Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2023 – 10:41 PM EDT

PDB ID	:	3HOS
Title	:	Crystal structure of the mariner Mos1 paired end complex with Mg
Authors	:	Richardson, J.M.; Walkinshaw, M.D.
Deposited on	:	2009-06-03
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

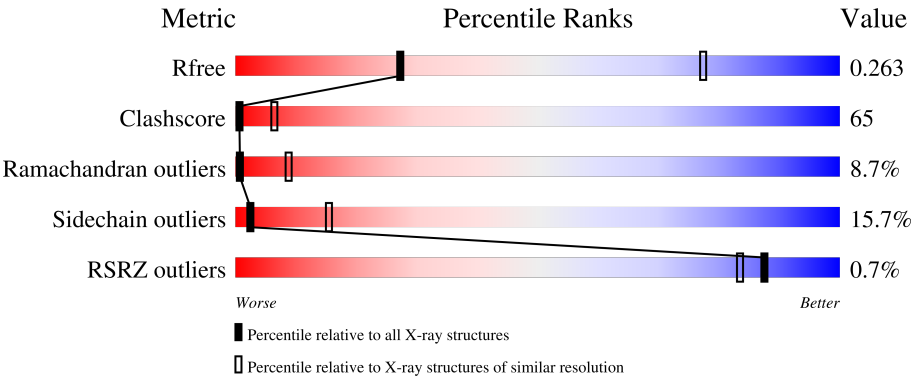
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	345	% 22% 60% 14%
1	B	345	% 22% 57% 17%
2	C	25	24% 76%
2	E	25	32% 64%
2	G	25	52% 44%

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Mol	Chain	Length	Quality of chain
3	D	28	32% 64%
3	F	28	29% 68%
3	H	28	7% 54% 39%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8885 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Transposable element mariner, complete cds.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2802	1778	507	507	10			
1	B	337	Total	C	N	O	S	0	0	0
			2812	1783	509	510	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	THR	LYS	SEE REMARK 999	UNP Q7JQ07
A	164	ASN	SER	SEE REMARK 999	UNP Q7JQ07
A	210	PRO	ARG	SEE REMARK 999	UNP Q7JQ07
A	216	ALA	THR	engineered mutation	UNP Q7JQ07
A	344	PHE	LEU	SEE REMARK 999	UNP Q7JQ07
B	45	THR	LYS	SEE REMARK 999	UNP Q7JQ07
B	164	ASN	SER	SEE REMARK 999	UNP Q7JQ07
B	210	PRO	ARG	SEE REMARK 999	UNP Q7JQ07
B	216	ALA	THR	engineered mutation	UNP Q7JQ07
B	344	PHE	LEU	SEE REMARK 999	UNP Q7JQ07

- Molecule 2 is a DNA chain called Mos1 NTS inverted repeat DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	25	Total	C	N	O	P	0	0	0
			520	248	94	153	25			
2	E	25	Total	C	N	O	P	0	0	0
			520	248	94	153	25			
2	G	25	Total	C	N	O	P	0	0	0
			520	248	94	153	25			

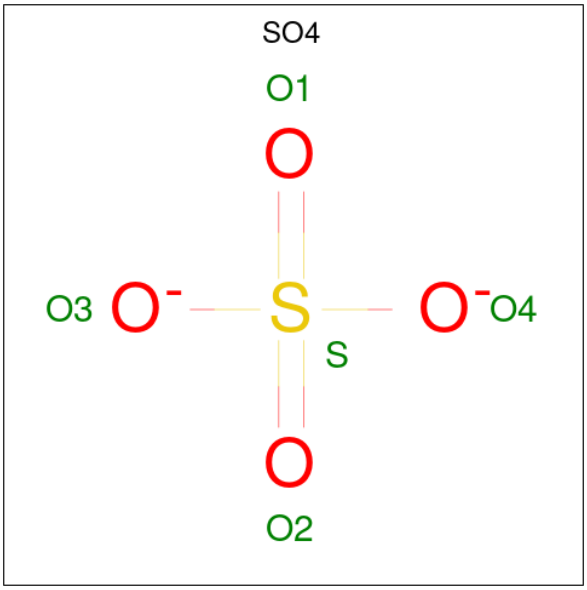
- Molecule 3 is a DNA chain called Mos1 TS inverted repeat DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	28	Total	C	N	O	P	0	0	0
			566	273	102	164	27			
3	F	28	Total	C	N	O	P	0	0	0
			566	273	102	164	27			
3	H	28	Total	C	N	O	P	0	0	0
			566	273	102	164	27			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		

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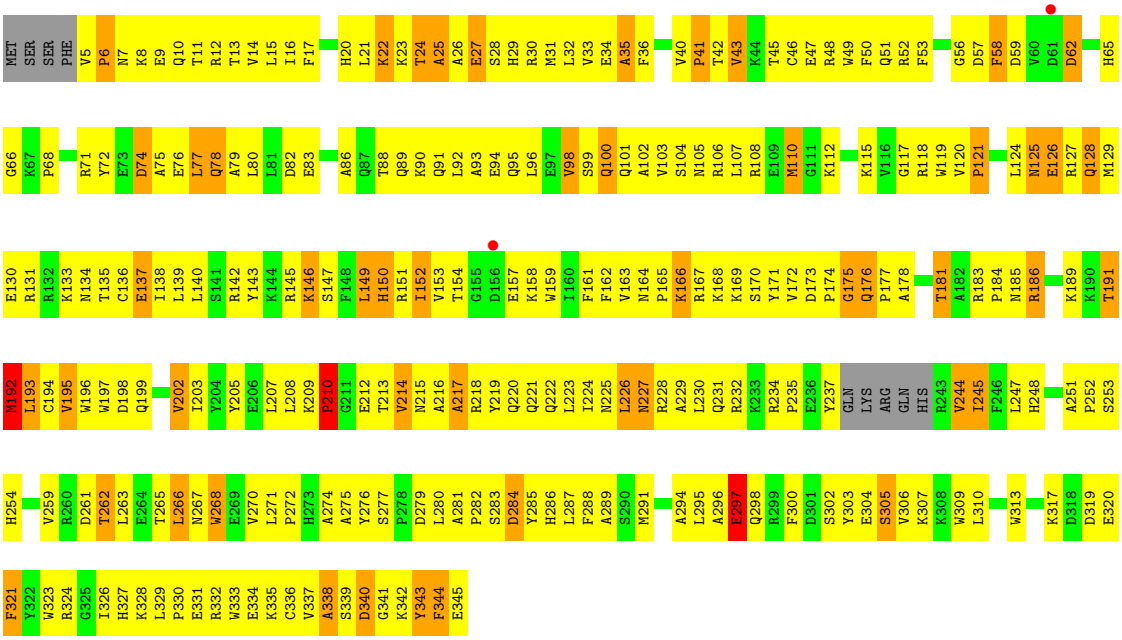
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

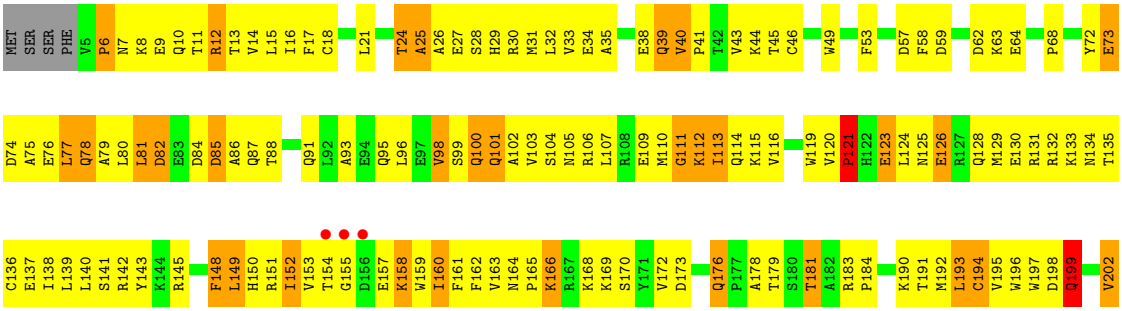
• Molecule 1: Transposable element mariner, complete cds

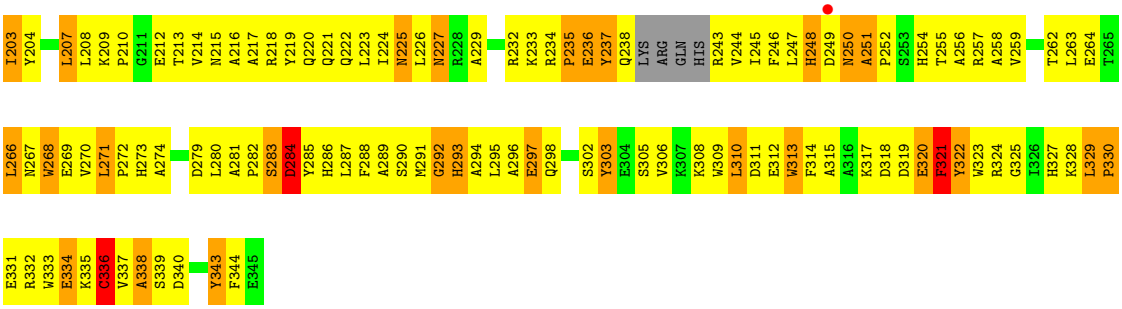
Chain A:



• Molecule 1: Transposable element mariner, complete cds

Chain B:





• Molecule 2: Mos1 NTS inverted repeat DNA

Chain C:

• Molecule 2: Mos1 NTS inverted repeat DNA

Chain E:

• Molecule 2: Mos1 NTS inverted repeat DNA

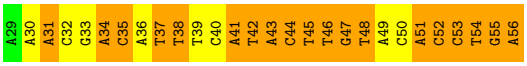
Chain G:

• Molecule 3: Mos1 TS inverted repeat DNA

Chain D:

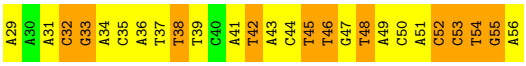
• Molecule 3: Mos1 TS inverted repeat DNA

Chain F:



• Molecule 3: Mos1 TS inverted repeat DNA

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	121.23Å 85.03Å 131.27Å 90.00° 98.93° 90.00°	Depositor
Resolution (Å)	29.87 – 3.50 29.87 – 3.50	Depositor EDS
% Data completeness (in resolution range)	96.7 (29.87-3.50) 96.7 (29.87-3.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 3.47Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.279 0.219 , 0.263	Depositor DCC
R_{free} test set	1647 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	89.1	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 116.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8885	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.81	0/2875	0.83	0/3881
1	B	0.74	0/2885	0.82	0/3893
2	C	1.41	1/583 (0.2%)	2.39	52/898 (5.8%)
2	E	1.52	5/583 (0.9%)	2.51	44/898 (4.9%)
2	G	1.25	2/583 (0.3%)	2.20	41/898 (4.6%)
3	D	1.54	4/634 (0.6%)	2.48	48/975 (4.9%)
3	F	1.54	8/634 (1.3%)	2.46	67/975 (6.9%)
3	H	1.11	0/634	1.85	24/975 (2.5%)
All	All	1.06	20/9411 (0.2%)	1.63	276/13393 (2.1%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	56	DA	N9-C4	-9.95	1.31	1.37
2	G	4	DG	OP3-P	-9.83	1.49	1.61
2	C	4	DG	OP3-P	-9.48	1.49	1.61
2	E	4	DG	OP3-P	-7.87	1.51	1.61
2	G	28	DT	C4-C5	-7.11	1.38	1.45
3	F	51	DA	N3-C4	-7.07	1.30	1.34
2	E	11	DA	N7-C5	-6.45	1.35	1.39
3	F	52	DC	N1-C6	-6.38	1.33	1.37
3	F	43	DA	N9-C4	-6.12	1.34	1.37
3	D	51	DA	C6-N1	-6.09	1.31	1.35
3	D	51	DA	N3-C4	-6.07	1.31	1.34
2	E	9	DA	N3-C4	-6.02	1.31	1.34
3	D	54	DT	N3-C4	-6.00	1.33	1.38
2	E	8	DT	N3-C4	-5.90	1.33	1.38
3	D	49	DA	N3-C4	-5.48	1.31	1.34
3	F	48	DT	C4-C5	-5.13	1.40	1.45
3	F	53	DC	O4'-C1'	-5.09	1.36	1.42
3	F	45	DT	N1-C2	-5.08	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	56	DA	N3-C4	-5.06	1.31	1.34
2	E	5	DG	C5-C4	-5.03	1.34	1.38

All (276) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	4	DG	OP1-P-OP2	-24.98	82.14	119.60
2	E	4	DG	O5'-P-OP2	-16.21	91.11	105.70
2	G	28	DT	N3-C4-O4	12.95	127.67	119.90
2	G	4	DG	N1-C6-O6	12.74	127.55	119.90
3	F	48	DT	N3-C4-O4	12.30	127.28	119.90
2	G	4	DG	O4'-C1'-N9	11.76	116.23	108.00
3	F	47	DG	C5-C6-O6	-11.75	121.55	128.60
3	D	34	DA	O4'-C1'-N9	11.22	115.85	108.00
2	E	19	DA	O4'-C1'-N9	-10.43	100.70	108.00
2	C	16	DT	N3-C4-O4	10.36	126.11	119.90
2	C	12	DA	N1-C6-N6	10.31	124.78	118.60
3	D	54	DT	O4'-C4'-C3'	10.02	112.01	106.00
2	G	28	DT	C4-C5-C7	-9.76	113.14	119.00
2	G	5	DG	N1-C6-O6	9.50	125.60	119.90
2	G	4	DG	C5-C6-O6	-9.50	122.90	128.60
3	F	48	DT	C5-C4-O4	-9.48	118.26	124.90
3	F	42	DT	N3-C4-O4	9.47	125.58	119.90
3	D	54	DT	C4-C5-C7	-9.42	113.35	119.00
2	C	8	DT	N3-C4-O4	9.41	125.55	119.90
2	E	14	DT	N3-C2-O2	9.03	127.72	122.30
3	D	42	DT	O4'-C4'-C3'	9.03	111.42	106.00
2	C	19	DA	O4'-C1'-N9	8.95	114.27	108.00
3	D	36	DA	N1-C6-N6	8.92	123.95	118.60
2	C	16	DT	C5-C4-O4	-8.88	118.69	124.90
3	F	55	DG	N1-C6-O6	8.84	125.20	119.90
3	H	29	DA	O4'-C1'-N9	8.82	114.18	108.00
2	C	20	DA	N1-C6-N6	8.79	123.87	118.60
2	E	26	DT	O4'-C1'-N1	8.75	114.13	108.00
3	D	35	DC	O4'-C1'-N1	8.71	114.10	108.00
3	F	48	DT	O4'-C1'-N1	8.68	114.08	108.00
2	G	5	DG	C5-C6-O6	-8.68	123.39	128.60
2	C	4	DG	O5'-P-OP1	-8.62	97.94	105.70
3	F	46	DT	P-O3'-C3'	-8.61	109.37	119.70
2	G	4	DG	C2-N3-C4	-8.58	107.61	111.90
3	F	43	DA	O4'-C1'-N9	-8.57	102.00	108.00
2	E	11	DA	N1-C6-N6	8.39	123.63	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	55	DG	N1-C6-O6	8.38	124.93	119.90
3	D	41	DA	N1-C6-N6	8.36	123.62	118.60
2	C	8	DT	C5-C4-O4	-8.34	119.06	124.90
2	G	4	DG	C6-C5-N7	-8.32	125.41	130.40
2	C	27	DT	O4'-C1'-N1	8.26	113.78	108.00
3	F	48	DT	C4-C5-C7	-8.21	114.08	119.00
2	G	28	DT	C5-C4-O4	-8.19	119.17	124.90
3	F	38	DT	O4'-C1'-N1	8.15	113.71	108.00
3	H	33	DG	O5'-P-OP2	-8.09	98.42	105.70
2	G	5	DG	O4'-C1'-N9	8.04	113.63	108.00
3	F	54	DT	N3-C4-O4	8.01	124.71	119.90
3	F	51	DA	O4'-C1'-N9	-7.92	102.46	108.00
3	F	34	DA	O4'-C1'-N9	7.91	113.54	108.00
3	F	31	DA	P-O3'-C3'	7.89	129.16	119.70
2	G	8	DT	N3-C4-O4	7.87	124.62	119.90
3	F	47	DG	N1-C6-O6	7.79	124.58	119.90
3	F	45	DT	N3-C2-O2	7.79	126.97	122.30
3	H	52	DC	O4'-C1'-C2'	-7.69	99.75	105.90
2	C	6	DT	C4-C5-C7	-7.60	114.44	119.00
3	D	45	DT	C5-C4-O4	-7.58	119.59	124.90
2	G	4	DG	OP1-P-OP2	-7.56	108.26	119.60
3	F	50	DC	O4'-C1'-C2'	-7.50	99.90	105.90
3	D	45	DT	N3-C4-O4	7.50	124.40	119.90
3	H	29	DA	N1-C6-N6	7.44	123.07	118.60
2	G	26	DT	N3-C4-O4	7.43	124.36	119.90
3	F	42	DT	C5-C4-O4	-7.40	119.72	124.90
2	E	13	DG	O4'-C1'-N9	7.36	113.15	108.00
2	G	8	DT	O5'-P-OP2	-7.34	99.09	105.70
3	F	45	DT	O4'-C4'-C3'	7.33	110.40	106.00
2	G	7	DG	O4'-C4'-C3'	-7.31	101.58	104.50
3	F	44	DC	O4'-C4'-C3'	7.27	110.36	106.00
3	F	55	DG	C6-C5-N7	-7.25	126.05	130.40
3	D	35	DC	O4'-C4'-C3'	-7.23	101.61	104.50
2	C	18	DA	O4'-C1'-N9	-7.21	102.95	108.00
2	G	8	DT	C5-C4-O4	-7.21	119.85	124.90
3	F	42	DT	C4-C5-C7	-7.17	114.70	119.00
2	C	13	DG	O4'-C1'-N9	7.12	112.98	108.00
2	E	10	DC	O4'-C1'-C2'	-7.10	100.22	105.90
2	E	25	DG	O4'-C1'-N9	7.06	112.94	108.00
2	C	21	DT	O4'-C1'-N1	-7.06	103.06	108.00
2	G	7	DG	N1-C6-O6	7.04	124.12	119.90
2	C	25	DG	O4'-C1'-N9	7.01	112.91	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	26	DT	N3-C4-O4	6.99	124.09	119.90
2	G	21	DT	C4-C5-C7	6.99	123.19	119.00
2	G	28	DT	C6-C5-C7	6.95	127.07	122.90
3	D	38	DT	C5-C6-N1	-6.92	119.55	123.70
2	E	25	DG	O4'-C4'-C3'	6.91	110.15	106.00
2	G	13	DG	O4'-C1'-N9	6.87	112.81	108.00
2	E	10	DC	P-O5'-C5'	-6.86	109.92	120.90
3	D	42	DT	N3-C4-O4	6.85	124.01	119.90
3	H	33	DG	P-O3'-C3'	-6.82	111.52	119.70
2	E	8	DT	C6-C5-C7	6.81	126.99	122.90
3	D	48	DT	P-O3'-C3'	-6.80	111.54	119.70
3	F	52	DC	C5-C6-N1	-6.80	117.60	121.00
2	G	26	DT	C5-C4-O4	-6.78	120.15	124.90
2	E	8	DT	O4'-C1'-N1	-6.76	103.27	108.00
2	E	8	DT	C4-C5-C7	-6.74	114.96	119.00
2	G	4	DG	C4-C5-N7	6.68	113.47	110.80
2	G	5	DG	OP2-P-O3'	6.68	119.90	105.20
2	C	19	DA	P-O3'-C3'	-6.66	111.71	119.70
3	H	33	DG	O4'-C1'-N9	-6.63	103.36	108.00
3	D	54	DT	OP1-P-OP2	6.59	129.49	119.60
2	C	17	DG	O4'-C1'-C2'	-6.58	100.63	105.90
3	D	42	DT	C6-N1-C2	-6.57	118.02	121.30
2	G	5	DG	C6-C5-N7	-6.55	126.47	130.40
2	E	13	DG	C4-C5-N7	6.54	113.42	110.80
3	F	55	DG	O4'-C1'-C2'	6.53	111.12	105.90
2	C	11	DA	N1-C6-N6	6.50	122.50	118.60
2	E	20	DA	C2-N3-C4	-6.50	107.35	110.60
2	E	14	DT	N1-C2-O2	-6.49	117.91	123.10
3	D	37	DT	N3-C4-O4	6.49	123.79	119.90
2	G	7	DG	C6-C5-N7	-6.49	126.51	130.40
2	G	5	DG	C5-N7-C8	-6.46	101.07	104.30
3	H	53	DC	N3-C4-N4	6.46	122.52	118.00
3	F	46	DT	N3-C4-O4	6.43	123.75	119.90
2	C	10	DC	O5'-P-OP1	-6.42	99.92	105.70
3	F	45	DT	N3-C4-O4	6.41	123.75	119.90
2	G	5	DG	C4-C5-N7	6.41	113.36	110.80
2	G	27	DT	N3-C4-O4	6.41	123.75	119.90
2	E	6	DT	C5-C4-O4	-6.41	120.41	124.90
3	F	56	DA	C1'-O4'-C4'	-6.39	103.71	110.10
3	D	31	DA	O4'-C1'-N9	6.39	112.47	108.00
2	E	25	DG	N3-C2-N2	-6.38	115.43	119.90
3	H	32	DC	P-O3'-C3'	-6.38	112.05	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	8	DT	O4'-C4'-C3'	6.33	109.80	106.00
2	C	19	DA	O4'-C4'-C3'	-6.31	101.98	104.50
2	E	28	DT	N3-C4-O4	6.29	123.67	119.90
2	G	28	DT	C6-N1-C2	-6.28	118.16	121.30
3	F	52	DC	C2-N3-C4	-6.28	116.76	119.90
2	C	6	DT	N3-C4-O4	6.28	123.67	119.90
2	E	10	DC	C2-N3-C4	-6.27	116.76	119.90
3	F	49	DA	C5-C6-N6	-6.26	118.69	123.70
2	C	26	DT	C5-C4-O4	-6.25	120.53	124.90
3	D	51	DA	P-O3'-C3'	-6.24	112.21	119.70
2	E	16	DT	P-O5'-C5'	-6.24	110.92	120.90
3	D	48	DT	C5-C4-O4	-6.23	120.54	124.90
2	E	6	DT	O4'-C1'-N1	6.21	112.35	108.00
2	G	6	DT	O5'-P-OP2	-6.20	100.12	105.70
3	D	54	DT	C5-C6-N1	-6.18	119.99	123.70
2	G	6	DT	C6-C5-C7	-6.18	119.19	122.90
2	C	24	DC	O4'-C1'-N1	6.17	112.32	108.00
3	D	44	DC	O4'-C4'-C3'	6.16	109.69	106.00
2	E	26	DT	C5-C4-O4	-6.15	120.59	124.90
2	C	5	DG	C5-C6-O6	-6.15	124.91	128.60
3	F	41	DA	C5-C6-N6	-6.13	118.79	123.70
3	D	36	DA	P-O5'-C5'	-6.13	111.10	120.90
3	F	46	DT	O4'-C1'-N1	6.11	112.28	108.00
2	C	4	DG	OP1-P-OP2	-6.08	110.47	119.60
2	E	6	DT	N3-C4-O4	6.08	123.55	119.90
3	D	50	DC	O3'-P-O5'	-6.06	92.49	104.00
3	F	45	DT	C5-C4-O4	-6.03	120.68	124.90
2	G	4	DG	C5-N7-C8	-6.02	101.29	104.30
2	C	20	DA	C5-C6-N1	-6.01	114.69	117.70
3	F	49	DA	O4'-C1'-N9	-5.98	103.81	108.00
2	E	21	DT	C6-C5-C7	-5.97	119.32	122.90
2	C	18	DA	N1-C6-N6	-5.95	115.03	118.60
2	C	16	DT	O4'-C1'-N1	-5.94	103.84	108.00
2	C	21	DT	C6-C5-C7	5.93	126.46	122.90
2	C	22	DG	O4'-C1'-N9	-5.93	103.85	108.00
3	D	51	DA	N1-C2-N3	5.92	132.26	129.30
3	D	42	DT	O4'-C1'-C2'	5.91	110.63	105.90
3	F	31	DA	N1-C6-N6	5.90	122.14	118.60
2	G	25	DG	OP2-P-O3'	5.90	118.19	105.20
2	G	5	DG	N7-C8-N9	5.89	116.05	113.10
2	C	12	DA	C5-C6-N6	-5.88	119.00	123.70
2	G	14	DT	C4-C5-C7	5.88	122.53	119.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	32	DC	O4'-C1'-N1	5.83	112.08	108.00
2	G	7	DG	N7-C8-N9	5.82	116.01	113.10
2	E	25	DG	P-O3'-C3'	5.81	126.67	119.70
3	F	48	DT	P-O3'-C3'	-5.80	112.75	119.70
2	C	26	DT	O4'-C1'-N1	5.79	112.05	108.00
2	E	11	DA	C6-C5-N7	-5.77	128.26	132.30
2	C	16	DT	C4-C5-C7	-5.75	115.55	119.00
3	H	42	DT	C4-C5-C7	5.75	122.45	119.00
3	D	29	DA	N1-C6-N6	5.75	122.05	118.60
3	F	53	DC	O3'-P-O5'	-5.74	93.10	104.00
3	H	48	DT	N3-C4-O4	5.74	123.34	119.90
3	H	45	DT	N3-C4-O4	5.72	123.33	119.90
3	F	42	DT	O5'-P-OP2	5.71	117.55	110.70
2	C	25	DG	C4-C5-N7	5.71	113.08	110.80
3	F	55	DG	C5-C6-N1	-5.70	108.65	111.50
2	C	6	DT	C6-C5-C7	5.70	126.32	122.90
2	C	21	DT	C5-C4-O4	-5.70	120.91	124.90
3	H	45	DT	O4'-C1'-N1	5.68	111.97	108.00
3	F	41	DA	N1-C6-N6	5.67	122.00	118.60
3	H	45	DT	O4'-C4'-C3'	5.67	109.41	106.00
3	F	56	DA	O4'-C1'-N9	5.67	111.97	108.00
3	F	51	DA	N1-C2-N3	5.64	132.12	129.30
2	E	13	DG	C5-N7-C8	-5.64	101.48	104.30
2	E	4	DG	P-O5'-C5'	-5.62	111.90	120.90
3	D	49	DA	O4'-C1'-N9	-5.62	104.07	108.00
3	D	48	DT	O4'-C1'-N1	5.61	111.93	108.00
3	F	48	DT	O5'-P-OP2	-5.61	100.66	105.70
2	E	17	DG	C6-C5-N7	-5.60	127.04	130.40
2	C	25	DG	C5-N7-C8	-5.57	101.51	104.30
2	C	28	DT	N3-C4-O4	5.57	123.24	119.90
2	C	16	DT	P-O5'-C5'	-5.57	112.00	120.90
3	F	55	DG	P-O5'-C5'	-5.57	112.00	120.90
3	D	38	DT	P-O5'-C5'	-5.56	112.01	120.90
3	D	48	DT	C4-C5-C7	-5.55	115.67	119.00
2	E	20	DA	O4'-C1'-N9	-5.54	104.12	108.00
3	F	51	DA	P-O3'-C3'	-5.54	113.05	119.70
3	H	48	DT	C5-C4-O4	-5.54	121.03	124.90
3	D	52	DC	O5'-P-OP2	-5.53	100.73	105.70
3	F	35	DC	O4'-C1'-N1	5.52	111.86	108.00
3	F	51	DA	OP2-P-O3'	5.52	117.33	105.20
3	F	41	DA	O4'-C1'-N9	5.51	111.86	108.00
2	C	25	DG	N1-C6-O6	5.51	123.21	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	55	DG	O4'-C1'-N9	-5.50	104.15	108.00
3	F	56	DA	C5-N7-C8	-5.50	101.15	103.90
3	H	53	DC	C5-C4-N4	-5.48	116.36	120.20
2	C	18	DA	C5-C6-N1	5.47	120.44	117.70
2	G	8	DT	O4'-C1'-N1	-5.47	104.17	108.00
2	G	7	DG	O4'-C1'-N9	5.47	111.83	108.00
2	E	12	DA	O4'-C1'-N9	5.47	111.83	108.00
3	F	47	DG	C4-C5-N7	5.43	112.97	110.80
3	F	51	DA	C6-N1-C2	-5.42	115.35	118.60
3	H	54	DT	N3-C4-O4	5.41	123.15	119.90
3	D	54	DT	C4-C5-C6	5.41	121.24	118.00
3	H	46	DT	C4-C5-C7	5.40	122.24	119.00
2	C	20	DA	C5-N7-C8	-5.39	101.21	103.90
3	D	52	DC	OP2-P-O3'	5.38	117.04	105.20
3	H	33	DG	N3-C2-N2	-5.37	116.14	119.90
2	C	18	DA	P-O3'-C3'	5.36	126.14	119.70
3	F	45	DT	OP2-P-O3'	5.36	116.99	105.20
3	D	38	DT	O4'-C4'-C3'	5.35	109.21	106.00
3	D	43	DA	C2-N3-C4	-5.34	107.93	110.60
2	C	10	DC	C6-N1-C2	5.33	122.43	120.30
2	G	21	DT	C6-C5-C7	-5.32	119.71	122.90
3	D	42	DT	C4-C5-C6	5.32	121.19	118.00
2	G	7	DG	C8-N9-C4	-5.30	104.28	106.40
2	E	10	DC	C5-C4-N4	-5.30	116.49	120.20
2	C	5	DG	N1-C6-O6	5.29	123.08	119.90
3	D	55	DG	C6-C5-N7	-5.29	127.23	130.40
2	E	8	DT	P-O5'-C5'	-5.29	112.44	120.90
3	D	43	DA	P-O5'-C5'	-5.28	112.45	120.90
3	H	52	DC	P-O5'-C5'	-5.27	112.46	120.90
3	F	45	DT	C4'-C3'-C2'	-5.26	98.36	103.10
2	E	23	DT	C4-C5-C7	5.26	122.16	119.00
3	D	49	DA	O3'-P-O5'	-5.26	94.01	104.00
3	H	52	DC	N3-C2-O2	-5.26	118.22	121.90
3	D	38	DT	C1'-O4'-C4'	-5.24	104.86	110.10
3	F	53	DC	O4'-C1'-N1	-5.24	104.34	108.00
3	F	49	DA	N1-C6-N6	5.23	121.74	118.60
2	C	26	DT	O3'-P-O5'	-5.21	94.09	104.00
3	D	50	DC	OP1-P-O3'	5.21	116.67	105.20
3	D	36	DA	O5'-P-OP2	-5.21	101.01	105.70
3	D	47	DG	C8-N9-C4	-5.21	104.32	106.40
2	C	22	DG	C5-N7-C8	-5.20	101.70	104.30
2	E	6	DT	C3'-C2'-C1'	-5.19	96.28	102.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	50	DC	C2-N3-C4	-5.18	117.31	119.90
3	F	43	DA	OP2-P-O3'	5.18	116.59	105.20
2	C	8	DT	O3'-P-O5'	-5.17	94.17	104.00
2	E	10	DC	N1-C2-O2	-5.17	115.80	118.90
3	F	52	DC	C4-C5-C6	5.17	119.99	117.40
3	D	52	DC	C1'-O4'-C4'	-5.16	104.94	110.10
3	F	49	DA	O5'-P-OP1	-5.15	101.06	105.70
3	H	38	DT	C6-C5-C7	-5.15	119.81	122.90
3	F	43	DA	C5-N7-C8	-5.13	101.33	103.90
2	C	20	DA	O4'-C1'-N9	-5.10	104.43	108.00
3	F	51	DA	C5-C6-N6	-5.10	119.62	123.70
2	C	14	DT	C6-C5-C7	-5.10	119.84	122.90
2	C	11	DA	OP1-P-OP2	5.09	127.24	119.60
3	D	55	DG	C5-C6-O6	-5.09	125.55	128.60
3	F	53	DC	N3-C4-N4	-5.09	114.44	118.00
2	E	10	DC	N3-C4-C5	5.08	123.93	121.90
3	F	37	DT	N3-C4-O4	5.08	122.95	119.90
3	F	49	DA	OP1-P-OP2	5.07	127.20	119.60
3	F	40	DC	O4'-C1'-N1	5.06	111.54	108.00
3	F	51	DA	O3'-P-O5'	-5.04	94.42	104.00
2	E	25	DG	N1-C2-N2	5.04	120.73	116.20
2	E	11	DA	P-O3'-C3'	-5.03	113.67	119.70
2	E	6	DT	OP1-P-O3'	5.03	116.26	105.20
2	E	13	DG	C5-C6-O6	-5.02	125.59	128.60
2	C	22	DG	C2-N3-C4	-5.01	109.39	111.90
3	F	46	DT	C5-C4-O4	-5.01	121.39	124.90
3	H	55	DG	C8-N9-C4	-5.01	104.39	106.40
3	H	51	DA	O5'-P-OP2	-5.01	101.19	105.70
3	D	42	DT	N3-C2-O2	-5.01	119.30	122.30
3	F	55	DG	O4'-C4'-C3'	5.00	109.00	106.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2802	0	2739	398	0
1	B	2812	0	2747	415	0
2	C	520	0	285	54	0
2	E	520	0	285	33	0
2	G	520	0	285	52	0
3	D	566	0	318	76	0
3	F	566	0	317	48	0
3	H	566	0	318	61	0
4	A	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
All	All	8885	0	7294	1044	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 65.

All (1044) 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)
1:A:174:PRO:HA	1:B:113:ILE:HD11	1.26	1.17
3:H:36:DA:H2”	3:H:37:DT:H5’	1.23	1.15
3:H:45:DT:H2”	3:H:46:DT:C5’	1.75	1.14
3:D:43:DA:H2”	3:D:44:DC:H5”	1.27	1.14
3:H:33:DG:H2”	3:H:34:DA:H5”	1.31	1.11
3:D:46:DT:H2”	3:D:47:DG:H5’	1.22	1.09
1:B:271:LEU:HD22	1:B:272:PRO:HD2	1.27	1.07
1:A:24:THR:HG23	1:A:27:GLU:HB2	1.05	1.05
1:A:149:LEU:H	1:A:149:LEU:HD22	1.23	1.03
1:B:24:THR:HG23	1:B:27:GLU:HB2	1.40	1.03
1:A:215:ASN:OD1	1:A:217:ALA:HB3	1.59	1.03
3:D:43:DA:H2”	3:D:44:DC:C5’	1.88	1.03
3:D:31:DA:H2”	3:D:32:DC:C5’	1.88	1.03
1:A:151:ARG:HD2	1:A:245:ILE:HD11	1.43	1.00
1:A:282:PRO:HG3	1:A:329:LEU:HD21	1.39	1.00
2:E:26:DT:H2”	2:E:27:DT:H5’	1.44	1.00
1:A:166:LYS:H	1:A:166:LYS:HD3	1.24	1.00
1:B:191:THR:HB	1:B:207:LEU:HD11	1.41	1.00
3:D:51:DA:H2”	3:D:52:DC:H5’	1.44	0.98
1:A:152:ILE:HD13	1:A:153:VAL:N	1.79	0.97
1:B:237:TYR:CD1	1:B:244:VAL:HG22	1.99	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:THR:HG23	1:A:27:GLU:CB	1.94	0.97
1:B:68:PRO:HD3	2:E:16:DT:O2	1.64	0.97
3:F:53:DC:H2"	3:F:54:DT:H5'	1.46	0.97
1:B:223:LEU:O	1:B:226:LEU:HB3	1.66	0.96
3:D:31:DA:H2"	3:D:32:DC:H5"	1.44	0.96
1:B:172:VAL:HG22	1:B:173:ASP:N	1.81	0.96
3:F:38:DT:H2"	3:F:39:DT:H5"	1.46	0.96
3:H:48:DT:H2"	3:H:49:DA:H5'	1.44	0.96
3:H:45:DT:H2"	3:H:46:DT:H5"	1.48	0.96
2:C:13:DG:H2"	2:C:14:DT:H5'	1.46	0.95
1:B:40:VAL:HG22	1:B:41:PRO:HD2	1.46	0.95
1:B:202:VAL:HG22	1:B:203:ILE:H	1.31	0.95
1:A:92:LEU:O	1:A:96:LEU:HD13	1.66	0.95
1:A:172:VAL:HG22	1:A:173:ASP:N	1.82	0.95
1:A:191:THR:HB	1:A:207:LEU:HD11	1.50	0.94
2:E:12:DA:H2"	2:E:13:DG:H5"	1.47	0.93
1:A:170:SER:HB3	1:B:86:ALA:HB2	1.50	0.93
1:A:30:ARG:O	1:A:33:VAL:HG12	1.69	0.93
1:A:193:LEU:HD12	1:A:194:CYS:N	1.82	0.92
1:A:166:LYS:HD2	1:A:297:GLU:HB3	1.49	0.92
1:A:24:THR:CG2	1:A:27:GLU:HB2	1.99	0.92
1:B:157:GLU:HB3	1:B:194:CYS:HB3	1.52	0.92
1:B:282:PRO:HG3	1:B:329:LEU:HD21	1.51	0.92
1:A:329:LEU:HD12	1:A:333:TRP:CZ2	2.04	0.92
2:G:7:DG:H1	3:H:50:DC:H42	1.09	0.92
1:A:337:VAL:HG13	1:A:338:ALA:N	1.84	0.91
1:A:146:LYS:HE3	1:A:146:LYS:HA	1.53	0.91
3:D:43:DA:C2'	3:D:44:DC:H5"	2.00	0.91
2:G:7:DG:H2'	2:G:8:DT:H72	1.49	0.91
1:B:166:LYS:H	1:B:166:LYS:HD3	1.35	0.91
3:D:34:DA:H2"	3:D:35:DC:H5"	1.53	0.91
1:A:209:LYS:O	1:A:212:GLU:HB2	1.71	0.90
3:H:32:DC:H4'	3:H:32:DC:OP1	1.73	0.89
1:A:150:HIS:HA	1:A:199:GLN:NE2	1.88	0.89
1:A:150:HIS:HA	1:A:199:GLN:HE22	1.38	0.89
3:F:36:DA:H2"	3:F:37:DT:H5'	1.55	0.89
1:B:337:VAL:HG13	1:B:338:ALA:H	1.35	0.89
1:B:136:CYS:HB3	1:B:333:TRP:HB3	1.54	0.89
1:B:151:ARG:NH1	1:B:245:ILE:HD11	1.87	0.88
1:A:166:LYS:HD3	1:A:166:LYS:N	1.89	0.88
3:D:54:DT:H2'	3:D:54:DT:O2	1.71	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:VAL:HG13	1:A:338:ALA:H	1.39	0.88
1:A:172:VAL:HG21	1:A:176:GLN:HG2	1.57	0.87
1:A:74:ASP:OD1	1:A:106:ARG:HD3	1.76	0.86
2:E:10:DC:H2"	2:E:11:DA:O5'	1.74	0.86
1:A:282:PRO:CG	1:A:329:LEU:HD21	2.05	0.85
2:E:4:DG:H5"	2:E:4:DG:N3	1.90	0.85
1:B:172:VAL:CG2	1:B:173:ASP:N	2.39	0.85
3:D:34:DA:C2'	3:D:35:DC:H5"	2.06	0.85
3:H:37:DT:H2"	3:H:38:DT:OP2	1.77	0.85
1:A:220:GLN:HG2	1:A:259:VAL:HG22	1.59	0.84
1:A:66:GLY:HA3	2:C:17:DG:N3	1.93	0.84
1:A:88:THR:O	1:A:92:LEU:HD12	1.78	0.83
3:D:54:DT:H72	3:D:55:DG:N1	1.93	0.83
1:B:191:THR:CB	1:B:207:LEU:HD11	2.07	0.83
3:H:33:DG:C2'	3:H:34:DA:H5"	2.09	0.83
3:F:38:DT:C2'	3:F:39:DT:H5"	2.08	0.83
3:D:54:DT:H72	3:D:55:DG:H1	1.45	0.82
2:E:26:DT:H2'	2:E:27:DT:H71	1.61	0.82
1:A:32:LEU:HG	1:A:40:VAL:HG21	1.59	0.82
2:G:5:DG:H2'	2:G:6:DT:H71	1.62	0.82
2:G:7:DG:H1	3:H:50:DC:N4	1.77	0.82
3:D:46:DT:H2"	3:D:47:DG:C5'	2.07	0.82
1:A:172:VAL:CG2	1:A:173:ASP:N	2.42	0.82
1:A:77:LEU:HD13	1:A:78:GLN:N	1.94	0.81
1:A:88:THR:H	1:A:91:GLN:HE21	1.28	0.81
1:B:282:PRO:CG	1:B:329:LEU:HD21	2.10	0.81
1:A:99:SER:O	1:A:102:ALA:HB3	1.80	0.81
2:C:25:DG:H1	3:D:32:DC:H42	1.28	0.80
1:B:271:LEU:CD2	1:B:272:PRO:HD2	2.10	0.80
3:D:31:DA:H2"	3:D:32:DC:H5'	1.62	0.80
3:F:41:DA:H1'	3:F:42:DT:H5"	1.63	0.79
1:A:106:ARG:HH21	1:A:106:ARG:HG3	1.47	0.79
1:B:271:LEU:HD22	1:B:272:PRO:CD	2.11	0.79
1:A:166:LYS:CD	1:A:297:GLU:HB3	2.12	0.79
1:B:33:VAL:HG13	1:B:34:GLU:H	1.47	0.79
1:B:193:LEU:HD12	1:B:194:CYS:N	1.96	0.79
2:C:4:DG:N3	2:C:4:DG:H2'	1.97	0.79
1:A:149:LEU:C	1:A:151:ARG:H	1.86	0.79
1:B:220:GLN:HG2	1:B:262:THR:HG21	1.64	0.79
3:D:44:DC:H2"	3:D:45:DT:H5'	1.65	0.79
1:A:5:VAL:CG1	1:A:6:PRO:HD2	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:ARG:HG3	1:B:49:TRP:CE2	2.17	0.78
1:B:266:LEU:O	1:B:266:LEU:HD12	1.83	0.78
1:A:142:ARG:HA	1:A:145:ARG:HD2	1.66	0.78
1:A:149:LEU:O	1:A:151:ARG:N	2.15	0.78
1:A:262:THR:O	1:A:266:LEU:HD11	1.84	0.78
1:B:220:GLN:HE22	1:B:258:ALA:HB1	1.48	0.78
1:A:284:ASP:HA	1:A:288:PHE:HD2	1.49	0.78
1:B:72:TYR:OH	1:B:106:ARG:HG3	1.83	0.77
1:A:77:LEU:HD13	1:A:77:LEU:C	2.04	0.77
1:B:7:ASN:CG	1:B:8:LYS:H	1.85	0.77
1:A:172:VAL:CG2	1:A:173:ASP:H	1.97	0.77
1:B:57:ASP:CG	1:B:58:PHE:H	1.87	0.77
2:C:27:DT:H2'	2:C:28:DT:H71	1.66	0.77
1:B:193:LEU:HD12	1:B:193:LEU:C	2.05	0.76
1:B:80:LEU:HD12	1:B:80:LEU:N	1.99	0.76
2:C:19:DA:H2'	2:C:20:DA:C8	2.20	0.76
1:A:265:THR:C	1:A:266:LEU:HD12	2.06	0.76
1:A:40:VAL:HG22	1:A:41:PRO:HD2	1.66	0.76
1:A:86:ALA:HB2	1:B:170:SER:CB	2.16	0.76
3:D:42:DT:H5"	3:D:42:DT:H6	1.48	0.76
2:G:7:DG:H8	2:G:7:DG:H5'	1.50	0.76
1:B:12:ARG:CZ	1:B:16:ILE:HD11	2.15	0.76
1:A:152:ILE:HD13	1:A:153:VAL:H	1.51	0.75
1:A:207:LEU:HB3	1:A:307:LYS:HE2	1.67	0.75
1:A:279:ASP:OD1	1:A:280:LEU:HD22	1.86	0.75
2:G:27:DT:H2"	2:G:28:DT:O5'	1.85	0.75
1:A:96:LEU:O	1:A:98:VAL:HG12	1.87	0.75
2:G:6:DT:H2"	2:G:7:DG:H5"	1.69	0.75
1:B:210:PRO:HD3	1:B:303:TYR:HD1	1.51	0.74
3:D:45:DT:H2'	3:D:46:DT:H71	1.69	0.74
1:B:286:HIS:NE2	1:B:321:PHE:CE2	2.56	0.74
3:H:33:DG:H8	3:H:33:DG:OP2	1.70	0.74
1:A:186:ARG:HG3	3:H:55:DG:H4'	1.68	0.74
1:A:5:VAL:HG13	1:A:6:PRO:HD2	1.67	0.74
1:A:139:LEU:HD21	1:A:272:PRO:HD2	1.70	0.73
3:H:53:DC:H2"	3:H:54:DT:O4'	1.88	0.73
1:A:337:VAL:CG1	1:A:338:ALA:H	2.01	0.73
3:F:33:DG:H2"	3:F:34:DA:H5'	1.69	0.73
2:G:8:DT:H2"	2:G:9:DA:C8	2.23	0.73
2:E:26:DT:H2"	2:E:27:DT:C5'	2.17	0.73
2:G:7:DG:H2'	2:G:8:DT:C7	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:13:DG:H22	3:H:45:DT:H3	1.37	0.73
1:B:244:VAL:HB	1:B:268:TRP:CD1	2.24	0.73
1:A:174:PRO:CA	1:B:113:ILE:HD11	2.14	0.72
1:B:15:LEU:N	1:B:15:LEU:HD12	2.05	0.72
2:G:13:DG:H2"	2:G:14:DT:O5'	1.88	0.72
2:C:4:DG:C6	3:D:54:DT:H73	2.25	0.72
1:A:208:LEU:HB3	1:A:212:GLU:HB3	1.72	0.72
1:A:223:LEU:O	1:A:226:LEU:HB3	1.89	0.72
1:A:120:VAL:HG23	1:A:121:PRO:HD2	1.71	0.72
1:B:220:GLN:HE22	1:B:258:ALA:CB	2.02	0.72
2:E:4:DG:OP2	2:E:4:DG:H4'	1.89	0.72
1:B:125:ASN:HB3	1:B:128:GLN:OE1	1.89	0.71
3:F:44:DC:H2"	3:F:45:DT:O5'	1.90	0.71
1:B:152:ILE:C	1:B:152:ILE:HD13	2.10	0.71
1:B:73:GLU:HB2	1:B:76:GLU:HB2	1.70	0.71
3:D:38:DT:H2"	3:D:39:DT:H5'	1.73	0.71
1:B:251:ALA:HB1	1:B:252:PRO:HD2	1.72	0.71
1:B:286:HIS:CD2	1:B:325:GLY:HA3	2.26	0.71
1:B:77:LEU:C	1:B:77:LEU:HD13	2.12	0.70
3:F:46:DT:H2"	3:F:47:DG:O5'	1.91	0.70
3:D:51:DA:H2"	3:D:52:DC:C5'	2.19	0.70
1:B:152:ILE:HA	1:B:245:ILE:HB	1.73	0.70
3:D:47:DG:H2"	3:D:48:DT:O5'	1.91	0.70
1:B:195:VAL:HG22	1:B:196:TRP:N	2.05	0.70
3:D:54:DT:H2"	3:D:55:DG:H5'	1.72	0.70
1:A:337:VAL:CG1	1:A:338:ALA:N	2.53	0.70
2:C:19:DA:C4'	2:C:19:DA:OP1	2.38	0.70
1:A:172:VAL:HG22	1:A:173:ASP:H	1.56	0.70
1:B:68:PRO:CD	2:E:16:DT:O2	2.38	0.70
1:B:168:LYS:HE3	1:B:179:THR:HG21	1.73	0.70
3:F:47:DG:H2"	3:F:48:DT:O4'	1.90	0.70
2:C:15:DA:H2"	2:C:16:DT:H5'	1.73	0.69
1:A:277:SER:HB3	1:A:280:LEU:HD23	1.73	0.69
1:B:152:ILE:HD13	1:B:153:VAL:N	2.07	0.69
2:G:20:DA:H1'	2:G:21:DT:H5"	1.73	0.69
1:B:15:LEU:HD21	1:B:46:CYS:SG	2.32	0.69
1:B:31:MET:O	1:B:35:ALA:N	2.24	0.69
3:D:44:DC:H2"	3:D:45:DT:C5'	2.22	0.69
1:A:42:THR:O	1:A:45:THR:HB	1.93	0.69
3:H:36:DA:C2'	3:H:37:DT:H5'	2.14	0.69
1:B:216:ALA:HB2	2:G:7:DG:OP1	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:7:DG:H5'	2:G:7:DG:C8	2.27	0.69
1:A:220:GLN:HG2	1:A:259:VAL:CG2	2.22	0.69
1:A:251:ALA:HB1	1:A:252:PRO:HD2	1.75	0.69
1:B:142:ARG:HG2	1:B:148:PHE:CE2	2.27	0.69
1:B:153:VAL:HG23	1:B:197:TRP:O	1.91	0.69
3:D:42:DT:H2'	3:D:43:DA:C8	2.28	0.69
1:B:221:GLN:HA	1:B:224:ILE:HD12	1.75	0.69
3:F:43:DA:H2"	3:F:44:DC:H5"	1.74	0.69
1:B:210:PRO:HD3	1:B:303:TYR:CD1	2.28	0.69
1:B:165:PRO:HG3	1:B:184:PRO:HB3	1.75	0.68
1:B:136:CYS:O	1:B:137:GLU:C	2.31	0.68
3:D:54:DT:O2	3:D:54:DT:C2'	2.36	0.68
3:H:53:DC:H2'	3:H:54:DT:C6	2.29	0.68
2:G:6:DT:H2"	2:G:7:DG:C5'	2.23	0.68
1:B:208:LEU:HB3	1:B:212:GLU:HB3	1.74	0.68
1:B:305:SER:O	1:B:308:LYS:HB3	1.94	0.68
3:D:56:DA:H4'	3:D:56:DA:OP1	1.92	0.68
1:A:78:GLN:HB2	1:A:110:MET:HE1	1.75	0.68
2:C:25:DG:N2	3:D:33:DG:C2	2.61	0.67
1:A:302:SER:OG	1:A:305:SER:HB2	1.95	0.67
1:B:286:HIS:NE2	1:B:321:PHE:HE2	1.92	0.67
1:A:50:PHE:HA	1:A:53:PHE:HD2	1.60	0.67
1:A:170:SER:CB	1:B:86:ALA:HB2	2.24	0.67
1:B:163:VAL:HG13	1:B:163:VAL:O	1.94	0.67
1:A:191:THR:CB	1:A:207:LEU:HD11	2.25	0.66
1:A:121:PRO:HG2	1:A:343:TYR:CE2	2.31	0.66
1:B:77:LEU:O	1:B:77:LEU:HD22	1.94	0.66
2:E:15:DA:H2"	2:E:16:DT:O5'	1.95	0.66
1:A:284:ASP:HA	1:A:288:PHE:CD2	2.28	0.66
1:B:43:VAL:HG13	1:B:44:LYS:N	2.10	0.66
1:A:120:VAL:CG2	1:A:121:PRO:HD2	2.25	0.66
1:A:133:LYS:O	1:A:137:GLU:HB2	1.95	0.66
1:B:166:LYS:HD2	1:B:297:GLU:HA	1.77	0.66
2:G:11:DA:C2	3:H:47:DG:C2	2.83	0.66
1:B:284:ASP:HA	1:B:288:PHE:HD2	1.60	0.66
3:D:30:DA:H2"	3:D:31:DA:O5'	1.95	0.66
1:B:80:LEU:N	1:B:80:LEU:CD1	2.58	0.66
1:B:296:ALA:C	1:B:298:GLN:H	1.98	0.66
3:H:45:DT:H2"	3:H:46:DT:O5'	1.94	0.66
1:B:202:VAL:HG22	1:B:203:ILE:N	2.05	0.66
2:C:25:DG:H1	3:D:32:DC:N4	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:45:DT:H5'	3:D:45:DT:H6	1.60	0.66
1:B:329:LEU:HD12	1:B:333:TRP:CZ2	2.31	0.66
1:B:93:ALA:HA	1:B:98:VAL:HG23	1.76	0.66
2:G:22:DG:C2	3:H:36:DA:C2	2.84	0.66
1:A:230:LEU:HD23	1:A:230:LEU:C	2.15	0.65
1:B:149:LEU:O	1:B:152:ILE:HG22	1.96	0.65
1:B:223:LEU:HD12	1:B:223:LEU:H	1.61	0.65
1:A:6:PRO:HA	1:A:10:GLN:NE2	2.11	0.65
1:A:152:ILE:CD1	1:A:153:VAL:N	2.56	0.65
1:B:26:ALA:O	1:B:30:ARG:HG3	1.97	0.65
1:B:101:GLN:O	1:B:104:SER:HB3	1.96	0.65
2:G:27:DT:H2'	2:G:28:DT:H71	1.78	0.65
1:B:163:VAL:O	1:B:165:PRO:HD3	1.97	0.65
1:A:95:GLN:C	1:A:96:LEU:HD12	2.16	0.65
1:A:215:ASN:O	1:A:216:ALA:C	2.35	0.65
1:B:191:THR:HB	1:B:207:LEU:CD1	2.21	0.65
3:F:51:DA:H2"	3:F:52:DC:O5'	1.97	0.65
1:B:208:LEU:HG	1:B:212:GLU:HG2	1.78	0.64
3:D:31:DA:C2'	3:D:32:DC:H5"	2.25	0.64
1:B:33:VAL:HG13	1:B:34:GLU:N	2.12	0.64
1:A:154:THR:HG23	1:A:283:SER:OG	1.97	0.64
2:C:18:DA:H2"	2:C:19:DA:O5'	1.96	0.64
2:C:22:DG:C2	3:D:36:DA:C2	2.85	0.64
3:F:54:DT:H2"	3:F:55:DG:H5'	1.78	0.64
1:A:33:VAL:HG13	1:A:34:GLU:N	2.12	0.64
1:A:103:VAL:O	1:A:104:SER:C	2.35	0.64
1:B:183:ARG:CG	1:B:184:PRO:HD2	2.28	0.64
1:B:295:LEU:HD23	1:B:309:TRP:CH2	2.31	0.64
2:G:20:DA:H2"	2:G:21:DT:C5'	2.27	0.64
2:C:13:DG:H2"	2:C:14:DT:C5'	2.23	0.64
2:E:25:DG:H2"	2:E:26:DT:O5'	1.98	0.64
1:B:215:ASN:H	1:B:218:ARG:HB3	1.63	0.64
1:B:263:LEU:O	1:B:266:LEU:HB3	1.98	0.64
2:E:19:DA:H1'	2:E:20:DA:H5'	1.78	0.64
1:B:244:VAL:HB	1:B:268:TRP:NE1	2.13	0.64
3:F:52:DC:H2"	3:F:53:DC:OP2	1.97	0.64
2:G:14:DT:H2"	2:G:15:DA:C8	2.32	0.64
1:A:169:LYS:O	1:B:86:ALA:HB1	1.98	0.63
1:B:337:VAL:O	1:B:340:ASP:N	2.22	0.63
1:A:339:SER:O	1:A:340:ASP:HB2	1.98	0.63
1:A:153:VAL:HG13	1:A:153:VAL:O	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:53:DC:C2'	3:H:54:DT:O4'	2.46	0.63
3:H:35:DC:H2"	3:H:36:DA:O5'	1.99	0.63
1:A:72:TYR:CE1	1:A:106:ARG:NE	2.67	0.63
1:A:344:PHE:O	1:A:345:GLU:HB2	1.98	0.63
1:B:176:GLN:CA	1:B:176:GLN:NE2	2.61	0.63
3:F:43:DA:C2'	3:F:44:DC:H5"	2.29	0.63
1:A:205:TYR:O	1:A:205:TYR:CG	2.51	0.62
1:B:333:TRP:O	1:B:335:LYS:N	2.31	0.62
1:B:43:VAL:HG13	1:B:44:LYS:H	1.64	0.62
1:B:96:LEU:HB3	1:B:98:VAL:HG22	1.81	0.62
1:B:124:LEU:HG	1:B:343:TYR:CE1	2.34	0.62
2:E:4:DG:H5"	2:E:4:DG:C4	2.34	0.62
1:A:45:THR:HA	1:A:48:ARG:HG3	1.81	0.62
1:B:63:LYS:HD3	1:B:64:GLU:H	1.64	0.62
1:B:159:TRP:CZ3	1:B:192:MET:HB2	2.34	0.62
1:B:172:VAL:CG2	1:B:173:ASP:H	2.12	0.62
1:B:225:ASN:H	1:B:225:ASN:HD22	1.47	0.62
3:H:38:DT:H2"	3:H:39:DT:H5'	1.81	0.62
1:B:176:GLN:NE2	1:B:176:GLN:HA	2.13	0.62
1:B:225:ASN:HD22	1:B:225:ASN:N	1.97	0.62
3:D:46:DT:C2'	3:D:47:DG:H5'	2.15	0.62
3:D:48:DT:H2"	3:D:49:DA:C8	2.34	0.62
1:A:92:LEU:O	1:A:96:LEU:CD1	2.46	0.62
1:A:227:ASN:HD21	1:A:231:GLN:NE2	1.97	0.62
3:F:38:DT:C3'	3:F:39:DT:H5"	2.29	0.62
1:A:21:LEU:O	1:A:23:LYS:N	2.33	0.62
1:B:57:ASP:CG	1:B:58:PHE:N	2.53	0.62
1:B:337:VAL:HG13	1:B:338:ALA:N	2.10	0.62
3:D:43:DA:H2"	3:D:44:DC:H5'	1.78	0.62
3:D:45:DT:H2"	3:D:46:DT:O5'	2.00	0.62
2:G:20:DA:H2"	2:G:21:DT:H5'	1.81	0.62
1:A:295:LEU:HD21	1:A:309:TRP:CZ3	2.35	0.62
1:B:62:ASP:OD1	2:E:20:DA:H5"	1.99	0.62
1:A:139:LEU:HD21	1:A:271:LEU:HD22	1.82	0.62
1:A:176:GLN:HG3	1:A:177:PRO:HD2	1.81	0.62
1:B:293:HIS:O	1:B:295:LEU:N	2.33	0.61
1:A:136:CYS:O	1:A:138:ILE:N	2.33	0.61
1:A:172:VAL:CG2	1:A:176:GLN:HG2	2.29	0.61
1:A:321:PHE:C	1:A:321:PHE:CD1	2.73	0.61
1:B:12:ARG:HE	1:B:12:ARG:C	2.02	0.61
1:B:303:TYR:C	1:B:303:TYR:CD2	2.72	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:GLN:O	1:B:13:THR:HB	2.00	0.61
1:B:279:ASP:OD1	1:B:280:LEU:HD23	2.00	0.61
2:C:23:DT:H2"	2:C:24:DC:H5'	1.82	0.61
1:B:295:LEU:HD23	1:B:309:TRP:CZ3	2.36	0.61
1:A:195:VAL:CG2	1:A:196:TRP:N	2.64	0.61
1:B:168:LYS:HE3	1:B:179:THR:CG2	2.29	0.61
2:C:18:DA:H2"	2:C:19:DA:H8	1.65	0.61
1:A:162:PHE:HD2	1:A:300:PHE:O	1.82	0.61
1:A:331:GLU:HG3	1:A:332:ARG:N	2.15	0.61
1:B:248:HIS:HD2	1:B:248:HIS:O	1.83	0.61
1:B:252:PRO:HA	1:B:255:THR:HG22	1.82	0.61
1:B:168:LYS:HE2	1:B:181:THR:CG2	2.30	0.61
2:C:4:DG:C6	3:D:54:DT:C7	2.84	0.61
1:B:164:ASN:ND2	1:B:295:LEU:HD13	2.15	0.61
1:B:303:TYR:C	1:B:303:TYR:HD2	2.03	0.61
1:A:12:ARG:HD2	1:A:59:ASP:HB3	1.82	0.61
1:A:53:PHE:O	1:A:56:GLY:N	2.34	0.61
2:C:15:DA:H2"	2:C:16:DT:C5'	2.29	0.61
2:G:23:DT:H1'	2:G:24:DC:H5"	1.82	0.61
1:B:7:ASN:CG	1:B:8:LYS:N	2.53	0.60
1:A:147:SER:OG	1:A:149:LEU:CD2	2.48	0.60
1:A:166:LYS:N	1:A:166:LYS:CD	2.63	0.60
1:B:284:ASP:HA	1:B:288:PHE:CD2	2.35	0.60
1:A:86:ALA:HB1	1:B:169:LYS:O	2.00	0.60
1:A:136:CYS:O	1:A:137:GLU:C	2.39	0.60
1:A:164:ASN:O	1:A:297:GLU:HA	2.00	0.60
1:B:176:GLN:CA	1:B:176:GLN:HE21	2.12	0.60
2:E:19:DA:H2"	2:E:20:DA:O5'	2.00	0.60
2:G:13:DG:N2	3:H:45:DT:H3	1.99	0.60
1:B:221:GLN:HA	1:B:224:ILE:CD1	2.31	0.60
3:H:32:DC:H2'	3:H:33:DG:N7	2.16	0.60
1:A:13:THR:HG21	1:B:10:GLN:HB3	1.84	0.60
1:A:151:ARG:HA	1:A:237:TYR:OH	2.02	0.60
1:B:40:VAL:CG2	1:B:41:PRO:HD2	2.25	0.60
1:B:149:LEU:HD22	1:B:149:LEU:H	1.66	0.60
1:A:125:ASN:O	1:A:128:GLN:N	2.35	0.60
1:A:281:ALA:HB3	1:A:284:ASP:HB2	1.83	0.60
1:A:227:ASN:OD1	1:A:266:LEU:HD23	2.02	0.60
1:B:220:GLN:HG3	1:B:259:VAL:HG22	1.84	0.60
2:G:15:DA:H2'	2:G:16:DT:H71	1.82	0.60
1:A:26:ALA:O	1:A:30:ARG:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:43:DA:H2"	3:F:44:DC:C5'	2.31	0.59
1:A:214:VAL:HG22	1:A:218:ARG:HG2	1.84	0.59
1:A:86:ALA:HB2	1:B:170:SER:CA	2.32	0.59
1:B:337:VAL:O	1:B:339:SER:N	2.35	0.59
2:G:27:DT:H6	2:G:27:DT:H5'	1.68	0.59
1:A:88:THR:H	1:A:91:GLN:NE2	1.99	0.59
1:A:100:GLN:O	1:A:101:GLN:C	2.40	0.59
1:A:108:ARG:NH2	2:C:10:DC:OP1	2.36	0.59
1:A:198:ASP:OD1	1:A:198:ASP:C	2.37	0.59
1:B:148:PHE:HD1	1:B:148:PHE:C	2.06	0.59
1:A:140:LEU:HD21	1:A:334:GLU:HA	1.84	0.59
1:A:288:PHE:O	1:A:291:MET:N	2.35	0.59
2:E:4:DG:N3	2:E:4:DG:H2'	2.17	0.59
1:A:291:MET:CE	1:A:295:LEU:HD11	2.33	0.59
1:B:208:LEU:HD23	1:B:212:GLU:HB3	1.84	0.58
1:A:100:GLN:CD	2:C:8:DT:H73	2.22	0.58
1:B:24:THR:O	1:B:27:GLU:HB3	2.03	0.58
1:B:158:LYS:HD2	3:D:56:DA:OP2	2.03	0.58
1:B:329:LEU:HB3	1:B:333:TRP:CZ2	2.38	0.58
1:A:166:LYS:CE	1:A:297:GLU:HB3	2.33	0.58
1:A:21:LEU:HD21	1:B:35:ALA:HB1	1.85	0.58
1:A:333:TRP:HA	1:A:336:CYS:HB3	1.84	0.58
1:B:75:ALA:HA	1:B:78:GLN:HB2	1.84	0.58
3:D:34:DA:C3'	3:D:35:DC:H5"	2.33	0.58
1:A:21:LEU:HD21	1:B:35:ALA:CB	2.34	0.58
1:A:139:LEU:CD2	1:A:271:LEU:HD22	2.34	0.58
1:B:328:LYS:C	1:B:330:PRO:HD2	2.24	0.58
2:G:6:DT:C2'	2:G:7:DG:H5"	2.34	0.58
3:H:32:DC:H2'	3:H:33:DG:C8	2.38	0.58
1:A:68:PRO:HD3	2:C:16:DT:O2	2.04	0.58
1:A:86:ALA:HB2	1:B:170:SER:HA	1.84	0.58
1:A:149:LEU:C	1:A:151:ARG:N	2.54	0.58
1:A:162:PHE:HD1	1:A:189:LYS:O	1.86	0.58
1:B:80:LEU:CD1	1:B:80:LEU:H	2.17	0.58
1:B:193:LEU:HD12	1:B:194:CYS:CA	2.34	0.58
1:A:152:ILE:CD1	1:A:152:ILE:C	2.72	0.57
1:B:72:TYR:CZ	1:B:106:ARG:HG3	2.38	0.57
1:B:160:ILE:HD11	1:B:193:LEU:HD23	1.84	0.57
1:B:212:GLU:HG3	1:B:213:THR:H	1.67	0.57
1:A:150:HIS:CA	1:A:199:GLN:HE22	2.15	0.57
1:B:183:ARG:HG2	1:B:184:PRO:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLN:NE2	2:C:8:DT:H3'	2.19	0.57
1:A:208:LEU:HB3	1:A:212:GLU:CB	2.34	0.57
3:H:52:DC:H2"	3:H:53:DC:O5'	2.04	0.57
1:B:124:LEU:HD11	1:B:132:ARG:HH11	1.69	0.57
3:D:55:DG:H2'	3:D:56:DA:O4'	2.04	0.57
2:G:17:DG:N2	3:H:41:DA:C2	2.72	0.57
1:B:33:VAL:HG23	1:B:38:GLU:HA	1.86	0.57
1:B:257:ARG:HB2	2:G:8:DT:H5'	1.85	0.57
2:C:20:DA:H2"	2:C:21:DT:H5'	1.87	0.57
1:A:7:ASN:HD21	1:A:9:GLU:HB3	1.69	0.57
1:A:149:LEU:H	1:A:149:LEU:CD2	2.03	0.57
1:A:186:ARG:CG	3:H:55:DG:H4'	2.34	0.57
1:A:227:ASN:O	1:A:228:ARG:C	2.42	0.57
2:E:10:DC:C2'	2:E:11:DA:O5'	2.50	0.57
3:H:43:DA:H2"	3:H:44:DC:O5'	2.04	0.57
3:H:45:DT:C2'	3:H:46:DT:H5"	2.30	0.57
1:B:282:PRO:HG3	1:B:329:LEU:CD2	2.31	0.57
1:A:163:VAL:HG13	1:A:163:VAL:O	2.05	0.57
1:B:319:ASP:O	1:B:320:GLU:C	2.42	0.57
2:C:20:DA:H1'	2:C:21:DT:H5"	1.85	0.57
3:F:43:DA:H1'	3:F:44:DC:H5"	1.86	0.57
1:A:106:ARG:HH21	1:A:106:ARG:CG	2.18	0.56
1:A:125:ASN:O	1:A:127:ARG:N	2.38	0.56
2:C:19:DA:H2'	2:C:20:DA:H8	1.66	0.56
1:A:262:THR:O	1:A:266:LEU:CD1	2.51	0.56
1:A:331:GLU:O	1:A:335:LYS:HG3	2.04	0.56
2:C:19:DA:OP1	2:C:19:DA:H4'	2.03	0.56
1:A:296:ALA:O	1:A:298:GLN:N	2.39	0.56
1:B:40:VAL:HG13	1:B:41:PRO:CD	2.34	0.56
1:B:99:SER:HB3	3:F:45:DT:OP2	2.05	0.56
1:A:7:ASN:OD1	1:A:10:GLN:N	2.38	0.56
1:A:71:ARG:HG3	3:D:44:DC:O5'	2.05	0.56
1:A:230:LEU:HD23	1:A:234:ARG:HB2	1.86	0.56
1:B:162:PHE:HE1	1:B:191:THR:HG23	1.70	0.56
1:A:282:PRO:HG3	1:A:329:LEU:CD2	2.25	0.56
1:B:168:LYS:HE2	1:B:181:THR:HG23	1.88	0.56
1:A:77:LEU:HD12	1:A:110:MET:CE	2.35	0.56
1:B:78:GLN:O	1:B:78:GLN:NE2	2.36	0.56
1:B:162:PHE:CE1	1:B:191:THR:HG23	2.41	0.56
1:B:166:LYS:H	1:B:166:LYS:CD	2.14	0.56
1:B:173:ASP:O	1:B:176:GLN:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:25:DG:N2	3:D:33:DG:N2	2.53	0.56
1:B:138:ILE:O	1:B:141:SER:HB3	2.06	0.56
3:H:53:DC:H2"	3:H:54:DT:O5'	2.05	0.56
1:A:175:GLY:O	1:A:176:GLN:NE2	2.38	0.56
1:B:148:PHE:C	1:B:148:PHE:CD1	2.77	0.56
1:A:281:ALA:CB	1:A:284:ASP:HB2	2.36	0.56
1:B:72:TYR:OH	1:B:106:ARG:CG	2.54	0.56
1:B:139:LEU:HD21	1:B:272:PRO:HG2	1.87	0.56
1:A:121:PRO:HD3	3:F:56:DA:N7	2.21	0.56
1:A:203:ILE:HD11	1:A:234:ARG:CZ	2.36	0.56
1:A:35:ALA:HB2	1:B:21:LEU:HD21	1.88	0.55
1:A:96:LEU:HD12	1:A:96:LEU:N	2.21	0.55
1:B:281:ALA:HB3	1:B:284:ASP:HB2	1.88	0.55
1:B:106:ARG:NH1	3:F:44:DC:OP1	2.39	0.55
1:B:124:LEU:HD21	1:B:343:TYR:OH	2.06	0.55
1:A:193:LEU:HD12	1:A:193:LEU:C	2.25	0.55
3:H:53:DC:C2'	3:H:54:DT:O5'	2.55	0.55
1:A:244:VAL:C	1:A:245:ILE:HD13	2.27	0.55
1:A:285:TYR:OH	1:A:329:LEU:HD22	2.06	0.55
1:B:197:TRP:HE1	1:B:283:SER:HB3	1.72	0.55
3:D:55:DG:H5'	3:D:55:DG:C8	2.41	0.55
1:A:100:GLN:O	1:A:103:VAL:N	2.39	0.55
1:B:49:TRP:HA	1:B:49:TRP:CE3	2.41	0.55
1:B:320:GLU:O	1:B:321:PHE:C	2.43	0.55
3:F:41:DA:C8	3:F:42:DT:H71	2.42	0.55
2:G:26:DT:H2"	2:G:27:DT:H71	1.89	0.55
3:H:45:DT:H2"	3:H:46:DT:H5'	1.81	0.55
3:D:42:DT:H2"	3:D:43:DA:O5'	2.07	0.55
1:A:191:THR:HG22	1:A:208:LEU:O	2.06	0.55
1:B:195:VAL:CG2	1:B:196:TRP:N	2.68	0.55
1:A:221:GLN:O	1:A:225:ASN:ND2	2.39	0.55
1:B:103:VAL:O	1:B:104:SER:C	2.45	0.55
3:D:38:DT:H2"	3:D:39:DT:C5'	2.36	0.55
1:B:84:ASP:O	1:B:87:GLN:HG3	2.06	0.55
1:B:221:GLN:O	1:B:225:ASN:ND2	2.40	0.54
2:G:18:DA:H2"	2:G:19:DA:OP2	2.07	0.54
1:A:158:LYS:HG2	1:A:159:TRP:N	2.21	0.54
1:A:230:LEU:HD23	1:A:230:LEU:O	2.07	0.54
1:A:24:THR:OG1	1:A:25:ALA:N	2.41	0.54
1:A:245:ILE:HD13	1:A:245:ILE:N	2.22	0.54
1:B:139:LEU:HD22	1:B:271:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:TRP:O	1:B:337:VAL:HG12	2.08	0.54
2:G:15:DA:H2"	2:G:16:DT:C6	2.42	0.54
1:A:33:VAL:CG1	1:A:34:GLU:N	2.71	0.54
1:A:263:LEU:HA	1:A:266:LEU:HD13	1.89	0.54
1:B:120:VAL:HG13	1:B:121:PRO:HD2	1.90	0.54
1:B:159:TRP:CE3	1:B:192:MET:HB2	2.42	0.54
1:B:246:PHE:HE2	1:B:248:HIS:ND1	2.06	0.54
1:B:248:HIS:O	1:B:248:HIS:CD2	2.61	0.54
1:B:293:HIS:C	1:B:295:LEU:H	2.09	0.54
1:B:333:TRP:O	1:B:336:CYS:N	2.41	0.54
1:B:125:ASN:O	1:B:126:GLU:C	2.46	0.54
1:A:68:PRO:HD2	3:D:42:DT:O2	2.08	0.54
1:B:120:VAL:HG11	1:B:343:TYR:CD1	2.43	0.54
2:E:22:DG:H8	2:E:22:DG:H5'	1.72	0.54
1:A:50:PHE:O	1:A:53:PHE:N	2.35	0.54
3:H:31:DA:H2"	3:H:32:DC:O5'	2.08	0.54
1:A:43:VAL:O	1:A:47:GLU:HG3	2.07	0.54
1:A:58:PHE:CG	1:A:58:PHE:O	2.61	0.54
1:A:80:LEU:HD22	1:A:96:LEU:HD11	1.90	0.54
1:A:21:LEU:HD23	1:A:21:LEU:N	2.23	0.53
3:D:32:DC:H2"	3:D:33:DG:C8	2.43	0.53
3:H:42:DT:H2"	3:H:43:DA:N7	2.23	0.53
3:H:48:DT:C2'	3:H:49:DA:H5'	2.29	0.53
1:A:317:LYS:HD2	1:A:321:PHE:CD2	2.42	0.53
1:A:10:GLN:O	1:A:13:THR:HB	2.08	0.53
1:B:12:ARG:NH1	1:B:59:ASP:HB3	2.23	0.53
1:A:267:ASN:O	1:A:268:TRP:C	2.46	0.53
1:A:313:TRP:CZ2	1:A:317:LYS:HE2	2.43	0.53
1:B:31:MET:O	1:B:34:GLU:HG2	2.07	0.53
1:B:322:TYR:O	1:B:323:TRP:C	2.46	0.53
2:C:19:DA:OP1	2:C:19:DA:O4'	2.27	0.53
3:D:54:DT:H2"	3:D:55:DG:C5'	2.37	0.53
1:B:24:THR:O	1:B:25:ALA:C	2.47	0.53
1:B:40:VAL:HG13	1:B:41:PRO:N	2.23	0.53
1:B:176:GLN:HE21	1:B:176:GLN:N	2.07	0.53
1:B:296:ALA:C	1:B:298:GLN:N	2.61	0.53
1:B:39:GLN:CD	1:B:39:GLN:H	2.11	0.53
2:C:20:DA:C2	2:C:21:DT:C2	2.96	0.53
1:A:139:LEU:HD21	1:A:272:PRO:CD	2.39	0.53
1:A:151:ARG:HG3	1:A:245:ILE:HG12	1.91	0.53
1:A:216:ALA:O	1:A:217:ALA:C	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ARG:HA	1:B:145:ARG:HH11	1.73	0.53
1:B:256:ALA:HB3	1:B:259:VAL:HG23	1.90	0.53
2:E:12:DA:C2'	2:E:13:DG:H5"	2.30	0.53
2:G:5:DG:C2'	2:G:6:DT:H71	2.35	0.53
3:H:38:DT:H2"	3:H:39:DT:C5'	2.39	0.53
1:A:86:ALA:CB	1:B:170:SER:HA	2.38	0.53
1:A:245:ILE:CG2	1:A:271:LEU:HG	2.39	0.53
1:A:271:LEU:HD23	1:A:272:PRO:HD3	1.91	0.53
1:A:291:MET:HE3	1:A:295:LEU:HD11	1.89	0.53
1:A:337:VAL:O	1:A:339:SER:N	2.42	0.53
1:B:219:TYR:O	1:B:223:LEU:HD12	2.08	0.53
2:C:5:DG:H2"	2:C:6:DT:H5"	1.91	0.53
1:A:31:MET:O	1:A:34:GLU:HG2	2.09	0.52
1:A:275:ALA:HB1	1:A:276:TYR:CD1	2.44	0.52
1:B:286:HIS:CE1	1:B:321:PHE:HE2	2.27	0.52
1:B:12:ARG:HG3	1:B:49:TRP:CD2	2.44	0.52
1:B:251:ALA:HB3	1:B:254:HIS:CD2	2.44	0.52
2:E:6:DT:H2'	2:E:6:DT:O5'	2.09	0.52
1:B:13:THR:HA	1:B:16:ILE:HD12	1.92	0.52
1:B:164:ASN:HD21	1:B:295:LEU:HD13	1.74	0.52
1:B:214:VAL:HA	1:B:218:ARG:HG2	1.91	0.52
1:B:220:GLN:O	1:B:224:ILE:HG13	2.10	0.52
1:A:11:THR:HG21	1:A:41:PRO:HG2	1.92	0.52
1:A:74:ASP:C	1:A:76:GLU:H	2.13	0.52
1:A:153:VAL:O	1:A:153:VAL:CG1	2.58	0.52
1:B:79:ALA:O	1:B:82:ASP:HB2	2.10	0.52
1:B:329:LEU:HB3	1:B:333:TRP:CH2	2.45	0.52
3:D:42:DT:H5"	3:D:42:DT:C6	2.38	0.52
3:F:32:DC:H2"	3:F:33:DG:C8	2.45	0.52
1:A:152:ILE:HD13	1:A:152:ILE:C	2.22	0.52
3:F:45:DT:C2'	3:F:46:DT:H71	2.40	0.52
1:B:96:LEU:HB3	1:B:98:VAL:CG2	2.40	0.52
1:B:134:ASN:HA	1:B:137:GLU:HB2	1.92	0.52
1:B:263:LEU:O	1:B:266:LEU:N	2.40	0.52
1:A:176:GLN:CA	1:A:176:GLN:HE21	2.23	0.52
1:A:183:ARG:NH1	1:B:119:TRP:HB3	2.25	0.52
2:C:24:DC:H2"	2:C:25:DG:C8	2.45	0.52
1:A:96:LEU:C	1:A:98:VAL:HG12	2.30	0.52
1:A:333:TRP:O	1:A:334:GLU:C	2.47	0.52
1:B:223:LEU:O	1:B:226:LEU:CB	2.49	0.52
2:C:20:DA:H2"	2:C:21:DT:C5'	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ARG:NH2	3:D:53:DC:OP2	2.42	0.52
3:D:44:DC:H2"	3:D:45:DT:OP2	2.09	0.52
2:G:7:DG:H2"	2:G:8:DT:C6	2.45	0.52
1:A:186:ARG:CB	3:H:55:DG:H4'	2.40	0.51
1:B:151:ARG:HD2	1:B:243:ARG:O	2.10	0.51
1:B:166:LYS:HD3	1:B:166:LYS:N	2.16	0.51
1:B:285:TYR:OH	1:B:329:LEU:HD22	2.10	0.51
3:H:33:DG:OP2	3:H:33:DG:C8	2.56	0.51
1:A:12:ARG:O	1:A:16:ILE:HG12	2.11	0.51
1:A:31:MET:O	1:A:35:ALA:N	2.40	0.51
1:B:161:PHE:CD1	3:H:56:DA:C6	2.98	0.51
1:A:166:LYS:HE3	1:A:297:GLU:OE2	2.10	0.51
1:B:279:ASP:C	1:B:280:LEU:HD22	2.31	0.51
1:B:110:MET:O	1:B:111:GLY:C	2.49	0.51
2:G:7:DG:H8	2:G:7:DG:C5'	2.20	0.51
1:A:149:LEU:HD22	1:A:149:LEU:N	2.08	0.51
1:B:43:VAL:O	1:B:44:LYS:C	2.46	0.51
1:B:77:LEU:HB2	1:B:96:LEU:HD21	1.93	0.51
3:D:33:DG:H2"	3:D:34:DA:O5'	2.11	0.51
3:H:45:DT:H4'	3:H:45:DT:OP1	2.11	0.51
1:B:79:ALA:HB3	1:B:80:LEU:HD12	1.92	0.51
1:B:29:HIS:O	1:B:33:VAL:HG12	2.11	0.51
1:A:11:THR:HG22	1:A:12:ARG:N	2.24	0.51
1:A:74:ASP:O	1:A:76:GLU:N	2.44	0.51
1:A:125:ASN:CB	1:A:128:GLN:HG3	2.41	0.51
1:A:271:LEU:CD2	1:A:272:PRO:HD3	2.41	0.51
1:B:219:TYR:O	1:B:222:GLN:HB2	2.11	0.51
1:B:333:TRP:O	1:B:334:GLU:C	2.49	0.51
1:A:329:LEU:HD12	1:A:333:TRP:CE2	2.45	0.51
1:B:217:ALA:O	1:B:218:ARG:C	2.48	0.51
1:A:71:ARG:N	3:D:44:DC:OP1	2.44	0.50
1:A:276:TYR:CD1	1:A:276:TYR:N	2.79	0.50
1:B:11:THR:HG22	1:B:12:ARG:N	2.26	0.50
2:E:4:DG:OP2	2:E:4:DG:C4'	2.57	0.50
1:A:62:ASP:OD1	2:C:20:DA:H5"	2.11	0.50
1:A:125:ASN:O	1:A:126:GLU:C	2.50	0.50
1:A:134:ASN:O	1:A:135:THR:C	2.49	0.50
1:A:172:VAL:O	1:B:113:ILE:HG13	2.10	0.50
1:A:183:ARG:HG3	1:A:183:ARG:HH11	1.76	0.50
1:A:208:LEU:CD2	1:A:213:THR:O	2.59	0.50
1:B:100:GLN:O	1:B:101:GLN:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLY:N	3:D:51:DA:OP1	2.39	0.50
3:D:44:DC:C2'	3:D:45:DT:OP2	2.58	0.50
1:A:333:TRP:C	1:A:335:LYS:N	2.64	0.50
1:B:237:TYR:CD1	1:B:244:VAL:CG2	2.85	0.50
1:A:323:TRP:NE1	1:A:327:HIS:NE2	2.59	0.50
1:B:29:HIS:C	1:B:29:HIS:CD2	2.85	0.50
1:B:289:ALA:O	1:B:290:SER:C	2.49	0.50
3:F:45:DT:H2"	3:F:46:DT:O5'	2.11	0.50
1:A:162:PHE:CD1	1:A:189:LYS:O	2.64	0.50
1:B:318:ASP:O	1:B:319:ASP:C	2.50	0.50
3:F:38:DT:H2"	3:F:39:DT:C5'	2.32	0.50
1:A:208:LEU:HD23	1:A:213:THR:O	2.12	0.50
1:B:227:ASN:OD1	1:B:266:LEU:HD11	2.12	0.50
1:B:237:TYR:HD1	1:B:244:VAL:HG22	1.70	0.50
2:G:7:DG:C8	2:G:7:DG:C5'	2.95	0.50
1:A:72:TYR:O	1:A:72:TYR:CD1	2.65	0.49
1:A:147:SER:OG	1:A:149:LEU:HD23	2.11	0.49
1:A:266:LEU:HD12	1:A:266:LEU:N	2.26	0.49
1:A:291:MET:O	1:A:294:ALA:HB3	2.12	0.49
1:B:220:GLN:HA	1:B:223:LEU:HD13	1.94	0.49
1:B:317:LYS:HB3	1:B:321:PHE:HD1	1.76	0.49
3:F:30:DA:H2"	3:F:31:DA:O5'	2.11	0.49
3:F:43:DA:C2	3:F:44:DC:C2	2.99	0.49
1:A:77:LEU:HD12	1:A:110:MET:HE3	1.94	0.49
1:A:176:GLN:HE21	1:A:176:GLN:HA	1.77	0.49
2:C:14:DT:H2"	2:C:15:DA:O5'	2.12	0.49
1:B:15:LEU:N	1:B:15:LEU:CD1	2.74	0.49
1:B:100:GLN:O	1:B:100:GLN:HG2	2.09	0.49
1:B:106:ARG:HH11	3:F:44:DC:P	2.35	0.49
3:F:41:DA:C1'	3:F:42:DT:H5"	2.37	0.49
1:A:280:LEU:O	1:A:282:PRO:HD3	2.12	0.49
1:B:198:ASP:C	1:B:198:ASP:OD1	2.51	0.49
1:B:291:MET:O	1:B:292:GLY:C	2.51	0.49
1:B:337:VAL:O	1:B:338:ALA:C	2.51	0.49
3:D:41:DA:OP2	3:D:41:DA:H8	1.95	0.49
2:G:20:DA:C1'	2:G:21:DT:H5"	2.42	0.49
1:A:89:GLN:HE22	2:C:8:DT:H3'	1.77	0.49
1:B:124:LEU:HG	1:B:343:TYR:HE1	1.77	0.49
1:B:331:GLU:HG3	1:B:332:ARG:N	2.26	0.49
1:A:193:LEU:HD11	1:A:195:VAL:HG12	1.94	0.49
1:A:274:ALA:O	1:A:277:SER:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:LEU:HD11	1:B:32:LEU:HD21	1.95	0.49
1:B:158:LYS:HE3	1:B:291:MET:CE	2.43	0.49
1:A:15:LEU:HD21	1:A:46:CYS:HB3	1.95	0.49
1:A:68:PRO:CD	3:D:42:DT:O2	2.60	0.49
1:A:91:GLN:O	1:A:95:GLN:HG3	2.12	0.49
1:A:226:LEU:O	1:A:227:ASN:C	2.50	0.49
1:B:138:ILE:HG22	1:B:139:LEU:N	2.28	0.49
1:B:293:HIS:C	1:B:295:LEU:N	2.66	0.49
1:A:11:THR:O	1:A:12:ARG:C	2.51	0.49
1:A:42:THR:O	1:A:45:THR:N	2.45	0.49
1:A:216:ALA:O	1:A:220:GLN:HG3	2.13	0.49
1:B:43:VAL:CG1	1:B:44:LYS:N	2.76	0.49
2:G:26:DT:C2'	2:G:27:DT:H71	2.43	0.49
1:A:86:ALA:HB2	1:B:170:SER:HB2	1.93	0.49
2:C:16:DT:H2"	2:C:17:DG:O4'	2.13	0.49
1:A:93:ALA:C	1:A:95:GLN:H	2.16	0.48
1:A:129:MET:O	1:A:130:GLU:C	2.50	0.48
1:A:222:GLN:HA	1:A:225:ASN:HD22	1.77	0.48
1:B:285:TYR:CD2	1:B:286:HIS:N	2.80	0.48
1:A:227:ASN:ND2	1:A:231:GLN:NE2	2.61	0.48
1:A:320:GLU:O	1:A:321:PHE:C	2.50	0.48
1:B:15:LEU:HD11	1:B:32:LEU:CD2	2.42	0.48
1:A:146:LYS:CE	1:A:147:SER:H	2.26	0.48
1:A:230:LEU:C	1:A:230:LEU:CD2	2.81	0.48
2:G:20:DA:C2'	2:G:21:DT:H5"	2.43	0.48
2:C:25:DG:C2	3:D:33:DG:N2	2.81	0.48
1:B:252:PRO:HA	1:B:255:THR:CG2	2.43	0.48
1:B:280:LEU:O	1:B:282:PRO:HD3	2.13	0.48
2:E:4:DG:N2	2:E:5:DG:C5	2.81	0.48
1:A:170:SER:CA	1:B:86:ALA:HB2	2.43	0.48
1:B:218:ARG:O	1:B:222:GLN:HG3	2.13	0.48
2:C:19:DA:H2"	2:C:20:DA:O5'	2.14	0.48
1:A:125:ASN:HB3	1:A:128:GLN:HG3	1.94	0.48
1:A:219:TYR:O	1:A:220:GLN:C	2.52	0.48
1:B:30:ARG:O	1:B:33:VAL:CG1	2.61	0.48
1:B:212:GLU:HG3	1:B:213:THR:N	2.28	0.48
1:B:335:LYS:O	1:B:336:CYS:C	2.51	0.48
3:F:41:DA:H2"	3:F:42:DT:OP2	2.13	0.48
1:A:171:TYR:CE2	1:B:114:GLN:HB2	2.49	0.48
1:B:143:TYR:CE1	1:B:149:LEU:HD21	2.49	0.48
1:B:271:LEU:HD13	1:B:272:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:VAL:O	1:A:105:ASN:N	2.47	0.48
1:B:63:LYS:HD3	1:B:64:GLU:N	2.29	0.48
1:B:123:GLU:OE2	1:B:123:GLU:HA	2.14	0.48
1:A:154:THR:HB	1:A:247:LEU:HB3	1.95	0.48
1:B:258:ALA:O	1:B:262:THR:N	2.47	0.48
2:C:4:DG:C5	3:D:54:DT:H73	2.48	0.48
3:D:44:DC:H1'	3:D:45:DT:H5"	1.96	0.48
2:G:15:DA:H2'	2:G:16:DT:C7	2.43	0.48
1:A:124:LEU:HB3	1:A:129:MET:HG3	1.95	0.47
1:B:16:ILE:HG12	1:B:53:PHE:CZ	2.49	0.47
1:B:142:ARG:HG2	1:B:148:PHE:HE2	1.78	0.47
1:B:236:GLU:C	1:B:238:GLN:H	2.18	0.47
1:B:43:VAL:CG1	1:B:44:LYS:H	2.27	0.47
1:B:334:GLU:O	1:B:337:VAL:HG13	2.14	0.47
2:C:19:DA:H2"	2:C:20:DA:C5'	2.45	0.47
1:A:45:THR:HG22	1:A:46:CYS:N	2.29	0.47
1:A:46:CYS:O	1:A:47:GLU:C	2.52	0.47
1:A:216:ALA:O	1:A:217:ALA:O	2.31	0.47
1:B:136:CYS:O	1:B:138:ILE:N	2.47	0.47
1:B:209:LYS:HA	1:B:303:TYR:HE1	1.78	0.47
2:C:26:DT:H2"	2:C:27:DT:H71	1.95	0.47
1:A:89:GLN:O	1:A:91:GLN:N	2.48	0.47
1:A:118:ARG:NH1	1:A:344:PHE:O	2.47	0.47
1:A:207:LEU:HD21	1:A:306:VAL:HG11	1.95	0.47
1:A:286:HIS:NE2	1:A:321:PHE:CE1	2.81	0.47
1:B:99:SER:OG	1:B:102:ALA:HB2	2.13	0.47
1:B:251:ALA:O	1:B:255:THR:HG22	2.15	0.47
3:H:35:DC:H2"	3:H:36:DA:H8	1.79	0.47
1:A:5:VAL:HG12	1:A:6:PRO:HD2	1.91	0.47
1:A:110:MET:O	1:A:112:LYS:N	2.46	0.47
1:B:249:ASP:O	1:B:251:ALA:N	2.45	0.47
2:C:4:DG:N2	2:C:5:DG:C4	2.82	0.47
1:A:170:SER:OG	1:A:178:ALA:HB1	2.15	0.47
1:A:98:VAL:CG2	1:A:102:ALA:CB	2.93	0.47
1:A:101:GLN:O	1:A:104:SER:HB3	2.15	0.47
1:A:115:LYS:HD2	1:B:176:GLN:O	2.15	0.47
1:A:146:LYS:HE2	1:A:147:SER:H	1.80	0.47
1:A:237:TYR:CD1	1:A:244:VAL:HG23	2.50	0.47
1:B:12:ARG:HG3	1:B:49:TRP:CZ2	2.50	0.47
1:B:251:ALA:HB1	1:B:252:PRO:CD	2.41	0.47
1:B:256:ALA:HB3	1:B:259:VAL:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:LEU:N	1:B:280:LEU:CD2	2.78	0.47
1:B:283:SER:O	1:B:287:LEU:HB3	2.14	0.47
2:C:4:DG:N3	2:C:4:DG:C2'	2.71	0.47
3:D:53:DC:H2"	3:D:54:DT:O2	2.13	0.47
3:F:43:DA:C1'	3:F:44:DC:H5"	2.44	0.47
1:B:323:TRP:CE2	1:B:327:HIS:CD2	3.03	0.47
2:C:5:DG:C2'	2:C:6:DT:H5"	2.44	0.47
2:C:21:DT:H2"	2:C:22:DG:O5'	2.13	0.47
3:D:34:DA:H2"	3:D:35:DC:C5'	2.35	0.47
1:A:45:THR:CA	1:A:48:ARG:HG3	2.45	0.47
1:B:158:LYS:HE3	1:B:291:MET:HE2	1.97	0.47
1:B:172:VAL:HG23	1:B:173:ASP:H	1.80	0.47
1:B:203:ILE:HG22	1:B:204:TYR:N	2.29	0.47
1:B:282:PRO:HG2	1:B:329:LEU:HD21	1.95	0.47
1:A:337:VAL:O	1:A:340:ASP:N	2.32	0.47
1:B:296:ALA:O	1:B:298:GLN:N	2.48	0.47
3:F:54:DT:H6	3:F:54:DT:H2'	1.49	0.47
1:B:159:TRP:O	1:B:160:ILE:HG12	2.14	0.46
1:B:193:LEU:C	1:B:193:LEU:CD1	2.75	0.46
1:B:321:PHE:O	1:B:322:TYR:C	2.51	0.46
1:A:197:TRP:HB3	1:A:202:VAL:HA	1.97	0.46
1:A:321:PHE:C	1:A:321:PHE:HD1	2.17	0.46
1:A:327:HIS:O	1:A:330:PRO:HD2	2.15	0.46
1:A:341:GLY:O	1:A:342:LYS:C	2.52	0.46
1:B:215:ASN:OD1	1:B:217:ALA:N	2.48	0.46
1:B:337:VAL:C	1:B:339:SER:N	2.66	0.46
1:B:311:ASP:O	1:B:312:GLU:C	2.52	0.46
1:B:285:TYR:O	1:B:289:ALA:CB	2.63	0.46
2:G:12:DA:C2	3:H:46:DT:N3	2.83	0.46
1:A:77:LEU:C	1:A:77:LEU:CD1	2.78	0.46
1:A:193:LEU:N	1:A:207:LEU:HD13	2.30	0.46
1:B:7:ASN:HD21	1:B:9:GLU:HB3	1.81	0.46
1:B:18:CYS:HB3	1:B:28:SER:OG	2.16	0.46
1:B:121:PRO:HB2	1:B:343:TYR:CZ	2.50	0.46
1:B:164:ASN:HD21	1:B:295:LEU:CD1	2.29	0.46
3:F:37:DT:H2"	3:F:38:DT:O5'	2.14	0.46
1:B:40:VAL:HG13	1:B:41:PRO:HD2	1.96	0.46
1:B:191:THR:OG1	1:B:207:LEU:HD11	2.14	0.46
1:B:259:VAL:HG12	1:B:263:LEU:CD1	2.45	0.46
2:C:18:DA:H2"	2:C:19:DA:C8	2.47	0.46
1:A:43:VAL:HA	1:A:46:CYS:SG	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:DT:H1'	2:E:28:DT:H5"	1.97	0.46
1:A:158:LYS:HG2	1:A:159:TRP:O	2.15	0.46
1:B:72:TYR:CE1	1:B:106:ARG:HG3	2.51	0.46
1:B:134:ASN:O	1:B:137:GLU:N	2.49	0.46
1:B:254:HIS:CD2	1:B:254:HIS:N	2.82	0.46
3:D:45:DT:H5'	3:D:45:DT:C6	2.45	0.46
1:B:151:ARG:HH11	1:B:245:ILE:HD11	1.73	0.46
3:H:33:DG:H2"	3:H:34:DA:H8	1.80	0.46
1:A:6:PRO:HG3	1:A:36:PHE:CD2	2.51	0.45
1:A:121:PRO:HD3	3:F:56:DA:C8	2.51	0.45
1:B:320:GLU:O	1:B:321:PHE:O	2.34	0.45
1:B:328:LYS:C	1:B:330:PRO:CD	2.85	0.45
3:F:44:DC:H2"	3:F:45:DT:C5'	2.46	0.45
1:A:77:LEU:HD21	1:A:107:LEU:HD21	1.97	0.45
1:A:105:ASN:O	1:A:108:ARG:N	2.50	0.45
1:B:220:GLN:NE2	1:B:258:ALA:CB	2.75	0.45
1:B:252:PRO:CA	1:B:255:THR:HG22	2.46	0.45
1:B:335:LYS:O	1:B:337:VAL:N	2.49	0.45
1:A:282:PRO:HA	1:A:285:TYR:CZ	2.50	0.45
3:H:33:DG:H2"	3:H:34:DA:C5'	2.23	0.45
1:A:251:ALA:HB3	1:A:254:HIS:CG	2.51	0.45
1:B:72:TYR:CE2	1:B:98:VAL:HG11	2.52	0.45
1:B:158:LYS:HD2	3:D:56:DA:P	2.57	0.45
1:B:202:VAL:CG2	1:B:203:ILE:H	2.15	0.45
1:B:235:PRO:O	1:B:236:GLU:C	2.54	0.45
1:B:271:LEU:HD13	1:B:272:PRO:CD	2.47	0.45
1:A:282:PRO:HA	1:A:285:TYR:CE1	2.51	0.45
1:B:88:THR:OG1	1:B:91:GLN:HG3	2.17	0.45
1:B:142:ARG:HG2	1:B:148:PHE:CD2	2.50	0.45
1:B:215:ASN:O	1:B:218:ARG:HB3	2.16	0.45
2:E:20:DA:C2	3:F:38:DT:O2	2.69	0.45
1:A:143:TYR:HE1	1:A:149:LEU:HD21	1.82	0.45
1:A:207:LEU:CD2	1:A:306:VAL:HG12	2.46	0.45
1:A:336:CYS:N	1:A:344:PHE:HE2	2.14	0.45
1:B:7:ASN:ND2	1:B:9:GLU:H	2.15	0.45
1:B:246:PHE:CE2	1:B:248:HIS:ND1	2.85	0.45
1:A:106:ARG:CG	1:A:106:ARG:NH2	2.78	0.45
1:A:271:LEU:HD22	1:A:272:PRO:HD2	1.99	0.45
1:B:293:HIS:O	1:B:296:ALA:N	2.50	0.45
1:A:15:LEU:N	1:A:15:LEU:HD12	2.32	0.45
1:A:170:SER:HB2	1:B:85:ASP:OD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:TRP:NE1	1:A:287:LEU:HD23	2.31	0.45
1:B:234:ARG:HB3	1:B:237:TYR:HD2	1.81	0.45
1:B:250:ASN:O	3:H:52:DC:H4'	2.17	0.45
1:A:207:LEU:HD21	1:A:306:VAL:CG1	2.47	0.45
1:B:15:LEU:HD12	1:B:15:LEU:H	1.77	0.45
1:B:101:GLN:H	1:B:101:GLN:NE2	2.15	0.45
2:E:26:DT:C5	2:E:27:DT:H73	2.52	0.45
3:F:46:DT:H4'	3:F:46:DT:OP1	2.17	0.45
1:A:78:GLN:O	1:A:78:GLN:NE2	2.50	0.45
1:A:165:PRO:HG3	1:A:184:PRO:HB3	1.98	0.44
1:B:29:HIS:O	1:B:29:HIS:HD2	2.01	0.44
1:A:5:VAL:CG1	1:A:6:PRO:CD	2.92	0.44
1:B:150:HIS:HA	1:B:199:GLN:OE1	2.17	0.44
1:B:245:ILE:HG23	1:B:269:GLU:HG2	1.99	0.44
1:A:47:GLU:O	1:A:50:PHE:HB2	2.18	0.44
1:A:229:ALA:O	1:A:230:LEU:C	2.55	0.44
1:A:263:LEU:O	1:A:266:LEU:HD13	2.17	0.44
1:A:266:LEU:O	1:A:267:ASN:HB3	2.17	0.44
1:B:285:TYR:HB2	3:D:55:DG:H21	1.82	0.44
1:B:302:SER:O	1:B:305:SER:HB2	2.18	0.44
2:E:21:DT:H2"	2:E:22:DG:OP2	2.17	0.44
2:E:22:DG:H5'	2:E:22:DG:C8	2.52	0.44
1:A:17:PHE:CE1	1:B:14:VAL:HG11	2.53	0.44
1:A:165:PRO:CG	1:A:184:PRO:HB3	2.48	0.44
1:A:324:ARG:O	1:A:328:LYS:HG3	2.17	0.44
1:B:14:VAL:O	1:B:17:PHE:HB3	2.16	0.44
1:B:101:GLN:H	1:B:101:GLN:CD	2.21	0.44
1:B:229:ALA:O	1:B:233:LYS:HB2	2.17	0.44
3:F:35:DC:H2"	3:F:36:DA:OP2	2.17	0.44
3:F:54:DT:C2'	3:F:55:DG:H5'	2.46	0.44
3:H:33:DG:C3'	3:H:34:DA:H5"	2.45	0.44
1:B:286:HIS:CE1	1:B:321:PHE:CE2	3.04	0.44
1:B:324:ARG:O	1:B:328:LYS:HG3	2.17	0.44
1:B:334:GLU:O	1:B:337:VAL:CG1	2.66	0.44
3:F:45:DT:H2"	3:F:46:DT:H71	2.00	0.44
1:B:249:ASP:HB2	3:H:53:DC:OP1	2.18	0.44
1:A:227:ASN:O	1:A:230:LEU:N	2.51	0.44
1:B:78:GLN:NE2	1:B:82:ASP:OD1	2.50	0.44
1:B:93:ALA:HB2	1:B:100:GLN:HA	1.98	0.44
1:B:132:ARG:O	1:B:133:LYS:C	2.53	0.44
1:A:21:LEU:O	1:A:22:LYS:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:MET:H	1:A:207:LEU:HD11	1.82	0.44
1:A:266:LEU:C	1:A:268:TRP:H	2.20	0.44
1:B:333:TRP:HA	1:B:336:CYS:HB3	2.00	0.44
1:A:49:TRP:CE3	1:A:49:TRP:HA	2.53	0.44
1:A:100:GLN:HE22	2:C:9:DA:H62	1.65	0.44
1:A:146:LYS:HA	1:A:146:LYS:CE	2.27	0.44
1:A:337:VAL:C	1:A:339:SER:N	2.71	0.44
1:B:84:ASP:HB3	1:B:87:GLN:NE2	2.33	0.44
1:B:161:PHE:CE1	3:H:56:DA:C4	3.06	0.44
1:B:333:TRP:C	1:B:335:LYS:N	2.70	0.44
2:E:23:DT:H2"	2:E:24:DC:O5'	2.18	0.44
1:A:21:LEU:C	1:A:23:LYS:N	2.70	0.43
1:A:328:LYS:O	1:A:332:ARG:HG2	2.17	0.43
1:B:121:PRO:HB2	1:B:343:TYR:CE2	2.53	0.43
1:B:151:ARG:HG3	1:B:245:ILE:HG12	2.00	0.43
2:C:6:DT:H2"	2:C:7:DG:O5'	2.18	0.43
2:C:8:DT:H2"	2:C:9:DA:O5'	2.18	0.43
1:A:106:ARG:HG3	1:A:106:ARG:NH2	2.24	0.43
1:A:195:VAL:HG23	1:A:196:TRP:N	2.33	0.43
1:B:313:TRP:O	1:B:315:ALA:N	2.51	0.43
2:C:15:DA:C8	2:C:16:DT:H72	2.53	0.43
1:A:11:THR:O	1:A:14:VAL:N	2.51	0.43
1:B:31:MET:HA	1:B:34:GLU:HG2	2.00	0.43
1:B:134:ASN:O	1:B:135:THR:C	2.56	0.43
1:B:232:ARG:HG3	1:B:233:LYS:N	2.33	0.43
1:B:247:LEU:HD11	1:B:273:HIS:HD2	1.84	0.43
2:G:20:DA:H2"	2:G:21:DT:H5"	2.00	0.43
1:A:142:ARG:HA	1:A:145:ARG:HH11	1.83	0.43
1:A:210:PRO:HD3	1:A:303:TYR:CD1	2.54	0.43
1:A:222:GLN:O	1:A:223:LEU:C	2.57	0.43
1:B:101:GLN:HG3	3:F:46:DT:H73	2.00	0.43
1:B:107:LEU:O	1:B:110:MET:O	2.36	0.43
1:B:110:MET:O	1:B:112:LYS:N	2.51	0.43
1:B:309:TRP:HA	1:B:312:GLU:OE1	2.17	0.43
1:B:332:ARG:O	1:B:333:TRP:C	2.56	0.43
1:A:98:VAL:HG22	1:A:99:SER:O	2.19	0.43
2:G:27:DT:C2'	2:G:28:DT:H71	2.48	0.43
1:A:50:PHE:HA	1:A:53:PHE:CD2	2.47	0.43
1:A:175:GLY:O	1:A:176:GLN:HB2	2.17	0.43
1:B:139:LEU:CD2	1:B:271:LEU:HD11	2.49	0.43
1:A:53:PHE:C	1:A:56:GLY:H	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:TYR:CE2	1:A:223:LEU:HD11	2.54	0.43
1:A:288:PHE:O	1:A:289:ALA:C	2.56	0.43
2:E:11:DA:H2"	2:E:12:DA:H5"	2.00	0.43
1:A:25:ALA:O	1:A:27:GLU:N	2.52	0.43
1:B:85:ASP:OD2	1:B:85:ASP:O	2.37	0.43
3:H:54:DT:H2"	3:H:55:DG:C5'	2.49	0.43
1:A:224:ILE:O	1:A:225:ASN:C	2.57	0.43
1:B:138:ILE:O	1:B:139:LEU:C	2.56	0.43
1:A:136:CYS:O	1:A:139:LEU:N	2.52	0.42
1:A:152:ILE:HD13	1:A:245:ILE:O	2.19	0.42
1:A:168:LYS:HE3	1:A:181:THR:HG21	2.00	0.42
1:B:43:VAL:O	1:B:46:CYS:N	2.52	0.42
3:H:54:DT:H2"	3:H:55:DG:O5'	2.19	0.42
1:A:207:LEU:C	1:A:207:LEU:HD12	2.40	0.42
1:A:326:ILE:O	1:A:326:ILE:HG22	2.18	0.42
1:B:220:GLN:O	1:B:221:GLN:C	2.55	0.42
1:B:235:PRO:O	1:B:238:GLN:N	2.51	0.42
3:F:38:DT:H2"	3:F:39:DT:O4'	2.19	0.42
2:G:22:DG:N3	3:H:36:DA:C2	2.87	0.42
3:H:42:DT:H2"	3:H:43:DA:C8	2.55	0.42
1:A:166:LYS:HD2	1:A:297:GLU:CB	2.35	0.42
1:B:209:LYS:O	1:B:212:GLU:HB2	2.18	0.42
1:B:264:GLU:C	1:B:266:LEU:H	2.22	0.42
3:D:42:DT:H2"	3:D:43:DA:C5'	2.49	0.42
1:A:279:ASP:O	1:A:280:LEU:HD13	2.20	0.42
1:B:161:PHE:CD1	3:H:56:DA:C5	3.07	0.42
1:B:197:TRP:HA	1:B:203:ILE:HG12	2.02	0.42
3:D:36:DA:H2"	3:D:37:DT:O5'	2.19	0.42
1:A:89:GLN:HB3	1:A:100:GLN:HG2	2.00	0.42
1:A:140:LEU:HD13	1:A:333:TRP:HB2	2.00	0.42
1:A:192:MET:H	1:A:207:LEU:CD1	2.33	0.42
1:A:259:VAL:HA	1:A:262:THR:OG1	2.20	0.42
1:A:271:LEU:HD22	1:A:272:PRO:CD	2.49	0.42
1:B:100:GLN:HE21	1:B:100:GLN:HB3	1.61	0.42
1:B:215:ASN:N	1:B:218:ARG:HB3	2.30	0.42
1:B:286:HIS:NE2	1:B:325:GLY:HA3	2.35	0.42
2:G:8:DT:H2"	2:G:9:DA:H8	1.76	0.42
2:G:26:DT:C6	2:G:27:DT:H73	2.55	0.42
3:H:46:DT:H2"	3:H:47:DG:O5'	2.19	0.42
1:A:20:HIS:HB3	1:B:35:ALA:O	2.19	0.42
1:B:24:THR:HG23	1:B:27:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LEU:CD2	1:B:334:GLU:HA	2.50	0.42
1:B:331:GLU:CG	1:B:332:ARG:N	2.82	0.42
2:G:24:DC:H2"	2:G:25:DG:C8	2.54	0.42
1:A:23:LYS:HA	1:A:23:LYS:HD3	1.89	0.42
1:A:107:LEU:O	1:A:108:ARG:C	2.57	0.42
1:A:173:ASP:O	1:A:176:GLN:HB2	2.19	0.42
1:A:209:LYS:O	1:A:210:PRO:O	2.37	0.42
1:B:115:LYS:HE3	3:D:51:DA:H5"	2.01	0.42
1:B:197:TRP:CB	1:B:202:VAL:HA	2.50	0.42
1:B:286:HIS:CE1	1:B:325:GLY:CA	3.03	0.42
1:A:77:LEU:CD1	1:A:110:MET:SD	3.08	0.42
1:A:209:LYS:O	1:A:210:PRO:C	2.58	0.42
1:B:24:THR:O	1:B:27:GLU:CB	2.68	0.42
1:B:29:HIS:O	1:B:29:HIS:CD2	2.73	0.42
1:A:7:ASN:CG	1:A:8:LYS:N	2.73	0.42
1:A:208:LEU:HD21	1:A:214:VAL:HG23	2.02	0.42
1:A:328:LYS:O	1:A:329:LEU:C	2.58	0.42
1:B:256:ALA:CB	1:B:259:VAL:HG23	2.50	0.42
1:B:329:LEU:O	1:B:333:TRP:CD2	2.73	0.42
2:C:24:DC:H6	2:C:24:DC:H2'	1.70	0.42
2:G:12:DA:H2	3:H:46:DT:N3	2.17	0.42
3:H:33:DG:H2"	3:H:34:DA:C8	2.55	0.42
1:A:6:PRO:HA	1:A:10:GLN:HE22	1.81	0.42
1:A:65:HIS:HB3	2:C:19:DA:H1'	2.01	0.42
1:A:89:GLN:C	1:A:91:GLN:N	2.72	0.42
1:A:333:TRP:O	1:A:335:LYS:N	2.52	0.42
1:B:81:LEU:N	1:B:81:LEU:CD2	2.82	0.42
2:E:14:DT:H2"	2:E:15:DA:C8	2.55	0.42
3:F:45:DT:H2'	3:F:46:DT:H71	2.02	0.42
1:A:28:SER:HA	1:A:31:MET:SD	2.60	0.41
1:A:100:GLN:HE21	1:A:100:GLN:HB3	1.69	0.41
1:A:140:LEU:HD21	1:A:334:GLU:CA	2.49	0.41
1:A:146:LYS:HE3	1:A:146:LYS:CA	2.38	0.41
1:A:158:LYS:HB3	1:A:288:PHE:CE1	2.55	0.41
1:A:170:SER:HA	1:B:86:ALA:HB2	2.02	0.41
1:B:282:PRO:O	1:B:283:SER:C	2.59	0.41
1:A:13:THR:CG2	1:B:10:GLN:HB3	2.50	0.41
1:A:285:TYR:CD2	1:A:286:HIS:N	2.89	0.41
1:B:215:ASN:H	1:B:218:ARG:CB	2.30	0.41
2:E:18:DA:H2"	2:E:19:DA:N7	2.35	0.41
3:F:46:DT:H2"	3:F:47:DG:C5'	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ALA:C	1:A:27:GLU:N	2.72	0.41
1:A:49:TRP:HZ3	1:A:52:ARG:HD2	1.85	0.41
1:A:79:ALA:HA	1:A:82:ASP:OD2	2.20	0.41
1:A:115:LYS:NZ	3:F:51:DA:OP2	2.40	0.41
1:A:186:ARG:HG3	3:H:55:DG:O3'	2.20	0.41
1:B:162:PHE:HD1	1:B:190:LYS:HA	1.85	0.41
1:B:285:TYR:CD2	1:B:286:HIS:HB2	2.55	0.41
1:A:29:HIS:O	1:A:30:ARG:C	2.59	0.41
1:A:168:LYS:HE3	1:A:181:THR:CG2	2.50	0.41
1:B:33:VAL:CG1	1:B:34:GLU:H	2.24	0.41
1:B:105:ASN:O	1:B:106:ARG:C	2.58	0.41
1:B:138:ILE:O	1:B:141:SER:N	2.53	0.41
1:B:279:ASP:O	1:B:280:LEU:HD22	2.21	0.41
1:B:329:LEU:CD2	1:B:329:LEU:H	2.33	0.41
1:B:38:GLU:O	1:B:40:VAL:N	2.53	0.41
1:B:172:VAL:O	1:B:173:ASP:C	2.59	0.41
1:B:197:TRP:CD1	1:B:197:TRP:N	2.87	0.41
2:G:23:DT:H2"	2:G:24:DC:C5'	2.50	0.41
1:A:89:GLN:O	1:A:90:LYS:C	2.58	0.41
1:A:261:ASP:O	1:A:263:LEU:N	2.53	0.41
1:B:132:ARG:HH21	1:B:280:LEU:HD21	1.85	0.41
1:B:151:ARG:NH1	1:B:245:ILE:CD1	2.71	0.41
1:B:251:ALA:HB3	1:B:254:HIS:CG	2.56	0.41
3:D:31:DA:H4'	3:D:31:DA:OP1	2.21	0.41
2:E:25:DG:N2	3:F:33:DG:C2	2.88	0.41
2:G:11:DA:C2	3:H:47:DG:N2	2.89	0.41
3:H:32:DC:C2'	3:H:33:DG:C8	3.03	0.41
1:A:15:LEU:CD2	1:A:46:CYS:HB3	2.50	0.41
1:A:195:VAL:HG22	1:A:196:TRP:N	2.34	0.41
1:A:77:LEU:CD1	1:A:78:GLN:N	2.76	0.41
1:A:98:VAL:HA	3:D:45:DT:OP1	2.21	0.41
1:A:134:ASN:O	1:A:138:ILE:HD12	2.20	0.41
1:A:193:LEU:HD22	1:A:310:LEU:HD11	2.03	0.41
1:B:87:GLN:OE1	1:B:95:GLN:NE2	2.53	0.41
1:B:160:ILE:CD1	1:B:193:LEU:HD23	2.50	0.41
3:D:54:DT:C5	3:D:55:DG:C6	3.09	0.41
2:G:21:DT:H2"	2:G:22:DG:H8	1.85	0.41
1:A:74:ASP:C	1:A:76:GLU:N	2.74	0.41
1:A:98:VAL:HG22	1:A:102:ALA:HB3	2.02	0.41
1:A:151:ARG:HG3	1:A:151:ARG:O	2.21	0.41
1:A:228:ARG:O	1:A:229:ALA:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LEU:CD2	1:A:309:TRP:CH2	3.04	0.41
1:B:99:SER:OG	1:B:102:ALA:CB	2.69	0.41
1:B:225:ASN:N	1:B:225:ASN:ND2	2.68	0.41
1:B:285:TYR:O	1:B:289:ALA:HB2	2.21	0.41
1:A:96:LEU:CD1	1:A:96:LEU:N	2.84	0.41
1:A:106:ARG:HH12	3:D:44:DC:P	2.43	0.41
1:A:117:GLY:HA2	1:B:178:ALA:HB3	2.03	0.41
1:A:138:ILE:O	1:A:139:LEU:C	2.57	0.41
1:B:99:SER:CB	3:F:45:DT:OP2	2.67	0.41
1:B:321:PHE:C	1:B:321:PHE:CD2	2.94	0.41
3:D:35:DC:H2"	3:D:36:DA:H8	1.85	0.41
3:H:43:DA:C2	3:H:44:DC:C4	3.09	0.41
1:A:86:ALA:HB2	1:B:170:SER:OG	2.21	0.40
1:B:73:GLU:HB2	1:B:76:GLU:CB	2.46	0.40
1:B:155:GLY:HA3	1:B:196:TRP:HA	2.03	0.40
2:C:13:DG:H2'	2:C:14:DT:H71	2.02	0.40
2:E:19:DA:H8	2:E:19:DA:O5'	2.04	0.40
1:A:222:GLN:HA	1:A:225:ASN:ND2	2.36	0.40
1:B:24:THR:HG23	1:B:27:GLU:CB	2.28	0.40
1:B:129:MET:O	1:B:130:GLU:C	2.58	0.40
2:C:7:DG:N2	3:D:51:DA:C2	2.89	0.40
2:G:5:DG:C8	2:G:6:DT:H73	2.56	0.40
1:A:230:LEU:HD21	1:A:237:TYR:HD2	1.87	0.40
1:A:245:ILE:HG21	1:A:271:LEU:HG	2.02	0.40
1:A:317:LYS:HD2	1:A:321:PHE:CE2	2.56	0.40
1:B:116:VAL:O	1:B:116:VAL:HG23	2.22	0.40
1:B:160:ILE:O	1:B:160:ILE:HG22	2.22	0.40
2:G:23:DT:H2"	2:G:24:DC:H5'	2.04	0.40
1:A:72:TYR:HE2	1:A:98:VAL:HG21	1.86	0.40
1:A:229:ALA:O	1:A:232:ARG:HG2	2.21	0.40
1:A:291:MET:HE2	1:A:295:LEU:HD11	2.04	0.40
1:B:195:VAL:CG2	1:B:196:TRP:H	2.33	0.40
1:B:220:GLN:HG2	1:B:262:THR:CG2	2.42	0.40
1:B:286:HIS:NE2	1:B:321:PHE:CD2	2.90	0.40
3:F:41:DA:H2"	3:F:42:DT:C5'	2.51	0.40
1:A:174:PRO:O	1:A:175:GLY:O	2.40	0.40
1:B:249:ASP:OD1	1:B:254:HIS:CE1	2.74	0.40
1:B:306:VAL:HG12	1:B:310:LEU:CD2	2.51	0.40
3:D:53:DC:O5'	3:D:53:DC:H2'	2.22	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	332/345 (96%)	224 (68%)	86 (26%)	22 (7%)	1 13
1	B	333/345 (96%)	235 (71%)	62 (19%)	36 (11%)	0 6
All	All	665/690 (96%)	459 (69%)	148 (22%)	58 (9%)	1 9

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	62	ASP
1	A	126	GLU
1	A	137	GLU
1	A	150	HIS
1	B	126	GLU
1	B	293	HIS
1	B	297	GLU
1	B	321	PHE
1	A	25	ALA
1	A	58	PHE
1	A	75	ALA
1	A	83	GLU
1	A	94	GLU
1	A	175	GLY
1	A	192	MET
1	A	217	ALA
1	A	297	GLU
1	B	25	ALA
1	B	39	GLN
1	B	85	ASP
1	B	111	GLY
1	B	112	LYS
1	B	235	PRO
1	B	250	ASN

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Mol	Chain	Res	Type
1	B	274	ALA
1	B	294	ALA
1	B	334	GLU
1	B	338	ALA
1	A	210	PRO
1	A	235	PRO
1	A	268	TRP
1	B	160	ILE
1	B	236	GLU
1	B	267	ASN
1	B	313	TRP
1	B	314	PHE
1	A	121	PRO
1	A	262	THR
1	B	6	PRO
1	B	199	GLN
1	B	237	TYR
1	B	292	GLY
1	B	320	GLU
1	B	322	TYR
1	B	330	PRO
1	A	35	ALA
1	A	41	PRO
1	A	338	ALA
1	B	73	GLU
1	B	121	PRO
1	B	202	VAL
1	B	203	ILE
1	B	251	ALA
1	B	284	ASP
1	B	336	CYS
1	B	343	TYR
1	B	329	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	298/307 (97%)	248 (83%)	50 (17%)	2 12
1	B	299/307 (97%)	255 (85%)	44 (15%)	3 18
All	All	597/614 (97%)	503 (84%)	94 (16%)	2 15

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PRO
1	A	24	THR
1	A	27	GLU
1	A	43	VAL
1	A	51	GLN
1	A	57	ASP
1	A	74	ASP
1	A	77	LEU
1	A	78	GLN
1	A	98	VAL
1	A	100	GLN
1	A	110	MET
1	A	119	TRP
1	A	125	ASN
1	A	128	GLN
1	A	131	ARG
1	A	146	LYS
1	A	149	LEU
1	A	152	ILE
1	A	157	GLU
1	A	161	PHE
1	A	166	LYS
1	A	176	GLN
1	A	181	THR
1	A	185	ASN
1	A	186	ARG
1	A	191	THR
1	A	192	MET
1	A	193	LEU
1	A	195	VAL
1	A	202	VAL
1	A	210	PRO
1	A	214	VAL
1	A	226	LEU
1	A	227	ASN

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Mol	Chain	Res	Type
1	A	244	VAL
1	A	245	ILE
1	A	248	HIS
1	A	253	SER
1	A	266	LEU
1	A	270	VAL
1	A	284	ASP
1	A	297	GLU
1	A	304	GLU
1	A	305	SER
1	A	319	ASP
1	A	321	PHE
1	A	340	ASP
1	A	343	TYR
1	A	344	PHE
1	B	6	PRO
1	B	12	ARG
1	B	24	THR
1	B	40	VAL
1	B	45	THR
1	B	74	ASP
1	B	77	LEU
1	B	78	GLN
1	B	81	LEU
1	B	82	ASP
1	B	98	VAL
1	B	100	GLN
1	B	101	GLN
1	B	109	GLU
1	B	113	ILE
1	B	121	PRO
1	B	123	GLU
1	B	131	ARG
1	B	148	PHE
1	B	149	LEU
1	B	152	ILE
1	B	154	THR
1	B	158	LYS
1	B	166	LYS
1	B	176	GLN
1	B	181	THR
1	B	193	LEU

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Mol	Chain	Res	Type
1	B	194	CYS
1	B	199	GLN
1	B	207	LEU
1	B	225	ASN
1	B	227	ASN
1	B	248	HIS
1	B	266	LEU
1	B	268	TRP
1	B	270	VAL
1	B	271	LEU
1	B	283	SER
1	B	284	ASP
1	B	303	TYR
1	B	310	LEU
1	B	321	PHE
1	B	336	CYS
1	B	344	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	20	HIS
1	A	91	GLN
1	A	100	GLN
1	A	114	GLN
1	A	125	ASN
1	A	150	HIS
1	A	176	GLN
1	A	185	ASN
1	A	199	GLN
1	A	221	GLN
1	A	225	ASN
1	A	227	ASN
1	A	293	HIS
1	B	10	GLN
1	B	87	GLN
1	B	95	GLN
1	B	100	GLN
1	B	101	GLN
1	B	150	HIS
1	B	164	ASN

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Mol	Chain	Res	Type
1	B	176	GLN
1	B	220	GLN
1	B	225	ASN
1	B	231	GLN
1	B	248	HIS
1	B	254	HIS
1	B	267	ASN
1	B	327	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
5	SO4	A	346	-	4,4,4	0.16	0	6,6,6	0.29	0
5	SO4	B	346	-	4,4,4	0.18	0	6,6,6	0.35	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	336/345 (97%)	-0.77	2 (0%) 89 86	14, 58, 131, 225	0
1	B	337/345 (97%)	-0.66	4 (1%) 79 73	18, 63, 137, 226	0
2	C	25/25 (100%)	-0.64	0 100 100	34, 53, 83, 122	0
2	E	25/25 (100%)	-0.56	0 100 100	35, 60, 80, 96	0
2	G	25/25 (100%)	-0.47	0 100 100	25, 94, 144, 156	0
3	D	28/28 (100%)	-0.75	0 100 100	36, 52, 76, 91	0
3	F	28/28 (100%)	-0.68	0 100 100	34, 62, 92, 105	0
3	H	28/28 (100%)	-0.45	0 100 100	28, 88, 150, 150	0
All	All	832/849 (97%)	-0.69	6 (0%) 87 83	14, 62, 136, 226	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	155	GLY	3.5
1	B	156	ASP	2.9
1	A	156	ASP	2.6
1	A	61	ASP	2.4
1	B	154	THR	2.1
1	B	249	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	B	346	5/5	0.93	0.17	103,112,125,135	0
5	SO4	A	346	5/5	0.95	0.32	117,126,130,139	0
4	MG	A	1001	1/1	0.97	0.16	2,2,2,2	0

6.5 Other polymers

There are no such residues in this entry.