MET:SD	10:K:355:ILE:HG12	2.35	0.66
6:F:133:DC:O3'	6:F:134:DG:C5'	2.42	0.66
9:I:883:PHE:CB	9:I:886:ILE:HD12	2.25	0.66
5:E:17:DG:P	5:E:17:DG:H5'	2.34	0.66
6:F:137:DC:O3'	6:F:138:DC:C5'	2.44	0.66
9:I:408:LYS:O	9:I:414:LEU:CG	2.44	0.66
5:E:67:DA:C3'	5:E:68:DG:P	2.82	0.66
9:I:439:HIS:H	9:I:439:HIS:CD2	2.13	0.66
1:A:278:GLN:H	1:A:278:GLN:NE2	1.93	0.66
9:I:455:LEU:HD13	9:I:455:LEU:C	2.16	0.66
9:I:241:PRO:HG3	9:I:496:MET:SD	2.34	0.65
9:I:666:ILE:HD11	9:I:701:CYS:CB	2.25	0.65
5:E:24:DG:C3'	5:E:25:DG:P	2.84	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:566:VAL:CG1	9:I:628:ILE:HG22	2.26	0.65
9:I:854:CYS:HB2	9:I:874:PHE:CZ	2.31	0.65
9:I:284:LEU:HA	9:I:287:VAL:HG22	1.78	0.65
9:I:569:GLN:HA	9:I:575:PHE:HB3	1.79	0.65
5:E:20:DG:O3'	5:E:21:DT:H5'	1.97	0.65
6:F:131:DC:O3'	6:F:132:DG:C5'	2.43	0.65
9:I:537:PHE:CG	9:I:544:LEU:HD13	2.31	0.65
1:A:214:PHE:CE1	5:E:15:DA:H1'	2.31	0.65
9:I:568:VAL:O	9:I:575:PHE:CB	2.40	0.65
5:E:41:DG:C3'	5:E:42:DT:P	2.84	0.65
5:E:68:DG:O3'	5:E:69:DA:H5'	1.96	0.65
9:I:723:PHE:CD2	9:I:754:PRO:HG3	2.31	0.65
5:E:28:DG:N2	6:F:134:DG:N2	2.45	0.65
5:E:43:DC:HO3'	5:E:44:DG:H5'	1.62	0.65
6:F:88:DC:C3'	6:F:89:DA:P	2.85	0.65
9:I:314:VAL:HA	9:I:921:TYR:CD1	2.32	0.65
10:J:250:PRO:CD	11:L:183:ARG:HD3	2.24	0.65
9:I:37:ASN:O	9:I:38:ILE:HB	1.96	0.65
9:I:38:ILE:HD13	9:I:45:VAL:CG1	2.26	0.65
9:I:314:VAL:HA	9:I:921:TYR:CE1	2.32	0.65
10:K:238:LYS:NZ	10:K:241:GLU:OE1	2.28	0.65
5:E:71:DG:OP1	7:G:877:GLY:CA	2.45	0.65
9:I:719:MET:HA	9:I:753:MET:SD	2.37	0.65
9:I:703:ALA:HB2	9:I:756:ALA:HA	1.78	0.65
10:J:238:LYS:NZ	11:L:175:LEU:CD2	2.53	0.64
10:J:220:GLN:CD	11:L:186:VAL:HG22	2.17	0.64
9:I:313:TYR:CE1	9:I:884:VAL:HG21	2.31	0.64
9:I:783:ASP:HB2	11:L:188:ARG:HH12	1.59	0.64
9:I:707:ASN:CB	9:I:712:THR:HG22	2.28	0.64
9:I:867:VAL:HG12	9:I:897:TYR:OH	1.92	0.64
7:G:835:LEU:HB3	7:G:846:ILE:HG21	1.77	0.64
9:I:634:MET:CG	9:I:664:GLU:HG3	2.27	0.64
6:F:138:DC:O3'	6:F:139:DC:C5'	2.45	0.64
9:I:751:LYS:CG	9:I:797:GLU:HB3	2.27	0.64
9:I:707:ASN:HB3	9:I:712:THR:HG22	1.79	0.64
9:I:43:LYS:HD3	9:I:163:VAL:CG1	2.27	0.64
5:E:26:DG:C3'	5:E:27:DC:P	2.85	0.64
6:F:142:DC:O3'	6:F:143:DC:P	2.56	0.64
9:I:324:ILE:HG13	9:I:327:THR:OG1	1.98	0.64
9:I:54:PHE:CZ	9:I:143:VAL:HG22	2.27	0.64
9:I:752:THR:HA	9:I:755:VAL:HB	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:806:VAL:HA	9:I:809:ALA:HB3	1.80	0.64
5:E:29:DC:HO3'	5:E:30:DG:H5'	1.60	0.64
9:I:413:LEU:HG	9:I:413:LEU:O	1.98	0.64
9:I:725:ARG:HB3	9:I:744:PHE:CE2	2.33	0.64
9:I:706:ALA:HA	9:I:760:LEU:HD13	1.80	0.64
9:I:795:ARG:O	9:I:799:ILE:HG12	1.96	0.64
9:I:919:VAL:HB	9:I:922:VAL:CG2	2.28	0.64
5:E:44:DG:C2	6:F:118:DG:C2	2.85	0.64
5:E:3:DG:O3'	5:E:4:DG:P	2.55	0.64
9:I:296:THR:HG22	9:I:296:THR:O	1.98	0.64
9:I:183:GLN:OE1	9:I:438:PRO:HA	1.98	0.64
5:E:25:DG:O3'	5:E:26:DG:C5'	2.45	0.63
9:I:666:ILE:HD11	9:I:701:CYS:SG	2.38	0.63
10:K:327:TRP:CD1	10:K:374:TYR:CE2	2.86	0.63
5:E:60:DG:C3'	5:E:61:DC:P	2.86	0.63
6:F:121:DT:H3'	6:F:122:DG:P	2.39	0.63
9:I:799:ILE:HG22	9:I:856:ARG:HB2	1.80	0.63
9:I:745:GLN:O	9:I:746:SER:OG	2.13	0.63
6:F:115:DC:C3'	6:F:116:DG:P	2.87	0.63
6:F:157:DC:O3'	6:F:158:DC:P	2.55	0.63
9:I:49:VAL:CG2	9:I:51:LEU:CD1	2.74	0.63
9:I:690:CYS:HB3	9:I:694:VAL:HG11	1.81	0.63
9:I:210:ALA:CB	9:I:232:LYS:HG3	2.27	0.63
5:E:37:DC:C3'	5:E:38:DT:P	2.86	0.63
10:J:223:TYR:CB	11:L:182:GLN:HE22	2.11	0.63
9:I:741:PHE:HD2	9:I:747:TYR:OH	1.80	0.63
9:I:35:ILE:HG21	9:I:45:VAL:CG1	2.27	0.63
5:E:65:DG:O3'	5:E:66:DC:H5'	1.98	0.63
5:E:66:DC:C3'	5:E:67:DA:P	2.87	0.63
6:F:87:DG:O3'	6:F:88:DC:H5'	1.98	0.63
9:I:537:PHE:CD2	9:I:625:LEU:HD22	2.33	0.63
10:J:223:TYR:H	11:L:182:GLN:NE2	1.97	0.62
9:I:531:PHE:CE1	9:I:638:ARG:CB	2.82	0.62
10:J:219:GLU:HG2	11:L:182:GLN:HG2	1.81	0.62
9:I:338:GLU:HB3	9:I:342:THR:OG1	1.99	0.62
5:E:42:DT:C3'	5:E:43:DC:P	2.87	0.62
6:F:101:DC:C3'	6:F:102:DT:P	2.86	0.62
5:E:70:DC:O4'	7:G:875:ARG:CZ	2.48	0.62
9:I:159:LEU:HB2	9:I:161:PHE:CE1	2.31	0.62
9:I:393:HIS:CG	9:I:659:VAL:HB	2.34	0.62
5:E:18:DG:N2	6:F:144:DC:O2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:123:DA:HO3'	6:F:124:DG:H5'	1.64	0.62
10:J:250:PRO:C	11:L:183:ARG:NE	2.53	0.62
9:I:161:PHE:CE2	9:I:177:VAL:CG2	2.75	0.62
6:F:137:DC:HO3'	6:F:138:DC:H5'	1.62	0.62
10:K:305:ILE:HD13	10:K:351:ILE:HD12	1.82	0.62
9:I:178:PHE:CG	9:I:309:ILE:CD1	2.83	0.62
9:I:159:LEU:CD2	9:I:179:SER:HB3	2.29	0.62
9:I:240:ILE:HG23	9:I:241:PRO:HD2	1.82	0.62
9:I:733:PRO:CD	11:L:192:ARG:CZ	2.77	0.62
9:I:706:ALA:O	9:I:707:ASN:HB2	1.99	0.62
5:E:33:DC:HO3'	5:E:34:DG:H5'	1.65	0.61
5:E:57:DC:C3'	5:E:58:DG:P	2.88	0.61
5:E:62:DC:HO3'	5:E:63:DG:H5'	1.64	0.61
9:I:240:ILE:HG13	9:I:495:GLN:O	2.00	0.61
9:I:443:TRP:NE1	9:I:969:CYS:CB	2.62	0.61
9:I:537:PHE:HB3	9:I:625:LEU:CD2	2.29	0.61
9:I:727:PHE:HE2	9:I:781:TYR:CD1	2.18	0.61
9:I:464:ILE:HB	9:I:511:SER:HB3	1.81	0.61
9:I:32:VAL:HG13	9:I:203:LYS:HB3	1.82	0.61
5:E:62:DC:O3'	5:E:63:DG:C5'	2.46	0.61
5:E:69:DA:HO3'	7:G:875:ARG:HD3	1.65	0.61
6:F:98:DC:C3'	6:F:99:DG:P	2.88	0.61
9:I:566:VAL:C	9:I:577:HIS:ND1	2.53	0.61
9:I:867:VAL:CG1	9:I:897:TYR:HH	1.90	0.61
7:G:680:GLY:H	9:I:475:LYS:CD	2.13	0.61
9:I:564:LEU:HD23	9:I:564:LEU:C	2.21	0.61
6:F:91:DG:C3'	6:F:92:DT:P	2.89	0.61
9:I:396:LYS:HG2	9:I:660:VAL:HG11	1.82	0.61
5:E:70:DC:H5'	7:G:875:ARG:HD3	1.82	0.61
9:I:703:ALA:CB	9:I:756:ALA:HA	2.30	0.61
10:J:250:PRO:CA	11:L:183:ARG:HD3	2.31	0.61
9:I:537:PHE:HB2	9:I:625:LEU:HD13	1.83	0.61
9:I:761:ARG:CG	9:I:808:PRO:HG2	2.31	0.61
6:F:93:DC:C3'	6:F:94:DT:P	2.88	0.61
9:I:267:HIS:CE1	9:I:277:LEU:HB3	2.35	0.61
6:F:103:DC:H3'	6:F:104:DG:P	2.41	0.61
9:I:784:ASN:CB	11:L:192:ARG:NH1	2.64	0.61
9:I:295:LEU:CD1	9:I:354:PHE:CZ	2.82	0.61
5:E:72:DT:C3'	5:E:73:DG:P	2.88	0.61
9:I:439:HIS:HB3	9:I:965:TRP:HE3	1.66	0.61
9:I:394:TRP:HE1	9:I:691:PHE:HB3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:570:GLU:HA	9:I:626:LEU:CD2	2.31	0.60
9:I:566:VAL:HG13	9:I:629:ARG:O	2.01	0.60
9:I:215:VAL:HG12	9:I:327:THR:HG21	1.83	0.60
9:I:267:HIS:CE1	9:I:277:LEU:CD2	2.84	0.60
9:I:633:ASP:H	9:I:661:ALA:HB2	1.66	0.60
10:J:381:ALA:HA	10:J:388:ILE:HD11	1.83	0.60
9:I:695:ARG:CB	9:I:749:LEU:HD22	2.26	0.60
9:I:653:LEU:HG	9:I:681:LEU:HD22	1.82	0.60
5:E:45:DC:HO3'	5:E:46:DG:H5'	1.66	0.60
5:E:46:DG:N2	6:F:116:DG:C2	2.69	0.60
6:F:137:DC:HO3'	6:F:138:DC:P	2.21	0.60
9:I:314:VAL:HG21	9:I:318:ALA:N	2.08	0.60
9:I:359:ILE:HB	9:I:498:VAL:HG21	1.83	0.60
5:E:53:DC:C3'	5:E:54:DA:P	2.89	0.60
9:I:707:ASN:O	9:I:708:SER:HB3	2.00	0.60
9:I:802:LEU:CD1	9:I:856:ARG:NH1	2.64	0.60
9:I:314:VAL:HG22	9:I:318:ALA:N	2.14	0.60
9:I:322:MET:HB3	9:I:329:LEU:HB3	1.84	0.60
9:I:720:LYS:HA	9:I:723:PHE:HB2	1.82	0.60
9:I:799:ILE:HG21	9:I:852:VAL:O	2.01	0.60
10:J:319:LEU:HA	10:J:326:HIS:CG	2.35	0.60
6:F:140:DA:H2''	6:F:141:DC:C6	2.37	0.60
10:J:223:TYR:CB	11:L:182:GLN:OE1	2.24	0.60
9:I:723:PHE:CE2	9:I:754:PRO:HG3	2.36	0.60
9:I:751:LYS:HE2	9:I:755:VAL:HG21	1.83	0.60
6:F:143:DC:H2''	6:F:144:DC:H6	1.63	0.60
9:I:38:ILE:HG21	9:I:251:ILE:HD13	1.83	0.60
4:D:3:TYR:C	4:D:5:LEU:H	2.05	0.60
9:I:154:GLN:HB3	9:I:155:PRO:HD3	1.83	0.60
9:I:577:HIS:O	9:I:578:THR:CB	2.49	0.60
9:I:267:HIS:CE1	9:I:277:LEU:HD23	2.35	0.60
9:I:49:VAL:HG13	9:I:51:LEU:CD1	2.32	0.60
9:I:898:THR:HG21	9:I:910:LEU:HD22	1.82	0.60
9:I:43:LYS:CD	9:I:163:VAL:HG13	2.31	0.60
5:E:29:DC:O3'	5:E:30:DG:C5'	2.45	0.60
9:I:396:LYS:HG3	9:I:399:LEU:HD23	1.83	0.60
9:I:153:ASP:HB2	9:I:156:LYS:HE3	1.84	0.60
9:I:725:ARG:CB	9:I:744:PHE:CZ	2.84	0.59
9:I:761:ARG:NE	9:I:808:PRO:HB2	2.16	0.59
9:I:396:LYS:HE2	9:I:399:LEU:CD2	2.32	0.59
5:E:70:DC:C4'	7:G:875:ARG:CZ	2.79	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:138:DC:H2''	6:F:139:DC:C6	2.37	0.59
9:I:630:ILE:HG12	9:I:648:MET:SD	2.42	0.59
10:J:219:GLU:CG	11:L:182:GLN:HG2	2.31	0.59
9:I:54:PHE:CZ	9:I:143:VAL:CG2	2.82	0.59
5:E:10:DA:H2''	5:E:11:DT:H5'	1.83	0.59
5:E:24:DG:O3'	5:E:25:DG:C5'	2.48	0.59
6:F:92:DT:C3'	6:F:93:DC:P	2.90	0.59
9:I:735:ILE:HD12	9:I:735:ILE:C	2.23	0.59
5:E:68:DG:C3'	5:E:69:DA:P	2.89	0.59
6:F:121:DT:O3'	6:F:122:DG:C5'	2.47	0.59
9:I:234:PHE:CD2	9:I:236:TYR:OH	2.54	0.59
5:E:22:DG:C2	6:F:140:DA:C2	2.90	0.59
5:E:54:DA:C2	6:F:108:DG:C2	2.90	0.59
9:I:919:VAL:HB	9:I:922:VAL:HG22	1.83	0.59
5:E:55:DC:C3'	5:E:56:DT:P	2.90	0.59
6:F:139:DC:H3'	6:F:140:DA:P	2.41	0.59
9:I:570:GLU:HA	9:I:626:LEU:HD22	1.83	0.59
9:I:630:ILE:CB	9:I:648:MET:SD	2.90	0.59
9:I:838:ASN:HD21	11:L:178:LYS:CB	2.13	0.59
9:I:161:PHE:CE1	9:I:177:VAL:CG2	2.86	0.59
9:I:35:ILE:CG2	9:I:45:VAL:HG12	2.30	0.59
5:E:17:DG:C1'	5:E:18:DG:C8	2.84	0.59
5:E:38:DT:C3'	5:E:39:DC:P	2.89	0.59
5:E:45:DC:C3'	5:E:46:DG:P	2.90	0.59
6:F:99:DG:C3'	6:F:100:DG:P	2.91	0.59
7:G:680:GLY:N	9:I:475:LYS:HD2	2.16	0.59
9:I:35:ILE:HG21	9:I:45:VAL:HG11	1.84	0.59
9:I:927:LEU:HD13	9:I:927:LEU:C	2.23	0.59
9:I:575:PHE:CE1	9:I:593:HIS:HB3	2.37	0.59
9:I:568:VAL:HG22	9:I:628:ILE:HG12	1.83	0.59
10:J:249:ASP:OD1	11:L:179:ALA:HB1	2.03	0.59
9:I:847:ARG:HB2	9:I:883:PHE:CZ	2.37	0.59
9:I:337:ASP:CB	9:I:789:PHE:CG	2.84	0.59
6:F:94:DT:C3'	6:F:95:DG:P	2.90	0.58
10:J:238:LYS:HZ2	11:L:175:LEU:CD2	2.16	0.58
10:K:370:TRP:CE3	10:K:371:THR:HA	2.38	0.58
6:F:139:DC:O3'	6:F:140:DA:C5'	2.49	0.58
9:I:178:PHE:HD1	9:I:250:ALA:HB1	1.67	0.58
5:E:7:DC:H2''	5:E:8:DC:O5'	2.02	0.58
7:G:678:SER:N	7:G:679:GLY:HA2	2.16	0.58
10:K:319:LEU:HD11	10:K:371:THR:HG1	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:25:DG:HO3'	5:E:26:DG:H5'	1.65	0.58
10:J:241:GLU:CG	11:L:172:TYR:CD1	2.78	0.58
9:I:301:TYR:CZ	9:I:325:PHE:CE2	2.91	0.58
10:J:241:GLU:OE1	11:L:175:LEU:HD23	2.03	0.58
9:I:806:VAL:HG11	9:I:860:VAL:HG11	1.86	0.58
9:I:806:VAL:HG13	9:I:860:VAL:HG13	1.85	0.58
4:D:87:LEU:HD11	4:D:89:LYS:CE	2.32	0.58
9:I:833:ILE:HG12	9:I:856:ARG:CG	2.32	0.58
9:I:258:VAL:HG23	9:I:266:THR:OG1	2.04	0.58
5:E:24:DG:HO3'	5:E:25:DG:H5'	1.66	0.58
6:F:120:DC:HO3'	6:F:121:DT:P	2.22	0.58
9:I:408:LYS:H	9:I:414:LEU:HD11	1.67	0.58
9:I:731:SER:HB2	9:I:735:ILE:CG1	2.33	0.58
9:I:313:TYR:CZ	9:I:884:VAL:CG2	2.86	0.58
6:F:101:DC:HO3'	6:F:102:DT:H5'	1.67	0.58
6:F:106:DG:C3'	6:F:107:DT:P	2.91	0.58
9:I:568:VAL:CG1	9:I:626:LEU:HB3	2.34	0.58
5:E:2:DG:H2''	5:E:3:DG:C8	2.39	0.58
9:I:747:TYR:CE1	9:I:794:TYR:CD1	2.91	0.58
9:I:729:CYS:SG	9:I:781:TYR:HE1	2.26	0.58
9:I:45:VAL:HB	9:I:152:LEU:HD22	1.85	0.58
6:F:117:DC:C3'	6:F:118:DG:P	2.92	0.58
9:I:575:PHE:HE1	9:I:593:HIS:HB3	1.68	0.58
9:I:843:LEU:HB2	9:I:844:PRO:HD3	1.84	0.58
5:E:43:DC:O3'	5:E:44:DG:C5'	2.46	0.58
9:I:566:VAL:HG12	9:I:577:HIS:ND1	2.18	0.58
9:I:761:ARG:HH22	9:I:809:ALA:HA	1.69	0.58
9:I:313:TYR:CZ	9:I:884:VAL:HG22	2.39	0.58
9:I:69:GLN:O	9:I:156:LYS:NZ	2.31	0.58
6:F:119:DA:C3'	6:F:120:DC:P	2.92	0.57
9:I:45:VAL:H	9:I:152:LEU:HB2	1.68	0.57
9:I:553:THR:O	9:I:553:THR:HG22	2.04	0.57
5:E:69:DA:O3'	7:G:875:ARG:CZ	2.52	0.57
3:C:332:GLU:HG2	3:C:334:VAL:CG2	2.33	0.57
9:I:274:LEU:N	9:I:275:PRO:HD2	2.19	0.57
9:I:725:ARG:CB	9:I:744:PHE:CE2	2.87	0.57
9:I:566:VAL:CA	9:I:579:LEU:HD12	2.31	0.57
4:D:32:LEU:O	4:D:36:VAL:HG23	2.05	0.57
1:A:159:SER:C	1:A:161:ILE:H	2.05	0.57
5:E:70:DC:C5'	7:G:875:ARG:CD	2.82	0.57
9:I:707:ASN:OD1	9:I:712:THR:CG2	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:69:DA:C3'	5:E:70:DC:P	2.92	0.57
5:E:34:DG:N2	6:F:128:DG:N3	2.52	0.57
9:I:240:ILE:CG1	9:I:495:GLN:O	2.52	0.57
9:I:969:CYS:HA	9:I:972:VAL:CB	2.33	0.57
9:I:744:PHE:CB	9:I:747:TYR:CZ	2.84	0.57
9:I:49:VAL:HG13	9:I:51:LEU:HD11	1.87	0.57
11:L:194:MET:O	11:L:197:THR:OG1	2.21	0.57
5:E:54:DA:C2	6:F:108:DG:N2	2.73	0.57
9:I:699:CYS:SG	9:I:752:THR:O	2.59	0.57
9:I:240:ILE:HG12	9:I:495:GLN:C	2.25	0.57
6:F:157:DC:H2''	6:F:158:DC:C5	2.39	0.57
5:E:31:DT:C3'	5:E:32:DT:P	2.93	0.57
6:F:139:DC:HO3'	6:F:140:DA:P	2.20	0.57
6:F:113:DA:HO3'	6:F:114:DT:H5'	1.70	0.56
5:E:59:DA:O3'	5:E:60:DG:C5'	2.47	0.56
5:E:64:DA:C3'	5:E:65:DG:P	2.92	0.56
6:F:120:DC:O3'	6:F:121:DT:C5'	2.49	0.56
6:F:87:DG:H2''	6:F:88:DC:C6	2.40	0.56
9:I:568:VAL:C	9:I:575:PHE:HB3	2.23	0.56
9:I:707:ASN:OD1	9:I:712:THR:HG22	2.05	0.56
9:I:631:ASP:OD1	9:I:635:SER:N	2.37	0.56
9:I:649:TRP:CZ2	9:I:668:ALA:CB	2.88	0.56
9:I:816:VAL:CA	9:I:864:ASN:HB3	2.34	0.56
9:I:383:LYS:HB3	9:I:391:TYR:HB3	1.87	0.56
6:F:96:DC:C3'	6:F:97:DT:P	2.93	0.56
5:E:57:DC:HO3'	5:E:58:DG:H5'	1.70	0.56
6:F:124:DG:C3'	6:F:125:DG:P	2.93	0.56
6:F:89:DA:C3'	6:F:90:DC:P	2.94	0.56
9:I:867:VAL:O	9:I:897:TYR:CE1	2.59	0.56
5:E:3:DG:HO3'	5:E:4:DG:H5'	1.69	0.56
10:J:406:VAL:HB	10:J:412:LEU:HD22	1.87	0.56
5:E:27:DC:HO3'	5:E:28:DG:H5'	1.68	0.56
6:F:105:DA:HO3'	6:F:106:DG:H5'	1.68	0.56
9:I:267:HIS:NE2	9:I:277:LEU:HG	2.20	0.56
9:I:720:LYS:HA	9:I:723:PHE:CB	2.35	0.56
5:E:8:DC:H2'	5:E:9:DT:C6	2.41	0.56
9:I:883:PHE:CE2	9:I:886:ILE:HA	2.38	0.56
9:I:802:LEU:HD13	9:I:856:ARG:NH1	2.20	0.56
8:H:140:LEU:O	8:H:143:VAL:HG22	2.06	0.56
5:E:46:DG:C2	6:F:116:DG:C2	2.94	0.56
10:J:219:GLU:HG3	11:L:182:GLN:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ILE:HD11	1:A:209:THR:HG1	1.66	0.56
9:I:911:LEU:CD1	9:I:930:LEU:CD2	2.82	0.56
9:I:531:PHE:HE1	9:I:638:ARG:HB3	1.69	0.56
4:D:54:ASN:ND2	4:D:83:GLU:OE2	2.39	0.56
5:E:51:DA:C3'	5:E:52:DA:P	2.94	0.56
9:I:567:THR:CA	9:I:577:HIS:HB3	2.25	0.56
9:I:730:LYS:CE	11:L:195:ALA:HB1	2.28	0.56
10:K:319:LEU:HD11	10:K:371:THR:OG1	2.05	0.56
5:E:26:DG:H2''	5:E:27:DC:C6	2.40	0.56
10:J:219:GLU:HB2	11:L:182:GLN:CG	2.35	0.56
5:E:4:DG:H2''	5:E:5:DC:C5	2.40	0.56
5:E:19:DG:C3'	5:E:20:DG:P	2.94	0.56
5:E:58:DG:C3'	5:E:59:DA:P	2.93	0.56
9:I:464:ILE:HA	9:I:511:SER:OG	2.05	0.56
9:I:84:PHE:HE2	9:I:126:LEU:HB3	1.59	0.56
5:E:71:DG:C3'	5:E:72:DT:P	2.93	0.56
6:F:159:DC:C2'	6:F:160:DT:H73	2.32	0.56
5:E:6:DG:C2'	5:E:7:DC:O5'	2.52	0.56
9:I:806:VAL:CG1	9:I:860:VAL:CG2	2.83	0.56
3:C:336:VAL:CG1	4:D:5:LEU:HG	2.36	0.56
3:C:372:GLY:HA2	4:D:58:PHE:O	2.06	0.56
9:I:257:LEU:HB2	9:I:274:LEU:HD11	1.88	0.55
9:I:706:ALA:O	9:I:707:ASN:CB	2.53	0.55
9:I:148:ILE:HG21	9:I:191:PRO:HG2	1.88	0.55
5:E:44:DG:C3'	5:E:45:DC:P	2.94	0.55
6:F:139:DC:H2''	6:F:140:DA:C8	2.42	0.55
9:I:788:LYS:CB	9:I:791:ASP:OD2	2.50	0.55
5:E:30:DG:HO3'	5:E:31:DT:H5'	1.71	0.55
10:J:250:PRO:CB	11:L:183:ARG:HD3	2.37	0.55
9:I:240:ILE:HG23	9:I:496:MET:CA	2.36	0.55
9:I:761:ARG:CZ	9:I:768:PRO:CB	2.84	0.55
5:E:33:DC:C3'	5:E:34:DG:P	2.94	0.55
5:E:34:DG:N3	6:F:128:DG:N2	2.54	0.55
9:I:314:VAL:HA	9:I:921:TYR:CG	2.42	0.55
9:I:670:GLU:OE2	9:I:700:PHE:HD2	1.89	0.55
5:E:61:DC:HO3'	5:E:62:DC:P	2.30	0.55
5:E:71:DG:OP1	7:G:877:GLY:N	2.40	0.55
5:E:77:DA:C2	6:F:85:DA:C2	2.94	0.55
6:F:107:DT:C3'	6:F:108:DG:P	2.94	0.55
6:F:114:DT:H2''	6:F:115:DC:C6	2.42	0.55
6:F:120:DC:H3'	6:F:121:DT:P	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:883:PHE:HE2	9:I:886:ILE:HA	1.72	0.55
7:G:819:ARG:NH1	7:G:819:ARG:HG3	2.16	0.55
9:I:314:VAL:HA	9:I:921:TYR:CZ	2.42	0.55
9:I:159:LEU:HD23	9:I:179:SER:CB	2.37	0.55
9:I:855:LEU:HA	9:I:858:ILE:CG2	2.37	0.55
1:A:204:ILE:H	1:A:204:ILE:HD12	1.72	0.55
9:I:156:LYS:HA	9:I:156:LYS:HE2	1.88	0.55
10:J:412:LEU:HG	10:J:413:SER:N	2.21	0.55
5:E:62:DC:H3'	5:E:63:DG:P	2.47	0.55
9:I:35:ILE:HD13	9:I:189:TRP:NE1	2.22	0.55
9:I:222:GLU:HG3	9:I:224:VAL:HG13	1.88	0.55
9:I:223:THR:OG1	9:I:234:PHE:CD2	2.55	0.55
9:I:741:PHE:CD1	9:I:791:ASP:HB3	2.42	0.55
9:I:153:ASP:O	9:I:156:LYS:HG2	2.07	0.55
6:F:105:DA:O3'	6:F:106:DG:C5'	2.51	0.54
5:E:50:DG:N2	6:F:112:DG:N3	2.55	0.54
6:F:97:DT:C3'	6:F:98:DC:P	2.95	0.54
9:I:324:ILE:HG13	9:I:327:THR:O	2.07	0.54
9:I:211:ALA:O	9:I:254:PHE:HD2	1.91	0.54
1:A:159:SER:HB2	1:A:161:ILE:HG12	1.89	0.54
10:J:310:THR:O	10:J:314:SER:HB2	2.07	0.54
5:E:34:DG:N2	6:F:128:DG:N2	2.51	0.54
6:F:115:DC:O3'	6:F:116:DG:C5'	2.51	0.54
6:F:140:DA:HO3'	6:F:141:DC:P	2.25	0.54
9:I:669:LEU:HD13	9:I:681:LEU:CD1	2.34	0.54
10:J:370:TRP:CE3	10:J:371:THR:HA	2.43	0.54
9:I:220:LEU:C	9:I:220:LEU:HD23	2.27	0.54
9:I:84:PHE:HE2	9:I:126:LEU:CD2	2.06	0.54
9:I:829:ILE:HG22	9:I:833:ILE:HD11	1.89	0.54
10:K:330:ARG:HE	10:K:371:THR:HG1	1.55	0.54
5:E:50:DG:N3	6:F:112:DG:N2	2.56	0.54
5:E:79:DG:C2	6:F:83:DG:N2	2.76	0.54
9:I:867:VAL:HG12	9:I:868:PRO:N	2.22	0.54
10:J:241:GLU:OE1	11:L:175:LEU:CD2	2.56	0.54
9:I:51:LEU:HD12	9:I:51:LEU:N	2.23	0.54
4:D:83:GLU:O	4:D:85:THR:N	2.40	0.54
5:E:31:DT:HO3'	5:E:32:DT:H5'	1.70	0.54
9:I:569:GLN:HA	9:I:575:PHE:CB	2.37	0.54
9:I:161:PHE:CD2	9:I:177:VAL:CG2	2.90	0.54
5:E:6:DG:H2''	5:E:7:DC:C5'	2.37	0.54
5:E:61:DC:O3'	5:E:62:DC:C5'	2.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:138:DC:H3'	6:F:139:DC:P	2.46	0.54
6:F:89:DA:H2''	6:F:90:DC:C6	2.43	0.54
4:D:90:VAL:HG22	4:D:92:LYS:H	1.73	0.54
9:I:84:PHE:C	9:I:84:PHE:HD1	2.09	0.54
9:I:267:HIS:NE2	9:I:277:LEU:CG	2.71	0.54
6:F:155:DC:H2'	6:F:156:DG:C8	2.43	0.54
9:I:670:GLU:CD	9:I:700:PHE:HD2	2.10	0.54
3:C:366:ILE:HG22	4:D:52:VAL:HG11	1.89	0.54
9:I:871:PRO:HG3	9:I:897:TYR:CE2	2.43	0.54
1:A:304:ILE:HD12	1:A:304:ILE:N	2.23	0.54
9:I:695:ARG:O	9:I:749:LEU:HD13	2.07	0.54
9:I:67:SER:HB2	9:I:126:LEU:CD1	2.32	0.54
5:E:51:DA:HO3'	5:E:52:DA:H5'	1.73	0.54
6:F:113:DA:C3'	6:F:114:DT:P	2.96	0.54
10:J:223:TYR:CD2	11:L:179:ALA:HA	2.42	0.54
9:I:761:ARG:NH2	9:I:809:ALA:HA	2.23	0.54
10:J:220:GLN:CD	11:L:186:VAL:CG2	2.76	0.54
9:I:408:LYS:O	9:I:414:LEU:HD12	2.07	0.53
9:I:761:ARG:CZ	9:I:768:PRO:HB2	2.38	0.53
7:G:829:GLN:OE1	7:G:866:ARG:HG3	2.07	0.53
10:J:396:LEU:HD13	10:J:427:LEU:HD13	1.90	0.53
10:K:291:ASP:OD1	10:K:339:GLN:NE2	2.35	0.53
5:E:57:DC:O3'	5:E:58:DG:C5'	2.49	0.53
9:I:568:VAL:CB	9:I:575:PHE:CD2	2.86	0.53
9:I:629:ARG:CD	9:I:651:TYR:HB2	2.33	0.53
11:L:178:LYS:HE2	11:L:182:GLN:NE2	2.24	0.53
9:I:747:TYR:CD2	9:I:794:TYR:HB2	2.43	0.53
6:F:123:DA:O3'	6:F:124:DG:C5'	2.51	0.53
10:J:222:LEU:CB	11:L:178:LYS:CE	2.83	0.53
6:F:155:DC:H2''	6:F:156:DG:H5'	1.90	0.53
5:E:33:DC:O3'	5:E:34:DG:C5'	2.47	0.53
3:C:336:VAL:HG11	4:D:5:LEU:O	2.09	0.53
6:F:137:DC:H2''	6:F:138:DC:C6	2.43	0.53
9:I:531:PHE:HD1	9:I:638:ARG:HB2	1.73	0.53
9:I:653:LEU:HG	9:I:681:LEU:CD2	2.37	0.53
3:C:374:ALA:HA	4:D:60:GLY:O	2.08	0.53
9:I:670:GLU:HG2	9:I:701:CYS:HA	1.91	0.53
10:K:227:ILE:HG21	10:K:246:ILE:HD11	1.91	0.53
1:A:204:ILE:H	1:A:204:ILE:CD1	2.21	0.53
9:I:931:THR:HG23	9:I:974:LEU:HG	1.91	0.53
6:F:136:DC:HO3'	6:F:137:DC:H5'	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1:DA:H2''	5:E:2:DG:C8	2.44	0.53
9:I:646:ASP:CB	9:I:675:PRO:HD2	2.39	0.53
9:I:891:LEU:O	9:I:894:VAL:HG12	2.09	0.53
5:E:28:DG:N3	6:F:134:DG:N2	2.57	0.53
6:F:114:DT:C3'	6:F:115:DC:P	2.97	0.53
9:I:630:ILE:CG1	9:I:648:MET:SD	2.97	0.53
9:I:32:VAL:HG22	9:I:203:LYS:HB3	1.91	0.53
1:A:294:ARG:NH1	5:E:12:DA:OP1	2.30	0.53
9:I:470:LEU:HA	9:I:473:PHE:CE2	2.44	0.53
5:E:45:DC:O3'	5:E:46:DG:C5'	2.51	0.53
6:F:121:DT:HO3'	6:F:122:DG:H5'	1.74	0.53
6:F:86:DG:C3'	6:F:87:DG:P	2.97	0.53
9:I:314:VAL:CB	9:I:921:TYR:CZ	2.92	0.53
9:I:38:ILE:CG1	9:I:207:THR:O	2.56	0.53
6:F:141:DC:C3'	6:F:142:DC:P	2.97	0.52
9:I:307:VAL:HG13	9:I:329:LEU:HD12	1.90	0.52
9:I:838:ASN:CG	11:L:178:LYS:CD	2.03	0.52
5:E:38:DT:H2''	5:E:39:DC:C6	2.44	0.52
5:E:1:DA:O3'	5:E:2:DG:P	2.67	0.52
9:I:75:VAL:HG13	9:I:128:ILE:HD12	1.88	0.52
2:B:18:ILE:O	2:B:22:ILE:HG12	2.09	0.52
9:I:27:LYS:HG2	9:I:198:GLU:OE2	2.09	0.52
9:I:575:PHE:CE2	9:I:576:ASN:O	2.61	0.52
9:I:725:ARG:NH1	9:I:749:LEU:HD23	2.23	0.52
4:D:79:VAL:HG21	4:D:93:VAL:HG12	1.91	0.52
9:I:344:ARG:HB2	9:I:378:TYR:CZ	2.45	0.52
9:I:396:LYS:NZ	9:I:660:VAL:HG11	2.25	0.52
5:E:61:DC:H2''	5:E:62:DC:C6	2.44	0.52
6:F:136:DC:O3'	6:F:137:DC:C5'	2.53	0.52
9:I:548:ILE:HB	9:I:581:ILE:HD13	1.90	0.52
5:E:43:DC:H3'	5:E:44:DG:P	2.49	0.52
5:E:59:DA:HO3'	5:E:60:DG:H5'	1.70	0.52
6:F:111:DC:HO3'	6:F:112:DG:H5'	1.73	0.52
6:F:115:DC:HO3'	6:F:116:DG:H5'	1.71	0.52
6:F:127:DC:HO3'	6:F:128:DG:H5'	1.73	0.52
9:I:578:THR:HG22	9:I:579:LEU:N	2.24	0.52
9:I:867:VAL:CB	9:I:868:PRO:CD	2.77	0.52
9:I:439:HIS:O	9:I:443:TRP:HD1	1.93	0.52
9:I:827:ARG:NH2	11:L:184:ARG:NH2	2.48	0.52
5:E:27:DC:O3'	5:E:28:DG:C5'	2.50	0.52
5:E:40:DA:O3'	5:E:41:DG:C5'	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:131:DC:C3'	6:F:132:DG:P	2.98	0.52
9:I:267:HIS:NE2	9:I:308:PHE:CE2	2.75	0.52
9:I:649:TRP:HB2	9:I:669:LEU:HD21	1.92	0.52
1:A:188:ARG:HH11	4:D:64:THR:HG21	1.75	0.52
5:E:71:DG:OP1	7:G:877:GLY:HA3	2.09	0.52
9:I:847:ARG:HB3	9:I:883:PHE:CE2	2.42	0.52
6:F:159:DC:H2''	6:F:160:DT:H71	1.78	0.52
9:I:741:PHE:CB	9:I:747:TYR:OH	2.54	0.52
9:I:337:ASP:HB2	9:I:789:PHE:CG	2.44	0.52
9:I:265:VAL:HG22	9:I:304:PHE:HB3	1.92	0.52
7:G:970:GLU:HG2	7:G:972:THR:O	2.08	0.52
5:E:22:DG:N2	6:F:140:DA:C2	2.78	0.52
5:E:54:DA:C3'	5:E:55:DC:P	2.98	0.52
6:F:121:DT:HO3'	6:F:122:DG:P	2.25	0.52
9:I:761:ARG:NE	9:I:808:PRO:CB	2.73	0.52
9:I:426:ASN:N	9:I:427:PRO:HD2	2.24	0.52
5:E:47:DA:HO3'	5:E:48:DT:H5'	1.74	0.52
5:E:53:DC:HO3'	5:E:54:DA:H5'	1.75	0.52
5:E:70:DC:H5'	7:G:875:ARG:NE	2.23	0.52
9:I:159:LEU:HD22	9:I:179:SER:HB3	1.91	0.52
9:I:300:PRO:HD3	9:I:358:PHE:CZ	2.45	0.52
5:E:52:DA:C3'	5:E:53:DC:P	2.98	0.52
9:I:344:ARG:CB	9:I:378:TYR:CZ	2.93	0.52
9:I:295:LEU:HD12	9:I:354:PHE:CE1	2.45	0.52
7:G:943:LYS:N	7:G:943:LYS:HZ2	2.08	0.52
6:F:94:DT:HO3'	6:F:95:DG:H5'	1.75	0.51
9:I:830:LEU:HA	9:I:833:ILE:HB	1.92	0.51
9:I:666:ILE:O	9:I:670:GLU:HG3	2.10	0.51
9:I:715:GLY:C	9:I:717:PRO:HD2	2.31	0.51
9:I:602:LYS:O	9:I:605:PRO:HD2	2.10	0.51
1:A:278:GLN:HG2	1:A:279:GLN:HE21	1.74	0.51
5:E:63:DG:C3'	5:E:64:DA:P	2.99	0.51
6:F:120:DC:H2''	6:F:121:DT:C6	2.45	0.51
5:E:28:DG:N2	6:F:134:DG:N3	2.58	0.51
9:I:761:ARG:HE	9:I:768:PRO:HB3	1.72	0.51
10:K:373:ARG:NH1	10:K:408:ASP:HB2	2.24	0.51
1:A:201:ILE:HD12	1:A:201:ILE:N	2.26	0.51
9:I:550:GLN:HG2	9:I:584:ASN:HA	1.91	0.51
9:I:548:ILE:CG1	9:I:581:ILE:CD1	2.75	0.51
9:I:531:PHE:CD2	9:I:564:LEU:HD12	2.45	0.51
9:I:287:VAL:O	9:I:291:TYR:CG	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:39:DC:O3'	5:E:40:DA:C5'	2.55	0.51
5:E:56:DT:C3'	5:E:57:DC:P	2.98	0.51
10:J:249:ASP:OD1	11:L:179:ALA:CB	2.59	0.51
9:I:806:VAL:CG1	9:I:860:VAL:CG1	2.89	0.51
1:A:301:VAL:HG21	5:E:12:DA:H5'	1.92	0.51
6:F:101:DC:O3'	6:F:102:DT:C5'	2.52	0.51
9:I:578:THR:O	9:I:579:LEU:HB2	2.11	0.51
9:I:744:PHE:HB2	9:I:747:TYR:OH	2.10	0.51
9:I:531:PHE:CE1	9:I:638:ARG:HG2	2.46	0.51
5:E:31:DT:O3'	5:E:32:DT:C5'	2.53	0.51
9:I:651:TYR:N	9:I:651:TYR:CD1	2.79	0.51
9:I:306:THR:HB	9:I:330:LEU:HD13	1.93	0.51
9:I:337:ASP:OD2	9:I:790:SER:HA	2.11	0.51
9:I:84:PHE:HE1	9:I:86:TYR:HB2	1.76	0.51
5:E:25:DG:H3'	5:E:26:DG:P	2.49	0.51
9:I:269:CYS:HB2	9:I:277:LEU:HD21	1.92	0.51
6:F:100:DG:C3'	6:F:101:DC:P	2.99	0.51
9:I:802:LEU:HD13	9:I:856:ARG:CZ	2.41	0.51
1:A:305:PHE:CD2	6:F:152:DA:H5'	2.45	0.51
3:C:331:THR:CG2	3:C:359:ASN:OD1	2.59	0.51
9:I:630:ILE:N	9:I:648:MET:SD	2.84	0.51
1:A:204:ILE:HD13	1:A:209:THR:H	1.75	0.51
10:J:406:VAL:HB	10:J:412:LEU:HD13	1.93	0.51
10:K:318:CYS:O	10:K:320:ARG:N	2.44	0.51
5:E:32:DT:H2''	5:E:33:DC:C6	2.46	0.51
6:F:118:DG:C3'	6:F:119:DA:P	2.98	0.51
5:E:40:DA:C2	6:F:122:DG:C2	2.99	0.51
5:E:31:DT:H2''	5:E:32:DT:C6	2.46	0.50
6:F:120:DC:HO3'	6:F:121:DT:H5'	1.74	0.50
6:F:139:DC:HO3'	6:F:140:DA:H5'	1.72	0.50
9:I:604:ILE:HA	9:I:606:LEU:H	1.76	0.50
9:I:219:ASP:HA	9:I:325:PHE:CE1	2.46	0.50
9:I:682:THR:HA	9:I:685:LEU:HD12	1.91	0.50
5:E:25:DG:H2''	5:E:26:DG:C8	2.46	0.50
5:E:78:DC:C3'	5:E:79:DG:P	2.99	0.50
9:I:269:CYS:SG	9:I:270:LEU:N	2.84	0.50
9:I:802:LEU:HD12	9:I:856:ARG:NH1	2.27	0.50
9:I:646:ASP:OD1	9:I:674:THR:HB	2.12	0.50
9:I:280:THR:O	9:I:284:LEU:HG	2.11	0.50
9:I:336:ILE:O	9:I:336:ILE:HG13	2.10	0.50
5:E:26:DG:O3'	5:E:27:DC:C5'	2.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:344:ARG:HA	9:I:378:TYR:CZ	2.47	0.50
5:E:59:DA:H3'	5:E:60:DG:P	2.51	0.50
5:E:70:DC:O3'	5:E:71:DG:C5'	2.55	0.50
9:I:722:LEU:HB3	9:I:725:ARG:HE	1.76	0.50
9:I:706:ALA:CA	9:I:760:LEU:HD13	2.41	0.50
9:I:344:ARG:HG2	9:I:378:TYR:CE2	2.46	0.50
1:A:278:GLN:H	1:A:278:GLN:HE21	1.59	0.50
7:G:796:GLU:HG3	8:H:29:ARG:NH1	2.26	0.50
9:I:240:ILE:N	9:I:240:ILE:HD12	2.26	0.50
9:I:36:ASN:O	9:I:38:ILE:N	2.45	0.50
9:I:35:ILE:HG22	9:I:45:VAL:CG1	2.41	0.50
9:I:284:LEU:HA	9:I:287:VAL:CG2	2.42	0.50
6:F:136:DC:C3'	6:F:137:DC:P	2.99	0.50
9:I:240:ILE:CG2	9:I:241:PRO:HD2	2.41	0.50
4:D:83:GLU:O	4:D:84:VAL:C	2.48	0.50
9:I:692:TYR:N	9:I:692:TYR:CD1	2.80	0.50
9:I:859:ARG:HA	9:I:862:GLN:HB3	1.92	0.50
6:F:133:DC:H3'	6:F:134:DG:P	2.51	0.50
6:F:90:DC:O3'	6:F:91:DG:C5'	2.56	0.50
9:I:274:LEU:H	9:I:275:PRO:HD2	1.76	0.50
9:I:443:TRP:CZ2	9:I:966:ARG:HA	2.46	0.50
7:G:1104:LEU:O	8:H:141:LYS:HG3	2.12	0.50
5:E:39:DC:HO3'	5:E:40:DA:H5'	1.74	0.50
5:E:59:DA:HO3'	5:E:60:DG:P	2.30	0.50
6:F:113:DA:O3'	6:F:114:DT:C5'	2.58	0.50
6:F:121:DT:H2''	6:F:122:DG:C8	2.47	0.50
5:E:69:DA:H1'	7:G:875:ARG:NH2	2.27	0.50
9:I:317:ALA:HB1	9:I:322:MET:SD	2.52	0.50
10:J:219:GLU:HG3	11:L:185:ASP:OD2	2.12	0.50
1:A:204:ILE:CD1	1:A:204:ILE:N	2.74	0.50
9:I:761:ARG:HD3	9:I:768:PRO:HA	1.94	0.50
6:F:105:DA:H3'	6:F:106:DG:P	2.52	0.50
6:F:98:DC:O3'	6:F:99:DG:C5'	2.54	0.50
9:I:659:VAL:HG11	9:I:691:PHE:CD2	2.47	0.50
9:I:332:SER:OG	9:I:333:ALA:N	2.44	0.50
5:E:63:DG:C2	6:F:99:DG:C2	3.00	0.49
9:I:806:VAL:HG22	9:I:806:VAL:O	2.11	0.49
9:I:843:LEU:CB	9:I:844:PRO:HD3	2.40	0.49
6:F:90:DC:H3'	6:F:91:DG:P	2.51	0.49
9:I:325:PHE:O	9:I:327:THR:N	2.45	0.49
5:E:7:DC:H2''	5:E:8:DC:C5'	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:396:LYS:HD3	9:I:660:VAL:HG21	1.94	0.49
1:A:228:GLU:HA	1:A:228:GLU:OE1	2.12	0.49
5:E:64:DA:HO3'	5:E:65:DG:H5'	1.75	0.49
6:F:133:DC:H2''	6:F:134:DG:C8	2.47	0.49
1:A:204:ILE:CD1	1:A:209:THR:OG1	2.48	0.49
4:D:5:LEU:HD13	4:D:98:CYS:SG	2.52	0.49
6:F:88:DC:H2''	6:F:89:DA:C8	2.48	0.49
5:E:3:DG:H2''	5:E:4:DG:H8	1.70	0.49
1:A:204:ILE:C	1:A:204:ILE:HD13	2.33	0.49
4:D:53:ARG:CG	4:D:53:ARG:O	2.58	0.49
9:I:126:LEU:N	9:I:126:LEU:HD12	2.27	0.49
5:E:37:DC:H2''	5:E:38:DT:C6	2.48	0.49
9:I:838:ASN:ND2	11:L:178:LYS:NZ	2.59	0.49
9:I:161:PHE:CG	9:I:177:VAL:HG23	2.47	0.49
9:I:761:ARG:HG3	9:I:808:PRO:CG	2.43	0.49
9:I:854:CYS:HB2	9:I:874:PHE:CE1	2.47	0.49
9:I:568:VAL:HG11	9:I:626:LEU:HB3	1.94	0.49
9:I:631:ASP:HB2	9:I:638:ARG:NH2	2.26	0.49
6:F:102:DT:O3'	6:F:103:DC:C5'	2.59	0.49
9:I:35:ILE:HG23	9:I:45:VAL:HG12	1.94	0.49
5:E:18:DG:O3'	5:E:19:DG:C5'	2.56	0.49
9:I:176:HIS:HB3	9:I:178:PHE:CE2	2.47	0.49
9:I:443:TRP:CE2	9:I:966:ARG:HA	2.48	0.49
9:I:953:LEU:C	9:I:953:LEU:HD23	2.32	0.49
5:E:44:DG:N2	6:F:118:DG:C2	2.81	0.49
5:E:69:DA:H2''	5:E:70:DC:C6	2.47	0.49
9:I:274:LEU:H	9:I:275:PRO:HD3	1.74	0.49
10:J:220:GLN:NE2	11:L:186:VAL:HG22	2.27	0.49
6:F:119:DA:H2''	6:F:120:DC:C6	2.48	0.48
10:J:222:LEU:HB3	11:L:178:LYS:HZ1	0.72	0.48
9:I:919:VAL:CG1	9:I:922:VAL:HG22	2.43	0.48
4:D:56:VAL:HG12	4:D:57:ASN:N	2.28	0.48
5:E:60:DG:H2''	5:E:61:DC:C6	2.47	0.48
5:E:70:DC:C5'	7:G:875:ARG:CG	2.77	0.48
5:E:79:DG:N2	6:F:83:DG:C2	2.81	0.48
10:J:219:GLU:HG2	11:L:182:GLN:CA	2.41	0.48
9:I:751:LYS:O	9:I:755:VAL:HG23	2.13	0.48
9:I:747:TYR:CE2	9:I:794:TYR:HB2	2.48	0.48
4:D:20:ASP:HA	4:D:23:ILE:HD12	1.94	0.48
6:F:91:DG:H2''	6:F:92:DT:C6	2.48	0.48
5:E:1:DA:N6	6:F:160:DT:N3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:666:ILE:CD1	9:I:701:CYS:HB2	2.43	0.48
1:A:189:ASN:OD1	4:D:64:THR:HA	2.13	0.48
9:I:472:VAL:HG11	9:I:507:ILE:HG12	1.94	0.48
8:H:75:GLU:HG2	8:H:87:LYS:HE3	1.95	0.48
5:E:78:DC:HO3'	5:E:79:DG:H5'	1.76	0.48
6:F:116:DG:H2''	6:F:117:DC:C6	2.49	0.48
9:I:210:ALA:HB1	9:I:232:LYS:HG3	1.94	0.48
4:D:81:PHE:HB2	4:D:88:ILE:HB	1.95	0.48
1:A:292:ILE:HD12	1:A:292:ILE:N	2.28	0.48
6:F:122:DG:O3'	6:F:123:DA:C5'	2.60	0.48
9:I:393:HIS:CE1	9:I:659:VAL:HG23	2.48	0.48
10:J:406:VAL:CB	10:J:412:LEU:HD22	2.43	0.48
10:K:366:GLU:OE1	10:K:402:ARG:NH2	2.46	0.48
9:I:731:SER:OG	9:I:735:ILE:HD11	2.13	0.48
10:J:370:TRP:CD1	10:J:412:LEU:HA	2.48	0.48
9:I:426:ASN:N	9:I:427:PRO:CD	2.76	0.48
4:D:16:GLN:HG2	4:D:37:LEU:HD21	1.94	0.48
5:E:42:DT:O3'	5:E:43:DC:C5'	2.59	0.48
5:E:61:DC:HO3'	5:E:62:DC:H5'	1.75	0.48
6:F:122:DG:H3'	6:F:123:DA:P	2.54	0.48
1:A:204:ILE:HD12	1:A:204:ILE:N	2.29	0.48
9:I:742:MET:C	9:I:744:PHE:N	2.67	0.48
9:I:548:ILE:HG21	9:I:581:ILE:HG21	1.95	0.48
3:C:348:LYS:HZ2	3:C:375:GLU:CD	2.17	0.48
5:E:49:DC:HO3'	5:E:50:DG:H5'	1.73	0.48
6:F:132:DG:HO3'	6:F:133:DC:H5'	1.79	0.48
6:F:92:DT:H2''	6:F:93:DC:C6	2.49	0.48
9:I:215:VAL:HG23	9:I:250:ALA:HB3	1.96	0.48
9:I:35:ILE:HG22	9:I:45:VAL:HG13	1.96	0.48
2:B:43:LYS:HE2	2:B:47:GLU:OE2	2.14	0.48
9:I:258:VAL:CA	9:I:266:THR:HG23	2.44	0.48
1:A:159:SER:HB2	1:A:161:ILE:H	1.78	0.48
9:I:434:SER:O	9:I:435:ILE:HG13	2.14	0.48
9:I:339:THR:HB	9:I:340:PRO:CD	2.43	0.48
5:E:53:DC:O3'	5:E:54:DA:C5'	2.54	0.48
5:E:69:DA:H1'	7:G:875:ARG:CZ	2.44	0.48
9:I:178:PHE:CZ	9:I:252:GLY:CA	2.97	0.48
3:C:359:ASN:HA	3:C:363:ARG:O	2.14	0.48
9:I:455:LEU:HD22	9:I:455:LEU:O	2.14	0.48
6:F:115:DC:H2''	6:F:116:DG:C8	2.49	0.47
9:I:215:VAL:CG1	9:I:327:THR:HG21	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:799:ILE:HG23	9:I:856:ARG:HD2	1.96	0.47
5:E:30:DG:O3'	5:E:31:DT:C5'	2.57	0.47
6:F:143:DC:H2''	6:F:144:DC:C5	2.48	0.47
9:I:570:GLU:OE2	9:I:604:ILE:CD1	2.62	0.47
10:J:223:TYR:CE2	11:L:179:ALA:CA	2.97	0.47
1:A:214:PHE:CZ	5:E:15:DA:H1'	2.49	0.47
9:I:568:VAL:H	9:I:577:HIS:HB2	1.78	0.47
9:I:215:VAL:HG22	9:I:250:ALA:HB3	1.95	0.47
9:I:537:PHE:CB	9:I:625:LEU:HD22	2.38	0.47
10:K:395:ARG:CD	10:K:399:GLU:OE1	2.62	0.47
5:E:18:DG:H3'	5:E:19:DG:P	2.53	0.47
5:E:30:DG:C3'	5:E:31:DT:P	3.02	0.47
5:E:70:DC:H3'	5:E:71:DG:P	2.53	0.47
6:F:102:DT:HO3'	6:F:103:DC:H5'	1.76	0.47
6:F:137:DC:H3'	6:F:138:DC:P	2.53	0.47
9:I:604:ILE:HG22	9:I:604:ILE:O	2.13	0.47
9:I:838:ASN:HB3	11:L:178:LYS:HZ2	1.80	0.47
9:I:751:LYS:HB2	9:I:797:GLU:HB3	1.95	0.47
6:F:158:DC:H2''	6:F:159:DC:C6	2.49	0.47
9:I:761:ARG:CG	9:I:808:PRO:CG	2.93	0.47
9:I:806:VAL:CG1	9:I:860:VAL:HG22	2.45	0.47
9:I:919:VAL:HA	9:I:920:PRO:HD3	1.71	0.47
9:I:461:GLU:O	9:I:465:SER:N	2.46	0.47
5:E:61:DC:H3'	5:E:62:DC:P	2.54	0.47
5:E:67:DA:H2''	5:E:68:DG:C8	2.50	0.47
6:F:102:DT:H2''	6:F:103:DC:C6	2.49	0.47
9:I:870:ASP:HB2	9:I:871:PRO:CD	2.44	0.47
9:I:531:PHE:HB2	9:I:638:ARG:HE	1.79	0.47
9:I:919:VAL:CB	9:I:922:VAL:HG22	2.44	0.47
5:E:78:DC:O3'	5:E:79:DG:C5'	2.56	0.47
6:F:86:DG:H2''	6:F:87:DG:C8	2.49	0.47
9:I:396:LYS:HE2	9:I:399:LEU:HD22	1.96	0.47
10:J:321:PRO:HD2	10:J:326:HIS:CE1	2.49	0.47
9:I:654:ARG:NH1	9:I:683:ASP:OD2	2.47	0.47
5:E:51:DA:O3'	5:E:52:DA:C5'	2.59	0.47
5:E:65:DG:C3'	5:E:66:DC:P	3.03	0.47
5:E:75:DC:HO3'	5:E:76:DT:H5'	1.79	0.47
5:E:58:DG:N2	6:F:104:DG:C2	2.82	0.47
6:F:129:DA:HO3'	6:F:130:DA:H5'	1.76	0.47
5:E:17:DG:C4	5:E:18:DG:C5	3.02	0.47
5:E:18:DG:H2''	5:E:19:DG:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:26:DG:HO3'	5:E:27:DC:H5'	1.79	0.47
5:E:41:DG:O3'	5:E:42:DT:C5'	2.57	0.47
6:F:87:DG:C3'	6:F:88:DC:P	3.02	0.47
9:I:215:VAL:HB	9:I:324:ILE:HD12	1.97	0.47
9:I:733:PRO:HD2	11:L:192:ARG:HH12	1.64	0.47
9:I:825:ASP:O	9:I:829:ILE:HG12	2.13	0.47
9:I:221:VAL:HG22	9:I:235:HIS:O	2.15	0.47
9:I:659:VAL:HB	9:I:691:PHE:CE2	2.50	0.47
9:I:256:ILE:HG22	9:I:268:PHE:CZ	2.50	0.47
6:F:124:DG:HO3'	6:F:125:DG:H5'	1.79	0.47
6:F:88:DC:O3'	6:F:89:DA:C5'	2.60	0.47
9:I:439:HIS:HD2	9:I:439:HIS:H	1.58	0.47
9:I:473:PHE:C	9:I:473:PHE:CD1	2.88	0.47
5:E:40:DA:H3'	5:E:41:DG:P	2.55	0.47
6:F:117:DC:O3'	6:F:118:DG:C5'	2.53	0.47
10:J:223:TYR:HE1	11:L:175:LEU:HD12	1.80	0.47
5:E:3:DG:O3'	5:E:4:DG:C5'	2.59	0.47
4:D:80:GLU:HG2	4:D:89:LYS:HG2	1.97	0.47
9:I:832:GLU:CB	9:I:856:ARG:NH1	2.77	0.47
9:I:911:LEU:HD11	9:I:930:LEU:HD23	1.92	0.47
3:C:338:GLN:HA	4:D:98:CYS:O	2.15	0.47
5:E:67:DA:H3'	5:E:68:DG:P	2.54	0.47
6:F:107:DT:O3'	6:F:108:DG:C5'	2.54	0.47
6:F:113:DA:H2''	6:F:114:DT:C6	2.49	0.47
6:F:140:DA:H3'	6:F:141:DC:P	2.55	0.47
6:F:95:DG:C3'	6:F:96:DC:P	3.03	0.47
9:I:832:GLU:HB3	9:I:856:ARG:NH1	2.30	0.47
9:I:265:VAL:HA	9:I:304:PHE:O	2.15	0.47
5:E:28:DG:HO3'	5:E:29:DC:H5'	1.77	0.46
5:E:70:DC:HO3'	5:E:71:DG:H5'	1.75	0.46
6:F:107:DT:HO3'	6:F:108:DG:H5'	1.76	0.46
9:I:301:TYR:CE1	9:I:325:PHE:CE2	3.03	0.46
9:I:325:PHE:O	9:I:326:SER:C	2.54	0.46
9:I:159:LEU:HD23	9:I:179:SER:HB2	1.96	0.46
9:I:548:ILE:CG2	9:I:581:ILE:HG21	2.45	0.46
5:E:10:DA:H2''	5:E:11:DT:C5'	2.46	0.46
9:I:448:MET:O	9:I:452:LYS:HB3	2.15	0.46
9:I:785:ARG:HD2	9:I:785:ARG:N	2.30	0.46
6:F:96:DC:HO3'	6:F:97:DT:H5'	1.77	0.46
9:I:577:HIS:NE2	9:I:579:LEU:CD2	2.76	0.46
10:J:220:GLN:OE1	11:L:186:VAL:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:451:CYS:HA	9:I:454:HIS:HB3	1.96	0.46
5:E:55:DC:O3'	5:E:56:DT:C5'	2.59	0.46
3:C:333:ASN:HA	3:C:359:ASN:O	2.15	0.46
7:G:865:LYS:O	7:G:868:LYS:HG2	2.15	0.46
9:I:574:SER:HB2	9:I:604:ILE:HG12	1.98	0.46
9:I:159:LEU:CB	9:I:161:PHE:CD1	2.97	0.46
9:I:313:TYR:CZ	9:I:884:VAL:HG21	2.50	0.46
5:E:65:DG:H2''	5:E:66:DC:C6	2.51	0.46
5:E:74:DC:HO3'	5:E:75:DC:H5'	1.80	0.46
9:I:566:VAL:HG13	9:I:628:ILE:HG22	1.97	0.46
10:J:219:GLU:CA	11:L:182:GLN:HG2	2.45	0.46
10:J:251:GLY:CA	11:L:183:ARG:HG2	2.45	0.46
9:I:161:PHE:CE1	9:I:177:VAL:HG23	2.49	0.46
9:I:791:ASP:C	9:I:791:ASP:OD1	2.54	0.46
9:I:75:VAL:HG13	9:I:128:ILE:CD1	2.43	0.46
4:D:63:ASN:OD1	4:D:64:THR:HG23	2.16	0.46
10:K:320:ARG:N	10:K:321:PRO:CD	2.78	0.46
10:K:365:ASP:HB3	10:K:368:THR:HG23	1.97	0.46
9:I:731:SER:O	9:I:735:ILE:HG13	2.15	0.46
3:C:350:LYS:HG2	3:C:373:ASP:OD1	2.16	0.46
10:K:304:LEU:O	10:K:308:VAL:HG23	2.16	0.46
5:E:36:DC:C3'	5:E:37:DC:P	3.03	0.46
6:F:117:DC:HO3'	6:F:118:DG:H5'	1.76	0.46
9:I:314:VAL:CA	9:I:921:TYR:CE1	2.99	0.46
9:I:531:PHE:CZ	9:I:636:VAL:HG21	2.51	0.46
9:I:189:TRP:CH2	9:I:249:LEU:HB2	2.50	0.46
9:I:162:VAL:HG13	9:I:166:VAL:HG23	1.97	0.46
7:G:968:LEU:HB2	7:G:989:ILE:HG13	1.98	0.46
5:E:32:DT:C3'	5:E:33:DC:P	3.02	0.46
5:E:47:DA:C3'	5:E:48:DT:P	3.03	0.46
9:I:640:VAL:HG13	9:I:640:VAL:O	2.15	0.46
5:E:70:DC:C5'	7:G:875:ARG:CZ	2.60	0.46
4:D:87:LEU:CD1	4:D:89:LYS:HE3	2.34	0.46
9:I:344:ARG:HD3	9:I:348:GLN:OE1	2.16	0.46
7:G:680:GLY:O	9:I:475:LYS:HD2	2.16	0.46
10:K:395:ARG:HD3	10:K:399:GLU:OE1	2.15	0.46
7:G:1084:LYS:HD2	7:G:1084:LYS:HA	1.66	0.46
5:E:47:DA:O3'	5:E:48:DT:C5'	2.56	0.46
5:E:58:DG:C2	6:F:104:DG:C2	3.04	0.46
6:F:115:DC:H3'	6:F:116:DG:P	2.55	0.46
6:F:85:DA:C3'	6:F:86:DG:P	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:838:ASN:HD22	11:L:178:LYS:HE3	1.57	0.46
9:I:258:VAL:HB	9:I:266:THR:HG23	1.97	0.46
9:I:469:MET:O	9:I:472:VAL:HB	2.15	0.46
5:E:67:DA:HO3'	5:E:68:DG:P	2.34	0.45
6:F:127:DC:O3'	6:F:128:DG:C5'	2.55	0.45
6:F:94:DT:O3'	6:F:95:DG:C5'	2.60	0.45
9:I:969:CYS:HA	9:I:972:VAL:CG2	2.46	0.45
9:I:344:ARG:CG	9:I:378:TYR:CE2	2.99	0.45
9:I:35:ILE:CG2	9:I:45:VAL:HG13	2.45	0.45
5:E:79:DG:C3'	5:E:80:DG:P	3.04	0.45
5:E:3:DG:C3'	5:E:4:DG:P	3.04	0.45
9:I:328:ASN:O	9:I:330:LEU:HD12	2.16	0.45
8:H:53:HIS:CG	8:H:105:PRO:HG2	2.51	0.45
5:E:44:DG:H2''	5:E:45:DC:C6	2.51	0.45
6:F:110:DT:HO3'	6:F:111:DC:H5'	1.81	0.45
9:I:314:VAL:HA	9:I:921:TYR:CD2	2.51	0.45
9:I:45:VAL:O	9:I:152:LEU:HD13	2.16	0.45
3:C:331:THR:HG21	3:C:359:ASN:OD1	2.16	0.45
1:A:267:PRO:HA	1:A:306:VAL:O	2.16	0.45
11:L:193:PHE:O	11:L:197:THR:HG23	2.16	0.45
6:F:122:DG:H2''	6:F:123:DA:C8	2.52	0.45
6:F:125:DG:C3'	6:F:126:DA:P	3.04	0.45
9:I:591:PRO:O	9:I:593:HIS:N	2.48	0.45
5:E:6:DG:H2'	5:E:7:DC:H6	1.81	0.45
4:D:79:VAL:HG12	4:D:80:GLU:N	2.31	0.45
9:I:295:LEU:HD13	9:I:354:PHE:CE1	2.52	0.45
9:I:472:VAL:HG11	9:I:507:ILE:CG1	2.47	0.45
5:E:27:DC:C3'	5:E:28:DG:P	3.04	0.45
5:E:52:DA:H2''	5:E:53:DC:C6	2.52	0.45
6:F:88:DC:H3'	6:F:89:DA:P	2.56	0.45
9:I:651:TYR:N	9:I:651:TYR:HD1	2.14	0.45
9:I:325:PHE:C	9:I:325:PHE:CD1	2.89	0.45
9:I:666:ILE:HA	9:I:669:LEU:HB2	1.97	0.45
9:I:731:SER:C	9:I:735:ILE:HG13	2.36	0.45
1:A:214:PHE:CD2	5:E:15:DA:H2''	2.51	0.45
9:I:634:MET:HG2	9:I:664:GLU:HG3	1.95	0.45
9:I:188:PHE:CZ	9:I:962:SER:HA	2.52	0.45
9:I:519:ILE:HA	9:I:522:TRP:CD1	2.52	0.45
10:J:241:GLU:CD	11:L:175:LEU:HD23	2.37	0.45
10:J:250:PRO:HD2	11:L:183:ARG:HD2	1.96	0.45
5:E:2:DG:H2''	5:E:3:DG:N7	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:707:ASN:CG	9:I:712:THR:HG22	2.37	0.45
10:J:381:ALA:HA	10:J:388:ILE:CD1	2.45	0.45
5:E:29:DC:C3'	5:E:30:DG:P	3.04	0.45
6:F:135:DC:HO3'	6:F:136:DC:H5'	1.78	0.45
9:I:577:HIS:CD2	9:I:578:THR:N	2.85	0.45
9:I:570:GLU:OE2	9:I:604:ILE:HD11	2.16	0.45
9:I:460:ILE:O	9:I:464:ILE:HG12	2.16	0.45
9:I:692:TYR:N	9:I:692:TYR:HD1	2.15	0.45
10:J:317:LEU:CD1	10:J:329:LEU:HD23	2.46	0.45
9:I:623:SER:N	9:I:624:PRO:HD2	2.31	0.45
6:F:104:DG:H2''	6:F:105:DA:C8	2.51	0.45
6:F:127:DC:C3'	6:F:128:DG:P	3.05	0.45
6:F:86:DG:HO3'	6:F:87:DG:P	2.37	0.45
9:I:784:ASN:HB3	11:L:192:ARG:NH1	2.23	0.45
9:I:306:THR:HA	9:I:328:ASN:O	2.16	0.45
9:I:260:PRO:O	9:I:261:TYR:HB2	2.17	0.45
10:J:335:ARG:HH12	10:J:382:GLU:CD	2.19	0.45
5:E:37:DC:H3'	5:E:38:DT:P	2.56	0.45
6:F:82:DC:O3'	6:F:83:DG:C5'	2.55	0.45
9:I:305:LYS:HB2	9:I:327:THR:HG22	1.99	0.45
10:J:249:ASP:HB3	11:L:183:ARG:HE	1.49	0.45
9:I:241:PRO:HG3	9:I:496:MET:HE3	1.92	0.45
9:I:725:ARG:H	9:I:744:PHE:HZ	1.64	0.45
9:I:344:ARG:CB	9:I:378:TYR:OH	2.55	0.45
9:I:917:ASP:N	9:I:918:PRO:HA	2.24	0.45
10:K:308:VAL:HG12	10:K:337:VAL:HG23	1.98	0.45
9:I:418:PHE:H	9:I:523:VAL:CG1	2.30	0.45
10:K:274:ASN:OD1	10:K:326:HIS:NE2	2.48	0.45
5:E:39:DC:H3'	5:E:40:DA:P	2.56	0.45
5:E:66:DC:H2''	5:E:67:DA:C8	2.52	0.45
6:F:124:DG:O3'	6:F:125:DG:C5'	2.57	0.45
9:I:32:VAL:CG1	9:I:203:LYS:HD3	2.47	0.45
10:K:286:VAL:HG13	10:K:304:LEU:HD13	1.99	0.45
2:B:17:VAL:O	2:B:21:VAL:HG23	2.15	0.45
5:E:40:DA:HO3'	5:E:41:DG:H5'	1.75	0.44
5:E:66:DC:O3'	5:E:67:DA:C5'	2.62	0.44
9:I:568:VAL:CA	9:I:575:PHE:HD2	2.30	0.44
9:I:314:VAL:HA	9:I:921:TYR:CE2	2.52	0.44
10:J:241:GLU:HB2	11:L:172:TYR:CE1	2.52	0.44
9:I:806:VAL:HG13	9:I:860:VAL:CG1	2.46	0.44
9:I:666:ILE:CD1	9:I:669:LEU:HD12	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:154:GLN:HB3	9:I:155:PRO:CD	2.47	0.44
2:B:11:PRO:O	2:B:15:ARG:HG2	2.17	0.44
5:E:18:DG:HO3'	5:E:19:DG:P	2.30	0.44
5:E:24:DG:N2	6:F:138:DC:O2	2.50	0.44
9:I:309:ILE:HG12	9:I:311:GLU:N	2.26	0.44
9:I:751:LYS:HD2	9:I:752:THR:HG23	1.98	0.44
1:A:204:ILE:CD1	1:A:209:THR:H	2.30	0.44
9:I:338:GLU:CD	9:I:342:THR:OG1	2.54	0.44
9:I:470:LEU:C	9:I:470:LEU:HD23	2.37	0.44
9:I:878:ALA:O	9:I:887:ARG:NH1	2.50	0.44
6:F:109:DT:C3'	6:F:110:DT:P	3.05	0.44
5:E:18:DG:N2	6:F:144:DC:C2	2.86	0.44
6:F:83:DG:HO3'	6:F:84:DT:H5'	1.80	0.44
6:F:158:DC:O3'	6:F:159:DC:H5'	2.18	0.44
10:J:412:LEU:HG	10:J:413:SER:H	1.81	0.44
9:I:309:ILE:CG2	9:I:329:LEU:HD11	2.47	0.44
10:J:250:PRO:HG2	11:L:183:ARG:HD2	1.96	0.44
4:D:79:VAL:HG21	4:D:93:VAL:CG1	2.48	0.44
3:C:331:THR:OG1	3:C:362:GLY:CA	2.63	0.44
5:E:18:DG:HO3'	5:E:19:DG:H5'	1.80	0.44
6:F:104:DG:O3'	6:F:105:DA:C5'	2.61	0.44
9:I:301:TYR:CE2	9:I:325:PHE:CE2	3.06	0.44
9:I:442:SER:CB	9:I:965:TRP:HB2	2.48	0.44
9:I:725:ARG:HB2	9:I:744:PHE:CE2	2.52	0.44
9:I:747:TYR:CD1	9:I:794:TYR:HD1	2.35	0.44
9:I:850:ILE:HA	9:I:853:SER:HB2	2.00	0.44
9:I:833:ILE:HG23	9:I:853:SER:O	2.17	0.44
9:I:806:VAL:HG11	9:I:860:VAL:CG1	2.45	0.44
9:I:917:ASP:N	9:I:918:PRO:CA	2.80	0.44
9:I:919:VAL:HB	9:I:922:VAL:HG21	1.99	0.44
7:G:722:LYS:HA	7:G:722:LYS:HD3	1.86	0.44
5:E:68:DG:H2''	5:E:69:DA:C8	2.52	0.44
6:F:99:DG:O3'	6:F:100:DG:C5'	2.60	0.44
9:I:722:LEU:HG	9:I:725:ARG:HD3	1.99	0.44
9:I:854:CYS:HB2	9:I:874:PHE:HZ	1.78	0.44
9:I:287:VAL:O	9:I:291:TYR:CD2	2.71	0.44
10:K:360:THR:OG1	10:K:391:LEU:HD13	2.17	0.44
6:F:98:DC:H3'	6:F:99:DG:P	2.58	0.44
9:I:751:LYS:CB	9:I:797:GLU:HB3	2.48	0.44
9:I:707:ASN:HD21	9:I:760:LEU:CD2	2.31	0.44
9:I:344:ARG:HD2	9:I:344:ARG:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:344:ARG:HD2	9:I:345:CYS:HA	2.00	0.44
3:C:334:VAL:HG12	3:C:335:VAL:N	2.33	0.44
10:K:355:ILE:CG2	10:K:359:PHE:CE2	3.01	0.44
1:A:214:PHE:CG	5:E:15:DA:H2''	2.53	0.44
10:K:247:ALA:HA	10:K:292:ASN:HB2	1.99	0.44
5:E:66:DC:HO3'	5:E:67:DA:H5'	1.82	0.44
6:F:123:DA:H3'	6:F:124:DG:P	2.57	0.44
9:I:666:ILE:HD12	9:I:669:LEU:CB	2.42	0.44
9:I:32:VAL:HG13	9:I:203:LYS:HD3	1.99	0.44
9:I:156:LYS:HD3	9:I:188:PHE:HB3	2.00	0.44
9:I:234:PHE:HB3	9:I:236:TYR:CZ	2.52	0.44
10:J:405:SER:O	10:J:409:GLY:HA3	2.17	0.44
7:G:711:LEU:HD22	7:G:768:LEU:HD22	1.99	0.44
5:E:33:DC:H2''	5:E:34:DG:C8	2.53	0.44
5:E:37:DC:O3'	5:E:38:DT:C5'	2.58	0.44
5:E:49:DC:O3'	5:E:50:DG:C5'	2.56	0.44
5:E:63:DG:N2	6:F:99:DG:C2	2.86	0.44
9:I:240:ILE:H	9:I:240:ILE:HD12	1.82	0.44
9:I:707:ASN:HD21	9:I:760:LEU:HD21	1.81	0.44
9:I:528:VAL:HG21	9:I:531:PHE:CE1	2.52	0.44
9:I:669:LEU:HD23	9:I:674:THR:HG21	2.00	0.44
10:K:405:SER:O	10:K:409:GLY:HA3	2.18	0.44
6:F:104:DG:H3'	6:F:105:DA:P	2.56	0.43
6:F:106:DG:O3'	6:F:107:DT:C5'	2.63	0.43
6:F:130:DA:HO3'	6:F:131:DC:H5'	1.78	0.43
10:J:223:TYR:CE2	11:L:179:ALA:HA	2.53	0.43
10:J:223:TYR:CB	11:L:182:GLN:NE2	2.67	0.43
9:I:273:LEU:O	9:I:277:LEU:CD1	2.66	0.43
9:I:31:GLN:OE1	9:I:49:VAL:HG21	2.18	0.43
6:F:150:DA:H2''	6:F:151:DT:H5'	2.00	0.43
9:I:130:VAL:HA	9:I:131:PRO:HD3	1.65	0.43
5:E:62:DC:H2''	5:E:63:DG:C8	2.52	0.43
6:F:116:DG:C3'	6:F:117:DC:P	3.05	0.43
9:I:570:GLU:N	9:I:575:PHE:HB2	2.33	0.43
9:I:731:SER:CB	9:I:735:ILE:HG12	2.38	0.43
9:I:190:PHE:N	9:I:190:PHE:CD1	2.86	0.43
9:I:814:ASN:O	9:I:815:GLU:CB	2.63	0.43
9:I:295:LEU:HD13	9:I:354:PHE:CZ	2.53	0.43
9:I:953:LEU:HD11	9:I:975:TYR:HA	2.00	0.43
9:I:487:LYS:O	9:I:488:PHE:HB2	2.18	0.43
6:F:84:DT:HO3'	6:F:85:DA:H5'	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:LEU:HD22	3:C:366:ILE:CD1	2.48	0.43
3:C:366:ILE:HG22	3:C:367:PHE:N	2.33	0.43
9:I:182:TYR:O	9:I:182:TYR:CG	2.71	0.43
10:K:239:ARG:NH2	10:K:285:MET:HB2	2.32	0.43
9:I:874:PHE:CD1	9:I:890:ALA:HA	2.53	0.43
5:E:37:DC:HO3'	5:E:38:DT:H5'	1.83	0.43
5:E:57:DC:H3'	5:E:58:DG:P	2.58	0.43
5:E:69:DA:O3'	7:G:875:ARG:HD3	2.17	0.43
9:I:307:VAL:HG13	9:I:329:LEU:CD1	2.48	0.43
9:I:753:MET:HB3	9:I:754:PRO:CD	2.43	0.43
9:I:328:ASN:O	9:I:330:LEU:CD1	2.67	0.43
9:I:612:VAL:HG22	9:I:612:VAL:O	2.18	0.43
6:F:103:DC:H2''	6:F:104:DG:C8	2.53	0.43
6:F:132:DG:C3'	6:F:133:DC:P	3.06	0.43
9:I:176:HIS:HB3	9:I:178:PHE:HE2	1.84	0.43
9:I:43:LYS:CD	9:I:163:VAL:CG1	2.94	0.43
5:E:49:DC:C3'	5:E:50:DG:P	3.06	0.43
9:I:566:VAL:HG11	9:I:628:ILE:HG23	1.83	0.43
9:I:727:PHE:CE2	9:I:781:TYR:CG	3.07	0.43
9:I:806:VAL:HG13	9:I:860:VAL:HG22	2.00	0.43
9:I:35:ILE:CD1	9:I:189:TRP:CZ2	3.01	0.43
9:I:464:ILE:HB	9:I:511:SER:CB	2.47	0.43
1:A:188:ARG:NH1	4:D:64:THR:HG21	2.34	0.43
5:E:72:DT:O3'	5:E:73:DG:C5'	2.60	0.43
5:E:4:DG:H2''	5:E:5:DC:H6	1.74	0.43
9:I:38:ILE:HG13	9:I:207:THR:O	2.17	0.43
5:E:66:DC:H3'	5:E:67:DA:P	2.59	0.43
5:E:58:DG:C2	6:F:104:DG:N2	2.87	0.43
6:F:104:DG:HO3'	6:F:105:DA:P	2.32	0.43
1:A:302:LEU:HB2	1:A:304:ILE:HD11	2.01	0.43
9:I:854:CYS:O	9:I:858:ILE:HG22	2.19	0.43
7:G:820:ALA:O	7:G:824:ILE:HG13	2.18	0.43
9:I:397:GLU:HG2	9:I:401:LYS:HE3	2.01	0.43
5:E:32:DT:HO3'	5:E:33:DC:H5'	1.82	0.43
5:E:50:DG:N2	6:F:112:DG:N2	2.60	0.43
9:I:161:PHE:CD1	9:I:177:VAL:CG2	3.00	0.43
5:E:7:DC:C1'	5:E:7:DC:O2	2.67	0.43
9:I:919:VAL:HG12	9:I:922:VAL:HG22	2.01	0.43
2:B:19:GLU:OE1	2:B:19:GLU:HA	2.19	0.43
3:C:351:PHE:CD1	3:C:351:PHE:N	2.87	0.43
5:E:36:DC:H2''	5:E:37:DC:C6	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:60:DG:O3'	5:E:61:DC:C5'	2.65	0.42
6:F:98:DC:HO3'	6:F:99:DG:H5'	1.77	0.42
9:I:406:GLU:HA	9:I:414:LEU:HD22	2.00	0.42
9:I:910:LEU:CD2	9:I:930:LEU:HD13	2.50	0.42
9:I:207:THR:HG22	9:I:231:LYS:HB3	2.01	0.42
9:I:297:CYS:SG	9:I:358:PHE:CE2	3.12	0.42
1:A:187:ALA:HB2	1:A:244:LEU:HD11	2.01	0.42
5:E:34:DG:C3'	5:E:35:DT:P	3.07	0.42
5:E:41:DG:H2''	5:E:42:DT:C6	2.54	0.42
6:F:119:DA:O3'	6:F:120:DC:C5'	2.63	0.42
9:I:666:ILE:HD12	9:I:669:LEU:HD12	2.00	0.42
4:D:19:LEU:O	4:D:23:ILE:HG13	2.19	0.42
5:E:58:DG:O3'	5:E:59:DA:C5'	2.65	0.42
6:F:97:DT:H2''	6:F:98:DC:C6	2.53	0.42
9:I:215:VAL:HG21	9:I:324:ILE:CD1	2.50	0.42
9:I:159:LEU:HD23	9:I:179:SER:HB3	1.98	0.42
9:I:241:PRO:HG3	9:I:496:MET:HE1	1.98	0.42
6:F:156:DG:O5'	6:F:156:DG:OP1	2.34	0.42
9:I:725:ARG:HD2	9:I:745:GLN:OE1	2.19	0.42
9:I:287:VAL:HG23	9:I:288:PHE:N	2.34	0.42
10:J:287:LYS:HZ2	10:J:291:ASP:CG	2.21	0.42
5:E:42:DT:H2''	5:E:43:DC:C6	2.54	0.42
6:F:111:DC:C3'	6:F:112:DG:P	3.07	0.42
6:F:141:DC:H2''	6:F:142:DC:C6	2.54	0.42
6:F:85:DA:HO3'	6:F:86:DG:H5'	1.79	0.42
5:E:63:DG:C2	6:F:99:DG:N2	2.87	0.42
6:F:159:DC:C2'	6:F:160:DT:C5	2.80	0.42
5:E:24:DG:H3'	5:E:25:DG:P	2.59	0.42
5:E:23:DG:C3'	5:E:24:DG:P	3.07	0.42
5:E:41:DG:HO3'	5:E:42:DT:P	2.34	0.42
6:F:94:DT:C5'	7:G:873:PHE:CZ	2.97	0.42
9:I:570:GLU:CD	9:I:604:ILE:HD11	2.40	0.42
9:I:324:ILE:CD1	9:I:327:THR:OG1	2.67	0.42
4:D:5:LEU:HD23	4:D:6:TYR:CZ	2.54	0.42
10:K:355:ILE:HG23	10:K:359:PHE:CE2	2.55	0.42
9:I:810:VAL:HG23	9:I:810:VAL:O	2.19	0.42
6:F:140:DA:O3'	6:F:141:DC:C5'	2.62	0.42
6:F:81:DC:HO3'	6:F:82:DC:H5'	1.81	0.42
9:I:753:MET:CB	9:I:754:PRO:HD3	2.42	0.42
9:I:747:TYR:CE1	9:I:794:TYR:CG	3.07	0.42
9:I:342:THR:HA	9:I:345:CYS:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:799:ILE:HG23	9:I:856:ARG:HB2	1.98	0.42
9:I:804:ASN:HA	9:I:808:PRO:HD3	2.01	0.42
9:I:461:GLU:OE2	9:I:469:MET:HG2	2.19	0.42
5:E:34:DG:H2"	5:E:35:DT:C6	2.54	0.42
5:E:54:DA:H2"	5:E:55:DC:C6	2.55	0.42
6:F:102:DT:H3'	6:F:103:DC:P	2.59	0.42
6:F:111:DC:O3'	6:F:112:DG:C5'	2.55	0.42
9:I:784:ASN:CG	11:L:192:ARG:NH1	2.72	0.42
3:C:331:THR:CG2	3:C:332:GLU:N	2.83	0.42
9:I:389:ASN:HB3	9:I:394:TRP:CH2	2.55	0.42
6:F:101:DC:H3'	6:F:102:DT:P	2.59	0.42
6:F:124:DG:HO3'	6:F:125:DG:P	2.37	0.42
9:I:870:ASP:CB	9:I:871:PRO:CD	2.98	0.42
5:E:1:DA:C6	6:F:160:DT:N3	2.63	0.42
10:K:243:LEU:HD13	10:K:284:ARG:HB3	2.02	0.42
5:E:32:DT:O3'	5:E:33:DC:C5'	2.63	0.42
5:E:71:DG:H2"	5:E:72:DT:C6	2.55	0.42
6:F:132:DG:H2"	6:F:133:DC:C6	2.54	0.42
9:I:442:SER:HB2	9:I:965:TRP:HB2	2.00	0.42
9:I:295:LEU:HG	9:I:381:TRP:HZ2	1.85	0.42
9:I:130:VAL:HG13	9:I:131:PRO:HD2	2.02	0.42
5:E:45:DC:H3'	5:E:46:DG:P	2.60	0.42
10:J:250:PRO:C	11:L:183:ARG:HG2	2.37	0.42
5:E:60:DG:HO3'	5:E:61:DC:P	2.33	0.41
6:F:114:DT:O3'	6:F:115:DC:C5'	2.63	0.41
6:F:125:DG:HO3'	6:F:126:DA:H5'	1.82	0.41
5:E:3:DG:H3'	5:E:4:DG:P	2.60	0.41
9:I:741:PHE:CZ	9:I:791:ASP:HB2	2.55	0.41
9:I:795:ARG:O	9:I:798:MET:HG2	2.20	0.41
9:I:37:ASN:O	9:I:38:ILE:CB	2.62	0.41
7:G:1086:GLU:OE2	7:G:1089:ARG:NH2	2.46	0.41
6:F:108:DG:HO3'	6:F:109:DT:H5'	1.83	0.41
6:F:85:DA:H2"	6:F:86:DG:C8	2.55	0.41
6:F:89:DA:HO3'	6:F:90:DC:P	2.39	0.41
9:I:161:PHE:CG	9:I:177:VAL:CG2	3.03	0.41
9:I:439:HIS:N	9:I:965:TRP:CE3	2.88	0.41
9:I:670:GLU:CD	9:I:700:PHE:CD2	2.92	0.41
9:I:917:ASP:H	9:I:918:PRO:CA	2.26	0.41
9:I:55:PRO:HG2	9:I:138:VAL:HG21	2.02	0.41
9:I:649:TRP:O	9:I:653:LEU:HD23	2.21	0.41
9:I:306:THR:HG22	9:I:328:ASN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:114:DT:HO3'	6:F:115:DC:H5'	1.84	0.41
9:I:273:LEU:O	9:I:277:LEU:HD13	2.21	0.41
9:I:344:ARG:HD2	9:I:345:CYS:N	2.35	0.41
9:I:652:GLN:HA	9:I:656:GLU:CG	2.47	0.41
5:E:52:DA:O3'	5:E:53:DC:C5'	2.65	0.41
6:F:135:DC:O3'	6:F:136:DC:C5'	2.60	0.41
9:I:751:LYS:CD	9:I:752:THR:HG23	2.51	0.41
9:I:695:ARG:HH21	9:I:746:SER:HB3	1.85	0.41
9:I:284:LEU:HD11	9:I:306:THR:HG21	2.02	0.41
6:F:82:DC:HO3'	6:F:83:DG:H5'	1.75	0.41
6:F:85:DA:O3'	6:F:86:DG:C5'	2.60	0.41
9:I:301:TYR:CG	9:I:325:PHE:CZ	3.09	0.41
9:I:274:LEU:HA	9:I:277:LEU:HD13	2.02	0.41
9:I:412:VAL:HA	9:I:413:LEU:HA	1.95	0.41
9:I:788:LYS:O	9:I:791:ASP:CG	2.59	0.41
10:K:213:ILE:CG1	10:K:224:TYR:CE1	3.04	0.41
3:C:344:ARG:NH2	6:F:148:DT:OP2	2.51	0.41
6:F:90:DC:H2''	6:F:91:DG:C8	2.56	0.41
9:I:570:GLU:OE1	9:I:594:SER:O	2.38	0.41
9:I:324:ILE:CG1	9:I:327:THR:OG1	2.66	0.41
5:E:7:DC:H1'	5:E:7:DC:O2	2.21	0.41
9:I:581:ILE:HG22	9:I:581:ILE:O	2.19	0.41
9:I:338:GLU:HB2	9:I:342:THR:OG1	2.18	0.41
9:I:282:SER:O	9:I:285:HIS:HB3	2.21	0.41
9:I:219:ASP:HA	9:I:325:PHE:CZ	2.56	0.41
9:I:159:LEU:HB3	9:I:161:PHE:CD1	2.50	0.41
9:I:833:ILE:O	9:I:853:SER:HB3	2.21	0.41
3:C:331:THR:HG23	3:C:359:ASN:OD1	2.20	0.41
6:F:147:DT:H2''	6:F:148:DT:H5'	2.03	0.41
5:E:38:DT:O3'	5:E:39:DC:C5'	2.66	0.41
5:E:53:DC:H3'	5:E:54:DA:P	2.61	0.41
1:A:196:ARG:NE	6:F:146:DT:OP1	2.54	0.41
5:E:20:DG:C3'	5:E:21:DT:P	3.09	0.41
6:F:135:DC:C3'	6:F:136:DC:P	3.09	0.41
6:F:93:DC:H2''	6:F:94:DT:C6	2.56	0.41
6:F:93:DC:O3'	6:F:94:DT:C5'	2.60	0.41
6:F:93:DC:H3'	6:F:94:DT:P	2.60	0.41
9:I:314:VAL:HG22	9:I:318:ALA:C	2.41	0.41
10:J:226:GLU:OE1	11:L:175:LEU:CD1	2.68	0.41
9:I:159:LEU:HB2	9:I:161:PHE:CD1	2.56	0.41
9:I:581:ILE:HA	9:I:586:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:537:PHE:CG	9:I:625:LEU:HD22	2.54	0.41
9:I:333:ALA:HA	9:I:336:ILE:HG21	2.02	0.41
10:K:213:ILE:HG13	10:K:224:TYR:CE1	2.56	0.41
7:G:647:GLY:HA3	7:G:789:ARG:HG2	2.03	0.41
4:D:67:PHE:CZ	4:D:70:ASN:HA	2.56	0.41
9:I:541:ARG:HB3	9:I:543:VAL:HG23	2.02	0.41
9:I:137:HIS:CG	9:I:137:HIS:O	2.73	0.41
5:E:30:DG:H2"	5:E:31:DT:C6	2.55	0.41
4:D:80:GLU:CD	4:D:89:LYS:HE2	2.41	0.41
9:I:378:TYR:O	9:I:378:TYR:CD1	2.74	0.41
9:I:830:LEU:HD23	9:I:833:ILE:HD12	2.02	0.41
7:G:679:GLY:C	9:I:475:LYS:HG3	2.40	0.41
9:I:761:ARG:HG3	9:I:808:PRO:CB	2.51	0.41
9:I:806:VAL:CG1	9:I:860:VAL:HG21	2.50	0.41
9:I:649:TRP:CE2	9:I:668:ALA:HB1	2.56	0.41
9:I:297:CYS:HB3	9:I:354:PHE:HE2	1.86	0.41
7:G:660:LEU:HD22	7:G:793:TYR:HB3	2.02	0.41
7:G:808:PRO:HD2	7:G:959:PHE:CD2	2.56	0.41
7:G:718:ALA:HA	8:H:85:PHE:O	2.21	0.41
5:E:64:DA:O3'	5:E:65:DG:C5'	2.59	0.40
5:E:67:DA:C2	6:F:95:DG:C2	3.09	0.40
9:I:577:HIS:CG	9:I:578:THR:N	2.89	0.40
9:I:257:LEU:HB3	9:I:267:HIS:HB3	2.02	0.40
9:I:31:GLN:CD	9:I:51:LEU:HG	2.42	0.40
5:E:51:DA:H2"	5:E:52:DA:C8	2.57	0.40
5:E:71:DG:P	7:G:877:GLY:CA	3.09	0.40
6:F:106:DG:HO3'	6:F:107:DT:H5'	1.80	0.40
6:F:110:DT:C3'	6:F:111:DC:P	3.08	0.40
6:F:143:DC:C2'	6:F:144:DC:C6	2.96	0.40
9:I:574:SER:HB3	9:I:604:ILE:HG13	2.03	0.40
1:A:209:THR:O	1:A:237:TYR:OH	2.39	0.40
1:A:159:SER:C	1:A:161:ILE:N	2.70	0.40
10:K:318:CYS:C	10:K:320:ARG:N	2.75	0.40
9:I:259:ASP:OD1	9:I:259:ASP:C	2.60	0.40
5:E:73:DG:C3'	5:E:74:DC:P	3.10	0.40
9:I:570:GLU:CD	9:I:594:SER:O	2.59	0.40
5:E:7:DC:C2'	5:E:8:DC:O5'	2.69	0.40
1:A:204:ILE:HD12	1:A:209:THR:O	2.21	0.40
9:I:531:PHE:CD1	9:I:638:ARG:HB2	2.45	0.40
9:I:207:THR:CG2	9:I:231:LYS:HB3	2.52	0.40
10:J:412:LEU:CG	10:J:413:SER:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:93:DC:HO3'	6:F:94:DT:H5'	1.85	0.40
9:I:722:LEU:HG	9:I:725:ARG:CD	2.51	0.40
9:I:779:ILE:HG12	9:I:802:LEU:HD22	2.03	0.40
9:I:355:PHE:CE2	9:I:476:LEU:HD23	2.57	0.40
1:A:301:VAL:HG11	5:E:11:DT:H4'	2.03	0.40
1:A:190:ALA:O	4:D:66:ARG:HA	2.21	0.40
9:I:28:LEU:HD23	9:I:53:ILE:HB	2.04	0.40
5:E:42:DT:HO3'	5:E:43:DC:H5'	1.80	0.40
5:E:53:DC:H2''	5:E:54:DA:C8	2.57	0.40
6:F:90:DC:HO3'	6:F:91:DG:P	2.39	0.40
9:I:437:HIS:O	9:I:439:HIS:N	2.55	0.40
9:I:393:HIS:ND1	9:I:659:VAL:HB	2.36	0.40
9:I:258:VAL:HB	9:I:266:THR:CG2	2.51	0.40
3:C:369:LYS:HE2	3:C:369:LYS:HB3	1.71	0.40
4:D:44:ILE:HG23	4:D:45:ASN:N	2.36	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	178/339 (52%)	175 (98%)	3 (2%)	0	100	100
2	B	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
3	C	45/47 (96%)	43 (96%)	2 (4%)	0	100	100
4	D	95/97 (98%)	87 (92%)	7 (7%)	1 (1%)	17	63
7	G	398/1893 (21%)	391 (98%)	7 (2%)	0	100	100
8	H	119/349 (34%)	117 (98%)	2 (2%)	0	100	100
9	I	910/1199 (76%)	753 (83%)	122 (13%)	35 (4%)	4	37
10	J	218/677 (32%)	185 (85%)	17 (8%)	16 (7%)	1	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	K	196/677 (29%)	163 (83%)	20 (10%)	13 (7%)	1	24
11	L	25/310 (8%)	25 (100%)	0	0	100	100
All	All	2225/5631 (40%)	1979 (89%)	181 (8%)	65 (3%)	9	43

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	84	VAL
9	I	222	GLU
9	I	413	LEU
9	I	438	PRO
9	I	577	HIS
9	I	578	THR
9	I	581	ILE
9	I	716	PRO
9	I	743	SER
9	I	746	SER
10	J	256	LEU
10	J	257	PRO
10	J	319	LEU
10	J	367	LYS
10	J	406	VAL
10	J	411	VAL
10	J	412	LEU
10	J	413	SER
10	K	256	LEU
10	K	257	PRO
10	K	260	SER
10	K	319	LEU
10	K	367	LYS
10	K	406	VAL
9	I	227	HIS
9	I	228	ASP
9	I	319	TYR
9	I	332	SER
9	I	339	THR
9	I	496	MET
9	I	570	GLU
9	I	609	GLY
9	I	707	ASN
9	I	817	ARG

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Mol	Chain	Res	Type
9	I	867	VAL
10	J	260	SER
10	J	408	ASP
10	J	410	PRO
10	K	317	LEU
9	I	37	ASN
9	I	260	PRO
9	I	340	PRO
9	I	883	PHE
9	I	963	HIS
10	J	235	CYS
10	J	349	ASN
10	J	414	ASN
10	K	217	SER
10	K	349	ASN
10	K	408	ASP
9	I	465	SER
9	I	601	LYS
9	I	633	ASP
10	K	235	CYS
10	K	405	SER
9	I	314	VAL
9	I	450	GLN
9	I	964	ASP
10	J	405	SER
10	K	321	PRO
9	I	813	ASN
10	J	321	PRO
9	I	38	ILE
9	I	336	ILE
9	I	715	GLY

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	155/293 (53%)	152 (98%)	3 (2%)	65 86
2	B	42/42 (100%)	41 (98%)	1 (2%)	57 82
3	C	42/42 (100%)	41 (98%)	1 (2%)	57 82
4	D	89/89 (100%)	87 (98%)	2 (2%)	60 83
7	G	355/1680 (21%)	331 (93%)	24 (7%)	20 57
8	H	113/322 (35%)	104 (92%)	9 (8%)	15 50
9	I	832/1083 (77%)	830 (100%)	2 (0%)	95 97
10	J	194/574 (34%)	177 (91%)	17 (9%)	12 45
10	K	176/574 (31%)	162 (92%)	14 (8%)	15 50
11	L	22/270 (8%)	22 (100%)	0	100 100
All	All	2020/4969 (41%)	1947 (96%)	73 (4%)	46 74

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	A	204	ILE
1	A	278	GLN
2	B	13	LEU
3	C	364	ASP
4	D	24	GLN
4	D	76	LEU
7	G	617	VAL
7	G	619	LEU
7	G	660	LEU
7	G	666	LYS
7	G	669	LYS
7	G	670	MET
7	G	675	ARG
7	G	699	LEU
7	G	701	LEU
7	G	748	THR
7	G	752	LEU
7	G	797	LEU
7	G	852	LYS
7	G	866	ARG
7	G	868	LYS

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Mol	Chain	Res	Type
7	G	869	LEU
7	G	878	MET
7	G	943	LYS
7	G	944	ILE
7	G	963	MET
7	G	1084	LYS
7	G	1093	LEU
7	G	1104	LEU
7	G	1108	THR
8	H	23	GLU
8	H	73	VAL
8	H	99	VAL
8	H	100	ASP
8	H	129	LYS
8	H	138	LEU
8	H	141	LYS
8	H	143	VAL
8	H	154	LYS
9	I	84	PHE
9	I	638	ARG
10	J	219	GLU
10	J	241	GLU
10	J	274	ASN
10	J	283	MET
10	J	294	THR
10	J	301	VAL
10	J	319	LEU
10	J	322	ASP
10	J	326	HIS
10	J	353	SER
10	J	370	TRP
10	J	377	ILE
10	J	399	GLU
10	J	406	VAL
10	J	412	LEU
10	J	415	ILE
10	J	425	SER
10	K	219	GLU
10	K	241	GLU
10	K	274	ASN
10	K	283	MET
10	K	294	THR

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Mol	Chain	Res	Type
10	K	301	VAL
10	K	319	LEU
10	K	322	ASP
10	K	326	HIS
10	K	353	SER
10	K	370	TRP
10	K	377	ILE
10	K	399	GLU
10	K	406	VAL

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

Mol	Chain	Res	Type
1	A	193	ASN
1	A	278	GLN
1	A	279	GLN
2	B	48	ASN
3	C	352	HIS
4	D	8	ASN
4	D	13	ASN
9	I	542	ASN
9	I	838	ASN
10	J	326	HIS
10	J	343	HIS
10	J	422	HIS
10	K	220	GLN
10	K	254	GLN
10	K	343	HIS
11	L	182	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	SEP	G	1105	7	7,9,10	1.81	2 (28%)	8,12,14	1.17	1 (12%)
7	TPO	G	1106	7	7,10,11	1.25	0	10,14,16	1.20	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SEP	G	1105	7	-	0/5/8/10	0/0/0/0
7	TPO	G	1106	7	-	0/8/11/13	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1105	SEP	P-O2P	2.05	1.61	1.54
7	G	1105	SEP	P-O1P	3.50	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1106	TPO	P-OG1-CB	-2.73	109.50	121.42
7	G	1105	SEP	OG-P-O1P	2.18	112.57	107.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.