



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:58 PM UTC

PDB ID : 1Z1G / pdb_00001z1g
Title : Crystal structure of a lambda integrase tetramer bound to a Holliday junction
Authors : Biswas, T.; Aihara, H.; Radman-Livaja, M.; Filman, D.; Landy, A.; Ellenberger, T.
Deposited on : 2005-03-03
Resolution : 4.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

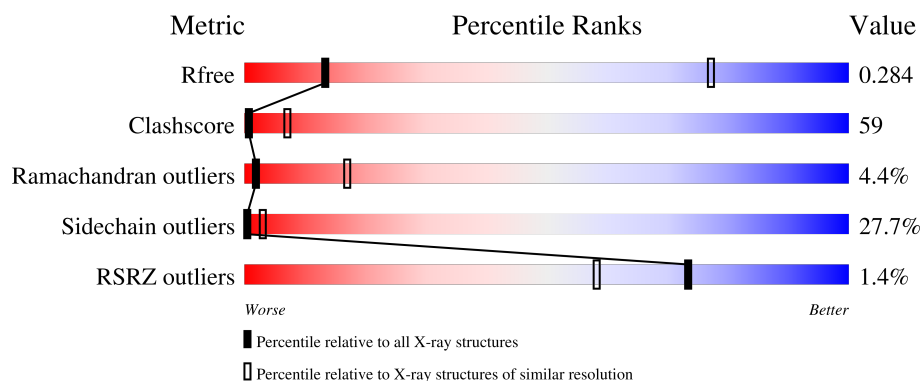
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.40 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}	180053	1088 (4.90-3.90)
Clashscore	190562	1135 (4.90-3.90)
Ramachandran outliers	187476	1026 (4.90-3.90)
Sidechain outliers	187428	1010 (4.90-3.90)
RSRZ outliers	180081	1084 (4.90-3.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	I	29	
2	J	29	
3	K	29	
4	L	29	
5	E	25	

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Mol	Chain	Length	Quality of chain
5	G	25	28%68% .
6	F	25	56%44%
6	H	25	28%68% .
7	A	356	32%41%18%6%.% .
7	B	356	28%38%23%6%6%3%
7	C	356	30%43%21%.%2% .
7	D	356	33%42%16%.%6% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15156 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 DNA chain called 29-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	29	Total	C	N	O	P	0	0	0
			588	284	103	173	28			

- Molecule 2 is a DNA chain called 29-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	29	Total	C	N	O	P	0	0	0
			594	286	110	170	28			

- Molecule 3 is a DNA chain called 29-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	29	Total	C	N	O	P	0	0	0
			590	285	102	175	28			

- Molecule 4 is a DNA chain called 29-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	29	Total	C	N	O	P	0	0	0
			594	285	111	170	28			

- Molecule 5 is a DNA chain called 5'-D(*AP*CP*AP*GP*GP*TP*CP*AP*CP*TP*AP*T
P*CP*AP*GP*TP*CP*AP*AP*AP*TP*AP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	24	Total	C	N	O	P	0	0	0
			487	234	93	137	23			
5	G	24	Total	C	N	O	P	0	0	0
			487	234	93	137	23			

- Molecule 6 is a DNA chain called 25-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	25	Total	C	N	O	P	0	0	0
			513	247	89	153	24			
6	H	25	Total	C	N	O	P	0	0	0
			513	247	89	153	24			

- Molecule 7 is a protein called Integrase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	A	349	Total	C	N	O	S	Se	0	0	0
			2763	1730	505	517	4	7			
7	B	336	Total	C	N	O	S	Se	0	0	0
			2630	1652	474	494	4	6			
7	C	349	Total	C	N	O	S	Se	0	0	0
			2767	1732	506	518	4	7			
7	D	336	Total	C	N	O	S	Se	0	0	0
			2630	1652	474	494	4	6			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P03700
A	101	MSE	MET	modified residue	UNP P03700
A	127	MSE	MET	modified residue	UNP P03700
A	203	MSE	MET	modified residue	UNP P03700
A	219	MSE	MET	modified residue	UNP P03700
A	255	MSE	MET	modified residue	UNP P03700
A	290	MSE	MET	modified residue	UNP P03700
A	338	MSE	MET	modified residue	UNP P03700
A	342	PHE	TYR	engineered mutation	UNP P03700
B	1	MSE	MET	modified residue	UNP P03700
B	101	MSE	MET	modified residue	UNP P03700
B	127	MSE	MET	modified residue	UNP P03700
B	203	MSE	MET	modified residue	UNP P03700
B	219	MSE	MET	modified residue	UNP P03700
B	255	MSE	MET	modified residue	UNP P03700
B	290	MSE	MET	modified residue	UNP P03700
B	338	MSE	MET	modified residue	UNP P03700
B	342	PHE	TYR	engineered mutation	UNP P03700
C	1	MSE	MET	modified residue	UNP P03700
C	101	MSE	MET	modified residue	UNP P03700
C	127	MSE	MET	modified residue	UNP P03700
C	203	MSE	MET	modified residue	UNP P03700
C	219	MSE	MET	modified residue	UNP P03700

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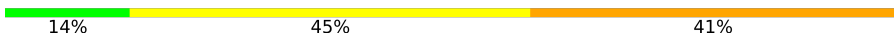
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Chain	Residue	Modelled	Actual	Comment	Reference
C	255	MSE	MET	modified residue	UNP P03700
C	290	MSE	MET	modified residue	UNP P03700
C	338	MSE	MET	modified residue	UNP P03700
C	342	PHE	TYR	engineered mutation	UNP P03700
D	1	MSE	MET	modified residue	UNP P03700
D	101	MSE	MET	modified residue	UNP P03700
D	127	MSE	MET	modified residue	UNP P03700
D	203	MSE	MET	modified residue	UNP P03700
D	219	MSE	MET	modified residue	UNP P03700
D	255	MSE	MET	modified residue	UNP P03700
D	290	MSE	MET	modified residue	UNP P03700
D	338	MSE	MET	modified residue	UNP P03700
D	342	PHE	TYR	engineered mutation	UNP P03700

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.

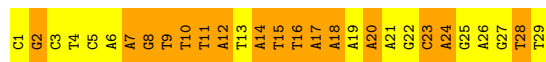
- Molecule 1: 29-MER

Chain I: 



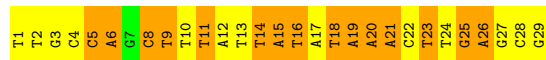
- Molecule 2: 29-MER

Chain J: 

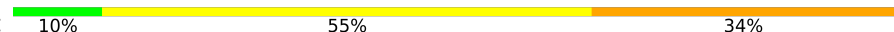


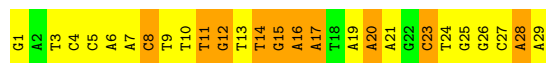
- Molecule 3: 29-MER

Chain K: 



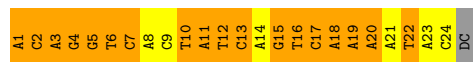
- Molecule 4: 29-MER

Chain L: 



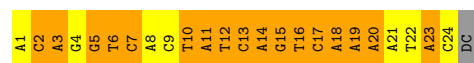
- Molecule 5: 5'-D(*AP*CP*AP*GP*GP*TP*CP*AP*CP*TP*AP*TP*CP*AP*GP*TP*CP*AP*AP*AP*TP*AP*CP*C)-3'

Chain E: 



- Molecule 5: 5'-D(*AP*CP*AP*GP*GP*TP*CP*AP*CP*TP*AP*TP*CP*AP*GP*TP*CP*AP*AP*AP*TP*AP*CP*C)-3'

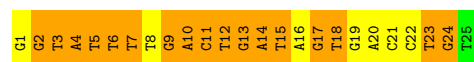
Chain G: 



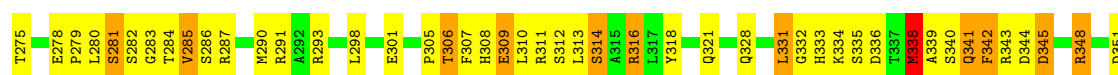
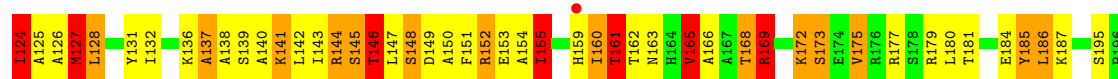
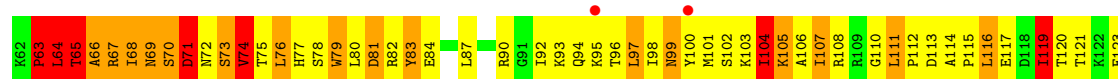
- Molecule 6: 25-MER



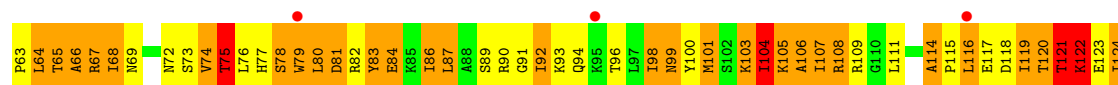
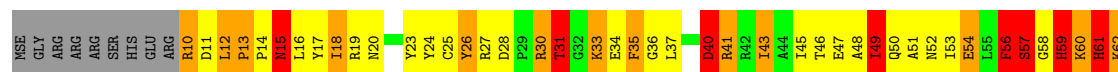
- Molecule 6: 25-MER

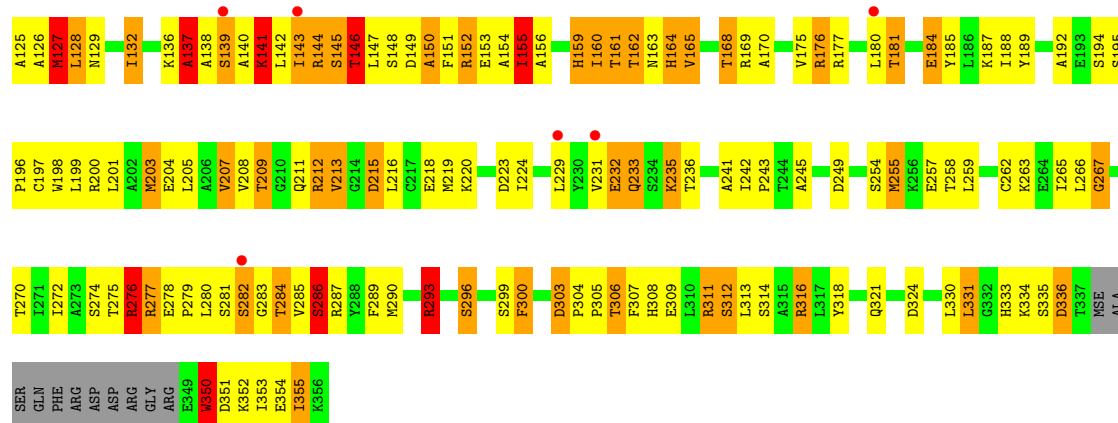


- Molecule 7: Integrase

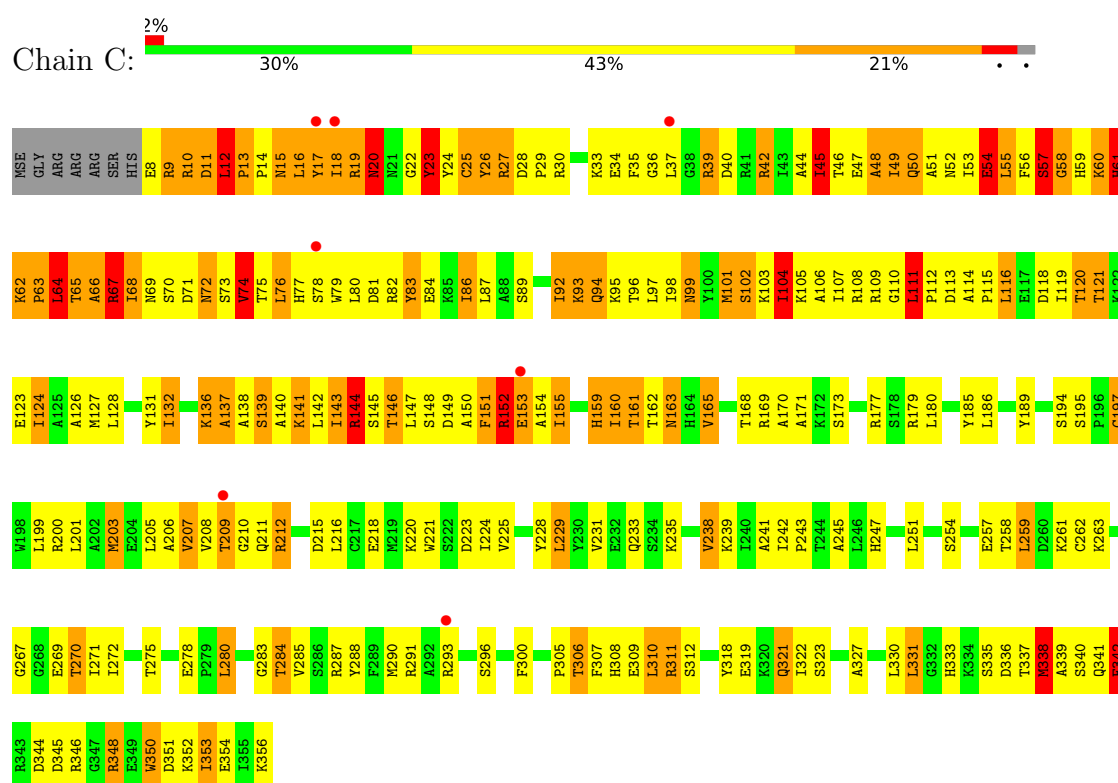


- Molecule 7: Integrase

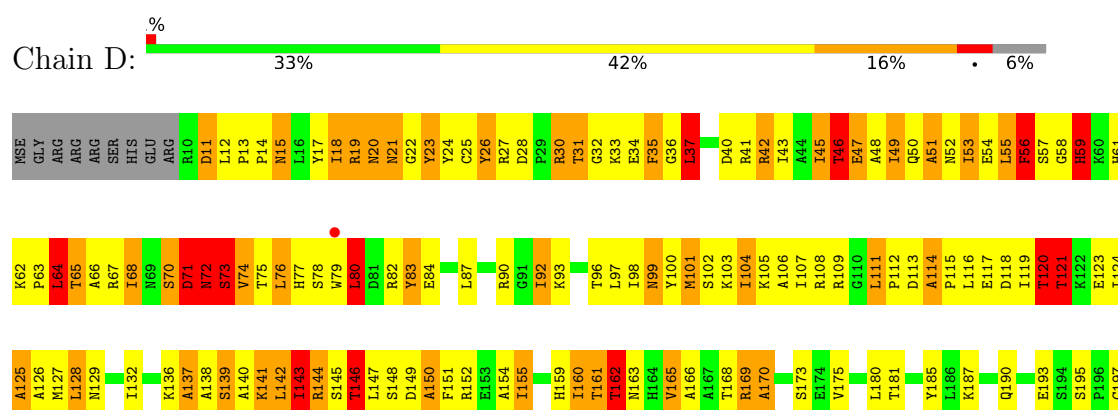


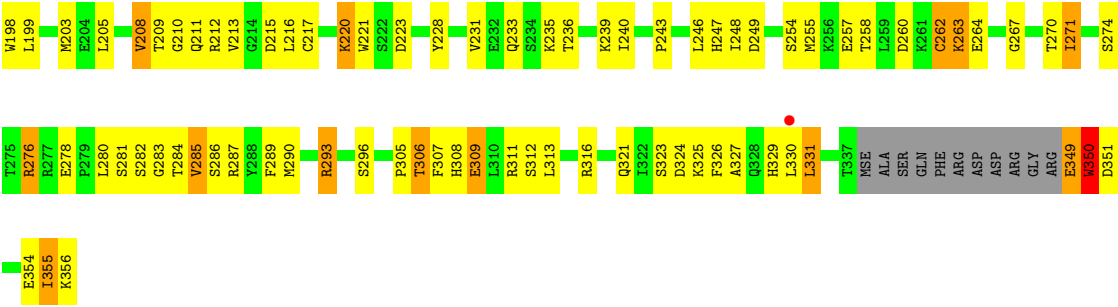


• Molecule 7: Integrase



• Molecule 7: Integrase





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	109.76Å 109.76Å 265.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 4.40 20.00 – 4.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-4.40) 98.9 (20.00-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 4.45Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.244 , 0.292 0.248 , 0.284	Depositor DCC
R_{free} test set	1158 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	241.9	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 129.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l 0.066 for h,-h-k,-l 0.044 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15156	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	I	0.86	1/658 (0.2%)	2.08	36/1013 (3.6%)
2	J	0.89	0/667	2.02	42/1028 (4.1%)
3	K	1.02	1/660 (0.2%)	2.24	47/1017 (4.6%)
4	L	0.89	1/667 (0.1%)	1.86	21/1028 (2.0%)
5	E	0.86	0/547	2.18	40/841 (4.8%)
5	G	1.06	0/547	2.35	39/841 (4.6%)
6	F	0.92	1/574 (0.2%)	2.06	25/886 (2.8%)
6	H	1.04	1/574 (0.2%)	2.34	39/886 (4.4%)
7	A	1.58	35/2804 (1.2%)	1.64	44/3762 (1.2%)
7	B	1.78	58/2670 (2.2%)	1.66	43/3589 (1.2%)
7	C	1.46	38/2808 (1.4%)	1.55	39/3767 (1.0%)
7	D	1.39	23/2670 (0.9%)	1.58	44/3589 (1.2%)
All	All	1.40	159/15846 (1.0%)	1.81	459/22247 (2.1%)

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
7	A	0	1
7	C	0	1
All	All	0	2

All (159) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	9	ARG	CA-C	16.45	1.61	1.52
7	B	124	ILE	CA-CB	-14.53	1.38	1.54
7	B	165	VAL	CA-CB	-12.75	1.39	1.54
7	B	119	ILE	CA-CB	-12.39	1.38	1.54
7	B	143	ILE	CA-CB	-11.87	1.41	1.54
7	B	64	LEU	CA-C	11.24	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	143	ILE	CA-CB	-11.20	1.42	1.54
7	A	31	THR	CA-CB	10.29	1.70	1.53
7	B	150	ALA	CA-CB	-9.95	1.37	1.53
7	D	155	ILE	CA-CB	-9.66	1.41	1.54
7	B	101	MSE	SE-CE	9.55	2.24	1.95
7	A	119	ILE	CA-CB	-9.39	1.42	1.54
7	A	168	THR	CA-CB	-9.39	1.37	1.53
7	A	338	MSE	SE-CE	9.21	2.23	1.95
7	A	71	ASP	CB-CG	9.19	1.75	1.52
7	B	155	ILE	CA-CB	-9.20	1.43	1.54
7	A	34	GLU	CA-C	-8.93	1.40	1.53
7	A	160	ILE	CA-C	-8.84	1.42	1.53
7	B	62	LYS	CA-C	8.75	1.62	1.52
7	C	152	ARG	NE-CZ	8.74	1.42	1.33
7	B	168	THR	CA-CB	-8.57	1.40	1.53
7	A	152	ARG	NE-CZ	8.49	1.42	1.33
7	B	355	ILE	CA-CB	8.38	1.64	1.54
7	B	104	ILE	CA-CB	-8.33	1.43	1.54
7	A	26	TYR	CA-C	-8.30	1.43	1.52
7	A	146	THR	CA-CB	-8.27	1.40	1.53
7	A	11	ASP	CA-CB	-8.05	1.42	1.53
7	A	334	LYS	CA-C	8.02	1.59	1.52
7	C	9	ARG	N-CA	7.94	1.55	1.45
6	H	15	DT	P-O5'	7.92	1.76	1.60
7	C	101	MSE	SE-CE	7.77	2.18	1.95
7	D	11	ASP	CA-CB	7.75	1.65	1.54
7	D	101	MSE	SE-CE	7.75	2.18	1.95
7	A	53	ILE	CA-CB	7.67	1.64	1.54
7	A	336	ASP	CA-C	7.66	1.62	1.52
7	C	155	ILE	CA-CB	-7.64	1.43	1.54
7	A	76	LEU	CA-C	-7.61	1.43	1.52
7	C	10	ARG	CA-C	7.42	1.61	1.52
7	C	34	GLU	CA-C	-7.37	1.42	1.53
7	B	31	THR	CA-CB	7.34	1.65	1.53
7	B	57	SER	C-O	7.34	1.32	1.24
7	C	54	GLU	CA-C	7.34	1.62	1.52
7	B	155	ILE	CA-C	-7.18	1.43	1.52
7	D	55	LEU	CA-C	-7.18	1.43	1.52
7	D	59	HIS	N-CA	7.14	1.55	1.46
7	B	120	THR	CA-C	-7.11	1.44	1.52
7	C	146	THR	CA-CB	-7.09	1.42	1.53
7	B	40	ASP	CA-C	-7.08	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	150	ALA	CA-CB	-7.05	1.42	1.53
7	C	86	ILE	CA-CB	-7.04	1.44	1.54
7	D	51	ALA	CA-C	-7.02	1.43	1.52
7	C	16	LEU	CA-C	-6.96	1.44	1.52
7	C	71	ASP	CB-CG	6.95	1.69	1.52
7	B	152	ARG	NE-CZ	6.92	1.40	1.33
7	B	159	HIS	CA-C	-6.80	1.43	1.52
7	B	79	TRP	CA-C	-6.71	1.43	1.52
7	A	124	ILE	CA-CB	-6.68	1.46	1.54
7	C	92	ILE	CA-C	-6.60	1.45	1.52
7	A	8	GLU	N-CA	6.56	1.58	1.46
7	A	10	ARG	N-CA	6.54	1.54	1.46
7	B	124	ILE	CA-C	-6.53	1.45	1.52
7	A	53	ILE	CB-CG2	6.45	1.73	1.52
7	B	336	ASP	CA-C	6.44	1.61	1.52
7	D	25	CYS	CA-C	6.37	1.60	1.52
7	D	72	ASN	CB-CG	6.26	1.67	1.52
7	B	57	SER	CA-C	6.25	1.60	1.52
7	C	26	TYR	N-CA	-6.23	1.38	1.46
7	B	83	TYR	CA-C	-6.22	1.45	1.52
7	C	336	ASP	CA-C	6.20	1.61	1.52
7	C	124	ILE	CA-CB	-6.20	1.47	1.54
7	A	119	ILE	CA-C	-6.17	1.45	1.52
7	C	104	ILE	CA-CB	-6.11	1.46	1.54
7	C	151	PHE	N-CA	-6.10	1.39	1.46
7	C	48	ALA	N-CA	-6.05	1.39	1.46
7	B	87	LEU	CA-C	-6.04	1.45	1.52
7	D	35	PHE	CB-CG	-6.00	1.36	1.50
7	D	11	ASP	CB-CG	5.94	1.66	1.52
7	B	59	HIS	CA-C	5.94	1.60	1.52
7	B	92	ILE	CA-CB	-5.93	1.46	1.54
7	D	46	THR	CA-CB	5.93	1.62	1.53
7	A	8	GLU	CA-C	5.91	1.65	1.52
1	I	15	DC	C1'-N1	5.91	1.67	1.49
7	A	71	ASP	CA-CB	5.90	1.63	1.53
7	C	48	ALA	CA-CB	-5.90	1.44	1.53
7	B	59	HIS	C-O	5.89	1.31	1.24
7	C	71	ASP	N-CA	5.88	1.53	1.46
4	L	27	DC	C1'-N1	5.85	1.67	1.49
7	B	169	ARG	NE-CZ	5.84	1.39	1.33
7	B	86	ILE	CA-CB	-5.80	1.47	1.54
7	A	71	ASP	N-CA	5.78	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	107	ILE	CA-CB	-5.78	1.47	1.54
7	D	155	ILE	CA-C	-5.77	1.44	1.52
7	A	9	ARG	C-N	5.76	1.40	1.33
7	C	64	LEU	CA-C	-5.74	1.45	1.52
7	B	276	ARG	NE-CZ	5.73	1.39	1.33
7	B	109	ARG	NE-CZ	5.73	1.39	1.33
7	B	146	THR	CA-CB	-5.71	1.44	1.53
7	B	92	ILE	CA-C	-5.71	1.45	1.52
7	B	143	ILE	N-CA	-5.67	1.40	1.46
7	D	61	HIS	CA-C	-5.67	1.45	1.52
7	B	98	ILE	CA-CB	5.65	1.61	1.54
7	C	68	ILE	CA-CB	-5.64	1.46	1.54
7	A	161	THR	CA-CB	-5.63	1.46	1.54
7	B	127	MSE	SE-CE	5.62	2.12	1.95
7	A	127	MSE	SE-CE	5.62	2.12	1.95
7	D	146	THR	CA-CB	-5.62	1.44	1.53
7	C	71	ASP	CA-CB	5.60	1.63	1.53
7	B	121	THR	N-CA	-5.60	1.39	1.46
7	C	10	ARG	N-CA	5.59	1.52	1.45
7	B	61	HIS	N-CA	-5.57	1.39	1.46
7	D	56	PHE	CD1-CE1	5.56	1.55	1.38
7	D	59	HIS	CA-CB	5.56	1.62	1.53
7	A	146	THR	CA-C	-5.55	1.45	1.52
7	B	10	ARG	NE-CZ	5.51	1.39	1.33
7	A	107	ILE	CA-CB	-5.51	1.48	1.54
7	C	17	TYR	CA-C	-5.49	1.46	1.52
7	A	153	GLU	CA-C	-5.48	1.45	1.52
7	C	153	GLU	N-CA	-5.47	1.39	1.46
7	B	355	ILE	CA-C	5.47	1.58	1.52
7	A	10	ARG	CA-C	5.46	1.59	1.52
7	B	106	ALA	CA-CB	-5.43	1.44	1.53
7	C	165	VAL	CA-CB	-5.41	1.48	1.54
3	K	16	DT	C1'-N1	5.39	1.65	1.49
7	C	152	ARG	CA-C	-5.39	1.45	1.52
7	B	33	LYS	CD-CE	5.37	1.68	1.52
7	C	143	ILE	CA-CB	-5.35	1.48	1.54
7	B	33	LYS	CG-CD	5.34	1.68	1.52
6	F	11	DC	C1'-N1	5.34	1.65	1.49
7	B	145	SER	N-CA	-5.33	1.39	1.46
7	B	122	LYS	CB-CG	5.32	1.68	1.52
7	B	105	LYS	CG-CD	5.30	1.68	1.52
7	A	54	GLU	CA-C	5.30	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	338	MSE	SE-CE	5.28	2.11	1.95
7	A	79	TRP	CA-CB	-5.28	1.45	1.53
7	B	165	VAL	N-CA	-5.26	1.40	1.46
7	D	37	LEU	CA-C	-5.26	1.48	1.52
7	C	26	TYR	CA-C	-5.26	1.46	1.52
7	B	124	ILE	N-CA	-5.25	1.40	1.46
7	C	159	HIS	CA-CB	-5.24	1.45	1.53
7	B	56	PHE	N-CA	-5.22	1.39	1.46
7	A	57	SER	CA-C	5.21	1.57	1.52
7	A	155	ILE	CA-CB	-5.20	1.47	1.54
7	D	74	VAL	CA-C	-5.20	1.46	1.52
7	B	141	LYS	N-CA	-5.18	1.40	1.46
7	B	137	ALA	CA-CB	-5.17	1.44	1.53
7	C	8	GLU	CA-C	5.14	1.63	1.52
7	B	72	ASN	CB-CG	5.13	1.64	1.52
7	C	160	ILE	CA-C	-5.13	1.45	1.53
7	B	84	GLU	CA-C	-5.12	1.46	1.52
7	C	153	GLU	CA-C	-5.10	1.46	1.52
7	B	236	THR	CA-CB	5.09	1.61	1.53
7	C	163	ASN	CA-C	-5.07	1.46	1.52
7	B	15	ASN	CB-CG	-5.07	1.39	1.52
7	D	26	TYR	CB-CG	-5.02	1.40	1.51
7	A	9	ARG	N-CA	5.02	1.52	1.46
7	D	64	LEU	CA-C	5.02	1.59	1.52
7	D	125	ALA	CA-CB	-5.01	1.45	1.53
7	C	30	ARG	NE-CZ	5.01	1.38	1.33
7	B	57	SER	CA-CB	5.00	1.59	1.53

All (459) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	14	DA	O3'-P-O5'	16.47	128.70	104.00
7	B	74	VAL	N-CA-C	-14.53	88.33	108.96
3	K	14	DT	N1-C1'-C2'	-13.78	92.83	113.50
3	K	16	DT	N1-C1'-C2'	12.50	132.25	113.50
7	A	74	VAL	N-CA-C	12.02	134.34	109.34
3	K	16	DT	C4'-C3'-O3'	-11.56	92.66	110.00
7	C	74	VAL	N-CA-C	11.11	132.44	109.34
6	H	15	DT	P-O5'-C5'	10.56	135.84	120.00
7	A	159	HIS	N-CA-C	-10.54	100.16	113.23
3	K	15	DA	O5'-C5'-C4'	10.51	126.56	110.80
7	A	30	ARG	N-CA-CB	-10.41	94.97	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	12	DT	O4'-C1'-N1	-10.29	92.97	108.40
7	A	10	ARG	N-CA-C	10.16	124.81	108.76
2	J	17	DA	C8-N9-C1'	10.13	142.25	127.05
2	J	16	DT	O5'-C5'-C4'	-10.11	95.63	110.80
1	I	27	DA	O4'-C1'-N9	10.09	123.54	108.40
1	I	12	DT	P-O3'-C3'	10.01	135.21	120.20
1	I	12	DT	N1-C1'-C2'	9.79	128.18	113.50
7	A	64	LEU	N-CA-C	-9.77	99.68	111.69
6	F	5	DT	O3'-P-O5'	-9.45	89.83	104.00
5	G	19	DA	O3'-P-O5'	-9.23	90.16	104.00
5	G	10	DT	C4'-C3'-O3'	-9.16	96.26	110.00
1	I	16	DA	N9-C1'-C2'	9.13	127.19	113.50
3	K	2	DT	C4'-C3'-O3'	-9.05	96.43	110.00
1	I	5	DC	C4'-C3'-O3'	-9.04	96.44	110.00
2	J	1	DC	C4'-C3'-O3'	-9.03	96.45	110.00
6	F	2	DG	N9-C1'-C2'	9.00	127.00	113.50
7	C	165	VAL	CB-CA-C	-8.99	100.25	112.02
7	C	61	HIS	N-CA-C	-8.97	93.96	108.41
5	G	5	DG	O4'-C1'-N9	8.96	121.84	108.40
7	B	161	THR	N-CA-CB	-8.89	95.40	110.51
7	B	159	HIS	N-CA-C	-8.87	102.47	113.28
2	J	9	DT	O5'-C5'-C4'	-8.83	97.55	110.80
7	B	35	PHE	N-CA-C	8.78	123.98	109.06
2	J	17	DA	N9-C1'-C2'	8.75	126.62	113.50
7	D	72	ASN	N-CA-C	-8.68	101.02	111.69
6	F	11	DC	O4'-C1'-N1	8.62	121.33	108.40
7	A	57	SER	N-CA-C	8.54	125.17	113.21
7	A	30	ARG	N-CA-C	-8.53	101.92	111.14
7	B	165	VAL	CB-CA-C	-8.52	101.07	111.97
5	G	1	DA	P-O3'-C3'	8.51	132.97	120.20
6	H	24	DG	P-O5'-C5'	8.47	132.70	120.00
1	I	28	DT	P-O5'-C5'	8.45	132.68	120.00
7	A	116	LEU	CA-CB-CG	-8.44	86.77	116.30
6	F	6	DT	O4'-C1'-N1	8.30	120.86	108.40
7	C	10	ARG	N-CA-C	8.25	122.54	109.50
3	K	21	DA	P-O3'-C3'	8.23	132.55	120.20
5	G	6	DT	O5'-C5'-C4'	-8.22	98.47	110.80
7	B	165	VAL	N-CA-CB	-8.21	100.94	110.55
3	K	20	DA	C4'-C3'-O3'	8.20	122.30	110.00
1	I	15	DC	N1-C1'-C2'	8.17	125.75	113.50
6	F	2	DG	C4-N9-C1'	-8.14	114.80	127.00
6	H	24	DG	P-O3'-C3'	8.13	132.40	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	27	DA	C4'-C3'-O3'	8.13	122.19	110.00
5	E	1	DA	N9-C1'-C2'	8.12	125.67	113.50
3	K	20	DA	P-O3'-C3'	8.07	132.31	120.20
7	A	132	ILE	CB-CA-C	-8.05	101.47	112.02
7	A	338	MSE	N-CA-C	8.03	123.61	112.93
5	E	6	DT	C5'-C4'-O4'	-8.02	97.36	109.40
5	G	11	DA	P-O5'-C5'	8.00	132.00	120.00
1	I	15	DC	C4'-C3'-O3'	-7.99	98.02	110.00
2	J	17	DA	C4-N9-C1'	-7.98	115.07	127.05
7	A	334	LYS	N-CA-C	7.98	123.06	112.13
7	D	26	TYR	CA-CB-CG	-7.88	99.71	113.90
5	E	6	DT	O5'-C5'-C4'	-7.86	99.02	110.80
1	I	16	DA	C4'-C3'-O3'	-7.84	98.25	110.00
6	H	14	DA	OP1-P-O3'	-7.82	84.53	108.00
6	H	2	DG	N9-C1'-C2'	7.82	125.23	113.50
6	F	16	DA	N9-C1'-C2'	-7.80	101.81	113.50
7	C	159	HIS	N-CA-C	-7.78	102.71	112.90
7	D	354	GLU	N-CA-C	-7.76	100.07	110.55
7	A	30	ARG	CA-CB-CG	7.76	129.62	114.10
6	H	6	DT	O4'-C1'-N1	7.75	120.03	108.40
6	H	9	DG	N9-C1'-C2'	7.69	125.03	113.50
7	C	339	ALA	N-CA-C	-7.62	103.72	112.87
6	H	15	DT	C3'-C2'-C1'	7.62	113.02	101.60
6	F	19	DG	P-O3'-C3'	7.59	131.59	120.20
1	I	15	DC	P-O5'-C5'	7.56	131.34	120.00
6	F	2	DG	C8-N9-C1'	7.54	138.30	127.00
7	A	165	VAL	CB-CA-C	-7.52	102.08	111.70
5	G	23	DA	O4'-C1'-N9	7.50	119.64	108.40
5	G	5	DG	O4'-C1'-C2'	-7.48	95.18	106.40
7	D	35	PHE	CA-CB-CG	-7.48	106.32	113.80
7	C	20	ASN	CA-C-N	-7.46	108.18	122.06
7	C	20	ASN	C-N-CA	-7.46	108.18	122.06
5	E	15	DG	C4'-C3'-O3'	-7.46	98.82	110.00
3	K	26	DA	P-O5'-C5'	-7.45	108.82	120.00
7	D	350	TRP	N-CA-C	7.45	121.13	109.96
5	G	23	DA	C5'-C4'-C3'	-7.42	103.77	114.90
7	C	350	TRP	N-CA-C	7.42	119.84	109.15
1	I	12	DT	C5'-C4'-C3'	7.42	126.03	114.90
6	F	7	DT	P-O3'-C3'	7.41	131.32	120.20
3	K	15	DA	O3'-P-O5'	7.41	115.11	104.00
6	H	2	DG	C5'-C4'-C3'	7.37	125.96	114.90
7	D	120	THR	CB-CA-C	-7.35	97.13	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	35	PHE	N-CA-C	7.32	121.47	109.24
6	H	23	DT	N1-C1'-C2'	7.32	124.48	113.50
5	E	5	DG	O4'-C1'-N9	7.30	119.36	108.40
5	G	6	DT	C4-C5-C7	-7.27	111.49	122.40
3	K	14	DT	O4'-C1'-N1	7.26	119.29	108.40
4	L	3	DT	N1-C1'-C2'	7.23	124.35	113.50
4	L	4	DC	C4'-C3'-O3'	-7.20	99.20	110.00
6	H	2	DG	C4'-C3'-O3'	-7.19	99.21	110.00
2	J	15	DT	C4'-C3'-C2'	-7.19	91.62	102.40
7	B	61	HIS	N-CA-C	-7.18	95.52	110.80
1	I	20	DA	P-O3'-C3'	7.16	130.94	120.20
5	E	3	DA	C4'-C3'-O3'	-7.14	99.28	110.00
5	G	5	DG	O5'-C5'-C4'	-7.10	100.15	110.80
3	K	14	DT	C2'-C3'-O3'	-7.09	100.86	111.50
2	J	17	DA	C5'-C4'-O4'	-7.07	98.80	109.40
7	A	332	GLY	N-CA-C	-7.05	105.48	115.43
5	G	20	DA	C4'-C3'-O3'	-7.03	99.45	110.00
7	D	58	GLY	N-CA-C	-7.03	101.73	112.84
3	K	20	DA	N9-C1'-C2'	-7.03	102.96	113.50
7	C	116	LEU	N-CA-C	7.03	119.54	111.11
5	G	14	DA	O4'-C1'-N9	7.02	118.93	108.40
2	J	7	DA	O3'-P-O5'	-7.02	93.47	104.00
6	F	12	DT	C4'-C3'-O3'	-7.02	99.47	110.00
7	B	121	THR	N-CA-CB	-7.00	98.65	110.49
5	G	23	DA	C5'-C4'-O4'	6.99	119.88	109.40
7	A	111	LEU	O-C-N	6.96	126.98	121.55
7	C	322	ILE	CB-CA-C	6.90	117.58	111.71
7	D	73	SER	N-CA-C	6.90	119.51	108.41
7	B	26	TYR	CA-CB-CG	-6.89	101.49	113.90
5	G	10	DT	O4'-C1'-N1	6.88	118.72	108.40
5	G	22	DT	P-O3'-C3'	6.86	130.49	120.20
5	E	19	DA	O4'-C1'-N9	6.86	118.69	108.40
7	B	197	CYS	N-CA-C	6.85	119.58	111.71
6	H	24	DG	OP1-P-O3'	-6.83	87.50	108.00
6	H	15	DT	C5'-C4'-O4'	6.83	119.64	109.40
7	C	342	PHE	N-CA-C	-6.80	103.57	112.41
4	L	19	DA	O3'-P-O5'	-6.79	93.81	104.00
3	K	29	DG	N9-C1'-C2'	6.78	123.66	113.50
2	J	28	DT	C4'-C3'-O3'	-6.76	99.86	110.00
6	H	12	DT	N1-C1'-C2'	6.75	123.63	113.50
6	F	23	DT	C1'-O4'-C4'	-6.75	99.58	109.70
1	I	13	DT	N1-C1'-C2'	6.74	123.60	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	17	DG	P-O3'-C3'	6.73	130.30	120.20
7	A	197	CYS	N-CA-C	6.72	119.46	111.33
7	D	165	VAL	CB-CA-C	-6.72	103.36	111.97
7	D	159	HIS	N-CA-C	-6.71	104.91	113.23
5	E	9	DC	N1-C1'-C2'	6.71	123.57	113.50
7	A	169	ARG	N-CA-C	6.71	120.34	109.40
2	J	15	DT	P-O3'-C3'	6.71	130.26	120.20
5	E	13	DC	O5'-C5'-C4'	6.71	120.86	110.80
5	G	23	DA	N9-C1'-C2'	-6.71	103.44	113.50
2	J	13	DT	N1-C1'-C2'	6.70	123.55	113.50
6	H	17	DG	C5'-C4'-O4'	-6.70	99.35	109.40
7	A	34	GLU	CB-CA-C	-6.69	98.13	109.83
3	K	1	DT	C4'-C3'-O3'	6.68	120.01	110.00
7	B	165	VAL	N-CA-C	6.67	116.83	110.42
7	B	120	THR	CB-CA-C	-6.67	98.75	109.75
7	A	26	TYR	N-CA-C	-6.66	99.37	109.95
3	K	25	DG	C4'-C3'-O3'	-6.65	100.03	110.00
7	D	21	ASN	N-CA-CB	-6.64	100.07	110.30
7	A	30	ARG	CB-CA-C	6.64	121.39	110.90
7	A	116	LEU	N-CA-C	6.63	122.25	111.37
6	H	4	DA	C5'-C4'-O4'	6.61	119.31	109.40
3	K	5	DC	P-O5'-C5'	6.60	129.90	120.00
6	H	18	DT	P-O5'-C5'	6.60	129.90	120.00
2	J	12	DA	P-O3'-C3'	6.59	130.09	120.20
4	L	27	DC	N1-C1'-C2'	6.59	123.38	113.50
6	H	7	DT	N1-C1'-C2'	6.58	123.38	113.50
6	H	11	DC	O4'-C1'-N1	6.57	118.26	108.40
7	C	26	TYR	N-CA-C	-6.57	99.01	109.59
4	L	23	DC	N1-C1'-C2'	6.54	123.31	113.50
7	C	83	TYR	N-CA-C	-6.54	103.04	111.02
4	L	28	DA	P-O5'-C5'	6.51	129.76	120.00
7	C	57	SER	N-CA-C	6.51	124.66	110.80
6	H	7	DT	P-O3'-C3'	6.50	129.95	120.20
6	F	23	DT	C5'-C4'-O4'	6.49	119.14	109.40
7	B	66	ALA	N-CA-C	-6.49	96.98	110.80
7	B	99	ASN	N-CA-C	-6.49	103.11	111.02
4	L	11	DT	P-O3'-C3'	6.48	129.92	120.20
4	L	14	DT	P-O5'-C5'	6.48	129.72	120.00
7	C	9	ARG	N-CA-C	6.48	118.42	108.12
6	H	3	DT	C4'-C3'-O3'	-6.48	100.29	110.00
7	C	142	LEU	CA-CB-CG	-6.47	93.64	116.30
7	A	331	LEU	N-CA-C	6.45	119.31	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	7	DC	O5'-C5'-C4'	-6.44	101.15	110.80
7	B	235	LYS	N-CA-C	6.42	118.07	111.14
6	H	23	DT	C4'-C3'-O3'	-6.41	100.39	110.00
7	D	73	SER	O-C-N	6.41	130.62	122.93
5	G	18	DA	O4'-C1'-C2'	-6.40	96.81	106.40
3	K	27	DG	P-O3'-C3'	6.39	129.78	120.20
7	D	61	HIS	N-CA-C	-6.38	99.38	109.07
7	C	55	LEU	N-CA-C	-6.37	104.39	111.71
7	D	121	THR	N-CA-CB	-6.37	99.73	110.49
7	A	20	ASN	CA-C-N	-6.37	111.25	122.26
7	A	20	ASN	C-N-CA	-6.37	111.25	122.26
1	I	7	DG	O3'-P-O5'	-6.36	94.47	104.00
7	C	321	GLN	CA-C-N	-6.36	116.74	122.97
7	C	321	GLN	C-N-CA	-6.36	116.74	122.97
5	G	6	DT	C6-N1-C1'	6.35	128.88	119.35
7	D	330	LEU	N-CA-C	6.34	117.99	111.14
2	J	18	DA	C4'-C3'-O3'	-6.34	100.49	110.00
5	E	14	DA	C4'-C3'-O3'	6.32	119.48	110.00
5	E	16	DT	O5'-C5'-C4'	6.32	120.28	110.80
7	D	74	VAL	O-C-N	6.32	129.76	123.00
7	B	143	ILE	N-CA-C	-6.32	104.17	110.30
7	A	54	GLU	N-CA-CB	-6.31	100.54	109.94
6	H	4	DA	O4'-C1'-N9	6.31	117.86	108.40
7	B	75	THR	CB-CA-C	-6.29	96.23	109.38
1	I	12	DT	O5'-C5'-C4'	6.28	120.22	110.80
7	D	99	ASN	N-CA-C	-6.27	103.37	111.02
3	K	2	DT	N1-C1'-C2'	6.26	122.89	113.50
7	B	124	ILE	CB-CA-C	-6.26	103.79	111.87
1	I	13	DT	O3'-P-O5'	-6.25	94.62	104.00
5	G	18	DA	C4'-C3'-O3'	-6.25	100.62	110.00
7	D	11	ASP	CA-CB-CG	6.25	118.85	112.60
5	E	3	DA	O3'-P-O5'	6.25	113.37	104.00
7	A	99	ASN	N-CA-C	-6.25	104.16	110.97
6	H	18	DT	N1-C1'-C2'	6.24	122.86	113.50
4	L	27	DC	P-O3'-C3'	6.24	129.56	120.20
4	L	15	DG	P-O3'-C3'	6.21	129.52	120.20
2	J	12	DA	O5'-C5'-C4'	6.20	120.10	110.80
1	I	13	DT	C2-N1-C1'	-6.18	110.08	119.35
3	K	9	DT	P-O5'-C5'	-6.17	110.75	120.00
5	E	18	DA	P-O5'-C5'	6.16	129.24	120.00
5	E	12	DT	C5'-C4'-O4'	6.16	118.63	109.40
7	C	13	PRO	N-CD-CG	-6.15	93.97	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	6	DA	P-O3'-C3'	6.15	129.42	120.20
3	K	6	DA	P-O5'-C5'	6.13	129.20	120.00
3	K	1	DT	O4'-C1'-N1	6.13	117.59	108.40
7	D	162	THR	N-CA-CB	-6.13	100.52	110.81
7	C	23	TYR	CB-CA-C	6.12	120.40	109.38
2	J	13	DT	O3'-P-O5'	-6.12	94.82	104.00
7	A	70	SER	N-CA-C	6.11	121.01	113.50
7	A	15	ASN	CB-CA-C	-6.10	98.28	110.42
1	I	27	DA	N9-C1'-C2'	-6.09	104.36	113.50
1	I	19	DA	C5'-C4'-O4'	-6.09	100.27	109.40
5	E	17	DC	P-O5'-C5'	-6.09	110.87	120.00
6	F	17	DG	N9-C1'-C2'	6.09	122.63	113.50
7	D	197	CYS	N-CA-C	6.08	118.69	111.33
7	C	99	ASN	N-CA-C	-6.07	103.61	111.02
2	J	15	DT	C4'-C3'-O3'	6.07	119.10	110.00
7	D	59	HIS	N-CA-CB	6.07	120.75	110.49
7	B	13	PRO	CA-C-N	6.02	126.04	119.90
7	B	13	PRO	C-N-CA	6.02	126.04	119.90
3	K	16	DT	O4'-C4'-C3'	-6.01	96.38	105.40
5	E	3	DA	OP1-P-O3'	-6.01	89.97	108.00
7	B	83	TYR	N-CA-C	-6.00	103.70	111.02
2	J	13	DT	C4'-C3'-O3'	-5.99	101.01	110.00
1	I	14	DA	O3'-P-O5'	5.96	112.95	104.00
2	J	15	DT	C5'-C4'-C3'	5.95	123.82	114.90
7	B	132	ILE	CB-CA-C	-5.94	104.24	112.02
6	H	4	DA	P-O3'-C3'	-5.93	111.30	120.20
5	G	2	DC	N1-C1'-C2'	5.92	122.39	113.50
6	H	24	DG	O3'-P-O5'	5.92	112.89	104.00
7	D	161	THR	N-CA-CB	-5.92	101.81	110.40
7	D	83	TYR	N-CA-C	-5.90	104.54	110.97
5	E	3	DA	P-O3'-C3'	5.89	129.03	120.20
3	K	14	DT	C4'-C3'-O3'	5.88	118.82	110.00
7	B	168	THR	CB-CA-C	-5.88	100.09	109.80
7	C	58	GLY	CA-C-N	5.87	130.23	121.72
7	C	58	GLY	C-N-CA	5.87	130.23	121.72
6	F	23	DT	C4'-C3'-O3'	-5.85	101.22	110.00
2	J	14	DA	P-O5'-C5'	5.84	128.77	120.00
1	I	14	DA	P-O5'-C5'	-5.84	111.24	120.00
6	H	5	DT	C5'-C4'-O4'	5.83	118.14	109.40
5	E	24	DC	N1-C1'-C2'	5.83	122.24	113.50
3	K	5	DC	O5'-C5'-C4'	5.82	119.53	110.80
4	L	20	DA	O3'-P-O5'	5.81	112.72	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	2	DG	O5'-C5'-C4'	5.81	119.51	110.80
7	B	61	HIS	CA-CB-CG	5.81	119.61	113.80
5	E	24	DC	P-O5'-C5'	5.81	128.71	120.00
7	A	69	ASN	N-CA-C	5.80	119.83	112.87
7	A	83	TYR	N-CA-C	-5.80	103.95	111.02
5	E	11	DA	P-O5'-C5'	5.80	128.69	120.00
5	E	1	DA	C4'-C3'-O3'	-5.79	101.31	110.00
7	A	21	ASN	CB-CA-C	5.79	119.72	109.65
7	C	197	CYS	N-CA-C	5.79	118.37	111.71
6	F	4	DA	C5'-C4'-O4'	5.78	118.07	109.40
5	G	23	DA	C3'-C2'-C1'	5.78	110.27	101.60
7	D	162	THR	N-CA-C	5.77	118.91	108.69
6	H	3	DT	O4'-C4'-C3'	-5.76	96.76	105.40
1	I	12	DT	C1'-O4'-C4'	-5.76	101.06	109.70
7	D	32	GLY	CA-C-O	5.75	125.54	119.04
6	F	16	DA	C2'-C3'-O3'	-5.75	102.88	111.50
7	B	162	THR	N-CA-CB	-5.75	101.17	110.71
6	F	1	DG	O5'-C5'-C4'	5.75	119.42	110.80
5	E	9	DC	C6-N1-C1'	5.74	128.31	119.70
2	J	24	DA	P-O3'-C3'	-5.74	111.59	120.20
2	J	14	DA	O4'-C1'-N9	5.73	117.00	108.40
7	B	111	LEU	N-CA-C	5.73	118.86	110.10
7	B	286	SER	CB-CA-C	-5.72	101.29	110.79
7	C	323	SER	N-CA-C	5.71	117.22	108.42
5	E	5	DG	O3'-P-O5'	-5.70	95.44	104.00
7	A	119	ILE	CB-CA-C	-5.70	103.84	110.91
7	C	152	ARG	CB-CA-C	-5.70	99.07	110.42
2	J	9	DT	P-O5'-C5'	-5.70	111.45	120.00
5	E	20	DA	C4'-C3'-O3'	-5.69	101.47	110.00
5	E	4	DG	O4'-C1'-N9	5.68	116.93	108.40
7	D	55	LEU	CA-CB-CG	-5.67	96.44	116.30
7	A	76	LEU	CA-CB-CG	-5.67	96.45	116.30
3	K	28	DC	P-O5'-C5'	5.65	128.48	120.00
3	K	15	DA	C4'-C3'-O3'	-5.64	101.54	110.00
7	D	72	ASN	CA-C-N	-5.64	114.92	122.42
7	D	72	ASN	C-N-CA	-5.64	114.92	122.42
3	K	16	DT	P-O3'-C3'	5.63	128.65	120.20
7	A	111	LEU	CA-C-N	5.62	125.64	119.90
7	A	111	LEU	C-N-CA	5.62	125.64	119.90
7	B	293	ARG	CB-CA-C	-5.61	102.31	110.96
3	K	16	DT	O3'-P-O5'	-5.61	95.58	104.00
7	D	61	HIS	CA-CB-CG	5.61	119.41	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	73	SER	CB-CA-C	5.61	120.06	110.81
2	J	11	DT	P-O3'-C3'	5.60	128.60	120.20
7	D	111	LEU	N-CA-C	5.60	118.67	110.10
1	I	15	DC	C2'-C3'-O3'	5.60	119.90	111.50
2	J	11	DT	C6-N1-C1'	5.60	127.75	119.35
2	J	11	DT	N1-C1'-C2'	5.60	121.90	113.50
3	K	24	DT	N1-C1'-C2'	5.60	121.89	113.50
5	E	1	DA	C2'-C3'-O3'	5.59	119.89	111.50
7	C	165	VAL	N-CA-C	5.59	115.79	110.53
7	C	173	SER	N-CA-C	5.58	117.62	108.52
1	I	11	DT	N1-C1'-C2'	5.57	121.86	113.50
3	K	15	DA	C5'-C4'-O4'	5.57	117.75	109.40
6	F	24	DG	O4'-C1'-C2'	-5.57	98.04	106.40
6	F	4	DA	C4'-C3'-O3'	-5.57	101.65	110.00
6	H	2	DG	C8-N9-C1'	5.57	135.35	127.00
7	D	40	ASP	CA-C-N	5.57	129.17	120.82
7	D	40	ASP	C-N-CA	5.57	129.17	120.82
3	K	11	DT	N1-C1'-C2'	5.56	121.84	113.50
4	L	15	DG	C2'-C3'-O3'	5.56	119.84	111.50
3	K	5	DC	P-O3'-C3'	5.55	128.52	120.20
3	K	20	DA	O3'-P-O5'	5.55	112.32	104.00
4	L	16	DA	O3'-P-O5'	-5.54	95.69	104.00
4	L	15	DG	C4'-C3'-C2'	-5.54	94.10	102.40
7	D	23	TYR	CB-CA-C	-5.54	100.14	109.72
2	J	23	DC	N1-C1'-C2'	5.53	121.79	113.50
3	K	21	DA	C3'-C2'-C1'	5.52	109.89	101.60
5	G	5	DG	C5'-C4'-C3'	-5.52	106.62	114.90
5	G	6	DT	O4'-C1'-N1	5.51	116.67	108.40
2	J	9	DT	C5'-C4'-O4'	-5.51	101.14	109.40
5	E	2	DC	N1-C1'-C2'	5.51	121.76	113.50
3	K	14	DT	N3-C4-O4	-5.50	114.34	122.60
5	E	11	DA	C8-N9-C1'	5.50	135.31	127.05
7	D	173	SER	N-CA-C	5.50	117.87	108.90
4	L	8	DC	C4'-C3'-O3'	5.49	118.23	110.00
5	E	4	DG	C5'-C4'-C3'	-5.48	106.67	114.90
3	K	5	DC	C5'-C4'-C3'	5.47	123.11	114.90
1	I	13	DT	C6-N1-C1'	5.47	127.56	119.35
5	G	12	DT	P-O5'-C5'	5.47	128.21	120.00
6	H	10	DA	C3'-C2'-C1'	-5.47	93.40	101.60
7	D	155	ILE	CB-CA-C	-5.47	103.41	112.26
3	K	23	DT	C5'-C4'-C3'	5.46	123.09	114.90
2	J	12	DA	O3'-P-O5'	-5.46	95.81	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	81	ASP	CA-C-N	-5.46	111.58	121.14
7	B	81	ASP	C-N-CA	-5.46	111.58	121.14
6	H	5	DT	O5'-C5'-C4'	5.46	118.99	110.80
5	G	14	DA	C4'-C3'-O3'	5.46	118.19	110.00
5	G	18	DA	C3'-C2'-C1'	-5.45	93.42	101.60
6	F	23	DT	O4'-C1'-N1	5.45	116.58	108.40
3	K	15	DA	OP1-P-O3'	-5.45	91.66	108.00
5	G	12	DT	C5'-C4'-O4'	5.45	117.57	109.40
2	J	15	DT	C1'-O4'-C4'	-5.44	101.54	109.70
5	E	6	DT	C4'-C3'-O3'	5.44	118.16	110.00
3	K	16	DT	C2'-C3'-O3'	5.43	119.64	111.50
7	D	40	ASP	N-CA-C	5.42	117.47	108.20
7	A	105	LYS	N-CA-C	-5.42	102.48	111.37
6	H	13	DG	O4'-C1'-N9	5.42	116.53	108.40
7	B	87	LEU	CA-CB-CG	-5.41	97.35	116.30
1	I	15	DC	P-O3'-C3'	5.40	128.31	120.20
3	K	15	DA	N9-C1'-C2'	5.40	121.59	113.50
7	C	323	SER	CA-C-N	5.39	127.50	120.28
7	C	323	SER	C-N-CA	5.39	127.50	120.28
3	K	8	DC	C5'-C4'-O4'	-5.39	101.31	109.40
5	E	20	DA	N9-C1'-C2'	5.39	121.58	113.50
7	C	238	VAL	CB-CA-C	5.39	119.45	111.26
1	I	13	DT	N3-C4-O4	-5.38	114.52	122.60
2	J	2	DG	O4'-C1'-N9	5.38	116.47	108.40
1	I	11	DT	C4-C5-C7	-5.38	114.34	122.40
2	J	12	DA	N9-C1'-C2'	5.38	121.56	113.50
1	I	3	DC	O4'-C1'-N1	5.37	116.46	108.40
7	B	65	THR	CA-C-N	5.37	131.80	121.54
7	B	65	THR	C-N-CA	5.37	131.80	121.54
4	L	27	DC	O4'-C1'-N1	5.37	116.45	108.40
2	J	17	DA	P-O5'-C5'	-5.36	111.96	120.00
7	A	124	ILE	CB-CA-C	-5.35	105.12	111.97
7	A	336	ASP	N-CA-C	5.34	121.64	113.19
1	I	16	DA	O5'-C5'-C4'	5.34	118.81	110.80
5	G	9	DC	N1-C1'-C2'	5.34	121.51	113.50
4	L	20	DA	C4'-C3'-O3'	5.33	117.99	110.00
5	G	17	DC	O3'-P-O5'	5.33	111.99	104.00
1	I	28	DT	C4'-C3'-O3'	5.31	117.97	110.00
7	A	341	GLN	N-CA-C	-5.31	107.34	112.97
6	F	25	DT	C4'-C3'-O3'	5.30	117.95	110.00
7	D	72	ASN	CB-CA-C	-5.30	101.01	110.70
7	B	69	ASN	N-CA-C	5.29	119.43	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	14	DA	O4'-C1'-N9	5.28	116.33	108.40
5	E	14	DA	O4'-C1'-N9	5.28	116.31	108.40
7	B	104	ILE	N-CA-CB	-5.27	102.53	111.23
1	I	15	DC	N3-C2-O2	-5.27	114.00	121.90
7	D	170	ALA	CA-C-N	-5.26	113.23	120.71
7	D	170	ALA	C-N-CA	-5.26	113.23	120.71
2	J	20	DA	C4'-C3'-O3'	5.26	117.89	110.00
6	H	15	DT	C1'-O4'-C4'	5.25	117.58	109.70
6	H	15	DT	O4'-C1'-N1	5.25	116.28	108.40
7	C	160	ILE	CB-CA-C	-5.24	104.01	111.19
4	L	28	DA	O4'-C1'-N9	5.24	116.26	108.40
5	G	7	DC	P-O3'-C3'	5.24	128.06	120.20
5	G	19	DA	O4'-C1'-C2'	-5.24	98.54	106.40
7	B	80	LEU	N-CA-C	-5.23	105.58	111.28
2	J	10	DT	C5'-C4'-O4'	-5.23	101.56	109.40
7	C	120	THR	N-CA-C	5.23	118.00	109.59
3	K	11	DT	C4-C5-C7	-5.22	114.56	122.40
7	B	233	GLN	N-CA-C	5.22	116.67	109.15
1	I	16	DA	C5'-C4'-O4'	5.22	117.23	109.40
7	C	111	LEU	N-CA-C	5.22	118.09	110.10
2	J	14	DA	O4'-C1'-C2'	-5.21	98.58	106.40
7	A	61	HIS	N-CA-C	-5.21	100.29	108.63
7	D	80	LEU	N-CA-C	-5.21	105.60	111.28
2	J	28	DT	N1-C1'-C2'	5.20	121.31	113.50
7	B	49	ILE	N-CA-CB	5.19	117.60	110.54
3	K	19	DA	C5'-C4'-C3'	-5.18	107.13	114.90
6	H	15	DT	O3'-P-O5'	5.18	111.77	104.00
7	D	11	ASP	OD1-CG-OD2	-5.17	110.48	122.90
5	G	7	DC	N1-C1'-C2'	5.16	121.24	113.50
2	J	18	DA	N9-C1'-C2'	5.16	121.24	113.50
5	G	15	DG	O3'-P-O5'	-5.16	96.26	104.00
5	E	15	DG	O3'-P-O5'	-5.15	96.27	104.00
2	J	6	DA	C4'-C3'-O3'	-5.15	102.27	110.00
5	G	13	DC	O3'-P-O5'	5.15	111.72	104.00
5	E	10	DT	O4'-C1'-N1	5.14	116.12	108.40
7	B	162	THR	N-CA-C	5.14	117.73	108.48
7	C	353	ILE	N-CA-C	-5.13	102.88	109.30
7	D	49	ILE	N-CA-CB	5.12	117.51	110.54
3	K	20	DA	C1'-O4'-C4'	-5.12	102.02	109.70
7	C	34	GLU	N-CA-C	-5.12	103.16	110.59
5	G	13	DC	O5'-C5'-C4'	5.11	118.47	110.80
6	H	6	DT	O4'-C1'-C2'	-5.10	98.75	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	33	LYS	CG-CD-CE	5.10	123.03	111.30
5	E	14	DA	O5'-C5'-C4'	5.10	118.45	110.80
7	B	103	LYS	N-CA-CB	-5.09	102.48	109.91
5	G	3	DA	O3'-P-O5'	5.08	111.62	104.00
7	A	111	LEU	N-CA-C	5.08	117.93	109.09
4	L	12	DG	P-O3'-C3'	5.07	127.81	120.20
3	K	18	DT	P-O5'-C5'	-5.06	112.40	120.00
7	A	53	ILE	CA-C-N	5.06	127.37	120.54
7	A	53	ILE	C-N-CA	5.06	127.37	120.54
7	C	261	LYS	N-CA-C	-5.06	105.95	111.82
1	I	13	DT	C1'-O4'-C4'	-5.06	102.11	109.70
6	H	10	DA	N9-C1'-C2'	5.05	121.08	113.50
6	F	1	DG	C4'-C3'-O3'	-5.04	102.44	110.00
2	J	14	DA	C4'-C3'-O3'	5.04	117.56	110.00
5	E	3	DA	O5'-C5'-C4'	-5.04	103.24	110.80
5	E	22	DT	P-O5'-C5'	5.04	127.55	120.00
5	G	16	DT	C5'-C4'-O4'	5.03	116.95	109.40
4	L	1	DG	O4'-C1'-N9	5.03	115.94	108.40
5	E	22	DT	P-O3'-C3'	5.03	127.74	120.20
5	G	24	DC	N1-C1'-C2'	5.02	121.03	113.50
4	L	17	DA	C5'-C4'-O4'	-5.02	101.87	109.40
7	A	9	ARG	N-CA-C	5.02	121.49	110.80
7	B	59	HIS	N-CA-C	5.02	121.49	110.80
2	J	8	DG	C5'-C4'-O4'	-5.02	101.88	109.40
5	E	23	DA	C4-N9-C1'	5.02	134.58	127.05
6	H	15	DT	O4'-C1'-C2'	-5.01	98.88	106.40
7	B	56	PHE	N-CA-C	5.01	117.49	107.62
6	F	2	DG	C5'-C4'-C3'	5.01	122.41	114.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	A	73	SER	Peptide
7	C	73	SER	Peptide

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	588	0	331	76	0
2	J	594	0	328	70	1
3	K	590	0	332	54	0
4	L	594	0	329	41	0
5	E	487	0	271	56	1
5	G	487	0	271	46	0
6	F	513	0	287	62	0
6	H	513	0	287	63	0
7	A	2763	0	2795	358	0
7	B	2630	0	2628	368	0
7	C	2767	0	2801	333	0
7	D	2630	0	2628	311	0
All	All	15156	0	13288	1681	1

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 59.

All (1681) 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)
7:A:71:ASP:CB	7:A:71:ASP:CG	1.75	1.58
7:C:101:MSE:CE	7:C:101:MSE:SE	2.18	1.41
7:D:101:MSE:CE	7:D:101:MSE:SE	2.18	1.40
1:I:13:DT:N3	2:J:17:DA:N6	1.69	1.39
1:I:13:DT:H3	2:J:17:DA:N6	1.12	1.39
7:A:338:MSE:CE	7:A:338:MSE:SE	2.23	1.36
7:B:101:MSE:SE	7:B:101:MSE:CE	2.24	1.34
7:D:169:ARG:C	7:D:169:ARG:HD2	1.43	1.32
7:D:165:VAL:O	7:D:168:THR:HG22	1.31	1.24
5:E:12:DT:H2''	5:E:13:DC:C5'	1.67	1.22
7:C:74:VAL:CG1	7:C:75:THR:H	1.49	1.22
1:I:12:DT:OP1	7:A:212:ARG:NH2	1.76	1.19
7:C:75:THR:CG2	7:C:78:SER:HB3	1.73	1.18
6:H:6:DT:H2''	6:H:7:DT:H5''	1.27	1.17
7:A:50:GLN:O	7:A:53:ILE:HG22	1.39	1.17
7:C:47:GLU:OE2	7:D:63:PRO:HD2	1.42	1.16
1:I:13:DT:C4	2:J:17:DA:N6	2.13	1.16
7:B:23:TYR:HD2	7:B:24:TYR:N	1.42	1.16
7:C:75:THR:HG23	7:C:78:SER:CB	1.74	1.16
7:A:61:HIS:NE2	7:D:47:GLU:OE1	1.77	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:14:DT:H4'	3:K:15:DA:OP1	1.46	1.14
7:C:148:SER:OG	7:C:152:ARG:NH2	1.80	1.13
7:B:120:THR:HG22	7:B:122:LYS:N	1.62	1.13
7:C:74:VAL:HG12	7:C:75:THR:N	1.47	1.13
7:D:306:THR:O	7:D:309:GLU:HB2	1.46	1.13
2:J:9:DT:H2''	2:J:10:DT:H5'	1.23	1.13
7:B:195:SER:HB3	7:B:199:LEU:CD2	1.78	1.12
2:J:16:DT:H2'	2:J:17:DA:H5''	1.24	1.12
7:C:47:GLU:HB3	7:D:63:PRO:HG2	1.32	1.11
7:D:101:MSE:HA	7:D:104:ILE:HD12	1.32	1.10
7:D:52:ASN:O	7:D:56:PHE:O	1.68	1.10
5:E:12:DT:C2'	5:E:13:DC:H5''	1.81	1.10
7:D:169:ARG:HD2	7:D:169:ARG:O	1.48	1.09
7:A:23:TYR:OH	7:A:36:GLY:HA2	1.52	1.09
7:C:19:ARG:HG2	7:C:19:ARG:HH11	0.98	1.09
7:D:211:GLN:C	7:D:311:ARG:HD2	1.77	1.09
7:B:76:LEU:O	7:B:80:LEU:HD12	1.51	1.08
3:K:23:DT:OP1	7:B:306:THR:OG1	1.71	1.08
7:A:75:THR:HG23	7:A:78:SER:HB2	1.33	1.07
7:B:195:SER:CB	7:B:199:LEU:HD22	1.85	1.07
7:D:104:ILE:HA	7:D:107:ILE:HD12	1.30	1.06
6:F:2:DG:H2''	6:F:3:DT:H71	1.33	1.05
7:B:27:ARG:CD	7:B:34:GLU:HG2	1.86	1.05
7:C:101:MSE:HA	7:C:104:ILE:HD12	1.37	1.05
7:A:28:ASP:OD2	7:A:30:ARG:HB3	1.57	1.05
7:B:76:LEU:HG	7:B:80:LEU:HD11	1.33	1.04
7:A:163:ASN:OD1	7:A:165:VAL:HB	1.57	1.03
1:I:18:DC:H2''	1:I:19:DA:H5''	1.06	1.03
5:E:12:DT:H2''	5:E:13:DC:H5''	1.04	1.03
7:C:14:PRO:O	7:C:15:ASN:HB2	1.57	1.03
2:J:19:DA:H2'	7:A:96:THR:CG2	1.90	1.02
6:F:6:DT:H2''	6:F:7:DT:H5''	1.36	1.02
7:D:144:ARG:NH2	7:D:168:THR:O	1.92	1.02
7:D:33:LYS:HA	7:D:33:LYS:HE3	1.38	1.02
7:D:169:ARG:C	7:D:169:ARG:CD	2.32	1.02
2:J:16:DT:H2'	2:J:16:DT:O2	1.56	1.01
7:D:144:ARG:HE	7:D:168:THR:HG23	1.26	1.01
7:B:306:THR:O	7:B:309:GLU:HB2	1.58	1.01
7:A:309:GLU:OE1	7:A:309:GLU:O	1.77	1.01
7:B:129:ASN:HA	7:B:132:ILE:HD12	1.38	1.01
7:D:154:ALA:HB3	7:D:160:ILE:HD11	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:6:DT:H2''	5:G:7:DC:H6	1.20	1.00
5:G:6:DT:H2''	5:G:7:DC:C6	1.96	1.00
7:D:31:THR:OG1	7:D:33:LYS:HG2	1.61	1.00
7:D:79:TRP:CZ2	7:D:154:ALA:HA	1.97	0.99
7:D:221:TRP:CH2	7:D:263:LYS:HB3	1.97	0.99
7:A:160:ILE:HG22	7:A:161:THR:N	1.74	0.98
7:B:195:SER:HB3	7:B:199:LEU:HD22	1.42	0.98
7:B:270:THR:OG1	7:B:272:ILE:O	1.80	0.98
6:F:9:DG:H2''	7:A:20:ASN:HD21	1.28	0.98
7:A:116:LEU:O	7:A:119:ILE:HD12	1.64	0.98
7:A:114:ALA:HB1	7:A:115:PRO:HD3	1.43	0.98
7:A:114:ALA:HB1	7:A:115:PRO:CD	1.93	0.97
7:B:155:ILE:HG13	7:B:160:ILE:HG12	1.42	0.97
3:K:9:DT:H2''	3:K:10:DT:H5''	1.45	0.97
7:C:23:TYR:HD2	7:C:24:TYR:N	1.63	0.97
1:I:13:DT:O4	2:J:17:DA:N6	1.98	0.97
7:C:19:ARG:HG2	7:C:19:ARG:NH1	1.64	0.96
2:J:19:DA:H2'	7:A:96:THR:HG21	1.47	0.96
7:B:60:LYS:O	7:B:61:HIS:HB3	1.63	0.96
1:I:8:DC:P	7:A:136:LYS:HZ3	1.87	0.96
7:B:205:LEU:O	7:B:208:VAL:HG12	1.65	0.96
1:I:5:DC:H1'	1:I:6:DT:H5'	1.47	0.96
3:K:12:DA:OP1	7:C:212:ARG:NH2	1.98	0.96
7:B:23:TYR:CD2	7:B:24:TYR:N	2.33	0.95
7:B:31:THR:OG1	7:B:33:LYS:HG2	1.66	0.95
7:D:76:LEU:HD12	7:D:76:LEU:O	1.65	0.95
7:C:26:TYR:CE1	7:C:51:ALA:HB3	2.01	0.95
6:F:6:DT:C2'	6:F:7:DT:H5''	1.96	0.94
2:J:16:DT:C2'	2:J:17:DA:H5''	1.97	0.94
7:B:213:VAL:HA	7:B:216:LEU:HD12	1.49	0.94
7:C:57:SER:O	7:C:59:HIS:N	1.99	0.94
7:C:160:ILE:HG22	7:C:161:THR:N	1.78	0.94
7:D:249:ASP:OD2	7:D:321:GLN:NE2	2.01	0.94
7:B:114:ALA:HB1	7:B:115:PRO:HD3	1.50	0.94
7:C:54:GLU:OE2	7:C:55:LEU:HD23	1.67	0.94
4:L:8:DC:H2'	4:L:9:DT:H71	1.48	0.94
1:I:8:DC:OP1	7:A:136:LYS:NZ	2.01	0.93
7:B:196:PRO:O	7:B:199:LEU:HD13	1.68	0.93
6:H:17:DG:C8	6:H:18:DT:H71	2.03	0.93
6:F:10:DA:N6	7:A:19:ARG:HH21	1.67	0.93
7:A:23:TYR:C	7:A:23:TYR:CD2	2.42	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:27:ARG:NH1	7:B:34:GLU:OE1	2.01	0.93
7:C:23:TYR:OH	7:C:36:GLY:HA2	1.68	0.92
7:B:120:THR:HG22	7:B:122:LYS:H	1.34	0.92
7:C:307:PHE:O	7:C:310:LEU:HG	1.69	0.92
7:A:57:SER:O	7:A:59:HIS:N	2.01	0.92
7:B:76:LEU:C	7:B:80:LEU:HD12	1.94	0.92
1:I:8:DC:P	7:A:136:LYS:NZ	2.42	0.92
7:B:84:GLU:HA	7:B:87:LEU:HD12	1.52	0.92
7:C:205:LEU:O	7:C:209:THR:HG23	1.71	0.91
7:C:111:LEU:HD22	7:C:112:PRO:HD2	1.52	0.91
7:B:149:ASP:HA	7:B:152:ARG:HD2	1.52	0.91
7:C:23:TYR:CD2	7:C:24:TYR:N	2.38	0.91
7:A:120:THR:HG22	7:A:123:GLU:HG3	1.52	0.91
7:D:27:ARG:HG3	7:D:34:GLU:HG2	1.51	0.91
7:B:205:LEU:HD23	7:B:272:ILE:HD11	1.53	0.91
7:A:211:GLN:C	7:A:311:ARG:HD2	1.96	0.90
7:A:116:LEU:HA	7:A:119:ILE:HD11	1.51	0.90
6:F:9:DG:C2'	7:A:20:ASN:HD21	1.85	0.90
7:C:23:TYR:OH	7:C:36:GLY:CA	2.19	0.90
7:B:50:GLN:HA	7:B:53:ILE:HD12	1.51	0.90
3:K:12:DA:H2'	3:K:13:DT:H72	1.52	0.90
7:D:70:SER:O	7:D:73:SER:N	2.05	0.90
7:D:80:LEU:CD2	7:D:104:ILE:HG23	2.01	0.90
7:B:155:ILE:CG1	7:B:160:ILE:HG12	2.01	0.89
1:I:18:DC:C2'	1:I:19:DA:H5''	1.99	0.89
7:C:354:GLU:HB2	7:C:356:LYS:HB2	1.53	0.89
7:B:79:TRP:CH2	7:B:154:ALA:HA	2.08	0.89
7:C:47:GLU:CB	7:D:63:PRO:HG2	2.03	0.89
7:B:155:ILE:HG13	7:B:160:ILE:CG1	2.01	0.89
7:D:19:ARG:HD3	7:D:20:ASN:H	1.36	0.88
4:L:13:DT:H5''	7:D:236:THR:HG21	1.53	0.88
7:C:74:VAL:CG1	7:C:75:THR:N	2.20	0.88
7:D:80:LEU:HD21	7:D:104:ILE:HG23	1.55	0.88
7:D:154:ALA:CB	7:D:160:ILE:HD11	2.02	0.88
7:D:169:ARG:O	7:D:169:ARG:CD	2.22	0.88
7:B:305:PRO:HB3	7:B:309:GLU:HG3	1.55	0.88
7:B:52:ASN:O	7:B:56:PHE:O	1.92	0.88
7:B:195:SER:CB	7:B:199:LEU:CD2	2.46	0.88
6:H:1:DG:H2''	6:H:2:DG:OP2	1.74	0.88
7:A:293:ARG:NH1	7:A:305:PRO:O	2.06	0.88
7:C:19:ARG:HH11	7:C:19:ARG:CG	1.87	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:27:ARG:HD3	7:B:34:GLU:HG2	1.54	0.87
7:B:114:ALA:HB1	7:B:115:PRO:CD	2.02	0.87
5:G:7:DC:H2'	5:G:8:DA:C8	2.08	0.87
7:D:76:LEU:HD12	7:D:76:LEU:C	1.94	0.87
7:A:76:LEU:HD12	7:A:76:LEU:N	1.87	0.87
7:B:155:ILE:HG22	7:B:155:ILE:O	1.71	0.87
7:B:195:SER:HB3	7:B:199:LEU:HD21	1.57	0.87
7:D:19:ARG:CD	7:D:20:ASN:N	2.38	0.87
6:H:17:DG:OP2	7:D:17:TYR:CE2	2.26	0.87
7:A:152:ARG:O	7:A:155:ILE:HB	1.74	0.87
7:B:27:ARG:HD3	7:B:34:GLU:CD	1.99	0.87
7:D:19:ARG:CD	7:D:20:ASN:H	1.87	0.87
7:D:211:GLN:HA	7:D:311:ARG:HH11	1.40	0.87
7:C:145:SER:O	7:C:148:SER:HB3	1.73	0.86
2:J:8:DG:O5'	7:B:136:LYS:HD3	1.75	0.86
7:B:195:SER:HB2	7:B:199:LEU:HD22	1.56	0.86
7:D:75:THR:HG23	7:D:78:SER:HB2	1.57	0.86
7:C:26:TYR:HE1	7:C:51:ALA:HB3	1.40	0.86
7:C:116:LEU:N	7:C:116:LEU:HD12	1.90	0.86
7:B:350:TRP:CZ3	7:C:239:LYS:HB3	2.10	0.86
6:H:13:DG:H2''	6:H:14:DA:O5'	1.75	0.86
7:A:160:ILE:CG2	7:A:161:THR:N	2.36	0.86
5:E:16:DT:O4	7:A:19:ARG:NH2	2.08	0.86
6:F:2:DG:H2''	6:F:3:DT:C7	2.04	0.86
7:C:114:ALA:HB1	7:C:115:PRO:CD	2.06	0.86
7:C:9:ARG:HD2	7:C:10:ARG:HE	1.41	0.86
7:B:47:GLU:OE1	7:C:61:HIS:NE2	2.08	0.86
7:D:23:TYR:CD2	7:D:24:TYR:N	2.43	0.86
6:H:8:DT:OP2	7:C:12:LEU:HD21	1.74	0.86
7:C:160:ILE:CG2	7:C:161:THR:N	2.36	0.86
7:C:224:ILE:HD11	7:C:271:ILE:HD11	1.57	0.86
7:A:110:GLY:O	7:A:111:LEU:HD23	1.75	0.85
7:A:165:VAL:HG12	7:A:166:ALA:N	1.89	0.85
7:B:45:ILE:O	7:B:48:ALA:HB3	1.75	0.85
7:C:40:ASP:OD2	7:C:42:ARG:HG3	1.77	0.85
7:A:210:GLY:O	7:A:311:ARG:NH1	2.10	0.85
5:E:10:DT:H2''	5:E:11:DA:N7	1.92	0.85
7:B:54:GLU:OE2	7:B:54:GLU:HA	1.74	0.85
7:A:75:THR:CG2	7:A:78:SER:HB2	2.06	0.84
7:A:76:LEU:O	7:A:80:LEU:HD12	1.76	0.84
7:A:179:ARG:NH1	7:A:312:SER:OG	2.09	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:84:GLU:HA	7:D:87:LEU:HD12	1.57	0.84
6:F:17:DG:OP2	7:B:17:TYR:CE2	2.30	0.84
7:B:155:ILE:HG13	7:B:160:ILE:CD1	2.08	0.84
1:I:8:DC:O5'	7:A:136:LYS:NZ	2.10	0.83
7:A:10:ARG:NH2	7:A:12:LEU:HD22	1.91	0.83
1:I:23:DT:OP1	7:D:306:THR:OG1	1.96	0.83
7:A:18:ILE:HG13	7:A:24:TYR:CE2	2.13	0.83
7:C:221:TRP:CH2	7:C:263:LYS:HB2	2.13	0.83
7:C:23:TYR:HD2	7:C:24:TYR:H	1.22	0.83
7:C:45:ILE:O	7:C:48:ALA:HB3	1.78	0.83
7:B:27:ARG:HD3	7:B:34:GLU:CG	2.08	0.83
1:I:16:DA:C6	4:L:15:DG:N2	2.47	0.83
7:A:18:ILE:HD11	7:A:22:GLY:HA2	1.61	0.83
7:D:19:ARG:HD3	7:D:20:ASN:N	1.92	0.83
7:A:169:ARG:HH21	7:B:152:ARG:HD3	1.44	0.83
7:B:49:ILE:O	7:B:53:ILE:HG13	1.79	0.82
1:I:12:DT:P	7:A:212:ARG:NH2	2.51	0.82
7:C:354:GLU:C	7:C:356:LYS:H	1.83	0.82
7:A:75:THR:HG23	7:A:78:SER:CB	2.09	0.82
5:G:2:DC:H2''	5:G:3:DA:N7	1.93	0.82
7:A:103:LYS:O	7:A:106:ALA:HB3	1.78	0.82
7:A:117:GLU:OE1	7:A:117:GLU:N	2.09	0.82
7:C:74:VAL:HG12	7:C:75:THR:H	0.68	0.82
5:G:15:DG:N7	7:C:19:ARG:HD2	1.93	0.82
7:D:50:GLN:HA	7:D:53:ILE:HD11	1.59	0.82
2:J:7:DA:H2''	2:J:8:DG:H5''	1.60	0.82
7:A:76:LEU:C	7:A:80:LEU:HD12	2.05	0.82
7:D:212:ARG:NE	7:D:233:GLN:OE1	2.13	0.82
7:A:165:VAL:O	7:A:168:THR:HG22	1.79	0.82
7:A:111:LEU:HD22	7:A:112:PRO:HD2	1.62	0.81
7:A:169:ARG:HH11	7:A:169:ARG:HG2	1.42	0.81
7:A:254:SER:O	7:A:258:THR:OG1	1.97	0.81
7:B:23:TYR:HD2	7:B:24:TYR:H	1.26	0.81
7:C:306:THR:O	7:C:309:GLU:HB2	1.81	0.81
1:I:24:DT:OP2	7:D:293:ARG:NH2	2.13	0.81
7:B:16:LEU:HD23	7:B:16:LEU:C	2.05	0.81
7:A:116:LEU:O	7:A:119:ILE:CD1	2.27	0.81
7:A:169:ARG:HG2	7:A:169:ARG:NH1	1.95	0.81
7:B:155:ILE:O	7:B:155:ILE:CG2	2.26	0.81
7:A:160:ILE:CG2	7:A:161:THR:H	1.94	0.81
7:A:309:GLU:OE1	7:A:312:SER:HB3	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:27:ARG:CD	7:B:34:GLU:CG	2.59	0.81
7:C:18:ILE:HD11	7:C:22:GLY:HA2	1.63	0.81
6:F:23:DT:H2''	6:F:24:DG:C8	2.16	0.80
7:D:15:ASN:HB2	7:D:26:TYR:HE1	1.46	0.80
2:J:9:DT:H2''	2:J:10:DT:C5'	2.10	0.80
5:G:6:DT:C2'	5:G:7:DC:H6	1.92	0.80
7:B:76:LEU:O	7:B:80:LEU:CD1	2.30	0.80
7:A:144:ARG:HE	7:A:168:THR:HG23	1.47	0.80
6:H:19:DG:H2'	6:H:20:DA:C8	2.16	0.80
7:C:57:SER:C	7:C:59:HIS:H	1.88	0.80
6:H:2:DG:OP2	6:H:2:DG:H8	1.64	0.80
7:B:62:LYS:O	7:B:65:THR:N	2.14	0.80
7:B:123:GLU:O	7:B:126:ALA:HB3	1.82	0.80
6:H:8:DT:H2''	6:H:9:DG:C8	2.17	0.79
7:B:203:MSE:O	7:B:207:VAL:HG23	1.82	0.79
7:A:77:HIS:HB2	7:A:113:ASP:OD1	1.83	0.79
7:B:19:ARG:HG2	7:B:20:ASN:H	1.47	0.79
7:B:101:MSE:HA	7:B:104:ILE:HD12	1.64	0.79
4:L:20:DA:H2''	4:L:21:DA:O4'	1.82	0.79
7:A:14:PRO:O	7:A:15:ASN:ND2	2.16	0.79
7:A:333:HIS:NE2	7:A:338:MSE:HB2	1.98	0.79
7:A:148:SER:HB2	7:A:165:VAL:HG11	1.64	0.79
7:D:180:LEU:O	7:D:316:ARG:NH2	2.16	0.78
3:K:8:DC:H2'	3:K:9:DT:H71	1.66	0.78
7:C:160:ILE:CG2	7:C:161:THR:H	1.95	0.78
7:A:54:GLU:OE2	7:A:55:LEU:N	2.16	0.78
2:J:16:DT:C2'	2:J:17:DA:C5'	2.62	0.78
6:H:6:DT:C6	6:H:7:DT:H72	2.18	0.78
7:A:57:SER:OG	7:A:59:HIS:CB	2.32	0.78
7:B:50:GLN:HA	7:B:53:ILE:CD1	2.13	0.78
7:A:69:ASN:O	7:A:73:SER:HB2	1.82	0.78
7:D:114:ALA:HB1	7:D:115:PRO:HD3	1.66	0.78
7:D:104:ILE:CA	7:D:107:ILE:HD12	2.12	0.77
6:H:15:DT:H2''	6:H:16:DA:O5'	1.84	0.77
7:B:163:ASN:OD1	7:B:165:VAL:HB	1.82	0.77
7:C:23:TYR:CE2	7:C:24:TYR:O	2.38	0.77
3:K:16:DT:H1'	3:K:17:DA:C8	2.20	0.77
1:I:13:DT:H2''	1:I:14:DA:H8	1.49	0.77
6:H:17:DG:C8	6:H:18:DT:C7	2.67	0.77
7:C:165:VAL:O	7:C:168:THR:HG22	1.84	0.77
7:C:120:THR:HG22	7:C:123:GLU:HG3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:7:DG:H2''	1:I:8:DC:H5''	1.66	0.76
7:C:92:ILE:CG2	7:C:96:THR:HB	2.15	0.76
7:B:19:ARG:HG2	7:B:20:ASN:N	2.01	0.76
2:J:18:DA:H2''	7:A:100:TYR:OH	1.86	0.76
7:C:79:TRP:CE2	7:C:154:ALA:HB2	2.19	0.76
2:J:19:DA:H2'	7:A:96:THR:HG23	1.66	0.76
5:G:6:DT:C2'	5:G:7:DC:C6	2.66	0.76
2:J:14:DA:H1'	2:J:15:DT:H5'	1.66	0.76
7:B:74:VAL:HG12	7:B:75:THR:N	2.00	0.76
7:D:141:LYS:C	7:D:141:LYS:CD	2.59	0.76
7:B:77:HIS:HA	7:B:80:LEU:HD12	1.67	0.76
7:A:101:MSE:HA	7:A:104:ILE:CD1	2.15	0.76
4:L:23:DC:H5''	7:C:306:THR:HG21	1.68	0.75
7:B:40:ASP:N	7:B:40:ASP:OD1	2.12	0.75
7:A:232:GLU:HG2	7:A:232:GLU:O	1.86	0.75
7:B:54:GLU:CG	7:C:65:THR:HG23	2.17	0.75
2:J:2:DG:H4'	7:B:276:ARG:NH2	2.01	0.75
7:A:57:SER:OG	7:A:59:HIS:HB2	1.85	0.75
1:I:10:DT:H5'	7:A:175:VAL:HG13	1.67	0.75
5:E:6:DT:H2'	5:E:7:DC:C6	2.21	0.75
7:B:41:ARG:O	7:B:45:ILE:HG13	1.86	0.75
1:I:10:DT:H2'	1:I:11:DT:H71	1.68	0.75
7:B:290:MSE:O	7:B:293:ARG:HB2	1.87	0.75
1:I:27:DA:H1'	1:I:28:DT:H5'	1.68	0.75
2:J:14:DA:H2''	2:J:15:DT:OP2	1.86	0.75
6:F:10:DA:N6	7:A:19:ARG:NH2	2.33	0.75
7:A:101:MSE:HA	7:A:104:ILE:HD12	1.68	0.75
7:A:338:MSE:C	7:A:340:SER:H	1.93	0.75
7:C:186:LEU:CD1	7:C:251:LEU:HD22	2.17	0.75
6:F:10:DA:H61	7:A:19:ARG:NH2	1.84	0.74
7:D:23:TYR:CE2	7:D:24:TYR:O	2.40	0.74
2:J:20:DA:H2''	2:J:21:DA:H5''	1.68	0.74
5:E:2:DC:H2''	5:E:3:DA:N7	2.01	0.74
5:E:12:DT:H2''	5:E:13:DC:H5'	1.66	0.74
7:B:212:ARG:HG3	7:B:215:ASP:OD2	1.86	0.74
7:D:15:ASN:HB2	7:D:26:TYR:CE1	2.22	0.74
7:C:56:PHE:O	7:C:57:SER:HB3	1.88	0.74
2:J:21:DA:H2'	2:J:22:DG:H8	1.52	0.74
7:A:104:ILE:O	7:A:107:ILE:N	2.20	0.74
7:A:306:THR:O	7:A:309:GLU:HB2	1.87	0.74
7:B:36:GLY:O	7:C:67:ARG:NH2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:87:LEU:HD12	7:C:87:LEU:N	2.03	0.74
7:D:36:GLY:C	7:D:37:LEU:HD23	2.12	0.74
7:A:211:GLN:HA	7:A:311:ARG:HH11	1.49	0.74
7:D:211:GLN:HA	7:D:311:ARG:NH1	2.02	0.74
7:A:9:ARG:HB2	7:A:10:ARG:HG3	1.70	0.74
7:A:23:TYR:C	7:A:23:TYR:HD2	1.95	0.74
7:C:47:GLU:HB3	7:D:63:PRO:CG	2.14	0.74
7:C:75:THR:CG2	7:C:78:SER:CB	2.49	0.74
7:A:144:ARG:NH2	7:A:168:THR:O	2.20	0.74
7:C:64:LEU:HD13	7:C:67:ARG:HD3	1.70	0.74
6:H:17:DG:OP2	7:D:17:TYR:HE2	1.68	0.74
7:B:37:LEU:HD12	7:B:37:LEU:N	2.01	0.74
7:B:205:LEU:CD2	7:B:272:ILE:HD11	2.18	0.73
6:H:19:DG:H2'	6:H:20:DA:H8	1.54	0.73
7:D:24:TYR:HE1	7:D:41:ARG:N	1.86	0.73
2:J:21:DA:H2'	2:J:22:DG:C8	2.24	0.73
7:A:103:LYS:O	7:A:104:ILE:C	2.29	0.73
7:C:14:PRO:O	7:C:15:ASN:CB	2.32	0.73
7:D:15:ASN:HA	7:D:17:TYR:CZ	2.24	0.73
7:B:104:ILE:O	7:B:107:ILE:N	2.21	0.73
7:C:242:ILE:HG23	7:C:330:LEU:HD11	1.70	0.73
3:K:26:DA:N6	7:B:287:ARG:NH2	2.37	0.73
6:F:9:DG:C2'	7:A:20:ASN:ND2	2.52	0.73
7:D:104:ILE:HA	7:D:107:ILE:CD1	2.12	0.73
5:G:12:DT:H2''	5:G:13:DC:H5'	1.71	0.73
7:A:45:ILE:HG22	7:A:46:THR:N	2.04	0.73
7:B:120:THR:O	7:B:121:THR:C	2.32	0.73
7:C:23:TYR:CD2	7:C:23:TYR:C	2.66	0.73
7:B:77:HIS:HA	7:B:80:LEU:CD1	2.19	0.73
7:B:207:VAL:O	7:B:314:SER:OG	2.06	0.73
7:C:23:TYR:HE2	7:C:24:TYR:O	1.72	0.73
7:D:45:ILE:O	7:D:48:ALA:HB3	1.88	0.73
7:B:28:ASP:OD2	7:B:30:ARG:HB2	1.89	0.73
7:D:76:LEU:C	7:D:76:LEU:CD1	2.61	0.73
7:B:84:GLU:CA	7:B:87:LEU:HD12	2.18	0.72
7:A:120:THR:CG2	7:A:123:GLU:HG3	2.18	0.72
7:C:72:ASN:ND2	7:C:72:ASN:H	1.84	0.72
7:D:23:TYR:HD2	7:D:24:TYR:N	1.86	0.72
7:A:104:ILE:HA	7:A:107:ILE:HD12	1.70	0.72
7:A:163:ASN:OD1	7:A:165:VAL:N	2.23	0.72
3:K:19:DA:H2''	3:K:20:DA:O4'	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:9:DG:H2''	6:F:10:DA:N7	2.04	0.72
6:H:2:DG:OP2	6:H:2:DG:C8	2.41	0.72
7:C:77:HIS:HA	7:C:80:LEU:HD12	1.71	0.72
7:C:306:THR:OG1	7:C:307:PHE:N	2.21	0.72
7:A:309:GLU:OE1	7:A:309:GLU:CA	2.38	0.72
7:D:83:TYR:CE1	7:D:150:ALA:HA	2.25	0.72
7:D:33:LYS:HA	7:D:33:LYS:CE	2.19	0.72
7:C:224:ILE:CD1	7:C:271:ILE:HD11	2.20	0.72
7:C:103:LYS:O	7:C:106:ALA:HB3	1.90	0.71
7:A:47:GLU:HB3	7:B:63:PRO:HG2	1.70	0.71
7:B:27:ARG:CG	7:B:34:GLU:HG2	2.19	0.71
7:B:103:LYS:O	7:B:104:ILE:C	2.31	0.71
7:D:24:TYR:OH	7:D:41:ARG:HB2	1.89	0.71
5:G:14:DA:H8	7:C:23:TYR:CE1	2.08	0.71
7:A:160:ILE:HG22	7:A:162:THR:H	1.53	0.71
1:I:24:DT:P	7:D:293:ARG:HH22	2.13	0.71
7:C:101:MSE:HA	7:C:104:ILE:CD1	2.17	0.71
7:D:23:TYR:CD2	7:D:23:TYR:C	2.66	0.71
2:J:2:DG:H2''	2:J:3:DC:OP2	1.90	0.71
7:C:212:ARG:HB2	7:C:215:ASP:OD2	1.90	0.71
7:C:79:TRP:CZ2	7:C:154:ALA:HB2	2.26	0.71
7:C:163:ASN:OD1	7:C:165:VAL:N	2.24	0.71
6:F:23:DT:C2'	6:F:24:DG:C8	2.73	0.71
7:D:306:THR:O	7:D:309:GLU:CB	2.33	0.71
3:K:12:DA:H2'	3:K:13:DT:C7	2.19	0.71
7:A:197:CYS:O	7:A:200:ARG:HG3	1.91	0.71
7:A:221:TRP:CH2	7:A:263:LYS:HB2	2.26	0.71
7:A:84:GLU:CA	7:A:87:LEU:HD12	2.20	0.70
7:B:77:HIS:CA	7:B:80:LEU:HD12	2.21	0.70
7:C:76:LEU:HG	7:C:80:LEU:HD11	1.71	0.70
7:A:148:SER:HA	7:A:165:VAL:HG21	1.74	0.70
7:A:168:THR:OG1	7:A:169:ARG:N	2.22	0.70
7:A:293:ARG:HH12	7:A:306:THR:HG22	1.56	0.70
7:D:258:THR:O	7:D:262:CYS:SG	2.48	0.70
7:A:68:ILE:HG22	7:A:69:ASN:N	2.06	0.70
7:B:54:GLU:HG3	7:C:65:THR:HG23	1.74	0.70
7:C:116:LEU:HB3	7:C:160:ILE:HD11	1.72	0.70
7:B:23:TYR:HD2	7:B:23:TYR:C	1.99	0.70
7:C:208:VAL:O	7:C:318:TYR:OH	2.09	0.70
7:D:144:ARG:HE	7:D:168:THR:CG2	2.03	0.70
7:B:36:GLY:C	7:B:37:LEU:HD12	2.16	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:17:TYR:HE1	7:D:27:ARG:HB3	1.57	0.70
7:A:84:GLU:HA	7:A:87:LEU:HD12	1.73	0.70
7:D:24:TYR:CE1	7:D:41:ARG:HA	2.27	0.70
1:I:27:DA:H2''	1:I:28:DT:OP2	1.91	0.70
5:E:15:DG:N7	7:A:19:ARG:HD2	2.06	0.70
7:A:9:ARG:CB	7:A:10:ARG:HG3	2.21	0.70
7:B:176:ARG:HG3	7:B:303:ASP:OD2	1.91	0.70
3:K:20:DA:H2''	3:K:21:DA:O4'	1.92	0.70
7:B:198:TRP:CE3	7:B:199:LEU:HD12	2.27	0.70
2:J:15:DT:H73	2:J:16:DT:H71	1.74	0.69
7:A:12:LEU:HD11	7:A:16:LEU:HD23	1.73	0.69
7:A:163:ASN:OD1	7:A:163:ASN:C	2.31	0.69
7:D:114:ALA:HB1	7:D:115:PRO:CD	2.22	0.69
4:L:6:DA:H2''	4:L:7:DA:OP2	1.92	0.69
5:E:5:DG:OP2	7:B:36:GLY:N	2.25	0.69
7:A:309:GLU:OE1	7:A:309:GLU:C	2.34	0.69
7:D:141:LYS:O	7:D:144:ARG:HB3	1.92	0.69
3:K:9:DT:C2'	3:K:10:DT:H5''	2.21	0.69
7:D:76:LEU:HD11	7:D:80:LEU:HD13	1.74	0.69
7:D:141:LYS:C	7:D:141:LYS:HD2	2.16	0.69
7:A:28:ASP:CG	7:A:30:ARG:HB3	2.16	0.69
7:A:215:ASP:OD2	7:A:233:GLN:HG3	1.93	0.69
6:F:10:DA:H2''	6:F:11:DC:OP2	1.93	0.69
7:C:45:ILE:HG22	7:C:46:THR:N	2.07	0.69
7:C:101:MSE:CA	7:C:104:ILE:HD12	2.18	0.69
7:D:23:TYR:HE2	7:D:24:TYR:O	1.76	0.69
7:A:94:GLN:O	7:A:98:ILE:HD12	1.93	0.68
7:B:105:LYS:O	7:B:106:ALA:C	2.35	0.68
7:C:92:ILE:HG22	7:C:93:LYS:N	2.06	0.68
7:D:144:ARG:NE	7:D:168:THR:HG23	2.05	0.68
7:D:313:LEU:HA	7:D:316:ARG:NH2	2.09	0.68
5:G:2:DC:H2''	5:G:3:DA:C8	2.28	0.68
7:C:160:ILE:HG22	7:C:162:THR:N	2.08	0.68
7:A:76:LEU:N	7:A:76:LEU:CD1	2.55	0.68
7:C:75:THR:HG23	7:C:78:SER:HB3	0.84	0.68
1:I:7:DG:C2	1:I:8:DC:C2	2.82	0.68
7:C:146:THR:O	7:C:147:LEU:C	2.34	0.68
4:L:9:DT:H2''	4:L:10:DT:H5''	1.75	0.68
7:A:146:THR:O	7:A:147:LEU:C	2.37	0.68
7:A:185:TYR:C	7:A:185:TYR:CD1	2.72	0.68
2:J:16:DT:H2'	2:J:17:DA:C5'	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:99:ASN:O	7:B:103:LYS:HG2	1.93	0.68
6:F:9:DG:H2'	7:A:20:ASN:ND2	2.10	0.67
7:B:121:THR:OG1	7:B:164:HIS:ND1	2.27	0.67
5:E:6:DT:H2''	5:E:7:DC:O4'	1.95	0.67
7:C:45:ILE:O	7:C:49:ILE:HG12	1.93	0.67
7:D:15:ASN:HA	7:D:17:TYR:OH	1.94	0.67
7:D:50:GLN:O	7:D:53:ILE:HG13	1.94	0.67
1:I:13:DT:H2''	1:I:14:DA:C8	2.29	0.67
5:E:6:DT:H2'	5:E:7:DC:H6	1.58	0.67
7:B:300:PHE:HE1	7:B:304:PRO:HB3	1.57	0.67
7:D:139:SER:O	7:D:143:ILE:HG13	1.94	0.67
7:A:16:LEU:C	7:A:17:TYR:CD2	2.73	0.67
7:B:213:VAL:CA	7:B:216:LEU:HD12	2.23	0.67
6:F:10:DA:N7	7:A:20:ASN:ND2	2.43	0.67
7:D:293:ARG:NH1	7:D:305:PRO:O	2.27	0.67
3:K:15:DA:C8	3:K:16:DT:H73	2.30	0.67
7:C:94:GLN:O	7:C:98:ILE:HD12	1.95	0.67
7:A:163:ASN:OD1	7:A:165:VAL:CB	2.41	0.67
7:A:114:ALA:CB	7:A:115:PRO:CD	2.66	0.67
7:A:151:PHE:O	7:A:152:ARG:C	2.38	0.67
7:C:186:LEU:CD1	7:C:251:LEU:CD2	2.73	0.67
6:F:7:DT:H5'	6:F:7:DT:H6	1.59	0.67
7:A:305:PRO:HB3	7:A:309:GLU:HG3	1.77	0.67
7:D:17:TYR:HE1	7:D:27:ARG:CB	2.08	0.67
7:A:67:ARG:NH1	7:D:36:GLY:O	2.27	0.66
7:C:270:THR:HB	7:C:272:ILE:O	1.94	0.66
2:J:19:DA:C2'	7:A:96:THR:HG21	2.23	0.66
7:C:51:ALA:O	7:C:54:GLU:HG3	1.96	0.66
2:J:11:DT:H4'	2:J:12:DA:OP1	1.95	0.66
7:A:55:LEU:HB3	7:A:56:PHE:HD1	1.58	0.66
7:C:104:ILE:O	7:C:107:ILE:N	2.28	0.66
7:D:19:ARG:CG	7:D:20:ASN:H	2.08	0.66
7:A:18:ILE:HG13	7:A:24:TYR:HE2	1.60	0.66
7:B:120:THR:HG21	7:B:122:LYS:HB3	1.78	0.66
7:B:84:GLU:HA	7:B:87:LEU:CD1	2.24	0.66
3:K:15:DA:N9	3:K:16:DT:H71	2.11	0.66
7:A:64:LEU:HD21	7:D:26:TYR:CD2	2.31	0.66
7:C:26:TYR:HD2	7:C:27:ARG:N	1.94	0.66
7:C:354:GLU:C	7:C:356:LYS:N	2.54	0.66
1:I:12:DT:H5''	7:A:235:LYS:NZ	2.11	0.66
3:K:3:DG:H2''	3:K:4:DC:OP2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:15:DA:C8	3:K:16:DT:C7	2.78	0.66
7:A:45:ILE:O	7:A:48:ALA:HB3	1.96	0.66
7:C:148:SER:O	7:C:151:PHE:HB2	1.96	0.66
7:C:160:ILE:HG22	7:C:162:THR:H	1.59	0.66
7:A:111:LEU:HD22	7:A:112:PRO:CD	2.26	0.66
7:B:83:TYR:O	7:B:86:ILE:HB	1.96	0.66
7:B:139:SER:O	7:B:140:ALA:C	2.37	0.66
7:C:114:ALA:HB1	7:C:115:PRO:HD3	1.78	0.66
7:D:31:THR:OG1	7:D:33:LYS:CG	2.42	0.66
7:A:104:ILE:HG22	7:A:105:LYS:N	2.09	0.65
5:E:21:DA:C8	5:E:22:DT:H71	2.31	0.65
7:B:293:ARG:O	7:B:296:SER:OG	2.12	0.65
7:D:212:ARG:HE	7:D:233:GLN:CD	2.04	0.65
6:F:18:DT:H2'	6:F:19:DG:C8	2.31	0.65
7:C:211:GLN:C	7:C:311:ARG:HD2	2.21	0.65
7:D:221:TRP:CZ2	7:D:263:LYS:HB3	2.30	0.65
1:I:8:DC:H2'	1:I:9:DT:H71	1.78	0.65
7:B:26:TYR:C	7:B:26:TYR:CD2	2.72	0.65
7:B:76:LEU:C	7:B:80:LEU:CD1	2.67	0.65
7:B:129:ASN:HA	7:B:132:ILE:CD1	2.22	0.65
7:B:146:THR:O	7:B:147:LEU:C	2.38	0.65
2:J:7:DA:C4	2:J:8:DG:C8	2.84	0.65
7:B:151:PHE:O	7:B:154:ALA:HB3	1.96	0.65
7:D:33:LYS:HE3	7:D:33:LYS:CA	2.21	0.65
6:F:19:DG:H2'	6:F:20:DA:C8	2.32	0.65
7:B:160:ILE:HD13	7:B:160:ILE:N	2.12	0.65
7:B:289:PHE:C	7:B:289:PHE:CD2	2.74	0.65
7:A:23:TYR:OH	7:A:36:GLY:CA	2.40	0.65
7:C:23:TYR:OH	7:C:36:GLY:HA3	1.95	0.65
3:K:9:DT:H2''	3:K:10:DT:C5'	2.23	0.65
7:A:169:ARG:NH2	7:B:152:ARG:HD3	2.12	0.65
7:A:309:GLU:OE1	7:A:309:GLU:HA	1.95	0.65
7:B:353:ILE:HD13	7:C:330:LEU:HD12	1.79	0.65
7:C:259:LEU:HD11	7:C:271:ILE:HD13	1.78	0.65
7:A:61:HIS:HE2	7:D:47:GLU:CD	1.98	0.65
7:A:67:ARG:NH2	7:D:36:GLY:O	2.30	0.65
7:D:120:THR:O	7:D:121:THR:C	2.40	0.65
7:C:105:LYS:HA	7:C:108:ARG:HG3	1.79	0.64
7:C:258:THR:O	7:C:262:CYS:SG	2.54	0.64
7:A:40:ASP:OD1	7:A:43:ILE:HG12	1.96	0.64
5:E:21:DA:C5	5:E:22:DT:H73	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:7:DG:C4	1:I:8:DC:C6	2.85	0.64
7:C:185:TYR:HD1	7:C:186:LEU:HD12	1.62	0.64
7:A:142:LEU:O	7:A:146:THR:OG1	2.16	0.64
7:A:160:ILE:HG22	7:A:162:THR:N	2.12	0.64
7:D:79:TRP:CZ2	7:D:154:ALA:CA	2.77	0.64
7:A:57:SER:OG	7:A:59:HIS:HB3	1.96	0.64
7:A:76:LEU:HD12	7:A:76:LEU:H	1.62	0.64
7:A:307:PHE:CD1	7:A:307:PHE:C	2.75	0.64
7:A:290:MSE:O	7:A:293:ARG:HB3	1.98	0.64
7:B:159:HIS:O	7:B:160:ILE:HG22	1.98	0.64
7:C:17:TYR:CE1	7:C:27:ARG:HB2	2.32	0.64
5:G:12:DT:H2'	5:G:13:DC:C6	2.33	0.64
7:A:26:TYR:CE2	7:A:51:ALA:HB1	2.33	0.64
7:A:57:SER:C	7:A:59:HIS:N	2.55	0.64
7:B:137:ALA:O	7:B:138:ALA:C	2.37	0.64
7:B:61:HIS:CE1	7:B:63:PRO:HA	2.33	0.64
7:C:353:ILE:HD11	7:D:240:ILE:HB	1.79	0.64
7:A:28:ASP:OD2	7:A:30:ARG:CB	2.41	0.64
7:B:74:VAL:CG1	7:B:75:THR:N	2.61	0.64
7:C:103:LYS:O	7:C:104:ILE:C	2.41	0.64
7:C:111:LEU:HD22	7:C:112:PRO:CD	2.26	0.64
2:J:15:DT:C7	2:J:16:DT:H71	2.27	0.63
4:L:5:DC:H2''	4:L:6:DA:C8	2.34	0.63
7:B:159:HIS:C	7:B:160:ILE:CG2	2.71	0.63
7:C:114:ALA:HB1	7:C:115:PRO:HD2	1.79	0.63
7:C:350:TRP:CE3	7:D:239:LYS:HB3	2.34	0.63
4:L:7:DA:C5	4:L:8:DC:C4	2.86	0.63
4:L:13:DT:H5''	7:D:236:THR:CG2	2.28	0.63
7:C:83:TYR:CE1	7:C:150:ALA:HA	2.33	0.63
3:K:16:DT:H1'	3:K:17:DA:H8	1.63	0.63
7:B:300:PHE:CE1	7:B:304:PRO:HB3	2.32	0.63
7:D:74:VAL:CG1	7:D:75:THR:N	2.61	0.63
6:H:17:DG:N7	6:H:18:DT:H73	2.13	0.63
7:C:92:ILE:CG2	7:C:93:LYS:N	2.60	0.63
7:C:144:ARG:HG2	7:C:145:SER:N	2.14	0.63
3:K:21:DA:H2'	3:K:22:DC:C6	2.34	0.63
5:E:11:DA:C8	5:E:12:DT:H73	2.33	0.63
1:I:19:DA:H2'	1:I:20:DA:C8	2.34	0.63
7:B:163:ASN:OD1	7:B:165:VAL:CB	2.45	0.63
7:A:10:ARG:HH22	7:A:12:LEU:HD22	1.63	0.63
7:D:80:LEU:HD23	7:D:104:ILE:HG23	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:20:DA:C2	6:H:21:DC:C2	2.87	0.63
1:I:21:DA:H62	7:D:99:ASN:ND2	1.98	0.62
7:B:84:GLU:O	7:B:87:LEU:HD12	1.99	0.62
7:B:104:ILE:O	7:B:105:LYS:C	2.41	0.62
5:E:10:DT:H2''	5:E:11:DA:C8	2.33	0.62
7:C:92:ILE:HG21	7:C:96:THR:HB	1.81	0.62
7:D:100:TYR:O	7:D:103:LYS:HG2	1.98	0.62
7:D:313:LEU:HA	7:D:316:ARG:CZ	2.29	0.62
1:I:7:DG:C6	1:I:8:DC:C4	2.87	0.62
1:I:19:DA:C6	1:I:20:DA:C6	2.88	0.62
2:J:20:DA:H2''	2:J:21:DA:O4'	1.99	0.62
6:H:17:DG:N7	6:H:18:DT:C7	2.61	0.62
7:B:103:LYS:O	7:B:106:ALA:HB3	2.00	0.62
7:C:18:ILE:HG12	7:C:19:ARG:N	2.13	0.62
7:C:97:LEU:HD23	7:C:98:ILE:HG13	1.81	0.62
1:I:12:DT:P	7:A:212:ARG:HH21	2.14	0.62
6:F:9:DG:H2''	6:F:10:DA:C8	2.33	0.62
7:B:121:THR:O	7:B:124:ILE:HB	1.99	0.62
7:C:64:LEU:O	7:C:65:THR:C	2.42	0.62
7:B:270:THR:HG21	7:B:279:PRO:HB3	1.81	0.62
7:C:186:LEU:HD12	7:C:251:LEU:HD22	1.80	0.62
1:I:12:DT:O5'	7:A:212:ARG:NH2	2.31	0.62
5:E:2:DC:H2''	5:E:3:DA:C8	2.33	0.62
7:D:111:LEU:HD22	7:D:112:PRO:HD2	1.82	0.62
7:B:25:CYS:SG	7:B:34:GLU:HB3	2.40	0.62
7:C:114:ALA:CB	7:C:115:PRO:CD	2.78	0.62
7:C:116:LEU:N	7:C:116:LEU:CD1	2.61	0.62
5:G:14:DA:H8	7:C:23:TYR:HE1	1.47	0.62
7:D:146:THR:O	7:D:147:LEU:C	2.42	0.62
7:C:77:HIS:HB2	7:C:113:ASP:OD2	2.00	0.61
2:J:23:DC:H2''	2:J:24:DA:C8	2.35	0.61
7:B:23:TYR:CD2	7:B:23:TYR:C	2.71	0.61
7:C:136:LYS:O	7:C:139:SER:HB2	1.99	0.61
7:C:147:LEU:HG	7:C:151:PHE:HE2	1.65	0.61
7:C:221:TRP:HH2	7:C:263:LYS:HB2	1.65	0.61
7:D:142:LEU:O	7:D:146:THR:OG1	2.17	0.61
7:D:211:GLN:CA	7:D:311:ARG:HH11	2.12	0.61
2:J:16:DT:H2''	2:J:17:DA:O5'	1.99	0.61
7:A:144:ARG:O	7:A:145:SER:C	2.43	0.61
7:D:151:PHE:O	7:D:154:ALA:HB3	1.99	0.61
3:K:19:DA:H2'	3:K:20:DA:H8	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:17:DG:OP2	7:B:17:TYR:CZ	2.53	0.61
7:C:87:LEU:HD12	7:C:87:LEU:H	1.64	0.61
7:C:287:ARG:O	7:C:290:MSE:HB3	2.01	0.61
5:E:21:DA:C5	5:E:22:DT:C7	2.84	0.61
7:A:10:ARG:HH21	7:A:12:LEU:HB2	1.65	0.61
7:B:59:HIS:O	7:B:60:LYS:O	2.17	0.61
7:D:212:ARG:NH2	7:D:233:GLN:OE1	2.33	0.61
7:A:18:ILE:HG13	7:A:24:TYR:CD2	2.35	0.61
7:A:98:ILE:HA	7:A:101:MSE:HB2	1.81	0.61
7:A:198:TRP:HB3	7:A:266:LEU:HD11	1.81	0.61
1:I:17:DA:C2	1:I:18:DC:C2	2.88	0.61
7:B:160:ILE:HD13	7:B:160:ILE:H	1.65	0.61
4:L:23:DC:H5''	7:C:306:THR:CG2	2.31	0.61
7:A:213:VAL:O	7:A:216:LEU:HB3	2.00	0.61
7:B:61:HIS:ND1	7:B:62:LYS:O	2.33	0.61
4:L:23:DC:H2''	4:L:24:DT:H71	1.82	0.61
7:A:105:LYS:O	7:A:106:ALA:C	2.43	0.61
7:B:181:THR:HG23	7:B:184:GLU:CD	2.26	0.61
7:C:47:GLU:OE2	7:D:63:PRO:CD	2.34	0.61
7:C:120:THR:CG2	7:C:123:GLU:HG3	2.31	0.61
7:C:199:LEU:O	7:C:203:MSE:CG	2.48	0.61
6:H:13:DG:C2'	6:H:14:DA:H8	2.13	0.60
7:A:103:LYS:O	7:A:106:ALA:N	2.34	0.60
7:C:83:TYR:O	7:C:87:LEU:CD1	2.49	0.60
6:H:9:DG:H2'	7:C:20:ASN:ND2	2.16	0.60
7:B:151:PHE:O	7:B:152:ARG:C	2.41	0.60
7:B:229:LEU:HD22	7:B:255:MSE:HE1	1.83	0.60
1:I:7:DG:C5	1:I:8:DC:C5	2.89	0.60
1:I:22:DG:H2''	1:I:23:DT:H5'	1.82	0.60
7:A:74:VAL:HG12	7:A:75:THR:HG22	1.83	0.60
7:D:290:MSE:O	7:D:293:ARG:HB2	2.01	0.60
1:I:9:DT:O2	1:I:10:DT:C6	2.54	0.60
3:K:25:DG:H1'	3:K:26:DA:H5''	1.83	0.60
7:B:159:HIS:C	7:B:160:ILE:HG23	2.26	0.60
6:H:23:DT:H2''	6:H:24:DG:N7	2.15	0.60
7:A:64:LEU:HB2	7:D:47:GLU:OE2	2.01	0.60
7:B:58:GLY:O	7:B:59:HIS:HB2	2.01	0.60
3:K:9:DT:C2	3:K:10:DT:C6	2.89	0.60
6:F:2:DG:C2'	6:F:3:DT:H71	2.19	0.60
7:C:151:PHE:O	7:C:152:ARG:C	2.42	0.60
7:C:307:PHE:O	7:C:308:HIS:C	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:83:TYR:CD2	7:D:87:LEU:HD11	2.36	0.60
7:D:97:LEU:O	7:D:100:TYR:HB2	2.01	0.60
6:H:14:DA:H2"	6:H:15:DT:C6	2.36	0.60
7:A:12:LEU:HD11	7:A:16:LEU:CD2	2.31	0.60
7:A:345:ASP:N	7:A:345:ASP:OD1	2.34	0.60
7:B:159:HIS:O	7:B:160:ILE:CG2	2.49	0.60
7:B:212:ARG:NH1	7:B:233:GLN:OE1	2.35	0.60
7:C:11:ASP:O	7:C:13:PRO:HD3	2.02	0.60
7:C:305:PRO:HB3	7:C:309:GLU:HG3	1.84	0.60
7:D:221:TRP:CE2	7:D:271:ILE:HG12	2.35	0.60
2:J:15:DT:C7	2:J:16:DT:C7	2.79	0.60
7:B:153:GLU:O	7:B:156:ALA:HB3	2.02	0.60
7:C:54:GLU:HG3	7:C:55:LEU:N	2.17	0.60
7:D:198:TRP:CE3	7:D:199:LEU:N	2.70	0.60
5:G:10:DT:H2"	5:G:11:DA:N7	2.17	0.60
7:A:55:LEU:HD22	7:A:56:PHE:HE1	1.65	0.60
7:A:104:ILE:O	7:A:105:LYS:C	2.45	0.59
6:F:7:DT:OP2	7:A:14:PRO:HA	2.02	0.59
7:B:283:GLY:O	7:B:287:ARG:HB2	2.01	0.59
7:D:34:GLU:C	7:D:35:PHE:CD1	2.80	0.59
4:L:20:DA:H2"	4:L:21:DA:H5"	1.84	0.59
6:F:11:DC:C5	6:F:12:DT:H73	2.37	0.59
7:A:76:LEU:CD1	7:A:76:LEU:H	2.14	0.59
4:L:7:DA:C5	4:L:8:DC:C5	2.90	0.59
7:A:83:TYR:CE1	7:A:150:ALA:HA	2.37	0.59
7:A:120:THR:HG22	7:A:123:GLU:CG	2.29	0.59
7:B:267:GLY:O	7:B:277:ARG:HG3	2.03	0.59
7:B:350:TRP:CE3	7:C:239:LYS:HB3	2.37	0.59
7:D:213:VAL:HB	7:D:307:PHE:CE1	2.37	0.59
3:K:26:DA:N6	7:B:287:ARG:HH22	2.01	0.59
7:B:25:CYS:HA	7:B:37:LEU:HD13	1.85	0.59
7:B:144:ARG:O	7:B:145:SER:C	2.45	0.59
7:C:152:ARG:O	7:C:155:ILE:HB	2.02	0.59
7:C:160:ILE:CG2	7:C:162:THR:H	2.15	0.59
7:C:338:MSE:C	7:C:340:SER:N	2.56	0.59
7:A:45:ILE:CG2	7:A:46:THR:N	2.66	0.59
7:A:203:MSE:O	7:A:207:VAL:HG23	2.02	0.59
7:C:151:PHE:O	7:C:154:ALA:N	2.36	0.59
7:C:186:LEU:HD11	7:C:251:LEU:CD2	2.33	0.59
7:C:120:THR:O	7:C:121:THR:C	2.46	0.59
7:C:338:MSE:C	7:C:340:SER:H	2.11	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:60:LYS:O	7:B:61:HIS:CB	2.45	0.59
7:C:79:TRP:CZ2	7:C:154:ALA:CA	2.86	0.59
2:J:16:DT:O2	2:J:17:DA:H5''	2.03	0.59
7:D:55:LEU:HD12	7:D:55:LEU:N	2.18	0.59
7:D:212:ARG:N	7:D:311:ARG:HD2	2.18	0.59
4:L:14:DT:H2''	4:L:15:DG:OP2	2.04	0.58
7:A:333:HIS:CE1	7:A:338:MSE:HB2	2.38	0.58
7:B:26:TYR:CD2	7:B:27:ARG:N	2.71	0.58
7:B:79:TRP:CZ2	7:B:154:ALA:CA	2.86	0.58
7:C:180:LEU:HD13	7:C:305:PRO:HB2	1.84	0.58
7:B:62:LYS:O	7:B:64:LEU:C	2.46	0.58
6:F:14:DA:H2''	6:F:15:DT:C6	2.38	0.58
7:A:160:ILE:HG22	7:A:161:THR:H	1.51	0.58
7:A:19:ARG:NH1	7:A:19:ARG:HG2	2.18	0.58
7:A:23:TYR:CD2	7:A:24:TYR:N	2.71	0.58
7:A:306:THR:O	7:A:309:GLU:CB	2.50	0.58
7:B:60:LYS:HE3	7:D:46:THR:CG2	2.34	0.58
2:J:24:DA:C2	2:J:25:DG:C6	2.92	0.58
4:L:7:DA:C4	4:L:8:DC:C6	2.92	0.58
7:B:75:THR:HA	7:B:115:PRO:HA	1.86	0.58
7:B:79:TRP:CZ2	7:B:154:ALA:HA	2.39	0.58
7:D:129:ASN:OD1	7:D:132:ILE:HD12	2.04	0.58
3:K:17:DA:H8	3:K:17:DA:H5'	1.69	0.58
6:H:13:DG:C2'	6:H:14:DA:C8	2.87	0.58
7:C:199:LEU:O	7:C:203:MSE:HG3	2.03	0.58
7:B:75:THR:HG22	7:B:114:ALA:C	2.29	0.58
7:C:83:TYR:O	7:C:87:LEU:HD13	2.03	0.58
7:D:37:LEU:HD23	7:D:37:LEU:N	2.19	0.58
7:A:116:LEU:HA	7:A:119:ILE:CD1	2.30	0.58
7:D:17:TYR:CE1	7:D:27:ARG:HB2	2.39	0.58
7:D:19:ARG:HD2	7:D:21:ASN:H	1.69	0.58
5:G:5:DG:N2	5:G:6:DT:C2	2.71	0.57
5:G:12:DT:H2'	5:G:13:DC:H6	1.68	0.57
7:A:75:THR:CG2	7:A:78:SER:CB	2.77	0.57
7:A:76:LEU:O	7:A:80:LEU:CD1	2.51	0.57
7:D:169:ARG:O	7:D:169:ARG:NE	2.36	0.57
4:L:7:DA:C8	4:L:8:DC:C5	2.92	0.57
7:B:74:VAL:CG1	7:B:75:THR:H	2.17	0.57
7:D:155:ILE:HG22	7:D:155:ILE:O	2.04	0.57
7:A:55:LEU:HB3	7:A:56:PHE:CD1	2.39	0.57
7:B:145:SER:O	7:B:148:SER:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:220:LYS:O	7:B:223:ASP:HB2	2.04	0.57
7:D:47:GLU:O	7:D:50:GLN:HB2	2.05	0.57
1:I:20:DA:C2	1:I:21:DA:C4	2.93	0.57
3:K:12:DA:C2'	3:K:13:DT:H72	2.29	0.57
5:E:4:DG:C4	5:E:5:DG:C8	2.92	0.57
6:F:13:DG:C4	6:F:14:DA:C8	2.92	0.57
1:I:16:DA:C5	4:L:15:DG:N2	2.73	0.57
7:A:27:ARG:HE	7:A:32:GLY:HA2	1.70	0.57
7:B:75:THR:OG1	7:B:78:SER:OG	2.03	0.57
7:C:79:TRP:O	7:C:83:TYR:N	2.34	0.57
7:D:215:ASP:OD2	7:D:233:GLN:HA	2.04	0.57
6:H:17:DG:C4	6:H:18:DT:C5	2.93	0.57
7:D:212:ARG:CZ	7:D:233:GLN:OE1	2.53	0.57
7:D:305:PRO:HB3	7:D:309:GLU:HG3	1.87	0.57
6:H:9:DG:O6	7:C:19:ARG:NH2	2.38	0.57
7:A:60:LYS:HZ2	7:B:67:ARG:CB	2.18	0.57
7:A:64:LEU:HD23	7:D:51:ALA:HB2	1.86	0.57
7:A:160:ILE:CG2	7:A:162:THR:H	2.17	0.57
7:A:311:ARG:NH2	7:A:331:LEU:HG	2.19	0.57
7:C:144:ARG:HE	7:C:168:THR:HG23	1.70	0.57
7:D:45:ILE:HG22	7:D:46:THR:N	2.19	0.57
6:F:17:DG:OP2	7:B:17:TYR:HE2	1.84	0.57
7:A:103:LYS:O	7:A:106:ALA:CB	2.49	0.57
7:D:221:TRP:HZ3	7:D:263:LYS:HZ1	1.53	0.57
7:B:27:ARG:HD3	7:B:34:GLU:OE1	2.05	0.56
7:C:77:HIS:HB2	7:C:113:ASP:CG	2.30	0.56
7:D:211:GLN:O	7:D:311:ARG:HD2	2.05	0.56
4:L:7:DA:H2''	4:L:8:DC:H5''	1.88	0.56
7:A:116:LEU:HB3	7:A:160:ILE:HD11	1.85	0.56
7:A:211:GLN:CA	7:A:311:ARG:HH11	2.18	0.56
7:D:121:THR:HA	7:D:124:ILE:HD12	1.87	0.56
2:J:8:DG:C5'	7:B:136:LYS:HD3	2.33	0.56
3:K:10:DT:H4'	7:C:177:ARG:NH1	2.19	0.56
3:K:12:DA:P	7:C:212:ARG:HH21	2.25	0.56
3:K:19:DA:H2'	3:K:20:DA:C8	2.40	0.56
3:K:21:DA:OP2	7:B:93:LYS:HD3	2.05	0.56
7:B:146:THR:O	7:B:149:ASP:N	2.37	0.56
7:B:181:THR:O	7:B:184:GLU:HG3	2.05	0.56
7:C:144:ARG:CG	7:C:145:SER:N	2.68	0.56
7:C:180:LEU:HD13	7:C:305:PRO:CB	2.35	0.56
7:C:220:LYS:O	7:C:223:ASP:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:11:DA:C2	5:E:12:DT:C4	2.93	0.56
7:A:101:MSE:CA	7:A:104:ILE:HD12	2.35	0.56
7:B:287:ARG:O	7:B:290:MSE:HB3	2.06	0.56
7:B:34:GLU:O	7:B:35:PHE:CD2	2.59	0.56
7:B:144:ARG:NH1	7:B:170:ALA:HB2	2.20	0.56
7:C:285:VAL:HG12	7:C:307:PHE:CE2	2.41	0.56
7:D:27:ARG:HG3	7:D:34:GLU:CG	2.31	0.56
7:D:54:GLU:HA	7:D:54:GLU:OE2	2.04	0.56
7:D:124:ILE:HG22	7:D:128:LEU:HD12	1.88	0.56
7:D:290:MSE:CG	7:D:293:ARG:HH21	2.18	0.56
7:D:327:ALA:O	7:D:331:LEU:HG	2.05	0.56
2:J:20:DA:C2	2:J:21:DA:C4	2.93	0.56
7:A:60:LYS:NZ	7:B:67:ARG:CB	2.68	0.56
6:H:6:DT:C5	6:H:7:DT:H72	2.41	0.56
7:A:55:LEU:HD22	7:A:56:PHE:CE1	2.40	0.56
7:A:307:PHE:O	7:A:308:HIS:C	2.47	0.56
7:B:62:LYS:C	7:B:64:LEU:N	2.58	0.56
7:B:198:TRP:CE3	7:B:199:LEU:N	2.74	0.56
7:D:123:GLU:O	7:D:126:ALA:HB3	2.06	0.56
2:J:15:DT:H73	2:J:16:DT:C7	2.36	0.56
7:A:143:ILE:O	7:A:144:ARG:C	2.46	0.56
7:A:148:SER:O	7:A:151:PHE:HB2	2.06	0.56
7:B:199:LEU:O	7:B:203:MSE:HG2	2.06	0.56
7:C:203:MSE:O	7:C:207:VAL:HG23	2.06	0.56
7:D:283:GLY:O	7:D:287:ARG:HB2	2.05	0.56
1:I:10:DT:H4'	7:A:177:ARG:NH1	2.21	0.56
3:K:9:DT:O2	3:K:10:DT:C6	2.59	0.56
6:H:17:DG:C5	6:H:18:DT:C5	2.94	0.56
6:H:23:DT:H2''	6:H:24:DG:C8	2.40	0.56
7:A:102:SER:OG	7:A:103:LYS:NZ	2.39	0.56
7:D:15:ASN:ND2	7:D:52:ASN:HD21	2.04	0.56
7:C:144:ARG:NH1	7:C:170:ALA:HB2	2.20	0.56
7:C:189:TYR:CZ	7:C:200:ARG:NH2	2.74	0.56
7:D:305:PRO:HB3	7:D:309:GLU:CG	2.35	0.56
5:E:7:DC:H2'	5:E:8:DA:C8	2.41	0.55
7:A:19:ARG:HG2	7:A:19:ARG:HH11	1.72	0.55
7:A:120:THR:O	7:A:121:THR:C	2.48	0.55
1:I:17:DA:H5'	1:I:17:DA:H8	1.71	0.55
4:L:28:DA:H2''	4:L:29:DA:OP2	2.05	0.55
7:B:27:ARG:HG3	7:B:34:GLU:HG2	1.86	0.55
7:C:40:ASP:CG	7:C:42:ARG:HG3	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:9:DG:H2''	6:H:10:DA:C8	2.41	0.55
7:C:107:ILE:O	7:C:108:ARG:C	2.49	0.55
7:C:224:ILE:HD13	7:C:259:LEU:HD21	1.89	0.55
7:D:212:ARG:N	7:D:311:ARG:HH11	2.05	0.55
7:B:114:ALA:CB	7:B:115:PRO:CD	2.76	0.55
7:D:15:ASN:HD21	7:D:52:ASN:ND2	2.04	0.55
7:D:27:ARG:CD	7:D:34:GLU:OE1	2.54	0.55
7:B:19:ARG:CG	7:B:20:ASN:H	2.19	0.55
7:C:57:SER:O	7:C:59:HIS:HB2	2.06	0.55
7:D:17:TYR:CE1	7:D:27:ARG:CB	2.89	0.55
3:K:12:DA:OP2	7:C:342:PHE:CE2	2.59	0.55
6:H:6:DT:C2'	6:H:7:DT:H5''	2.17	0.55
7:A:211:GLN:HA	7:A:311:ARG:NH1	2.18	0.55
7:B:27:ARG:HD2	7:B:34:GLU:HG2	1.82	0.55
7:B:61:HIS:HD1	7:B:62:LYS:C	2.13	0.55
7:B:124:ILE:HG22	7:B:125:ALA:N	2.19	0.55
7:C:131:TYR:N	7:C:131:TYR:HD1	2.03	0.55
7:C:307:PHE:O	7:C:310:LEU:CG	2.50	0.55
7:D:50:GLN:HA	7:D:53:ILE:CD1	2.32	0.55
7:D:53:ILE:HG22	7:D:57:SER:HB2	1.89	0.55
7:A:51:ALA:O	7:A:54:GLU:HB3	2.06	0.55
7:B:153:GLU:HA	7:B:156:ALA:HB2	1.89	0.55
7:B:200:ARG:HA	7:B:203:MSE:HG3	1.89	0.55
7:C:201:LEU:HD22	7:C:262:CYS:SG	2.46	0.55
2:J:9:DT:C2'	2:J:10:DT:H5'	2.17	0.55
3:K:23:DT:H4'	7:B:306:THR:HG21	1.87	0.55
6:F:2:DG:H2'	6:F:2:DG:OP2	2.07	0.55
7:B:138:ALA:O	7:B:139:SER:C	2.48	0.55
7:B:312:SER:HB2	7:B:316:ARG:HH21	1.70	0.55
7:C:147:LEU:HG	7:C:151:PHE:CE2	2.42	0.55
4:L:10:DT:H2'	4:L:11:DT:C6	2.42	0.55
7:A:83:TYR:O	7:A:84:GLU:C	2.50	0.55
7:A:145:SER:O	7:A:148:SER:HB3	2.07	0.55
7:D:141:LYS:NZ	7:D:145:SER:HB2	2.22	0.55
7:D:210:GLY:C	7:D:311:ARG:HG2	2.32	0.55
2:J:20:DA:H2''	2:J:21:DA:C5'	2.37	0.55
6:H:9:DG:C6	6:H:10:DA:N6	2.75	0.55
1:I:19:DA:H2'	1:I:20:DA:H8	1.72	0.54
5:E:1:DA:C2	5:E:2:DC:C2	2.95	0.54
7:A:169:ARG:HH21	7:B:152:ARG:CD	2.17	0.54
7:A:212:ARG:N	7:A:311:ARG:HD2	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:232:GLU:CG	7:B:232:GLU:O	2.54	0.54
7:B:281:SER:O	7:B:284:THR:OG1	2.18	0.54
7:D:24:TYR:CE1	7:D:41:ARG:CA	2.89	0.54
7:A:125:ALA:O	7:A:128:LEU:N	2.40	0.54
7:B:120:THR:CG2	7:B:122:LYS:H	2.12	0.54
7:B:144:ARG:HH11	7:B:170:ALA:HB2	1.72	0.54
3:K:12:DA:P	7:C:212:ARG:NH2	2.80	0.54
4:L:21:DA:H62	7:C:99:ASN:ND2	2.05	0.54
6:H:17:DG:OP2	7:D:17:TYR:CZ	2.60	0.54
7:A:180:LEU:N	7:A:309:GLU:OE2	2.37	0.54
7:B:15:ASN:HB2	7:B:26:TYR:CZ	2.43	0.54
7:B:255:MSE:HE3	7:B:259:LEU:HD11	1.89	0.54
7:C:9:ARG:HD2	7:C:10:ARG:NE	2.18	0.54
7:C:18:ILE:HG13	7:C:24:TYR:CE2	2.42	0.54
7:C:221:TRP:CH2	7:C:263:LYS:CB	2.89	0.54
7:D:105:LYS:HA	7:D:108:ARG:HD2	1.88	0.54
2:J:4:DT:H2''	2:J:5:DC:OP2	2.07	0.54
3:K:15:DA:C1'	3:K:16:DT:H71	2.38	0.54
5:E:4:DG:C6	5:E:5:DG:C5	2.95	0.54
7:A:25:CYS:HB2	7:A:34:GLU:OE2	2.07	0.54
7:B:293:ARG:NH1	7:B:305:PRO:O	2.38	0.54
7:D:103:LYS:O	7:D:104:ILE:C	2.50	0.54
7:B:205:LEU:O	7:B:209:THR:OG1	2.25	0.54
7:C:54:GLU:HG3	7:C:55:LEU:H	1.70	0.54
7:D:105:LYS:O	7:D:106:ALA:C	2.50	0.54
4:L:8:DC:C5'	7:D:136:LYS:HD3	2.38	0.54
7:B:25:CYS:SG	7:B:35:PHE:N	2.80	0.54
7:D:14:PRO:HG2	7:D:52:ASN:HD22	1.73	0.54
7:D:19:ARG:CG	7:D:20:ASN:N	2.69	0.54
3:K:17:DA:C8	3:K:17:DA:H5'	2.42	0.54
5:E:7:DC:C2'	5:E:8:DA:C8	2.90	0.54
7:A:11:ASP:O	7:A:13:PRO:HD3	2.07	0.54
7:A:114:ALA:CB	7:A:115:PRO:HD3	2.20	0.54
7:A:163:ASN:CG	7:A:165:VAL:HB	2.29	0.54
7:B:61:HIS:ND1	7:B:62:LYS:C	2.66	0.54
7:B:84:GLU:C	7:B:87:LEU:HD12	2.33	0.54
7:D:220:LYS:O	7:D:223:ASP:HB2	2.07	0.54
7:D:276:ARG:HH22	7:D:278:GLU:CD	2.14	0.54
2:J:16:DT:C2'	2:J:17:DA:O5'	2.55	0.54
7:A:144:ARG:HE	7:A:168:THR:CG2	2.18	0.54
7:B:140:ALA:O	7:B:141:LYS:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:224:ILE:HD11	7:C:271:ILE:CD1	2.35	0.54
6:F:6:DT:C6	6:F:7:DT:H72	2.42	0.54
6:H:13:DG:H2'	6:H:14:DA:C8	2.43	0.54
7:B:15:ASN:HA	7:B:17:TYR:CZ	2.43	0.54
7:C:131:TYR:N	7:C:131:TYR:CD1	2.73	0.54
2:J:2:DG:C4'	7:B:276:ARG:NH2	2.69	0.53
6:F:9:DG:H2''	7:A:20:ASN:ND2	2.09	0.53
6:H:13:DG:C2	6:H:14:DA:C4	2.96	0.53
7:A:205:LEU:O	7:A:208:VAL:HG12	2.09	0.53
7:B:262:CYS:O	7:B:266:LEU:HB2	2.07	0.53
7:D:162:THR:HG22	7:D:162:THR:O	2.02	0.53
7:D:285:VAL:HG12	7:D:286:SER:N	2.22	0.53
5:E:21:DA:C4	5:E:22:DT:C5	2.96	0.53
7:A:239:LYS:HB3	7:D:350:TRP:CE3	2.43	0.53
7:B:155:ILE:HG13	7:B:160:ILE:HD11	1.86	0.53
4:L:8:DC:OP1	7:D:136:LYS:NZ	2.40	0.53
7:A:18:ILE:HG12	7:A:19:ARG:N	2.23	0.53
7:B:49:ILE:O	7:B:50:GLN:C	2.52	0.53
7:C:120:THR:HG23	7:C:123:GLU:H	1.73	0.53
7:D:74:VAL:HG12	7:D:75:THR:N	2.23	0.53
3:K:10:DT:H2''	3:K:11:DT:O5'	2.08	0.53
7:C:327:ALA:O	7:C:331:LEU:HD22	2.08	0.53
7:D:198:TRP:HE3	7:D:199:LEU:N	2.07	0.53
4:L:7:DA:N7	4:L:8:DC:C5	2.76	0.53
7:C:83:TYR:CE2	7:C:87:LEU:HD21	2.43	0.53
7:D:18:ILE:HD11	7:D:22:GLY:HA2	1.91	0.53
7:D:144:ARG:O	7:D:145:SER:C	2.52	0.53
7:A:63:PRO:O	7:A:67:ARG:HB2	2.09	0.53
7:B:142:LEU:HD12	7:B:142:LEU:N	2.24	0.53
7:C:68:ILE:HG22	7:C:69:ASN:N	2.21	0.53
7:C:144:ARG:O	7:C:145:SER:C	2.51	0.53
7:B:27:ARG:CD	7:B:34:GLU:OE1	2.56	0.53
7:C:60:LYS:NZ	7:C:60:LYS:HB2	2.23	0.53
7:C:210:GLY:C	7:C:311:ARG:HG2	2.34	0.53
1:I:9:DT:C2	1:I:10:DT:C5	2.97	0.53
1:I:21:DA:H62	7:D:99:ASN:HD21	1.57	0.53
7:C:79:TRP:CH2	7:C:154:ALA:HA	2.44	0.53
7:C:120:THR:HG22	7:C:123:GLU:CG	2.38	0.53
7:D:307:PHE:O	7:D:308:HIS:C	2.49	0.53
2:J:8:DG:H2'	2:J:9:DT:H71	1.90	0.53
7:A:92:ILE:CG2	7:A:93:LYS:N	2.70	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:45:ILE:O	7:B:48:ALA:CB	2.54	0.53
7:B:74:VAL:HG12	7:B:75:THR:H	1.69	0.53
7:B:100:TYR:HA	7:B:103:LYS:HG3	1.91	0.53
7:C:76:LEU:O	7:C:80:LEU:HG	2.09	0.53
7:C:18:ILE:HG13	7:C:24:TYR:CD2	2.44	0.52
7:C:26:TYR:CE1	7:C:51:ALA:CB	2.86	0.52
7:D:18:ILE:HG12	7:D:19:ARG:N	2.24	0.52
7:D:169:ARG:HD2	7:D:170:ALA:N	2.16	0.52
1:I:13:DT:C7	7:A:338:MSE:HE3	2.39	0.52
2:J:15:DT:C5	2:J:16:DT:H73	2.44	0.52
3:K:15:DA:C8	3:K:16:DT:H71	2.43	0.52
5:E:16:DT:C4	5:E:17:DC:N4	2.77	0.52
7:C:307:PHE:CE1	7:C:310:LEU:HD12	2.44	0.52
3:K:11:DT:H1'	3:K:12:DA:H5''	1.91	0.52
6:F:8:DT:H2''	6:F:9:DG:C8	2.44	0.52
7:A:184:GLU:OE2	7:A:298:LEU:HD23	2.10	0.52
7:B:61:HIS:HE1	7:B:63:PRO:HA	1.72	0.52
7:B:285:VAL:CG1	7:B:307:PHE:CE2	2.92	0.52
7:B:307:PHE:O	7:B:308:HIS:C	2.50	0.52
7:C:82:ARG:O	7:C:83:TYR:C	2.49	0.52
1:I:9:DT:C2	1:I:10:DT:C6	2.97	0.52
6:F:13:DG:OP2	6:F:13:DG:H8	1.91	0.52
7:D:24:TYR:CE1	7:D:41:ARG:N	2.74	0.52
5:E:3:DA:H2'	5:E:4:DG:H8	1.74	0.52
7:A:184:GLU:OE2	7:A:298:LEU:CD2	2.57	0.52
7:B:185:TYR:CE2	7:B:203:MSE:HE2	2.45	0.52
7:C:74:VAL:HB	7:C:116:LEU:HD13	1.92	0.52
7:A:14:PRO:O	7:A:15:ASN:CG	2.52	0.52
3:K:14:DT:C4'	3:K:15:DA:OP1	2.37	0.52
5:E:16:DT:C5	5:E:17:DC:N4	2.78	0.52
7:A:83:TYR:CD2	7:A:87:LEU:HD11	2.44	0.52
7:C:87:LEU:H	7:C:87:LEU:CD1	2.22	0.52
7:D:49:ILE:O	7:D:50:GLN:C	2.53	0.52
1:I:19:DA:N6	1:I:20:DA:N6	2.58	0.52
7:B:125:ALA:O	7:B:128:LEU:N	2.43	0.52
7:C:98:ILE:O	7:C:102:SER:OG	2.28	0.52
7:D:180:LEU:HB2	7:D:309:GLU:HG3	1.92	0.52
1:I:18:DC:H6	1:I:18:DC:H5'	1.74	0.52
4:L:12:DG:C8	4:L:13:DT:H72	2.45	0.52
7:B:35:PHE:O	7:B:37:LEU:HD12	2.10	0.52
7:D:141:LYS:O	7:D:141:LYS:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:17:DA:C2	1:I:18:DC:N3	2.78	0.52
7:C:147:LEU:CG	7:C:151:PHE:HE2	2.23	0.52
7:C:199:LEU:O	7:C:203:MSE:HG2	2.08	0.52
7:D:152:ARG:HA	7:D:155:ILE:HD12	1.91	0.52
7:A:61:HIS:C	7:A:61:HIS:CD2	2.88	0.51
7:B:48:ALA:O	7:B:51:ALA:HB3	2.09	0.51
7:B:115:PRO:O	7:B:118:ASP:HB2	2.10	0.51
7:B:216:LEU:HA	7:B:219:MSE:SE	2.60	0.51
7:B:293:ARG:NH1	7:B:304:PRO:HB2	2.25	0.51
7:C:79:TRP:CZ2	7:C:154:ALA:CB	2.93	0.51
5:E:4:DG:C2	5:E:5:DG:C4	2.99	0.51
7:A:12:LEU:CD1	7:A:16:LEU:CD2	2.88	0.51
7:C:105:LYS:O	7:C:106:ALA:C	2.53	0.51
7:C:144:ARG:HG2	7:C:145:SER:H	1.75	0.51
7:C:148:SER:HG	7:C:152:ARG:NH2	2.01	0.51
4:L:23:DC:C2'	4:L:24:DT:H71	2.40	0.51
6:H:13:DG:H2'	6:H:14:DA:H8	1.74	0.51
7:B:293:ARG:CZ	7:B:304:PRO:HB2	2.39	0.51
7:C:228:TYR:HD2	7:C:241:ALA:HB1	1.75	0.51
6:F:23:DT:H2'	6:F:24:DG:C8	2.44	0.51
7:A:26:TYR:CE2	7:A:51:ALA:CB	2.93	0.51
7:A:169:ARG:HH11	7:A:169:ARG:CG	2.21	0.51
7:B:66:ALA:O	7:B:68:ILE:N	2.34	0.51
7:B:309:GLU:HA	7:B:312:SER:HG	1.76	0.51
6:H:1:DG:C2'	6:H:2:DG:OP2	2.48	0.51
7:B:96:THR:O	7:B:99:ASN:HB2	2.11	0.51
7:D:23:TYR:HD2	7:D:23:TYR:C	2.11	0.51
7:D:101:MSE:O	7:D:104:ILE:HB	2.10	0.51
4:L:20:DA:C2	4:L:21:DA:C4	2.99	0.51
7:C:63:PRO:O	7:C:66:ALA:HB3	2.10	0.51
7:C:83:TYR:O	7:C:84:GLU:C	2.54	0.51
7:C:116:LEU:HA	7:C:119:ILE:HD12	1.92	0.51
7:D:48:ALA:O	7:D:51:ALA:HB3	2.10	0.51
5:E:5:DG:H2''	5:E:6:DT:H6	1.76	0.51
5:E:21:DA:N7	5:E:22:DT:H73	2.25	0.51
7:B:18:ILE:HG12	7:B:19:ARG:N	2.26	0.51
7:B:79:TRP:CH2	7:B:154:ALA:CA	2.88	0.51
7:C:163:ASN:OD1	7:C:163:ASN:C	2.53	0.51
1:I:7:DG:C5	1:I:8:DC:C4	2.99	0.51
3:K:15:DA:N9	3:K:16:DT:C7	2.73	0.51
5:E:1:DA:C4	5:E:2:DC:C6	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:23:DA:C2	6:H:4:DA:C2	2.99	0.51
7:B:79:TRP:O	7:B:83:TYR:N	2.42	0.51
7:B:255:MSE:CE	7:B:259:LEU:HD11	2.41	0.51
7:B:307:PHE:CD1	7:B:307:PHE:C	2.88	0.51
7:D:148:SER:HA	7:D:165:VAL:HG21	1.93	0.51
7:D:23:TYR:CD2	7:D:24:TYR:O	2.63	0.51
2:J:2:DG:H4'	7:B:276:ARG:CZ	2.41	0.50
7:A:117:GLU:H	7:A:117:GLU:CD	2.13	0.50
7:B:137:ALA:O	7:B:140:ALA:N	2.44	0.50
7:B:208:VAL:HG13	7:B:209:THR:HG23	1.92	0.50
7:C:76:LEU:HD22	7:C:119:ILE:CD1	2.40	0.50
7:C:229:LEU:O	7:C:229:LEU:HG	2.01	0.50
7:D:28:ASP:OD2	7:D:30:ARG:HB2	2.11	0.50
7:D:34:GLU:C	7:D:35:PHE:CG	2.88	0.50
7:D:154:ALA:HB1	7:D:160:ILE:HD11	1.91	0.50
5:G:4:DG:H2''	5:G:5:DG:O4'	2.10	0.50
7:B:199:LEU:HD12	7:B:199:LEU:H	1.76	0.50
7:B:208:VAL:HA	7:B:318:TYR:OH	2.12	0.50
7:D:107:ILE:O	7:D:108:ARG:C	2.55	0.50
7:D:163:ASN:OD1	7:D:166:ALA:N	2.35	0.50
7:D:205:LEU:O	7:D:208:VAL:HG12	2.11	0.50
6:H:5:DT:H2''	6:H:6:DT:O4'	2.11	0.50
7:A:67:ARG:CZ	7:D:36:GLY:O	2.59	0.50
7:B:306:THR:O	7:B:309:GLU:N	2.44	0.50
2:J:19:DA:P	7:A:90:ARG:HH21	2.35	0.50
6:F:19:DG:C2'	6:F:20:DA:C8	2.95	0.50
5:G:15:DG:OP2	7:C:36:GLY:N	2.45	0.50
7:C:79:TRP:NE1	7:C:154:ALA:HB2	2.26	0.50
3:K:9:DT:C2	3:K:10:DT:C5	3.00	0.50
6:F:14:DA:C2'	6:F:15:DT:C6	2.95	0.50
7:B:77:HIS:O	7:B:81:ASP:OD2	2.29	0.50
7:B:120:THR:HG22	7:B:121:THR:C	2.32	0.50
7:B:125:ALA:O	7:B:126:ALA:C	2.55	0.50
5:E:6:DT:C2'	5:E:7:DC:O4'	2.60	0.50
6:F:16:DA:H3'	7:B:17:TYR:OH	2.12	0.50
7:A:64:LEU:HD21	7:D:26:TYR:HD2	1.74	0.50
7:A:82:ARG:O	7:A:83:TYR:C	2.53	0.50
7:B:153:GLU:HA	7:B:156:ALA:CB	2.42	0.50
7:B:208:VAL:HG13	7:B:209:THR:N	2.27	0.50
7:C:116:LEU:HD12	7:C:116:LEU:H	1.69	0.50
7:D:155:ILE:HG23	7:D:160:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:203:MSE:HE3	7:D:289:PHE:HE1	1.76	0.50
7:A:23:TYR:HD2	7:A:23:TYR:O	1.94	0.50
7:A:138:ALA:O	7:A:141:LYS:HB3	2.11	0.50
7:B:66:ALA:C	7:B:68:ILE:H	2.18	0.50
7:C:120:THR:N	7:C:123:GLU:OE1	2.29	0.50
7:C:179:ARG:NH1	7:C:344:ASP:O	2.44	0.50
7:D:141:LYS:CD	7:D:141:LYS:O	2.60	0.50
1:I:18:DC:OP1	7:C:169:ARG:NH2	2.45	0.50
5:G:2:DC:C2	5:G:3:DA:C6	3.00	0.50
6:H:21:DC:C2	6:H:22:DC:C6	3.00	0.50
7:A:137:ALA:O	7:A:138:ALA:C	2.54	0.50
1:I:16:DA:H1'	1:I:17:DA:C8	2.47	0.49
7:A:185:TYR:HD1	7:A:186:LEU:N	2.10	0.49
7:B:208:VAL:CG1	7:B:209:THR:N	2.74	0.49
7:B:274:SER:OG	7:B:275:THR:N	2.45	0.49
7:C:17:TYR:CE1	7:C:27:ARG:CB	2.95	0.49
7:D:18:ILE:HG12	7:D:19:ARG:H	1.77	0.49
7:A:307:PHE:C	7:A:307:PHE:HD1	2.16	0.49
7:C:116:LEU:CD1	7:C:116:LEU:H	2.23	0.49
7:C:350:TRP:O	7:C:352:LYS:N	2.44	0.49
7:D:92:ILE:HD11	7:D:97:LEU:HD13	1.92	0.49
7:A:15:ASN:HB2	7:A:26:TYR:CE1	2.46	0.49
7:A:338:MSE:C	7:A:340:SER:N	2.61	0.49
7:B:83:TYR:O	7:B:84:GLU:C	2.53	0.49
7:B:124:ILE:O	7:B:127:MSE:HE2	2.12	0.49
7:C:76:LEU:CD1	7:C:80:LEU:HD11	2.42	0.49
7:D:15:ASN:O	7:D:17:TYR:CE1	2.64	0.49
1:I:10:DT:H2''	1:I:11:DT:O5'	2.12	0.49
2:J:16:DT:O2	2:J:17:DA:C8	2.65	0.49
5:G:10:DT:H2''	5:G:11:DA:C8	2.47	0.49
6:H:8:DT:OP2	7:C:12:LEU:CD2	2.54	0.49
7:A:138:ALA:O	7:A:139:SER:C	2.54	0.49
7:A:139:SER:O	7:A:140:ALA:C	2.56	0.49
7:A:84:GLU:HA	7:A:87:LEU:CD1	2.41	0.49
7:A:344:ASP:OD1	7:B:334:LYS:HD3	2.13	0.49
7:B:314:SER:O	7:B:318:TYR:CD2	2.65	0.49
7:A:180:LEU:O	7:A:313:LEU:HD13	2.12	0.49
7:C:11:ASP:O	7:C:13:PRO:CD	2.59	0.49
7:C:199:LEU:HD22	7:C:288:TYR:HB3	1.95	0.49
5:E:11:DA:C6	5:E:12:DT:O4	2.65	0.49
7:A:114:ALA:HB1	7:A:115:PRO:HD2	1.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:27:DA:H1'	1:I:28:DT:C5'	2.42	0.49
4:L:7:DA:C6	4:L:8:DC:C4	3.00	0.49
5:G:5:DG:C2	5:G:6:DT:C6	3.01	0.49
6:H:19:DG:H2''	6:H:20:DA:O5'	2.13	0.49
7:B:198:TRP:CD2	7:B:199:LEU:HD12	2.48	0.49
7:B:229:LEU:HD23	7:B:242:ILE:HB	1.95	0.49
6:F:16:DA:H3'	7:B:17:TYR:HH	1.78	0.49
7:A:77:HIS:CB	7:A:113:ASP:OD1	2.58	0.49
7:C:79:TRP:CZ2	7:C:154:ALA:HA	2.47	0.49
7:D:151:PHE:O	7:D:152:ARG:C	2.53	0.49
7:D:254:SER:HB3	7:D:257:GLU:HB2	1.95	0.49
3:K:12:DA:C2'	3:K:13:DT:C7	2.87	0.49
5:E:18:DA:H4'	5:E:19:DA:OP1	2.12	0.49
6:H:17:DG:C4	6:H:18:DT:C6	3.01	0.49
7:B:82:ARG:O	7:B:83:TYR:C	2.55	0.49
7:C:64:LEU:CD1	7:C:67:ARG:HD3	2.40	0.49
7:D:83:TYR:CZ	7:D:87:LEU:HD21	2.48	0.49
7:D:100:TYR:C	7:D:103:LYS:HG2	2.37	0.49
7:D:137:ALA:O	7:D:138:ALA:C	2.54	0.49
2:J:7:DA:C6	2:J:8:DG:C5	3.01	0.48
2:J:20:DA:C2'	2:J:21:DA:H5''	2.40	0.48
7:B:286:SER:O	7:B:289:PHE:HB3	2.13	0.48
7:C:76:LEU:HD22	7:C:119:ILE:HD11	1.93	0.48
5:G:3:DA:H2'	5:G:4:DG:H8	1.78	0.48
7:A:10:ARG:HH21	7:A:12:LEU:HD22	1.77	0.48
7:A:216:LEU:C	7:A:216:LEU:HD23	2.38	0.48
7:B:37:LEU:N	7:B:37:LEU:CD1	2.71	0.48
7:B:163:ASN:OD1	7:B:165:VAL:CG2	2.61	0.48
7:C:350:TRP:HE3	7:D:239:LYS:HB3	1.76	0.48
7:D:146:THR:O	7:D:149:ASP:N	2.46	0.48
6:H:9:DG:H2''	6:H:10:DA:H8	1.78	0.48
7:A:120:THR:HG23	7:A:123:GLU:H	1.78	0.48
7:C:205:LEU:O	7:C:208:VAL:HG12	2.14	0.48
7:C:350:TRP:CD1	7:C:350:TRP:H	2.31	0.48
7:D:313:LEU:HD12	7:D:316:ARG:HH12	1.78	0.48
7:B:199:LEU:H	7:B:199:LEU:CD1	2.26	0.48
7:C:49:ILE:O	7:C:52:ASN:HB2	2.14	0.48
7:C:104:ILE:O	7:C:105:LYS:C	2.56	0.48
2:J:26:DA:H2'	2:J:27:DG:C8	2.48	0.48
5:E:4:DG:C2	5:E:5:DG:N9	2.81	0.48
7:A:26:TYR:CZ	7:A:51:ALA:HB3	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:160:ILE:CD1	7:B:160:ILE:N	2.76	0.48
7:D:141:LYS:C	7:D:141:LYS:HD3	2.36	0.48
2:J:16:DT:O2	2:J:16:DT:C2'	2.38	0.48
6:F:19:DG:H2'	6:F:20:DA:N7	2.28	0.48
5:G:3:DA:C2'	5:G:4:DG:H8	2.26	0.48
6:H:2:DG:H4'	6:H:3:DT:OP1	2.12	0.48
7:A:16:LEU:HD23	7:A:16:LEU:C	2.39	0.48
7:B:15:ASN:HA	7:B:17:TYR:OH	2.14	0.48
7:B:198:TRP:CZ3	7:B:199:LEU:HD12	2.48	0.48
7:D:96:THR:O	7:D:99:ASN:HB2	2.14	0.48
7:B:155:ILE:HG12	7:B:160:ILE:O	2.13	0.48
7:D:42:ARG:HB3	7:D:42:ARG:CZ	2.43	0.48
7:D:104:ILE:O	7:D:105:LYS:C	2.56	0.48
1:I:21:DA:N6	7:D:99:ASN:HD21	2.12	0.48
7:B:98:ILE:O	7:B:99:ASN:C	2.57	0.48
7:B:205:LEU:C	7:B:208:VAL:HG12	2.36	0.48
7:D:19:ARG:HG2	7:D:20:ASN:H	1.79	0.48
7:A:306:THR:OG1	7:A:307:PHE:N	2.44	0.48
7:B:35:PHE:O	7:B:37:LEU:CD1	2.61	0.48
7:B:290:MSE:O	7:B:293:ARG:CB	2.61	0.48
7:D:79:TRP:CH2	7:D:154:ALA:HA	2.44	0.48
5:G:5:DG:OP2	7:D:36:GLY:N	2.43	0.48
7:A:83:TYR:CZ	7:A:87:LEU:HD21	2.48	0.48
7:B:27:ARG:HD2	7:B:34:GLU:CG	2.38	0.48
7:B:101:MSE:O	7:B:104:ILE:HB	2.13	0.48
7:B:285:VAL:HG12	7:B:307:PHE:CE2	2.49	0.48
7:C:16:LEU:C	7:C:17:TYR:CD2	2.92	0.48
7:C:81:ASP:OD2	7:C:108:ARG:NH2	2.47	0.48
7:C:98:ILE:HA	7:C:101:MSE:HB2	1.94	0.48
7:D:287:ARG:O	7:D:290:MSE:HB3	2.14	0.48
7:A:207:VAL:O	7:A:314:SER:HB2	2.14	0.47
7:B:83:TYR:CZ	7:B:87:LEU:HD21	2.49	0.47
7:B:124:ILE:O	7:B:125:ALA:C	2.55	0.47
7:B:125:ALA:C	7:B:129:ASN:HD22	2.22	0.47
7:C:59:HIS:C	7:C:60:LYS:HD3	2.39	0.47
7:C:103:LYS:O	7:C:106:ALA:N	2.47	0.47
6:F:17:DG:OP2	7:B:17:TYR:OH	2.31	0.47
7:A:15:ASN:ND2	7:A:52:ASN:OD1	2.47	0.47
7:A:211:GLN:O	7:A:311:ARG:HD2	2.15	0.47
7:A:283:GLY:O	7:A:287:ARG:HB2	2.14	0.47
7:B:309:GLU:HA	7:B:312:SER:OG	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:16:LEU:HD22	7:C:48:ALA:HB2	1.96	0.47
6:F:17:DG:C8	6:F:18:DT:C7	2.97	0.47
6:H:6:DT:H2''	6:H:7:DT:C5'	2.19	0.47
7:A:107:ILE:O	7:A:108:ARG:C	2.55	0.47
7:A:121:THR:O	7:A:124:ILE:HB	2.14	0.47
7:B:285:VAL:HG12	7:B:307:PHE:CD2	2.49	0.47
7:D:185:TYR:CD1	7:D:185:TYR:C	2.92	0.47
6:H:10:DA:N6	7:C:19:ARG:HH21	2.12	0.47
6:H:17:DG:OP2	7:D:15:ASN:HA	2.14	0.47
7:D:15:ASN:HD21	7:D:52:ASN:HD21	1.62	0.47
2:J:23:DC:H5''	7:A:306:THR:OG1	2.15	0.47
3:K:20:DA:C2	3:K:21:DA:C4	3.02	0.47
6:F:6:DT:OP2	7:A:27:ARG:NH1	2.47	0.47
6:F:7:DT:H5'	6:F:7:DT:C6	2.44	0.47
6:F:20:DA:C2	6:F:21:DC:C2	3.02	0.47
7:B:27:ARG:CD	7:B:34:GLU:CD	2.77	0.47
7:B:61:HIS:CE1	7:B:62:LYS:O	2.67	0.47
7:B:103:LYS:HG2	7:B:103:LYS:H	1.25	0.47
7:B:208:VAL:O	7:B:318:TYR:OH	2.31	0.47
7:B:351:ASP:OD1	7:B:352:LYS:N	2.47	0.47
7:C:72:ASN:ND2	7:C:72:ASN:N	2.56	0.47
6:F:11:DC:C4	6:F:12:DT:H73	2.49	0.47
7:A:67:ARG:HH22	7:D:36:GLY:N	2.13	0.47
7:A:116:LEU:O	7:A:119:ILE:CG1	2.62	0.47
7:B:116:LEU:HA	7:B:119:ILE:HD12	1.97	0.47
7:B:229:LEU:O	7:B:241:ALA:HA	2.15	0.47
7:B:331:LEU:HB3	7:B:333:HIS:HD2	1.79	0.47
7:C:139:SER:O	7:C:140:ALA:C	2.57	0.47
1:I:2:DA:H2''	1:I:3:DC:OP2	2.14	0.47
3:K:8:DC:H2'	3:K:9:DT:C6	2.49	0.47
5:E:7:DC:H2''	5:E:8:DA:C8	2.50	0.47
6:F:10:DA:H61	7:A:19:ARG:HH21	1.38	0.47
6:F:17:DG:P	7:B:17:TYR:HE2	2.38	0.47
6:H:1:DG:H2''	6:H:2:DG:C8	2.49	0.47
7:A:13:PRO:O	7:A:16:LEU:HB3	2.15	0.47
7:A:16:LEU:O	7:A:17:TYR:HD2	1.98	0.47
7:B:43:ILE:HD12	7:B:46:THR:OG1	2.15	0.47
7:B:63:PRO:C	7:B:65:THR:H	2.23	0.47
2:J:11:DT:C4'	2:J:12:DA:OP1	2.62	0.47
7:A:26:TYR:CZ	7:A:51:ALA:CB	2.98	0.47
7:A:81:ASP:O	7:A:84:GLU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:239:LYS:HD2	7:D:349:GLU:HA	1.95	0.47
7:B:136:LYS:O	7:B:137:ALA:C	2.58	0.47
7:C:68:ILE:O	7:C:69:ASN:C	2.58	0.47
7:D:34:GLU:O	7:D:35:PHE:CD2	2.68	0.47
5:G:6:DT:C2	5:G:7:DC:C6	3.03	0.47
7:A:77:HIS:CE1	7:A:108:ARG:HG3	2.50	0.47
7:C:283:GLY:O	7:C:287:ARG:HB2	2.14	0.47
1:I:14:DA:H8	1:I:14:DA:H5'	1.80	0.46
2:J:2:DG:H4'	7:B:276:ARG:HH22	1.78	0.46
5:G:17:DC:H2''	5:G:18:DA:C8	2.50	0.46
6:H:14:DA:H2'	6:H:15:DT:H72	1.96	0.46
7:A:101:MSE:O	7:A:104:ILE:HB	2.15	0.46
7:B:204:GLU:O	7:B:205:LEU:C	2.58	0.46
7:C:310:LEU:N	7:C:310:LEU:HD23	2.30	0.46
7:D:211:GLN:C	7:D:311:ARG:HH11	2.23	0.46
1:I:12:DT:C5'	7:A:235:LYS:HZ3	2.28	0.46
5:E:3:DA:H2''	5:E:4:DG:O5'	2.14	0.46
5:G:11:DA:H2''	5:G:12:DT:O5'	2.14	0.46
7:A:152:ARG:O	7:A:155:ILE:N	2.48	0.46
7:C:60:LYS:HB2	7:C:60:LYS:HZ3	1.78	0.46
7:D:104:ILE:O	7:D:107:ILE:N	2.48	0.46
5:G:16:DT:O4	7:C:19:ARG:NH2	2.48	0.46
7:A:65:THR:O	7:A:66:ALA:C	2.58	0.46
7:B:82:ARG:O	7:B:86:ILE:HG13	2.15	0.46
7:C:10:ARG:HB3	7:C:12:LEU:CD1	2.45	0.46
7:C:160:ILE:HG23	7:C:161:THR:H	1.76	0.46
7:C:186:LEU:HD11	7:C:251:LEU:HD23	1.96	0.46
7:C:243:PRO:C	7:C:245:ALA:H	2.23	0.46
7:D:75:THR:CG2	7:D:78:SER:HB2	2.36	0.46
7:D:151:PHE:O	7:D:154:ALA:N	2.49	0.46
7:D:165:VAL:O	7:D:168:THR:CG2	2.27	0.46
5:E:11:DA:C4	5:E:12:DT:C5	3.04	0.46
5:G:7:DC:C2'	5:G:8:DA:C8	2.89	0.46
7:A:92:ILE:CG2	7:A:96:THR:HB	2.46	0.46
7:A:95:LYS:O	7:A:96:THR:C	2.58	0.46
7:A:285:VAL:HG12	7:A:286:SER:N	2.31	0.46
7:B:105:LYS:O	7:B:108:ARG:HB2	2.16	0.46
7:B:185:TYR:CD1	7:B:185:TYR:C	2.92	0.46
7:B:211:GLN:C	7:B:311:ARG:HD2	2.40	0.46
7:B:313:LEU:HD13	7:B:316:ARG:NH1	2.31	0.46
7:C:54:GLU:CG	7:C:55:LEU:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:61:HIS:C	7:C:61:HIS:CD2	2.93	0.46
7:C:138:ALA:O	7:C:141:LYS:HB2	2.15	0.46
3:K:11:DT:C2	3:K:12:DA:C8	3.03	0.46
7:A:14:PRO:C	7:A:15:ASN:CG	2.84	0.46
7:A:243:PRO:C	7:A:245:ALA:H	2.21	0.46
7:B:116:LEU:HB3	7:B:160:ILE:HG21	1.97	0.46
7:C:212:ARG:CB	7:C:215:ASP:OD2	2.62	0.46
2:J:24:DA:C2	2:J:25:DG:C5	3.04	0.46
3:K:8:DC:C2'	3:K:9:DT:H71	2.42	0.46
4:L:16:DA:C2'	4:L:17:DA:H5''	2.45	0.46
5:G:2:DC:C2'	5:G:3:DA:N7	2.72	0.46
7:A:16:LEU:HG	7:A:17:TYR:N	2.31	0.46
7:B:100:TYR:O	7:B:103:LYS:N	2.48	0.46
7:D:17:TYR:CD1	7:D:27:ARG:HB2	2.51	0.46
6:F:2:DG:C2'	6:F:3:DT:C7	2.86	0.46
7:B:103:LYS:O	7:B:106:ALA:N	2.48	0.46
7:B:199:LEU:O	7:B:203:MSE:CG	2.63	0.46
7:D:139:SER:O	7:D:140:ALA:C	2.57	0.46
7:A:147:LEU:HD12	7:A:147:LEU:O	2.16	0.46
7:A:338:MSE:O	7:A:342:PHE:HB2	2.16	0.46
7:B:306:THR:O	7:B:309:GLU:CB	2.47	0.46
7:B:350:TRP:HZ3	7:C:239:LYS:HB3	1.72	0.46
7:D:307:PHE:CD1	7:D:307:PHE:C	2.94	0.46
5:E:12:DT:C2'	5:E:13:DC:H6	2.28	0.46
7:A:98:ILE:O	7:A:99:ASN:C	2.59	0.46
7:A:313:LEU:HA	7:A:316:ARG:HH21	1.80	0.46
7:B:211:GLN:NE2	7:B:330:LEU:O	2.42	0.46
5:G:6:DT:C2	5:G:7:DC:C5	3.04	0.46
7:A:65:THR:HG23	7:D:54:GLU:CD	2.41	0.46
7:A:67:ARG:NH2	7:D:36:GLY:N	2.63	0.46
7:A:79:TRP:O	7:A:83:TYR:N	2.42	0.46
7:B:99:ASN:HB3	7:B:103:LYS:HZ3	1.81	0.46
7:B:127:MSE:O	7:B:128:LEU:C	2.58	0.46
7:B:215:ASP:O	7:B:218:GLU:HB2	2.16	0.46
7:C:306:THR:O	7:C:309:GLU:N	2.47	0.46
7:D:163:ASN:OD1	7:D:165:VAL:N	2.49	0.46
5:E:1:DA:H1'	5:E:2:DC:O4'	2.16	0.45
5:G:11:DA:C4	5:G:12:DT:C5	3.04	0.45
7:A:92:ILE:HG23	7:A:96:THR:HB	1.98	0.45
7:B:243:PRO:C	7:B:245:ALA:H	2.24	0.45
7:A:149:ASP:O	7:A:150:ALA:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:76:LEU:CG	7:C:80:LEU:HD11	2.42	0.45
7:C:99:ASN:O	7:C:103:LYS:HG2	2.16	0.45
7:C:308:HIS:C	7:C:310:LEU:N	2.74	0.45
3:K:4:DC:H2''	3:K:5:DC:OP2	2.17	0.45
7:B:15:ASN:HB2	7:B:26:TYR:CE1	2.51	0.45
7:B:189:TYR:O	7:B:192:ALA:HB3	2.15	0.45
7:B:307:PHE:C	7:B:307:PHE:HD1	2.25	0.45
7:C:72:ASN:H	7:C:72:ASN:HD22	1.63	0.45
7:C:280:LEU:HA	7:C:280:LEU:HD23	1.49	0.45
7:D:121:THR:O	7:D:124:ILE:HB	2.16	0.45
7:D:129:ASN:O	7:D:132:ILE:HB	2.17	0.45
1:I:10:DT:C2	1:I:11:DT:C5	3.04	0.45
5:E:11:DA:C4	5:E:12:DT:C4	3.04	0.45
7:A:127:MSE:O	7:A:128:LEU:C	2.58	0.45
7:A:274:SER:N	7:A:280:LEU:HD11	2.31	0.45
7:B:11:ASP:O	7:B:13:PRO:HD3	2.17	0.45
7:D:62:LYS:O	7:D:65:THR:N	2.49	0.45
7:D:121:THR:CA	7:D:124:ILE:HD12	2.47	0.45
7:D:143:ILE:O	7:D:144:ARG:C	2.60	0.45
1:I:21:DA:N6	7:D:99:ASN:ND2	2.63	0.45
2:J:20:DA:H8	7:A:96:THR:HG23	1.81	0.45
4:L:16:DA:H2'	4:L:17:DA:H5''	1.97	0.45
5:E:17:DC:H6	5:E:17:DC:H2'	1.49	0.45
7:A:104:ILE:CG2	7:A:105:LYS:N	2.70	0.45
7:A:221:TRP:NE1	7:A:271:ILE:HA	2.32	0.45
7:C:95:LYS:O	7:C:96:THR:C	2.60	0.45
7:D:290:MSE:HG3	7:D:293:ARG:HH21	1.81	0.45
3:K:20:DA:C4	3:K:21:DA:C8	3.05	0.45
4:L:20:DA:O3'	7:C:235:LYS:HG3	2.16	0.45
7:C:13:PRO:HA	7:C:14:PRO:HD3	1.78	0.45
1:I:12:DT:C5'	7:A:235:LYS:NZ	2.79	0.45
1:I:21:DA:H2'	1:I:22:DG:C8	2.52	0.45
7:A:147:LEU:C	7:A:147:LEU:HD12	2.42	0.45
7:C:111:LEU:CD2	7:C:112:PRO:HD2	2.35	0.45
4:L:5:DC:H2''	4:L:6:DA:H8	1.81	0.45
5:G:19:DA:H2''	5:G:20:DA:H8	1.81	0.45
5:G:19:DA:C5	5:G:20:DA:N7	2.85	0.45
7:A:17:TYR:CD2	7:A:17:TYR:N	2.79	0.45
7:A:50:GLN:HE22	7:A:61:HIS:CB	2.30	0.45
7:B:99:ASN:O	7:B:100:TYR:C	2.59	0.45
7:C:103:LYS:O	7:C:106:ALA:CB	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:45:ILE:O	7:D:46:THR:C	2.58	0.45
3:K:5:DC:H2''	3:K:6:DA:OP2	2.16	0.45
7:A:127:MSE:HE3	7:A:128:LEU:CA	2.46	0.45
7:A:281:SER:O	7:A:282:SER:C	2.60	0.45
7:A:308:HIS:C	7:A:310:LEU:N	2.73	0.45
7:B:54:GLU:OE2	7:B:54:GLU:CA	2.56	0.45
7:B:60:LYS:HE3	7:D:46:THR:HG22	1.97	0.45
7:B:79:TRP:CZ2	7:B:154:ALA:HB2	2.52	0.45
7:C:186:LEU:HD11	7:C:251:LEU:HD22	1.92	0.45
5:G:4:DG:C4	5:G:5:DG:C8	3.05	0.45
7:A:124:ILE:O	7:A:127:MSE:HE2	2.16	0.45
7:B:47:GLU:OE2	7:C:64:LEU:HB2	2.16	0.45
7:B:66:ALA:C	7:B:68:ILE:N	2.75	0.45
7:C:49:ILE:HG12	7:C:49:ILE:H	1.26	0.45
7:A:84:GLU:C	7:A:87:LEU:HD12	2.42	0.44
7:A:355:ILE:HG22	7:A:355:ILE:O	2.17	0.44
7:C:14:PRO:C	7:C:16:LEU:H	2.24	0.44
7:C:16:LEU:HD12	7:C:16:LEU:N	2.31	0.44
7:C:97:LEU:HD22	7:C:98:ILE:CD1	2.48	0.44
7:D:75:THR:HA	7:D:115:PRO:HA	1.99	0.44
7:D:141:LYS:HZ2	7:D:145:SER:HB2	1.81	0.44
5:E:21:DA:N7	5:E:22:DT:C7	2.80	0.44
7:A:9:ARG:HB3	7:A:10:ARG:HG3	1.99	0.44
7:A:14:PRO:O	7:A:15:ASN:CB	2.64	0.44
7:B:12:LEU:HA	7:B:13:PRO:HD2	1.71	0.44
7:B:77:HIS:HA	7:B:80:LEU:HD13	1.96	0.44
7:B:138:ALA:O	7:B:141:LYS:HB2	2.17	0.44
7:C:36:GLY:C	7:C:37:LEU:HD23	2.43	0.44
7:D:163:ASN:OD1	7:D:165:VAL:HB	2.16	0.44
1:I:5:DC:C1'	1:I:6:DT:H5'	2.33	0.44
6:H:10:DA:H61	7:C:19:ARG:HH21	1.66	0.44
7:C:92:ILE:CG2	7:C:96:THR:CB	2.92	0.44
7:C:242:ILE:CG2	7:C:330:LEU:HD11	2.44	0.44
2:J:20:DA:C8	7:A:96:THR:HG23	2.53	0.44
6:F:12:DT:H1'	6:F:13:DG:C8	2.52	0.44
7:B:100:TYR:O	7:B:103:LYS:CG	2.66	0.44
7:C:10:ARG:HB3	7:C:12:LEU:HD12	1.98	0.44
7:C:18:ILE:HG12	7:C:19:ARG:H	1.81	0.44
7:D:37:LEU:N	7:D:37:LEU:CD2	2.80	0.44
2:J:7:DA:C2	2:J:8:DG:C4	3.05	0.44
2:J:8:DG:H2'	2:J:9:DT:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:21:DA:C8	5:E:22:DT:C7	2.99	0.44
7:A:131:TYR:N	7:A:131:TYR:CD1	2.86	0.44
7:A:212:ARG:NH1	7:A:233:GLN:OE1	2.50	0.44
7:C:345:ASP:OD1	7:C:348:ARG:HB2	2.18	0.44
7:D:63:PRO:C	7:D:65:THR:H	2.26	0.44
1:I:7:DG:C4	1:I:8:DC:C5	3.05	0.44
2:J:10:DT:C2	2:J:11:DT:C5	3.06	0.44
7:A:165:VAL:HG12	7:A:166:ALA:CA	2.46	0.44
7:B:163:ASN:OD1	7:B:163:ASN:C	2.60	0.44
7:D:36:GLY:C	7:D:37:LEU:CD2	2.86	0.44
7:D:50:GLN:NE2	7:D:53:ILE:HD11	2.33	0.44
6:F:18:DT:OP1	7:B:10:ARG:NH2	2.51	0.44
7:B:100:TYR:O	7:B:103:LYS:HG2	2.17	0.44
7:B:151:PHE:O	7:B:154:ALA:N	2.51	0.44
7:C:10:ARG:HB2	7:C:12:LEU:HD13	1.99	0.44
7:D:243:PRO:HG2	7:D:246:LEU:CD1	2.47	0.44
2:J:26:DA:C2'	2:J:27:DG:C8	3.01	0.44
3:K:19:DA:C6	3:K:20:DA:C6	3.06	0.44
6:H:13:DG:N3	6:H:14:DA:C4	2.86	0.44
7:B:144:ARG:NH2	7:B:168:THR:O	2.51	0.44
7:C:149:ASP:O	7:C:150:ALA:C	2.60	0.44
7:D:138:ALA:O	7:D:139:SER:C	2.58	0.44
7:C:121:THR:O	7:C:124:ILE:HB	2.17	0.44
7:C:331:LEU:HD23	7:C:333:HIS:HD2	1.83	0.44
7:D:116:LEU:HA	7:D:116:LEU:HD23	1.67	0.44
2:J:27:DG:C2	2:J:28:DT:C2	3.06	0.43
7:B:155:ILE:HA	7:B:160:ILE:HD13	2.00	0.43
7:C:123:GLU:O	7:C:126:ALA:HB3	2.17	0.43
7:C:205:LEU:HD23	7:C:216:LEU:HD11	1.99	0.43
1:I:1:DA:C4	1:I:2:DA:N7	2.86	0.43
1:I:14:DA:C8	1:I:14:DA:H5'	2.52	0.43
7:A:10:ARG:HH21	7:A:12:LEU:CB	2.31	0.43
7:A:64:LEU:HD12	7:A:64:LEU:HA	1.61	0.43
7:A:99:ASN:O	7:A:100:TYR:C	2.61	0.43
7:A:120:THR:N	7:A:123:GLU:OE1	2.34	0.43
7:A:314:SER:O	7:A:318:TYR:CD2	2.71	0.43
7:B:53:ILE:O	7:B:57:SER:N	2.51	0.43
7:B:147:LEU:O	7:B:148:SER:C	2.60	0.43
7:B:278:GLU:HB3	7:B:279:PRO:CD	2.48	0.43
7:C:284:THR:HA	7:C:287:ARG:HB2	2.00	0.43
7:D:49:ILE:O	7:D:52:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1:DA:H2''	1:I:2:DA:O5'	2.18	0.43
6:F:12:DT:H2''	6:F:13:DG:OP2	2.18	0.43
7:A:49:ILE:O	7:A:50:GLN:C	2.60	0.43
7:A:111:LEU:CD2	7:A:112:PRO:HD2	2.40	0.43
7:B:47:GLU:O	7:B:50:GLN:HB2	2.19	0.43
7:B:155:ILE:N	7:B:160:ILE:HD11	2.32	0.43
7:B:199:LEU:HD12	7:B:199:LEU:N	2.32	0.43
7:C:64:LEU:HA	7:C:67:ARG:HD3	2.01	0.43
7:C:208:VAL:HG13	7:C:209:THR:HG22	2.00	0.43
7:D:13:PRO:HG3	7:D:45:ILE:HG13	1.99	0.43
7:D:27:ARG:HD2	7:D:34:GLU:OE1	2.18	0.43
7:D:83:TYR:O	7:D:84:GLU:C	2.61	0.43
4:L:7:DA:C6	4:L:8:DC:N3	2.86	0.43
5:E:19:DA:C6	5:E:20:DA:C6	3.06	0.43
6:F:6:DT:C2'	6:F:7:DT:C5'	2.83	0.43
7:A:125:ALA:O	7:A:126:ALA:C	2.61	0.43
7:A:256:LYS:HD2	7:A:256:LYS:HA	1.73	0.43
7:A:307:PHE:C	7:A:309:GLU:N	2.76	0.43
7:B:61:HIS:CE1	7:B:63:PRO:CA	3.01	0.43
7:B:149:ASP:O	7:B:150:ALA:C	2.59	0.43
1:I:12:DT:H5''	7:A:235:LYS:HZ3	1.82	0.43
2:J:10:DT:H4'	7:B:177:ARG:NH1	2.33	0.43
6:F:17:DG:C8	6:F:18:DT:H71	2.53	0.43
7:C:74:VAL:HG21	7:C:159:HIS:CD2	2.53	0.43
7:C:99:ASN:C	7:C:103:LYS:HZ3	2.25	0.43
7:C:103:LYS:HG2	7:C:103:LYS:H	1.50	0.43
7:C:153:GLU:O	7:C:154:ALA:C	2.61	0.43
7:C:308:HIS:O	7:C:310:LEU:N	2.52	0.43
7:D:18:ILE:HG13	7:D:24:TYR:CD2	2.53	0.43
7:D:71:ASP:N	7:D:71:ASP:OD1	2.52	0.43
3:K:8:DC:C2	3:K:9:DT:C7	3.01	0.43
7:A:67:ARG:NH2	7:D:36:GLY:H	2.17	0.43
7:D:128:LEU:HD21	7:D:144:ARG:HB2	2.00	0.43
7:D:180:LEU:HD22	7:D:309:GLU:HB3	2.01	0.43
7:D:260:ASP:HA	7:D:263:LYS:HG2	2.00	0.43
7:D:293:ARG:HH12	7:D:306:THR:HG22	1.83	0.43
5:G:3:DA:H2''	5:G:4:DG:O5'	2.18	0.43
7:A:141:LYS:O	7:A:144:ARG:HB3	2.17	0.43
7:B:13:PRO:HA	7:B:14:PRO:HD2	1.53	0.43
7:B:176:ARG:O	7:B:177:ARG:C	2.61	0.43
7:D:77:HIS:HB2	7:D:113:ASP:CG	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:83:TYR:CE2	7:D:87:LEU:HD11	2.54	0.43
7:D:145:SER:O	7:D:148:SER:HB3	2.18	0.43
7:D:247:HIS:HB3	7:D:254:SER:HA	2.01	0.43
6:H:19:DG:H5''	7:D:20:ASN:ND2	2.34	0.43
7:A:12:LEU:HA	7:A:13:PRO:HD2	1.88	0.43
7:A:306:THR:O	7:A:309:GLU:N	2.49	0.43
7:A:308:HIS:O	7:A:309:GLU:C	2.62	0.43
7:B:47:GLU:OE1	7:C:61:HIS:CE1	2.69	0.43
7:B:93:LYS:O	7:B:94:GLN:C	2.61	0.43
7:B:209:THR:O	7:B:211:GLN:HG2	2.19	0.43
7:C:136:LYS:O	7:C:137:ALA:C	2.61	0.43
7:D:306:THR:O	7:D:309:GLU:N	2.49	0.43
7:A:76:LEU:HD11	7:A:119:ILE:HD11	2.01	0.43
7:A:77:HIS:ND1	7:A:108:ARG:HG3	2.34	0.43
7:C:84:GLU:O	7:C:87:LEU:HB2	2.19	0.43
5:E:11:DA:N9	5:E:12:DT:C7	2.82	0.43
6:F:13:DG:C2	6:F:14:DA:C4	3.07	0.43
7:A:27:ARG:HD3	7:A:28:ASP:C	2.44	0.43
7:C:306:THR:O	7:C:307:PHE:C	2.61	0.43
7:D:26:TYR:CD1	7:D:27:ARG:N	2.87	0.43
7:A:136:LYS:O	7:A:137:ALA:C	2.60	0.42
7:C:45:ILE:O	7:C:49:ILE:CG1	2.64	0.42
7:C:80:LEU:O	7:C:83:TYR:HB3	2.19	0.42
7:D:136:LYS:O	7:D:137:ALA:C	2.62	0.42
7:D:281:SER:O	7:D:282:SER:C	2.61	0.42
5:G:14:DA:H2''	5:G:15:DG:O5'	2.20	0.42
7:A:79:TRP:CZ2	7:A:154:ALA:HA	2.54	0.42
7:D:313:LEU:CA	7:D:316:ARG:NH2	2.81	0.42
5:E:4:DG:N1	5:E:5:DG:C4	2.87	0.42
6:H:11:DC:H2''	6:H:12:DT:O5'	2.16	0.42
7:A:39:ARG:HD2	7:A:39:ARG:HA	1.47	0.42
7:A:76:LEU:HD13	7:A:114:ALA:O	2.19	0.42
7:B:56:PHE:HD2	7:B:56:PHE:HA	1.34	0.42
7:B:100:TYR:O	7:B:103:LYS:CB	2.66	0.42
7:C:51:ALA:O	7:C:54:GLU:CG	2.66	0.42
7:C:185:TYR:CD1	7:C:186:LEU:HD12	2.49	0.42
7:D:149:ASP:O	7:D:150:ALA:C	2.61	0.42
3:K:18:DT:H6	3:K:18:DT:H5'	1.84	0.42
4:L:8:DC:O5'	7:D:136:LYS:HD3	2.19	0.42
6:F:22:DC:H2''	6:F:23:DT:O4'	2.19	0.42
7:B:100:TYR:O	7:B:103:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:121:THR:O	7:B:122:LYS:C	2.62	0.42
7:B:180:LEU:O	7:B:313:LEU:HD13	2.19	0.42
7:B:212:ARG:O	7:B:216:LEU:HG	2.18	0.42
7:D:168:THR:OG1	7:D:169:ARG:N	2.52	0.42
7:D:311:ARG:NH2	7:D:331:LEU:HB3	2.35	0.42
5:G:5:DG:N3	5:G:6:DT:C6	2.88	0.42
7:A:262:CYS:O	7:A:266:LEU:HB2	2.20	0.42
7:B:198:TRP:HA	7:B:201:LEU:HD12	2.02	0.42
7:C:42:ARG:O	7:C:45:ILE:HB	2.19	0.42
7:D:74:VAL:O	7:D:115:PRO:HA	2.19	0.42
7:D:228:TYR:HD2	7:D:243:PRO:HA	1.85	0.42
1:I:17:DA:H5'	1:I:17:DA:C8	2.51	0.42
1:I:23:DT:H2''	1:I:24:DT:H5''	2.01	0.42
4:L:24:DT:H2''	4:L:25:DG:OP2	2.19	0.42
6:F:8:DT:P	7:A:10:ARG:HH22	2.42	0.42
7:A:66:ALA:O	7:A:68:ILE:N	2.53	0.42
7:A:77:HIS:CD2	7:A:113:ASP:HA	2.54	0.42
7:B:15:ASN:ND2	7:B:26:TYR:OH	2.50	0.42
7:B:107:ILE:HD13	7:B:147:LEU:HD13	2.02	0.42
7:B:127:MSE:HE3	7:B:128:LEU:HD12	2.02	0.42
7:C:120:THR:O	7:C:123:GLU:N	2.52	0.42
7:C:205:LEU:HB3	7:C:216:LEU:HD11	2.02	0.42
7:D:12:LEU:HA	7:D:13:PRO:HD2	1.85	0.42
1:I:19:DA:H2''	1:I:20:DA:O4'	2.19	0.42
2:J:4:DT:H1'	2:J:5:DC:H5'	2.01	0.42
2:J:16:DT:H2''	2:J:17:DA:C5'	2.45	0.42
3:K:12:DA:OP2	7:C:342:PHE:CZ	2.73	0.42
5:E:5:DG:C2'	5:E:6:DT:H6	2.33	0.42
6:H:2:DG:P	6:H:2:DG:H2'	2.59	0.42
6:H:9:DG:C5	6:H:10:DA:N6	2.88	0.42
7:A:15:ASN:C	7:A:17:TYR:CE2	2.97	0.42
7:D:26:TYR:HD1	7:D:26:TYR:HA	1.59	0.42
7:D:98:ILE:O	7:D:99:ASN:C	2.62	0.42
7:D:124:ILE:O	7:D:125:ALA:C	2.60	0.42
7:D:147:LEU:O	7:D:148:SER:C	2.63	0.42
6:H:8:DT:H2''	6:H:9:DG:N7	2.33	0.42
7:A:11:ASP:O	7:A:13:PRO:CD	2.67	0.42
7:A:121:THR:O	7:A:124:ILE:N	2.53	0.42
7:B:122:LYS:O	7:B:123:GLU:C	2.62	0.42
7:C:94:GLN:O	7:C:97:LEU:HB3	2.20	0.42
7:D:293:ARG:HD3	7:D:305:PRO:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:25:DG:H2''	4:L:26:DG:O4'	2.20	0.42
5:E:12:DT:H2'	5:E:13:DC:C6	2.54	0.42
6:F:19:DG:C2'	6:F:20:DA:H8	2.33	0.42
5:G:14:DA:C8	7:C:23:TYR:CE1	2.99	0.42
7:A:287:ARG:O	7:A:290:MSE:HB3	2.20	0.42
7:B:25:CYS:SG	7:B:35:PHE:O	2.77	0.42
7:C:306:THR:HG1	7:C:307:PHE:N	2.18	0.42
7:D:15:ASN:HA	7:D:17:TYR:HH	1.85	0.42
7:D:53:ILE:HG13	7:D:53:ILE:H	1.57	0.42
5:E:12:DT:C1'	5:E:13:DC:H5''	2.47	0.42
7:A:14:PRO:C	7:A:16:LEU:H	2.28	0.42
7:A:64:LEU:O	7:A:65:THR:C	2.63	0.42
7:A:144:ARG:HG2	7:A:145:SER:N	2.35	0.42
7:A:147:LEU:HD11	7:A:151:PHE:CE1	2.55	0.42
7:B:155:ILE:HG12	7:B:160:ILE:C	2.45	0.42
7:B:281:SER:O	7:B:282:SER:C	2.62	0.42
7:C:12:LEU:HA	7:C:13:PRO:HD2	1.89	0.42
7:C:44:ALA:O	7:C:45:ILE:C	2.62	0.42
7:D:100:TYR:HA	7:D:103:LYS:HG2	2.02	0.42
4:L:8:DC:H2'	4:L:9:DT:C7	2.34	0.41
6:F:13:DG:H1'	6:F:14:DA:O4'	2.20	0.41
6:H:4:DA:H2''	6:H:5:DT:O5'	2.20	0.41
7:C:25:CYS:HB3	7:C:35:PHE:O	2.19	0.41
7:D:70:SER:C	7:D:72:ASN:N	2.77	0.41
2:J:27:DG:H2''	2:J:28:DT:OP2	2.19	0.41
3:K:16:DT:O2	3:K:17:DA:C8	2.73	0.41
5:G:3:DA:C2'	5:G:4:DG:C8	3.04	0.41
7:A:266:LEU:HD13	7:A:273:ALA:H	1.85	0.41
7:D:155:ILE:HG13	7:D:160:ILE:CD1	2.50	0.41
4:L:16:DA:C2'	4:L:17:DA:C5'	2.98	0.41
6:H:17:DG:C5	6:H:18:DT:C4	3.08	0.41
7:A:146:THR:O	7:A:149:ASP:N	2.53	0.41
7:A:172:LYS:HD2	7:A:173:SER:H	1.85	0.41
7:B:16:LEU:C	7:B:16:LEU:CD2	2.78	0.41
7:B:79:TRP:CZ2	7:B:154:ALA:N	2.87	0.41
7:B:83:TYR:HA	7:B:86:ILE:HD12	2.03	0.41
7:B:120:THR:CG2	7:B:122:LYS:N	2.54	0.41
7:B:127:MSE:HE3	7:B:128:LEU:CA	2.50	0.41
7:B:143:ILE:O	7:B:144:ARG:C	2.62	0.41
7:C:97:LEU:CD2	7:C:98:ILE:HG13	2.50	0.41
7:C:203:MSE:HE3	7:C:203:MSE:HB3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:28:ASP:OD2	7:D:28:ASP:C	2.61	0.41
6:F:17:DG:C4	6:F:18:DT:C5	3.08	0.41
7:B:104:ILE:H	7:B:104:ILE:HG13	1.44	0.41
7:B:165:VAL:H	7:B:165:VAL:HG23	1.16	0.41
7:C:79:TRP:CZ2	7:C:154:ALA:N	2.88	0.41
7:C:132:ILE:HD11	7:C:171:ALA:HB2	2.01	0.41
7:D:125:ALA:O	7:D:126:ALA:C	2.63	0.41
7:D:246:LEU:HD21	7:D:326:PHE:HZ	1.86	0.41
4:L:23:DC:H5''	7:C:306:THR:OG1	2.21	0.41
6:F:11:DC:C5	6:F:12:DT:C7	3.02	0.41
7:A:220:LYS:O	7:A:223:ASP:HB2	2.20	0.41
7:B:77:HIS:N	7:B:80:LEU:HD12	2.30	0.41
7:B:198:TRP:O	7:B:199:LEU:C	2.64	0.41
7:D:35:PHE:O	7:D:37:LEU:HD23	2.20	0.41
7:D:41:ARG:HG2	7:D:45:ILE:HD13	2.02	0.41
7:D:305:PRO:HB3	7:D:309:GLU:HG2	2.00	0.41
5:E:4:DG:C6	5:E:5:DG:N7	2.89	0.41
6:F:17:DG:C5	6:F:18:DT:C4	3.08	0.41
6:F:19:DG:C2	6:F:20:DA:C5	3.08	0.41
6:H:17:DG:H5'	7:D:17:TYR:HE2	1.86	0.41
7:C:82:ARG:O	7:C:86:ILE:HD12	2.19	0.41
7:C:116:LEU:C	7:C:118:ASP:N	2.78	0.41
7:C:165:VAL:HG13	7:C:168:THR:HG21	2.03	0.41
7:C:308:HIS:O	7:C:311:ARG:N	2.46	0.41
7:D:125:ALA:O	7:D:128:LEU:N	2.54	0.41
7:A:84:GLU:O	7:A:87:LEU:HB2	2.20	0.41
7:B:23:TYR:CE2	7:B:24:TYR:O	2.73	0.41
7:B:254:SER:O	7:B:258:THR:OG1	2.36	0.41
7:C:39:ARG:HD3	7:C:39:ARG:HA	1.80	0.41
7:C:49:ILE:O	7:C:50:GLN:C	2.62	0.41
7:C:203:MSE:O	7:C:206:ALA:HB3	2.21	0.41
7:D:75:THR:HG23	7:D:78:SER:CB	2.39	0.41
1:I:18:DC:H5'	1:I:18:DC:C6	2.55	0.41
5:G:20:DA:H1'	5:G:21:DA:O5'	2.20	0.41
7:A:94:GLN:O	7:A:98:ILE:CD1	2.65	0.41
7:A:314:SER:O	7:A:318:TYR:HD2	2.04	0.41
7:C:28:ASP:OD2	7:C:29:PRO:HD2	2.20	0.41
7:D:62:LYS:C	7:D:64:LEU:N	2.76	0.41
7:D:79:TRP:O	7:D:83:TYR:N	2.44	0.41
7:D:163:ASN:OD1	7:D:163:ASN:C	2.63	0.41
7:D:190:GLN:O	7:D:193:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:209:THR:HG22	7:D:255:MSE:HE3	2.03	0.41
7:D:243:PRO:HG2	7:D:246:LEU:HD11	2.03	0.41
1:I:11:DT:H1'	7:A:235:LYS:HZ3	1.85	0.41
5:E:11:DA:N3	5:E:12:DT:C4	2.89	0.41
5:E:12:DT:H2'	5:E:13:DC:H6	1.86	0.41
5:G:17:DC:H6	5:G:17:DC:H2'	1.66	0.41
7:A:97:LEU:O	7:A:100:TYR:HB2	2.20	0.41
7:A:124:ILE:O	7:A:125:ALA:C	2.62	0.41
7:A:127:MSE:HE3	7:A:128:LEU:N	2.36	0.41
7:A:131:TYR:N	7:A:131:TYR:HD1	2.19	0.41
7:A:259:LEU:O	7:A:262:CYS:HB2	2.21	0.41
7:A:278:GLU:HB3	7:A:279:PRO:HD2	2.03	0.41
7:A:313:LEU:HA	7:A:316:ARG:NH2	2.36	0.41
7:B:15:ASN:ND2	7:B:52:ASN:ND2	2.68	0.41
7:B:163:ASN:OD1	7:B:165:VAL:HG23	2.20	0.41
7:B:188:ILE:O	7:B:189:TYR:C	2.62	0.41
7:C:137:ALA:O	7:C:138:ALA:C	2.63	0.41
5:G:12:DT:H2''	5:G:13:DC:C5'	2.45	0.41
7:A:92:ILE:HG22	7:A:93:LYS:N	2.33	0.41
7:A:101:MSE:HA	7:A:104:ILE:HD13	1.99	0.41
7:A:221:TRP:CZ3	7:A:263:LYS:HD2	2.56	0.41
7:B:53:ILE:HA	7:B:56:PHE:O	2.20	0.41
7:B:100:TYR:HD1	7:B:100:TYR:H	1.67	0.41
7:B:201:LEU:HD12	7:B:266:LEU:HD11	2.03	0.41
7:D:228:TYR:HE2	7:D:243:PRO:HB3	1.85	0.41
5:G:23:DA:N3	6:H:4:DA:C2	2.89	0.40
6:H:17:DG:C6	6:H:18:DT:C4	3.09	0.40
6:H:19:DG:C2'	6:H:20:DA:O5'	2.69	0.40
7:A:12:LEU:CD1	7:A:16:LEU:HD23	2.47	0.40
7:B:120:THR:CG2	7:B:122:LYS:HB3	2.49	0.40
7:D:74:VAL:HG13	7:D:75:THR:H	1.87	0.40
2:J:7:DA:C5	2:J:8:DG:N7	2.89	0.40
2:J:19:DA:H3'	7:A:96:THR:HG21	2.03	0.40
5:E:4:DG:H2''	5:E:5:DG:O5'	2.20	0.40
5:G:14:DA:H8	7:C:23:TYR:CD1	2.39	0.40
7:A:163:ASN:CG	7:A:166:ALA:H	2.29	0.40
7:B:25:CYS:HG	7:B:35:PHE:C	2.29	0.40
7:B:83:TYR:CD2	7:B:87:LEU:HD11	2.57	0.40
7:B:147:LEU:HD12	7:B:147:LEU:HA	1.85	0.40
7:B:205:LEU:HD12	7:B:205:LEU:HA	1.84	0.40
7:D:23:TYR:HD2	7:D:24:TYR:C	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:15:DT:C7	2:J:16:DT:H73	2.51	0.40
5:G:2:DC:C2'	5:G:3:DA:C8	3.03	0.40
7:A:74:VAL:O	7:A:75:THR:HB	2.22	0.40
7:C:211:GLN:HA	7:C:311:ARG:HH11	1.85	0.40
7:D:66:ALA:C	7:D:68:ILE:H	2.28	0.40
7:A:75:THR:HA	7:A:114:ALA:O	2.21	0.40
7:B:163:ASN:OD1	7:B:165:VAL:N	2.55	0.40
7:C:110:GLY:O	7:C:111:LEU:HD23	2.22	0.40
7:C:143:ILE:O	7:C:144:ARG:C	2.64	0.40
7:C:144:ARG:NH2	7:C:168:THR:O	2.55	0.40
7:D:313:LEU:HD13	7:D:316:ARG:HH22	1.85	0.40
7:D:349:GLU:N	7:D:349:GLU:OE2	2.54	0.40
1:I:8:DC:C2'	1:I:9:DT:H71	2.48	0.40
1:I:10:DT:N1	1:I:11:DT:H71	2.37	0.40
4:L:21:DA:OP2	7:C:93:LYS:HD3	2.22	0.40
5:E:11:DA:C2'	5:E:12:DT:H71	2.51	0.40
6:H:14:DA:H2'	6:H:15:DT:C7	2.51	0.40
7:B:307:PHE:C	7:B:309:GLU:N	2.79	0.40
7:C:62:LYS:HA	7:C:63:PRO:HD2	1.95	0.40
7:C:229:LEU:HD23	7:C:242:ILE:HB	2.04	0.40
7:D:221:TRP:NE1	7:D:271:ILE:HG12	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:29:DT:OP2	5:E:1:DA:O5'[1_565]	1.99	0.21

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	
7	A	347/356 (98%)	286 (82%)	45 (13%)	16 (5%)	2	17
7	B	332/356 (93%)	277 (83%)	42 (13%)	13 (4%)	2	18
7	C	347/356 (98%)	286 (82%)	44 (13%)	17 (5%)	1	16
7	D	332/356 (93%)	285 (86%)	33 (10%)	14 (4%)	2	17
All	All	1358/1424 (95%)	1134 (84%)	164 (12%)	60 (4%)	2	17

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	A	63	PRO
7	A	67	ARG
7	A	74	VAL
7	A	335	SER
7	A	348	ARG
7	B	60	LYS
7	B	61	HIS
7	B	67	ARG
7	B	350	TRP
7	C	57	SER
7	C	58	GLY
7	C	70	SER
7	C	74	VAL
7	C	351	ASP
7	D	59	HIS
7	D	67	ARG
7	D	68	ILE
7	D	70	SER
7	A	58	GLY
7	A	104	ILE
7	A	267	GLY
7	B	68	ILE
7	B	104	ILE
7	B	121	THR
7	B	267	GLY
7	C	45	ILE
7	C	67	ARG
7	C	267	GLY
7	C	341	GLN
7	D	104	ILE
7	D	137	ALA
7	D	267	GLY
7	D	355	ILE

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Mol	Chain	Res	Type
7	A	66	ALA
7	B	59	HIS
7	C	12	LEU
7	C	63	PRO
7	C	104	ILE
7	C	144	ARG
7	D	65	THR
7	D	71	ASP
7	D	121	THR
7	A	45	ILE
7	A	65	THR
7	A	137	ALA
7	A	144	ARG
7	A	339	ALA
7	B	137	ALA
7	C	121	THR
7	C	137	ALA
7	D	144	ARG
7	A	351	ASP
7	B	144	ARG
7	C	66	ALA
7	D	64	LEU
7	A	59	HIS
7	C	65	THR
7	D	114	ALA
7	B	91	GLY
7	B	114	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	A	292/292 (100%)	213 (73%)	79 (27%)	0	3
7	B	273/292 (94%)	196 (72%)	77 (28%)	0	3
7	C	293/292 (100%)	214 (73%)	79 (27%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	D	273/292 (94%)	195 (71%)	78 (29%)	0	3
All	All	1131/1168 (97%)	818 (72%)	313 (28%)	0	3

All (313) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	A	10	ARG
7	A	11	ASP
7	A	17	TYR
7	A	18	ILE
7	A	19	ARG
7	A	23	TYR
7	A	39	ARG
7	A	42	ARG
7	A	45	ILE
7	A	46	THR
7	A	49	ILE
7	A	53	ILE
7	A	54	GLU
7	A	55	LEU
7	A	57	SER
7	A	61	HIS
7	A	63	PRO
7	A	64	LEU
7	A	65	THR
7	A	68	ILE
7	A	70	SER
7	A	71	ASP
7	A	72	ASN
7	A	74	VAL
7	A	81	ASP
7	A	97	LEU
7	A	104	ILE
7	A	119	ILE
7	A	124	ILE
7	A	127	MSE
7	A	128	LEU
7	A	141	LYS
7	A	145	SER
7	A	146	THR
7	A	148	SER
7	A	155	ILE

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Mol	Chain	Res	Type
7	A	161	THR
7	A	165	VAL
7	A	169	ARG
7	A	172	LYS
7	A	173	SER
7	A	175	VAL
7	A	181	THR
7	A	185	TYR
7	A	186	LEU
7	A	187	LYS
7	A	195	SER
7	A	200	ARG
7	A	207	VAL
7	A	212	ARG
7	A	213	VAL
7	A	218	GLU
7	A	225	VAL
7	A	231	VAL
7	A	232	GLU
7	A	247	HIS
7	A	254	SER
7	A	258	THR
7	A	274	SER
7	A	275	THR
7	A	281	SER
7	A	284	THR
7	A	285	VAL
7	A	291	ARG
7	A	301	GLU
7	A	306	THR
7	A	309	GLU
7	A	314	SER
7	A	316	ARG
7	A	321	GLN
7	A	328	GLN
7	A	338	MSE
7	A	341	GLN
7	A	342	PHE
7	A	343	ARG
7	A	345	ASP
7	A	348	ARG
7	A	353	ILE

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Mol	Chain	Res	Type
7	A	354	GLU
7	B	12	LEU
7	B	15	ASN
7	B	18	ILE
7	B	30	ARG
7	B	31	THR
7	B	40	ASP
7	B	41	ARG
7	B	43	ILE
7	B	49	ILE
7	B	54	GLU
7	B	56	PHE
7	B	57	SER
7	B	61	HIS
7	B	73	SER
7	B	75	THR
7	B	78	SER
7	B	89	SER
7	B	90	ARG
7	B	92	ILE
7	B	108	ARG
7	B	116	LEU
7	B	117	GLU
7	B	122	LYS
7	B	127	MSE
7	B	128	LEU
7	B	139	SER
7	B	141	LYS
7	B	146	THR
7	B	155	ILE
7	B	160	ILE
7	B	161	THR
7	B	162	THR
7	B	164	HIS
7	B	175	VAL
7	B	176	ARG
7	B	181	THR
7	B	184	GLU
7	B	187	LYS
7	B	194	SER
7	B	203	MSE
7	B	207	VAL

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Mol	Chain	Res	Type
7	B	209	THR
7	B	212	ARG
7	B	213	VAL
7	B	215	ASP
7	B	224	ILE
7	B	231	VAL
7	B	232	GLU
7	B	235	LYS
7	B	249	ASP
7	B	255	MSE
7	B	257	GLU
7	B	263	LYS
7	B	265	ILE
7	B	276	ARG
7	B	277	ARG
7	B	280	LEU
7	B	282	SER
7	B	284	THR
7	B	286	SER
7	B	293	ARG
7	B	296	SER
7	B	299	SER
7	B	300	PHE
7	B	303	ASP
7	B	306	THR
7	B	311	ARG
7	B	312	SER
7	B	316	ARG
7	B	321	GLN
7	B	324	ASP
7	B	331	LEU
7	B	335	SER
7	B	336	ASP
7	B	350	TRP
7	B	354	GLU
7	B	355	ILE
7	C	11	ASP
7	C	12	LEU
7	C	15	ASN
7	C	18	ILE
7	C	19	ARG
7	C	20	ASN

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Mol	Chain	Res	Type
7	C	23	TYR
7	C	25	CYS
7	C	27	ARG
7	C	33	LYS
7	C	39	ARG
7	C	42	ARG
7	C	45	ILE
7	C	49	ILE
7	C	50	GLN
7	C	53	ILE
7	C	54	GLU
7	C	60	LYS
7	C	61	HIS
7	C	62	LYS
7	C	64	LEU
7	C	67	ARG
7	C	72	ASN
7	C	76	LEU
7	C	89	SER
7	C	93	LYS
7	C	94	GLN
7	C	102	SER
7	C	109	ARG
7	C	111	LEU
7	C	127	MSE
7	C	128	LEU
7	C	132	ILE
7	C	136	LYS
7	C	139	SER
7	C	141	LYS
7	C	144	ARG
7	C	152	ARG
7	C	161	THR
7	C	194	SER
7	C	195	SER
7	C	197	CYS
7	C	203	MSE
7	C	207	VAL
7	C	209	THR
7	C	212	ARG
7	C	218	GLU
7	C	225	VAL

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Mol	Chain	Res	Type
7	C	229	LEU
7	C	231	VAL
7	C	233	GLN
7	C	238	VAL
7	C	247	HIS
7	C	254	SER
7	C	257	GLU
7	C	259	LEU
7	C	269	GLU
7	C	270	THR
7	C	275	THR
7	C	278	GLU
7	C	280	LEU
7	C	284	THR
7	C	291	ARG
7	C	293	ARG
7	C	296	SER
7	C	300	PHE
7	C	306	THR
7	C	310	LEU
7	C	311	ARG
7	C	312	SER
7	C	319	GLU
7	C	321	GLN
7	C	331	LEU
7	C	335	SER
7	C	337	THR
7	C	338	MSE
7	C	342	PHE
7	C	346	ARG
7	C	348	ARG
7	D	11	ASP
7	D	15	ASN
7	D	18	ILE
7	D	19	ARG
7	D	20	ASN
7	D	30	ARG
7	D	31	THR
7	D	37	LEU
7	D	42	ARG
7	D	43	ILE
7	D	45	ILE

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Mol	Chain	Res	Type
7	D	46	THR
7	D	47	GLU
7	D	53	ILE
7	D	56	PHE
7	D	59	HIS
7	D	71	ASP
7	D	72	ASN
7	D	73	SER
7	D	76	LEU
7	D	80	LEU
7	D	82	ARG
7	D	90	ARG
7	D	92	ILE
7	D	93	LYS
7	D	102	SER
7	D	109	ARG
7	D	117	GLU
7	D	118	ASP
7	D	119	ILE
7	D	120	THR
7	D	127	MSE
7	D	128	LEU
7	D	139	SER
7	D	141	LYS
7	D	142	LEU
7	D	143	ILE
7	D	146	THR
7	D	160	ILE
7	D	161	THR
7	D	162	THR
7	D	169	ARG
7	D	175	VAL
7	D	181	THR
7	D	187	LYS
7	D	195	SER
7	D	208	VAL
7	D	216	LEU
7	D	217	CYS
7	D	220	LYS
7	D	231	VAL
7	D	235	LYS
7	D	248	ILE

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Mol	Chain	Res	Type
7	D	262	CYS
7	D	263	LYS
7	D	264	GLU
7	D	270	THR
7	D	271	ILE
7	D	274	SER
7	D	276	ARG
7	D	280	LEU
7	D	284	THR
7	D	285	VAL
7	D	293	ARG
7	D	296	SER
7	D	306	THR
7	D	309	GLU
7	D	312	SER
7	D	323	SER
7	D	324	ASP
7	D	325	LYS
7	D	329	HIS
7	D	331	LEU
7	D	349	GLU
7	D	350	TRP
7	D	351	ASP
7	D	355	ILE
7	D	356	LYS

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

Mol	Chain	Res	Type
7	A	15	ASN
7	A	20	ASN
7	A	50	GLN
7	A	72	ASN
7	A	99	ASN
7	B	15	ASN
7	B	20	ASN
7	B	21	ASN
7	B	99	ASN
7	B	129	ASN
7	B	308	HIS
7	B	333	HIS
7	C	20	ASN

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Mol	Chain	Res	Type
7	C	72	ASN
7	C	99	ASN
7	C	308	HIS
7	C	333	HIS
7	D	15	ASN
7	D	20	ASN
7	D	21	ASN
7	D	50	GLN
7	D	72	ASN
7	D	99	ASN
7	D	321	GLN
7	D	329	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 oligosaccharides 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.

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, 95th 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	I	29/29 (100%)	-0.03	0 100 100	108, 108, 108, 108	0
2	J	29/29 (100%)	0.07	0 100 100	108, 108, 108, 108	0
3	K	29/29 (100%)	0.11	0 100 100	108, 108, 108, 108	0
4	L	29/29 (100%)	-0.02	0 100 100	108, 108, 108, 108	0
5	E	24/25 (96%)	-0.22	0 100 100	108, 108, 108, 108	0
5	G	24/25 (96%)	-0.20	0 100 100	108, 108, 108, 108	0
6	F	25/25 (100%)	-0.26	0 100 100	108, 108, 108, 108	0
6	H	25/25 (100%)	-0.13	0 100 100	108, 108, 108, 108	0
7	A	342/356 (96%)	-0.05	4 (1%) 76 62	108, 108, 108, 200	0
7	B	330/356 (92%)	-0.04	9 (2%) 56 44	108, 108, 108, 108	0
7	C	342/356 (96%)	-0.05	7 (2%) 65 51	108, 108, 108, 200	0
7	D	330/356 (92%)	-0.26	2 (0%) 85 73	103, 108, 108, 108	0
All	All	1558/1640 (95%)	-0.10	22 (1%) 73 58	103, 108, 108, 200	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	B	231	VAL	5.1
7	C	209	THR	3.8
7	B	95	LYS	3.3
7	C	293	ARG	3.0
7	B	139	SER	2.8
7	C	17	TYR	2.5
7	C	18	ILE	2.5
7	B	180	LEU	2.5
7	A	20	ASN	2.4
7	D	79	TRP	2.3
7	B	282	SER	2.3

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Mol	Chain	Res	Type	RSRZ
7	C	78	SER	2.2
7	A	95	LYS	2.2
7	B	229	LEU	2.2
7	D	330	LEU	2.2
7	C	37	LEU	2.2
7	B	79	TRP	2.1
7	B	143	ILE	2.1
7	A	100	TYR	2.0
7	A	159	HIS	2.0
7	C	153	GLU	2.0
7	B	116	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.