



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:55 PM UTC

PDB ID : 6LA8 / pdb_00006la8
Title : 349 bp di-nucleosome harboring cohesive DNA termini assembled with linker histone H1.0
Authors : Adhireksan, Z.; Lee, P.L.; Sharma, D.; Davey, C.A.
Deposited on : 2019-11-12
Resolution : 3.40 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
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

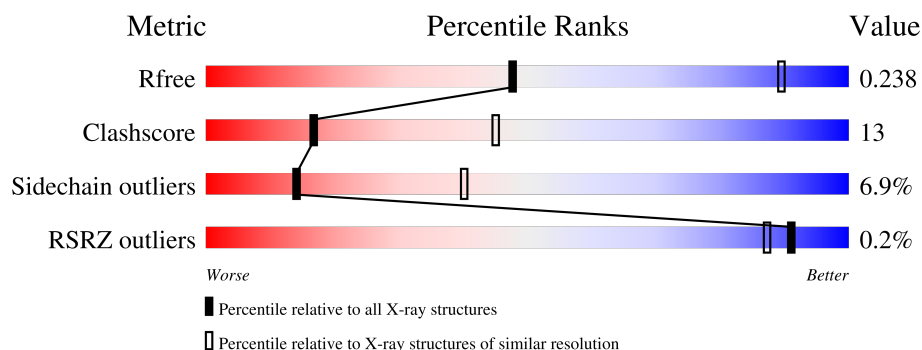
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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.



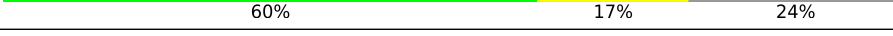
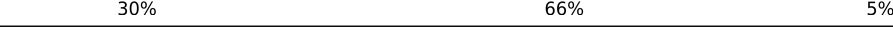
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	A	136	57% 16% 26%
1	E	136	57% 16% 27%
1	K	136	58% 15% 27%
1	O	136	60% 12% 28%
2	B	103	63% 16% 21%
2	F	103	66% 14% 20%

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Mol	Chain	Length	Quality of chain
2	L	103	
2	P	103	
3	C	130	
3	G	130	
3	M	130	
3	Q	130	
4	D	126	
4	H	126	
4	N	126	
4	R	126	
5	I	349	
6	J	349	
7	S	194	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 27058 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	100	Total	C	N	O	S	0	0	0
			825	520	160	141	4			
1	E	99	Total	C	N	O	S	0	0	0
			816	514	158	140	4			
1	K	99	Total	C	N	O	S	0	0	0
			816	514	158	140	4			
1	O	98	Total	C	N	O	S	0	0	0
			807	508	156	139	4			

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	81	Total	C	N	O	S	0	0	0
			646	407	126	112	1			
2	F	82	Total	C	N	O	S	0	0	0
			653	412	127	113	1			
2	L	80	Total	C	N	O	S	0	0	0
			638	401	125	111	1			
2	P	80	Total	C	N	O	S	0	0	0
			638	401	125	111	1			

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	110	Total	C	N	O	0	0	0
			849	535	168	146			
3	G	105	Total	C	N	O	0	0	0
			810	511	158	141			
3	M	106	Total	C	N	O	0	0	0
			819	517	160	142			
3	Q	105	Total	C	N	O	0	0	0
			812	512	158	142			

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	H	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	N	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			
4	R	96	Total	C	N	O	S	0	0	0
			755	474	138	141	2			

- Molecule 5 is a DNA chain called DNA (349-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	349	Total	C	N	O	P	0	0	0
			7149	3389	1357	2054	349			

- Molecule 6 is a DNA chain called DNA (349-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	349	Total	C	N	O	P	0	0	0
			7162	3407	1270	2136	349			

- Molecule 7 is a protein called Histone H1.0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	S	74	Total	C	N	O	S	0	0	0
			568	354	107	106	1			

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	1	Total	Ca	0	0
			1	1		
8	I	11	Total	Ca	0	0
			11	11		
8	J	10	Total	Ca	0	0
			10	10		
8	M	1	Total	Ca	0	0
			1	1		

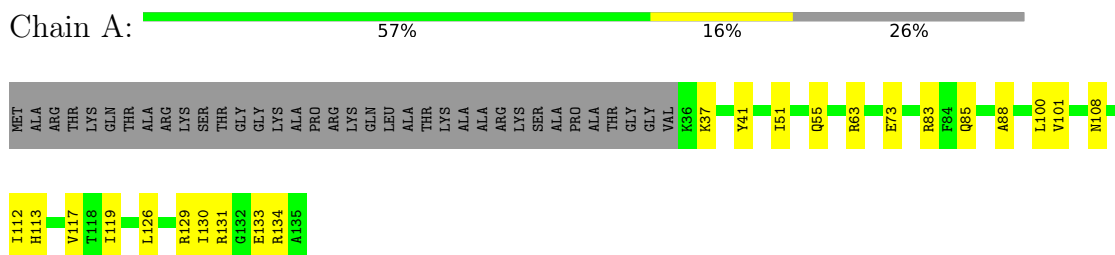
- Molecule 9 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	I	2	Total 2	K 2	0	0
9	J	5	Total 5	K 5	0	0

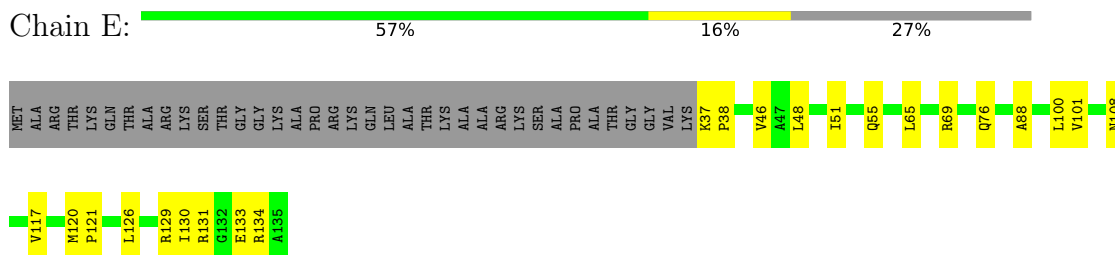
3 Residue-property plots [i](#)

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

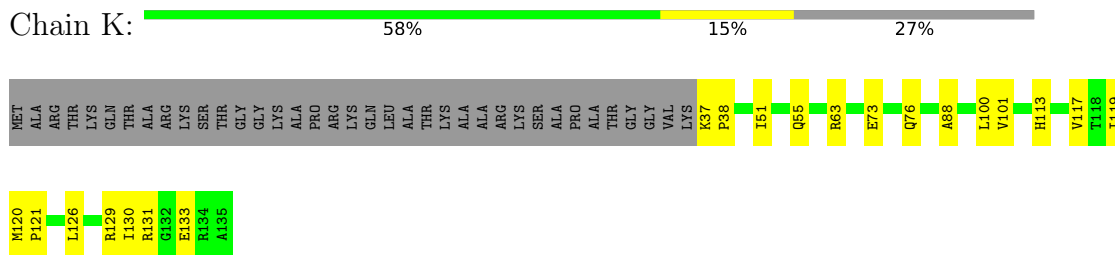
- Molecule 1: Histone H3.1



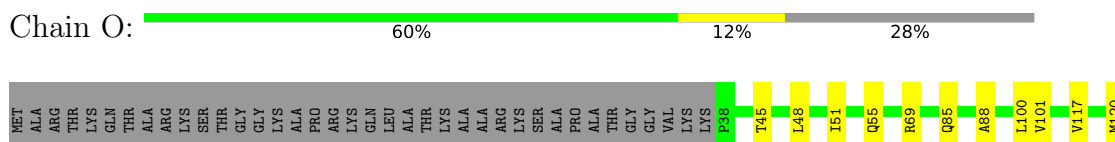
- Molecule 1: Histone H3.1

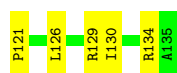


- Molecule 1: Histone H3.1



- Molecule 1: Histone H3.1





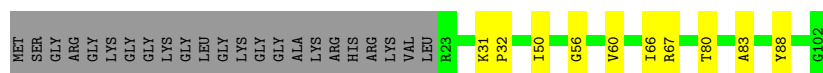
- Molecule 2: Histone H4



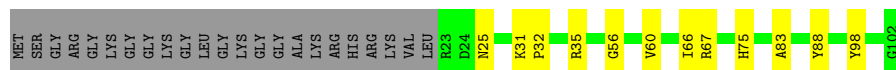
- Molecule 2: Histone H4



- Molecule 2: Histone H4



- Molecule 2: Histone H4



- Molecule 3: Histone H2A type 1-B/E

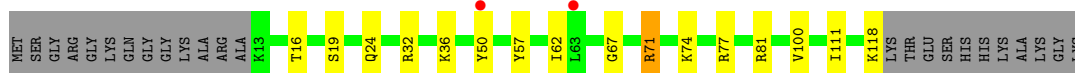


- Molecule 3: Histone H2A type 1-B/E



- Molecule 3: Histone H2A type 1-B/E

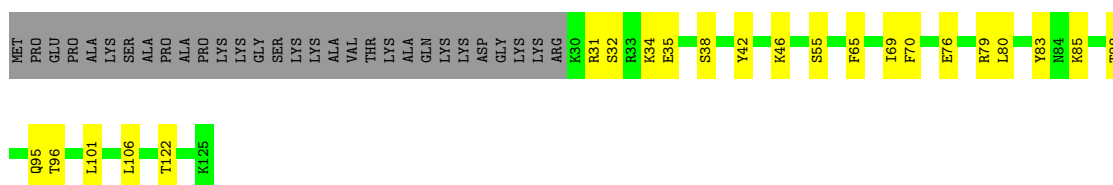




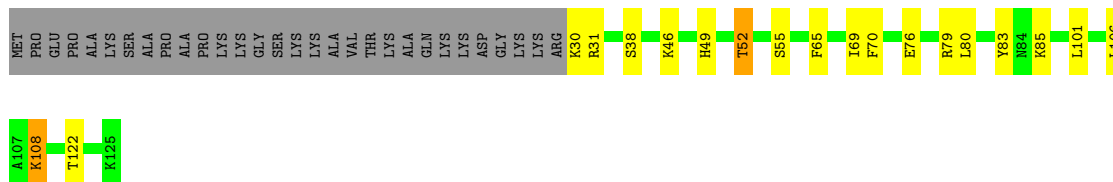
- Molecule 3: Histone H2A type 1-B/E



- Molecule 4: Histone H2B type 1-J



- Molecule 4: Histone H2B type 1-J



- Molecule 4: Histone H2B type 1-J



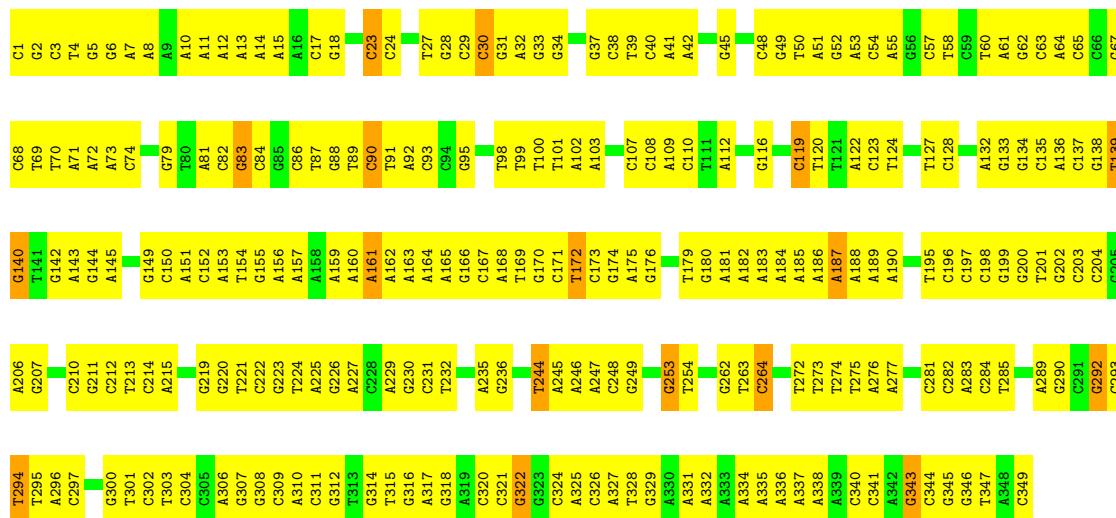
- Molecule 4: Histone H2B type 1-J





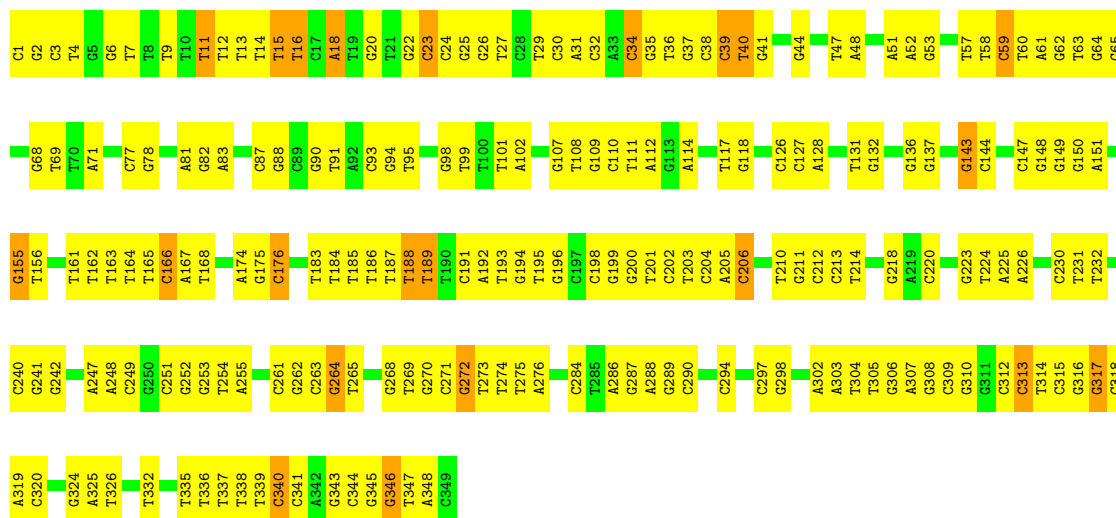
• Molecule 5: DNA (349-MER)

Chain I: 30% 66% 5%



• Molecule 6: DNA (349-MER)

Chain J: 40% 53% 6%



• Molecule 7: Histone H1.0

Chain S: 23% 11% 62%



LYS	T64
LYS	V87
LEU	G58
ALA	
ALA	
THR	P93
PRO	R94
LYS	L95
LYS	A96
ALA	K97
ALA	SER
LYS	ASP
PRO	GLU
LYS	PRO
THR	LYS
VAL	LYS
LYS	SER
ALA	VAL
LYS	ALA
PRO	PHE
VAL	LYS
LYS	LYS
ALA	THR
SER	LYS
LYS	LYS
PRO	GLU
LYS	ILE
LYS	LYS
ALA	LYS
LYS	VAL
PRO	VAL
VAL	THR
LYS	PRO
PRO	LYS
LYS	LYS
ALA	LYS
LYS	ALA
LYS	SER
SER	LYS
LYS	PRO
LYS	LYS
ALA	LYS
ARG	LYS
ALA	ALA
GLY	SER
LYS	LYS
LYS	ALA
LYS	PRO
	THR
	LYS
	PRO
	VAL
	LYS
	LYS
	ALA
	THR
	PRO
	VAL
	LYS
	LYS
	ALA
	LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.06Å 184.07Å 223.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 3.40 49.32 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.32-3.40) 99.7 (49.32-3.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.206 , 0.265 (Not available) , 0.238	Depositor DCC
R_{free} test set	1381 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	126.8	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 90.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	27058	wwPDB-VP
Average B, all atoms (Å ²)	160.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.07% 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

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.97	0/837	1.54	1/1120 (0.1%)
1	E	0.95	0/828	1.54	1/1109 (0.1%)
1	K	0.95	0/828	1.53	1/1109 (0.1%)
1	O	0.96	0/819	1.55	1/1097 (0.1%)
2	B	0.95	0/653	1.53	2/873 (0.2%)
2	F	0.96	0/660	1.54	3/883 (0.3%)
2	L	0.95	0/645	1.52	0/862
2	P	0.96	0/645	1.54	0/862
3	C	0.99	0/859	1.52	2/1157 (0.2%)
3	G	0.95	0/820	1.50	0/1107
3	M	0.97	0/829	1.49	0/1118
3	Q	0.96	0/822	1.51	0/1110
4	D	0.99	0/766	1.51	0/1026
4	H	0.99	0/766	1.53	0/1026
4	N	0.99	0/766	1.52	0/1026
4	R	0.98	0/766	1.51	0/1026
5	I	0.48	1/8032 (0.0%)	0.87	23/12384 (0.2%)
6	J	0.45	0/8022	0.91	31/12387 (0.3%)
7	S	1.11	0/574	1.64	0/765
All	All	0.74	1/28937 (0.0%)	1.19	65/42047 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	306	DA	O3'-P	-6.03	1.52	1.61

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	23	DC	C2'-C3'-O3'	-8.71	98.43	111.50
6	J	22	DG	C2'-C3'-O3'	-8.71	98.43	111.50
5	I	90	DC	C2'-C3'-O3'	7.85	123.28	111.50
6	J	143	DG	C2'-C3'-O3'	7.44	122.67	111.50
6	J	15	DT	C2'-C3'-O3'	7.44	122.66	111.50
6	J	313	DC	C2'-C3'-O3'	7.21	122.31	111.50
6	J	340	DC	C2'-C3'-O3'	7.15	122.22	111.50
5	I	23	DC	C2'-C3'-O3'	6.69	121.54	111.50
6	J	255	DA	C2'-C3'-O3'	-6.60	101.60	111.50
6	J	346	DG	C4'-C3'-O3'	-6.60	100.11	110.00
6	J	317	DG	C2'-C3'-O3'	6.56	121.35	111.50
6	J	63	DT	C2'-C3'-O3'	6.52	121.28	111.50
5	I	292	DG	C2'-C3'-O3'	6.47	121.21	111.50
6	J	346	DG	N9-C1'-C2'	6.41	123.12	113.50
5	I	187	DA	C2'-C3'-O3'	6.36	121.04	111.50
5	I	140	DG	C4'-C3'-O3'	6.14	119.22	110.00
6	J	220	DC	C2'-C3'-O3'	6.11	120.67	111.50
2	F	101	GLY	CA-C-O	-6.07	118.08	122.45
1	A	117	VAL	N-CA-C	-6.04	107.97	113.71
1	O	117	VAL	N-CA-C	-6.00	108.01	113.71
6	J	155	DG	C4'-C3'-O3'	5.86	118.78	110.00
6	J	16	DT	N1-C1'-C2'	5.85	122.27	113.50
5	I	161	DA	C2'-C3'-O3'	-5.79	102.81	111.50
5	I	172	DT	C2'-C3'-O3'	-5.74	102.89	111.50
6	J	206	DC	C4'-C3'-O3'	-5.72	101.42	110.00
3	C	15	LYS	CA-C-N	5.70	128.80	120.71
3	C	15	LYS	C-N-CA	5.70	128.80	120.71
5	I	139	DT	C2'-C3'-O3'	5.67	120.01	111.50
5	I	343	DG	C2'-C3'-O3'	5.64	119.95	111.50
6	J	34	DC	C2'-C3'-O3'	5.61	119.91	111.50
5	I	119	DC	C2'-C3'-O3'	-5.60	103.10	111.50
5	I	244	DT	C2'-C3'-O3'	5.60	119.89	111.50
1	E	117	VAL	N-CA-C	-5.59	108.40	113.71
1	K	117	VAL	N-CA-C	-5.58	108.41	113.71
6	J	189	DT	C4'-C3'-O3'	-5.56	101.66	110.00
6	J	40	DT	C2'-C3'-O3'	5.55	119.82	111.50
5	I	79	DG	C2'-C3'-O3'	-5.50	103.25	111.50
5	I	300	DG	C2'-C3'-O3'	-5.48	103.28	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	264	DG	C2'-C3'-O3'	5.43	119.64	111.50
6	J	18	DA	C2'-C3'-O3'	5.42	119.63	111.50
5	I	253	DG	C2'-C3'-O3'	-5.41	103.38	111.50
6	J	176	DC	C4'-C3'-O3'	5.41	118.11	110.00
5	I	30	DC	C2'-C3'-O3'	5.38	119.58	111.50
5	I	322	DG	C2'-C3'-O3'	-5.38	103.42	111.50
5	I	294	DT	C2'-C3'-O3'	-5.35	103.47	111.50
6	J	59	DC	C2'-C3'-O3'	-5.31	103.53	111.50
6	J	284	DC	C2'-C3'-O3'	5.31	119.46	111.50
6	J	294	DC	N1-C1'-C2'	5.31	121.46	113.50
6	J	4	DT	C2'-C3'-O3'	5.30	119.46	111.50
5	I	84	DC	C2'-C3'-O3'	-5.30	103.55	111.50
5	I	32	DA	C2'-C3'-O3'	5.28	119.42	111.50
2	B	29	ILE	CA-C-N	5.21	128.62	120.75
2	B	29	ILE	C-N-CA	5.21	128.62	120.75
6	J	188	DT	C4'-C3'-O3'	5.18	117.77	110.00
6	J	39	DC	C2'-C3'-O3'	5.17	119.26	111.50
5	I	264	DC	C2'-C3'-O3'	5.15	119.23	111.50
6	J	166	DC	C2'-C3'-O3'	5.15	119.22	111.50
5	I	83	DG	C4'-C3'-O3'	-5.10	102.35	110.00
6	J	11	DT	C2'-C3'-O3'	5.08	119.13	111.50
2	F	29	ILE	CA-C-N	5.06	128.38	120.75
2	F	29	ILE	C-N-CA	5.06	128.38	120.75
6	J	272	DG	N9-C1'-C2'	5.02	121.03	113.50
6	J	143	DG	N9-C1'-C2'	5.02	121.03	113.50
5	I	307	DG	C4'-C3'-O3'	-5.01	102.48	110.00
5	I	169	DT	C2'-C3'-O3'	5.01	119.01	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	14	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	825	0	869	19	0
1	E	816	0	856	15	0
1	K	816	0	856	12	0
1	O	807	0	844	10	0
2	B	646	0	687	16	0
2	F	653	0	696	7	0
2	L	638	0	676	8	0
2	P	638	0	676	9	0
3	C	849	0	915	5	0
3	G	810	0	866	7	0
3	M	819	0	879	11	0
3	Q	812	0	868	4	0
4	D	755	0	784	14	0
4	H	755	0	784	16	0
4	N	755	0	784	14	0
4	R	755	0	784	15	0
5	I	7149	0	3902	245	1
6	J	7162	0	3943	243	1
7	S	568	0	597	22	1
8	G	1	0	0	0	0
8	I	11	0	0	0	0
8	J	10	0	0	0	0
8	M	1	0	0	0	0
9	I	2	0	0	0	0
9	J	5	0	0	0	0
All	All	27058	0	21266	610	2

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

All (610) 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)
6:J:318:DC:H2''	6:J:319:DA:C8	1.60	1.35
5:I:346:DG:H2''	5:I:347:DT:OP2	1.41	1.14
5:I:153:DA:H2''	5:I:154:DT:OP2	1.51	1.08
4:H:49:HIS:HB3	4:H:52:THR:CG2	1.85	1.05
6:J:35:DG:H2'	6:J:36:DT:H72	1.34	1.04
6:J:202:DC:H2''	6:J:203:DT:OP2	1.58	1.02
4:R:49:HIS:HB3	4:R:52:THR:CG2	1.89	1.02
6:J:253:DG:H2''	6:J:254:DT:H72	1.38	1.02
6:J:345:DG:H4'	6:J:346:DG:OP1	1.59	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:73:GLU:O	1:K:76:GLN:HG2	1.61	1.00
5:I:262:DG:H2''	5:I:263:DT:OP2	1.64	0.95
6:J:318:DC:H2''	6:J:319:DA:N7	1.84	0.93
5:I:119:DC:H2''	5:I:120:DT:OP2	1.69	0.92
5:I:171:DC:H2''	5:I:172:DT:O5'	1.70	0.91
6:J:15:DT:H2'	6:J:16:DT:C6	2.05	0.91
5:I:230:DG:H2''	5:I:231:DC:OP2	1.68	0.91
6:J:23:DC:H2''	6:J:24:DC:OP2	1.72	0.90
6:J:162:DT:H2''	6:J:163:DT:C5'	2.02	0.89
6:J:346:DG:H4'	6:J:347:DT:OP1	1.69	0.89
4:H:49:HIS:HB3	4:H:52:THR:HG23	1.53	0.88
6:J:24:DC:H2''	6:J:25:DG:O5'	1.74	0.88
6:J:162:DT:H2''	6:J:163:DT:H5'	1.55	0.88
5:I:340:DC:H2''	5:I:341:DC:OP2	1.74	0.88
5:I:134:DG:H2''	5:I:135:DC:C6	2.09	0.88
6:J:193:DT:H2'	6:J:194:DG:C8	2.10	0.87
6:J:15:DT:H2''	6:J:16:DT:O5'	1.73	0.86
5:I:154:DT:H2''	5:I:155:DG:OP2	1.76	0.85
6:J:198:DC:H2''	6:J:199:DG:C8	2.11	0.85
5:I:303:DT:H2''	5:I:304:DC:OP2	1.76	0.85
4:R:49:HIS:HB3	4:R:52:THR:HG23	1.58	0.85
6:J:35:DG:H2'	6:J:36:DT:C7	2.06	0.84
6:J:339:DT:H4'	6:J:340:DC:OP1	1.76	0.84
6:J:253:DG:H2''	6:J:254:DT:C7	2.09	0.83
6:J:345:DG:C4'	6:J:346:DG:OP1	2.27	0.82
3:G:71:ARG:HH21	4:H:52:THR:HG22	1.43	0.82
5:I:28:DG:H2''	5:I:29:DC:OP2	1.77	0.82
6:J:15:DT:H2''	6:J:16:DT:C5'	2.10	0.81
6:J:163:DT:H2''	6:J:164:DT:O5'	1.80	0.81
6:J:24:DC:H2'	6:J:25:DG:C8	2.17	0.80
7:S:47:ARG:NH2	7:S:48:GLN:OE1	2.15	0.80
5:I:112:DA:H8	5:I:112:DA:P	2.03	0.80
5:I:175:DA:H2''	5:I:176:DG:OP2	1.82	0.79
6:J:192:DA:H2''	6:J:193:DT:O4'	1.84	0.78
6:J:162:DT:C2'	6:J:163:DT:H5'	2.14	0.78
6:J:175:DG:OP2	6:J:175:DG:H2'	1.83	0.77
5:I:346:DG:C2'	5:I:347:DT:OP2	2.29	0.77
7:S:36:ILE:HD11	7:S:95:LEU:HD11	1.67	0.76
5:I:165:DA:H2''	5:I:166:DG:OP2	1.84	0.76
1:E:76:GLN:HE22	2:F:21:VAL:HG12	1.50	0.76
6:J:14:DT:H2''	6:J:15:DT:OP2	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:340:DC:H2''	6:J:341:DC:OP2	1.87	0.75
6:J:264:DG:H2''	6:J:265:DT:OP2	1.84	0.75
6:J:313:DC:H2''	6:J:314:DT:OP2	1.85	0.75
6:J:347:DT:H4'	6:J:348:DA:OP1	1.87	0.74
5:I:37:DG:H2''	5:I:38:DC:OP2	1.87	0.74
5:I:134:DG:H2''	5:I:135:DC:H6	1.52	0.74
5:I:48:DC:H2''	5:I:49:DG:OP2	1.88	0.74
6:J:188:DT:H1'	6:J:189:DT:H5'	1.70	0.73
6:J:318:DC:C2'	6:J:319:DA:C8	2.56	0.73
6:J:52:DA:H1'	6:J:53:DG:C8	2.24	0.73
5:I:68:DC:C2'	5:I:69:DT:H5'	2.19	0.72
5:I:6:DG:H2''	5:I:7:DA:O5'	1.89	0.72
5:I:132:DA:N6	6:J:214:DT:O4	2.20	0.72
6:J:211:DG:H2''	6:J:212:DC:OP2	1.90	0.72
3:M:50:TYR:OH	4:N:95:GLN:NE2	2.22	0.72
6:J:15:DT:C2'	6:J:16:DT:C6	2.74	0.71
5:I:101:DT:H2''	5:I:102:DA:C8	2.26	0.71
7:S:43:ALA:O	7:S:84:THR:HG21	1.90	0.70
5:I:344:DC:H2''	5:I:345:DG:O4'	1.90	0.70
5:I:244:DT:H2''	5:I:245:DA:OP2	1.89	0.70
3:M:32:ARG:NH1	4:N:35:GLU:OE2	2.24	0.70
6:J:38:DC:H2''	6:J:39:DC:OP2	1.90	0.70
7:S:28:TYR:O	7:S:32:ILE:HG12	1.92	0.70
4:H:108:LYS:HA	4:H:108:LYS:HE2	1.74	0.70
5:I:309:DC:H2'	5:I:310:DA:C8	2.27	0.69
5:I:253:DG:H2''	5:I:254:DT:H72	1.74	0.69
6:J:253:DG:C2'	6:J:254:DT:H72	2.17	0.69
4:D:42:TYR:OH	5:I:33:DG:OP2	2.07	0.69
5:I:273:DT:H2''	5:I:274:DT:OP2	1.91	0.69
5:I:311:DC:H2''	5:I:312:DG:OP2	1.91	0.69
5:I:3:DC:H2''	5:I:4:DT:OP2	1.93	0.69
5:I:321:DC:H2''	5:I:322:DG:C8	2.28	0.69
5:I:30:DC:H2''	5:I:31:DG:OP2	1.93	0.68
5:I:226:DG:H1'	5:I:227:DA:C8	2.28	0.68
5:I:343:DG:H2''	5:I:344:DC:OP2	1.92	0.68
5:I:11:DA:H1'	5:I:12:DA:O5'	1.94	0.68
5:I:139:DT:H2''	5:I:140:DG:OP2	1.93	0.68
6:J:251:DC:H2''	6:J:252:DG:O5'	1.93	0.68
1:A:119:ILE:HG13	2:B:50:ILE:HD12	1.76	0.68
6:J:15:DT:H2'	6:J:16:DT:H6	1.55	0.68
6:J:318:DC:C2'	6:J:319:DA:N7	2.55	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:289:DA:H2''	5:I:290:DG:OP2	1.94	0.67
7:S:50:ILE:O	7:S:54:ILE:HG13	1.94	0.67
5:I:155:DG:OP2	5:I:155:DG:H8	1.77	0.67
5:I:164:DA:H2''	5:I:165:DA:OP2	1.92	0.67
6:J:186:DT:H2''	6:J:187:DT:OP2	1.92	0.67
5:I:292:DG:H2''	5:I:293:DC:OP2	1.94	0.67
5:I:13:DA:C8	5:I:13:DA:H5''	2.30	0.66
5:I:14:DA:C2'	5:I:15:DA:O5'	2.43	0.66
6:J:156:DT:OP1	1:O:45:THR:HG21	1.95	0.66
6:J:198:DC:H1'	6:J:199:DG:C8	2.30	0.66
5:I:207:DG:OP2	4:N:42:TYR:OH	2.14	0.66
1:E:37:LYS:NZ	6:J:332:DT:OP1	2.29	0.65
5:I:68:DC:H2''	5:I:69:DT:H5'	1.77	0.65
6:J:269:DT:H1'	6:J:270:DG:H5'	1.77	0.65
5:I:1:DC:H2''	5:I:2:DG:OP2	1.94	0.65
5:I:119:DC:C2'	5:I:120:DT:OP2	2.45	0.65
6:J:90:DG:H2''	6:J:91:DT:OP2	1.96	0.65
6:J:204:DC:H2''	6:J:205:DA:OP2	1.96	0.64
5:I:294:DT:H4'	5:I:295:DT:OP1	1.97	0.64
6:J:143:DG:H8	6:J:143:DG:OP2	1.81	0.64
5:I:29:DC:H2''	5:I:30:DC:OP2	1.96	0.64
5:I:2:DG:OP2	5:I:2:DG:H8	1.81	0.64
6:J:37:DG:H2''	6:J:38:DC:OP2	1.99	0.63
6:J:335:DT:H2''	6:J:336:DT:C5	2.33	0.63
6:J:188:DT:H4'	6:J:189:DT:OP1	1.99	0.63
5:I:134:DG:H2''	5:I:135:DC:C5	2.34	0.62
6:J:335:DT:H2''	6:J:336:DT:C6	2.33	0.62
4:H:49:HIS:CB	4:H:52:THR:HG23	2.28	0.62
5:I:174:DG:OP2	5:I:174:DG:H2'	1.98	0.62
6:J:175:DG:H4'	6:J:176:DC:OP1	1.99	0.62
6:J:344:DC:H2''	6:J:345:DG:O5'	1.98	0.62
1:A:73:GLU:CD	2:B:22:LEU:HB2	2.25	0.62
5:I:272:DT:H2''	5:I:273:DT:OP2	1.98	0.62
5:I:274:DT:H2''	5:I:275:DT:OP2	2.00	0.62
5:I:334:DA:H2''	5:I:335:DA:OP2	1.99	0.62
6:J:188:DT:H1'	6:J:189:DT:C5'	2.29	0.62
3:C:32:ARG:NH1	4:D:35:GLU:OE2	2.32	0.61
5:I:127:DT:H2''	5:I:128:DC:C6	2.35	0.61
5:I:6:DG:C2'	5:I:7:DA:O5'	2.49	0.61
6:J:198:DC:C2'	6:J:199:DG:C8	2.83	0.61
3:G:15:LYS:HB2	6:J:218:DG:OP1	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:318:DC:H2''	6:J:319:DA:H8	1.54	0.61
7:S:87:VAL:HG22	7:S:88:GLY:H	1.64	0.61
5:I:153:DA:C2'	5:I:154:DT:OP2	2.30	0.61
4:H:108:LYS:HA	4:H:108:LYS:CE	2.31	0.61
6:J:183:DT:H4'	6:J:184:DT:OP1	2.00	0.61
6:J:98:DG:H2''	6:J:99:DT:OP2	2.00	0.60
6:J:223:DG:H1'	6:J:224:DT:H5'	1.83	0.60
6:J:347:DT:C4'	6:J:348:DA:OP1	2.49	0.60
6:J:191:DC:H2''	6:J:192:DA:O4'	2.01	0.60
6:J:253:DG:H2''	6:J:254:DT:OP2	2.01	0.60
6:J:24:DC:C2'	6:J:25:DG:C8	2.84	0.60
5:I:69:DT:H2''	5:I:70:DT:OP2	2.00	0.60
5:I:99:DT:H2''	5:I:100:DT:OP2	2.02	0.60
6:J:127:DC:H2''	6:J:128:DA:C8	2.37	0.60
6:J:6:DG:C8	6:J:7:DT:H72	2.37	0.60
5:I:276:DA:H1'	5:I:277:DA:C8	2.36	0.60
6:J:94:DG:H2''	6:J:95:DT:H5'	1.83	0.60
6:J:316:DG:H1'	6:J:317:DG:C5	2.37	0.60
1:A:108:ASN:HD21	3:G:115:LEU:HD11	1.66	0.60
5:I:156:DA:H2''	5:I:157:DA:OP2	2.02	0.60
5:I:149:DG:H2''	5:I:150:DC:OP2	2.02	0.59
6:J:202:DC:C2'	6:J:203:DT:OP2	2.37	0.59
7:S:95:LEU:N	7:S:95:LEU:HD22	2.17	0.59
5:I:13:DA:C8	5:I:13:DA:C5'	2.86	0.59
5:I:301:DT:H2''	5:I:302:DC:OP2	2.02	0.59
6:J:25:DG:H2''	6:J:26:DG:OP2	2.03	0.59
5:I:296:DA:H1'	5:I:297:DC:H5'	1.83	0.59
5:I:13:DA:C5'	5:I:13:DA:H8	2.15	0.59
5:I:248:DC:H1'	5:I:249:DG:H5'	1.85	0.58
6:J:194:DG:H2''	6:J:195:DT:H5'	1.84	0.58
6:J:187:DT:H2''	6:J:188:DT:OP2	2.02	0.58
5:I:52:DG:H1'	5:I:53:DA:C8	2.38	0.58
6:J:199:DG:C2'	6:J:200:DG:O5'	2.51	0.58
5:I:41:DA:H2''	5:I:42:DA:C8	2.39	0.58
1:K:37:LYS:HB3	1:K:38:PRO:HD2	1.85	0.58
5:I:281:DC:H2'	5:I:282:DC:C6	2.39	0.58
6:J:315:DC:OP2	6:J:315:DC:H6	1.87	0.58
5:I:180:DG:H2''	5:I:181:DA:OP2	2.03	0.58
4:R:49:HIS:CB	4:R:52:THR:HG23	2.32	0.58
1:E:69:ARG:NH2	5:I:103:DA:OP2	2.37	0.58
5:I:221:DT:H2''	5:I:222:DC:OP2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:230:DG:C2'	5:I:231:DC:OP2	2.46	0.58
6:J:241:DG:OP2	6:J:241:DG:H2'	2.04	0.57
5:I:308:DG:H2''	5:I:309:DC:C6	2.39	0.57
6:J:30:DC:H2''	6:J:31:DA:OP2	2.04	0.57
5:I:11:DA:H2''	5:I:12:DA:OP2	2.04	0.57
6:J:162:DT:H2''	6:J:163:DT:O4'	2.03	0.57
6:J:340:DC:C2'	6:J:341:DC:OP2	2.53	0.57
1:E:37:LYS:CG	1:E:38:PRO:HD2	2.34	0.57
1:A:119:ILE:HD12	2:B:50:ILE:HD13	1.87	0.57
6:J:1:DC:H2'	6:J:2:DG:C8	2.39	0.57
6:J:347:DT:H1'	6:J:348:DA:C8	2.39	0.57
5:I:235:DA:H1'	5:I:236:DG:C8	2.40	0.57
5:I:1:DC:H2''	5:I:2:DG:C8	2.40	0.56
6:J:198:DC:H2''	6:J:199:DG:N7	2.20	0.56
5:I:174:DG:H2'	5:I:174:DG:P	2.45	0.56
5:I:329:DG:C2	6:J:18:DA:C2	2.92	0.56
7:S:32:ILE:HD11	7:S:68:ILE:HG23	1.87	0.56
5:I:14:DA:H2''	5:I:15:DA:O5'	2.03	0.56
5:I:137:DC:H2''	5:I:138:DG:OP2	2.04	0.56
6:J:268:DG:H2''	6:J:269:DT:H5'	1.87	0.56
6:J:12:DT:H2''	6:J:13:DT:OP2	2.04	0.56
6:J:15:DT:H2''	6:J:16:DT:H5'	1.87	0.56
6:J:317:DG:H2''	6:J:318:DC:O4'	2.05	0.56
6:J:230:DC:H2''	6:J:231:DT:OP2	2.06	0.56
3:Q:42:ARG:O	4:R:88:THR:HA	2.06	0.56
3:Q:71:ARG:HH21	4:R:52:THR:HG22	1.71	0.56
1:A:119:ILE:HG13	2:B:50:ILE:CD1	2.36	0.56
6:J:114:DA:OP1	2:L:80:THR:OG1	2.21	0.56
6:J:117:DT:H2'	6:J:118:DG:C8	2.41	0.55
6:J:264:DG:C2'	6:J:265:DT:OP2	2.54	0.55
6:J:241:DG:H1'	6:J:242:DG:C8	2.41	0.55
6:J:15:DT:H2'	6:J:16:DT:H71	1.88	0.55
6:J:131:DT:H2''	6:J:132:DG:N7	2.21	0.55
5:I:244:DT:C2'	5:I:245:DA:OP2	2.55	0.55
5:I:263:DT:H2''	5:I:264:DC:OP2	2.07	0.55
6:J:275:DT:H2''	6:J:276:DA:C8	2.42	0.55
5:I:112:DA:P	5:I:112:DA:C8	2.94	0.55
7:S:32:ILE:HG23	7:S:50:ILE:HD12	1.88	0.55
6:J:193:DT:H2'	6:J:194:DG:N9	2.21	0.55
6:J:240:DC:H2''	6:J:241:DG:OP2	2.07	0.55
5:I:225:DA:H1'	5:I:226:DG:H5'	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:37:LYS:HB3	1:K:38:PRO:CD	2.37	0.54
7:S:36:ILE:CD1	7:S:95:LEU:HD11	2.37	0.54
5:I:253:DG:H2''	5:I:254:DT:C7	2.37	0.54
5:I:327:DA:N3	6:J:20:DG:N2	2.55	0.54
4:D:65:PHE:CE1	4:D:69:ILE:CD1	2.90	0.54
1:E:46:VAL:HB	5:I:95:DG:OP1	2.07	0.54
5:I:41:DA:C2	6:J:306:DG:N2	2.76	0.54
5:I:28:DG:C2'	5:I:29:DC:OP2	2.52	0.54
5:I:247:DA:H1'	5:I:248:DC:H5'	1.88	0.54
6:J:198:DC:C1'	6:J:199:DG:C8	2.90	0.54
6:J:336:DT:H2''	6:J:337:DT:OP2	2.07	0.54
5:I:122:DA:H2''	5:I:123:DC:OP2	2.08	0.54
6:J:162:DT:C3'	6:J:163:DT:H5'	2.38	0.54
6:J:346:DG:C4'	6:J:347:DT:OP1	2.48	0.54
6:J:136:DG:C6	6:J:137:DG:C6	2.96	0.54
5:I:90:DC:H2''	5:I:91:DT:OP2	2.08	0.53
5:I:58:DT:C2	6:J:289:DG:N2	2.76	0.53
5:I:331:DA:H2''	5:I:332:DA:OP2	2.08	0.53
5:I:82:DC:H2''	5:I:83:DG:C8	2.42	0.53
6:J:15:DT:C2'	6:J:16:DT:H6	2.20	0.53
5:I:185:DA:H2''	5:I:186:DA:OP2	2.08	0.53
4:R:65:PHE:CE1	4:R:69:ILE:CD1	2.91	0.53
5:I:273:DT:H1'	5:I:274:DT:O5'	2.09	0.53
6:J:262:DG:H8	6:J:262:DG:OP2	1.91	0.53
5:I:23:DC:H2''	5:I:24:DC:OP2	2.08	0.53
5:I:73:DA:C2	5:I:74:DC:C2	2.97	0.53
1:A:41:TYR:HA	5:I:156:DA:H5''	1.90	0.53
5:I:39:DT:H2''	5:I:40:DC:OP2	2.08	0.53
5:I:223:DG:H2''	5:I:224:DT:OP2	2.09	0.53
6:J:271:DC:H2''	6:J:272:DG:OP2	2.09	0.53
5:I:112:DA:H8	5:I:112:DA:O5'	1.92	0.53
5:I:138:DG:H2''	5:I:139:DT:OP2	2.09	0.53
6:J:143:DG:H2''	6:J:144:DC:C6	2.44	0.53
4:H:65:PHE:CE1	4:H:69:ILE:CD1	2.91	0.52
5:I:135:DC:H2'	5:I:136:DA:C8	2.45	0.52
4:N:65:PHE:CE1	4:N:69:ILE:CD1	2.91	0.52
5:I:245:DA:H2''	5:I:246:DA:OP2	2.08	0.52
5:I:54:DC:H2''	5:I:55:DA:C8	2.45	0.52
5:I:81:DA:H2''	5:I:82:DC:C6	2.44	0.52
5:I:174:DG:H2'	5:I:174:DG:O5'	2.09	0.52
5:I:317:DA:H2'	5:I:318:DG:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:195:DT:H2''	6:J:196:DG:OP2	2.09	0.52
6:J:231:DT:H2''	6:J:232:DT:OP2	2.09	0.52
5:I:160:DA:H2''	5:I:161:DA:OP2	2.08	0.52
5:I:174:DG:H4'	5:I:175:DA:OP1	2.09	0.52
6:J:82:DG:H2''	6:J:83:DA:C8	2.45	0.52
6:J:165:DT:H4'	6:J:166:DC:OP1	2.09	0.52
6:J:254:DT:OP2	6:J:254:DT:H73	2.09	0.52
6:J:337:DT:H2''	6:J:338:DT:OP2	2.09	0.52
5:I:38:DC:H2''	5:I:39:DT:OP2	2.09	0.52
5:I:92:DA:H2''	5:I:93:DC:C6	2.44	0.52
6:J:52:DA:H1'	6:J:53:DG:N7	2.24	0.52
5:I:87:DT:H2''	5:I:88:DG:OP2	2.08	0.52
5:I:202:DG:H2''	5:I:203:DC:OP2	2.09	0.52
6:J:319:DA:H2''	6:J:320:DC:C6	2.45	0.52
3:M:100:VAL:HG11	2:P:98:TYR:CE2	2.44	0.52
5:I:183:DA:H1'	5:I:184:DA:O5'	2.10	0.52
1:A:112:ILE:HG23	3:G:114:VAL:HG21	1.91	0.51
6:J:77:DC:H2''	6:J:78:DG:OP2	2.10	0.51
7:S:25:HIS:O	7:S:31:MET:HE3	2.10	0.51
6:J:289:DG:H2''	6:J:290:DC:C6	2.45	0.51
5:I:109:DA:H2''	5:I:110:DC:OP2	2.10	0.51
5:I:151:DA:C2	6:J:196:DG:C2	2.98	0.51
5:I:154:DT:C2'	5:I:155:DG:OP2	2.53	0.51
5:I:180:DG:H1'	5:I:181:DA:OP2	2.11	0.51
6:J:62:DG:OP1	1:O:85:GLN:HA	2.10	0.51
1:K:119:ILE:HG13	2:L:50:ILE:HD12	1.93	0.51
5:I:183:DA:C1'	5:I:184:DA:O5'	2.58	0.51
2:B:98:TYR:CE2	3:G:100:VAL:HG11	2.45	0.51
6:J:35:DG:C2'	6:J:36:DT:H72	2.24	0.51
5:I:324:DC:H2''	5:I:325:DA:OP2	2.10	0.51
6:J:193:DT:C2'	6:J:194:DG:C8	2.91	0.51
6:J:23:DC:C2'	6:J:24:DC:OP2	2.53	0.51
6:J:223:DG:H2''	6:J:224:DT:OP2	2.10	0.51
1:A:119:ILE:C	2:B:50:ILE:HD11	2.35	0.50
4:H:49:HIS:CB	4:H:52:THR:CG2	2.76	0.50
6:J:15:DT:H2'	6:J:16:DT:C5	2.44	0.50
6:J:126:DC:H1'	6:J:127:DC:H5''	1.92	0.50
3:C:11:ARG:HG3	3:C:12:ALA:N	2.26	0.50
5:I:282:DC:H2'	5:I:283:DA:C8	2.46	0.50
5:I:327:DA:C2'	5:I:328:DT:O5'	2.60	0.50
6:J:251:DC:H2''	6:J:252:DG:C5'	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:272:DG:H2''	6:J:273:DT:OP2	2.11	0.50
5:I:231:DC:H2''	5:I:232:DT:OP2	2.12	0.50
7:S:83:GLN:HA	7:S:93:PHE:HA	1.94	0.50
5:I:155:DG:C2	6:J:192:DA:C2	3.00	0.50
5:I:175:DA:C4	5:I:176:DG:C8	2.99	0.50
5:I:340:DC:C2'	5:I:341:DC:OP2	2.49	0.50
6:J:87:DC:H2''	6:J:88:DG:OP2	2.12	0.50
6:J:224:DT:H2''	6:J:225:DA:C8	2.47	0.50
6:J:315:DC:H2''	6:J:316:DG:C8	2.46	0.50
7:S:27:LYS:HB3	7:S:30:ASP:HB2	1.94	0.50
4:N:80:LEU:CD1	4:N:96:THR:HB	2.42	0.50
1:A:88:ALA:HA	2:B:83:ALA:HA	1.93	0.50
5:I:67:DG:H2''	5:I:68:DC:O5'	2.12	0.50
5:I:98:DT:H2''	5:I:99:DT:OP2	2.12	0.50
6:J:223:DG:H1'	6:J:224:DT:C5'	2.42	0.50
5:I:180:DG:C2'	5:I:181:DA:OP2	2.59	0.49
6:J:61:DA:H2''	6:J:62:DG:C8	2.48	0.49
3:M:62:ILE:HD11	4:N:65:PHE:CE1	2.47	0.49
3:G:15:LYS:HD2	3:G:20:ARG:HE	1.76	0.49
5:I:64:DA:C2	5:I:65:DC:C2	3.00	0.49
5:I:289:DA:H1'	5:I:290:DG:H5'	1.95	0.49
6:J:155:DG:H4'	6:J:156:DT:OP1	2.12	0.49
4:D:80:LEU:CD1	4:D:96:THR:HB	2.41	0.49
5:I:61:DA:H2''	5:I:62:DG:C8	2.48	0.49
5:I:199:DG:H2''	5:I:200:DG:OP2	2.13	0.49
2:B:88:TYR:CE1	4:D:83:TYR:CE1	3.01	0.49
5:I:214:DC:H4'	5:I:215:DA:OP1	2.12	0.49
6:J:174:DA:H2''	6:J:175:DG:C8	2.47	0.49
5:I:1:DC:C2'	5:I:2:DG:OP2	2.61	0.49
6:J:35:DG:H2''	6:J:36:DT:C6	2.48	0.49
6:J:254:DT:H6	6:J:254:DT:O5'	1.95	0.49
1:A:85:GLN:HA	5:I:62:DG:OP1	2.13	0.49
5:I:143:DA:C2'	5:I:144:DG:C8	2.95	0.49
6:J:161:DT:H1'	6:J:162:DT:O5'	2.12	0.49
6:J:288:DA:C6	6:J:289:DG:C6	3.00	0.49
6:J:297:DC:H2''	6:J:298:DG:C8	2.48	0.49
3:M:71:ARG:HB3	3:M:71:ARG:HH11	1.76	0.49
5:I:229:DA:H2''	5:I:230:DG:OP2	2.12	0.49
6:J:64:DG:H1'	6:J:65:DG:H5'	1.95	0.49
4:D:76:GLU:OE2	4:D:79:ARG:NH1	2.46	0.48
5:I:170:DG:H2''	5:I:171:DC:OP2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:132:DA:H2''	5:I:133:DG:N7	2.27	0.48
2:P:88:TYR:CD1	4:R:83:TYR:CZ	3.02	0.48
4:R:76:GLU:OE2	4:R:79:ARG:NH1	2.46	0.48
5:I:4:DT:H2''	5:I:5:DG:OP2	2.12	0.48
5:I:27:DT:H2''	5:I:28:DG:OP2	2.13	0.48
1:K:88:ALA:HA	2:L:83:ALA:HA	1.95	0.48
5:I:162:DA:H2''	5:I:163:DA:OP2	2.13	0.48
1:O:69:ARG:HB3	2:P:25:ASN:OD1	2.13	0.48
5:I:163:DA:H2''	5:I:164:DA:OP2	2.13	0.48
6:J:304:DT:H2''	6:J:305:DT:OP2	2.14	0.48
6:J:319:DA:C5	6:J:320:DC:N4	2.82	0.48
6:J:64:DG:H1'	6:J:65:DG:C5'	2.43	0.48
6:J:149:DG:H1'	6:J:150:DG:C8	2.49	0.48
6:J:302:DA:H2''	6:J:303:DA:OP2	2.13	0.48
1:O:88:ALA:HA	2:P:83:ALA:HA	1.95	0.48
5:I:337:DA:H2''	5:I:338:DA:OP2	2.13	0.48
5:I:3:DC:C2'	5:I:4:DT:OP2	2.61	0.48
5:I:317:DA:C2'	5:I:318:DG:C8	2.96	0.48
6:J:269:DT:H2''	6:J:270:DG:H5'	1.96	0.48
4:R:49:HIS:CB	4:R:52:THR:CG2	2.79	0.48
2:P:75:HIS:HB2	4:R:96:THR:HG21	1.96	0.47
6:J:167:DA:H2''	6:J:168:DT:OP2	2.13	0.47
6:J:194:DG:H2'	6:J:195:DT:C6	2.49	0.47
6:J:263:DC:H2''	6:J:264:DG:OP2	2.14	0.47
1:A:113:HIS:CG	1:E:126:LEU:HD22	2.49	0.47
5:I:10:DA:C2	6:J:337:DT:C2	3.02	0.47
5:I:314:DG:H4'	5:I:315:DT:OP1	2.14	0.47
5:I:325:DA:N3	5:I:326:DC:C6	2.83	0.47
6:J:188:DT:H2'	6:J:189:DT:H71	1.97	0.47
5:I:63:DC:H2''	5:I:64:DA:O5'	2.13	0.47
4:R:30:LYS:O	4:R:30:LYS:HG2	2.15	0.47
5:I:310:DA:H2''	5:I:311:DC:C6	2.49	0.47
1:E:37:LYS:HG2	1:E:38:PRO:HD2	1.95	0.47
5:I:316:DG:H2''	5:I:317:DA:N7	2.30	0.47
4:N:76:GLU:OE2	4:N:79:ARG:NH1	2.47	0.47
2:P:88:TYR:CE1	4:R:83:TYR:CE1	3.03	0.47
7:S:32:ILE:HD12	7:S:50:ILE:HD11	1.97	0.47
1:A:100:LEU:O	1:A:101:VAL:C	2.58	0.47
5:I:92:DA:N6	6:J:253:DG:C6	2.83	0.47
5:I:112:DA:H8	5:I:112:DA:OP2	1.97	0.47
5:I:69:DT:C2'	5:I:70:DT:OP2	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:72:DA:C2	5:I:73:DA:C4	3.02	0.47
6:J:163:DT:H2''	6:J:164:DT:C5'	2.44	0.47
6:J:319:DA:N7	6:J:320:DC:N4	2.62	0.47
4:D:65:PHE:CE1	4:D:69:ILE:HD11	2.50	0.46
5:I:134:DG:C2'	5:I:135:DC:C5	2.98	0.46
6:J:26:DG:H2''	6:J:27:DT:OP2	2.14	0.46
6:J:325:DA:H2''	6:J:326:DT:OP2	2.14	0.46
1:E:100:LEU:O	1:E:101:VAL:C	2.58	0.46
4:D:32:SER:OG	5:I:116:DG:OP1	2.27	0.46
5:I:179:DT:H2'	5:I:180:DG:C8	2.51	0.46
1:A:51:ILE:O	1:A:55:GLN:HG3	2.16	0.46
4:H:76:GLU:OE2	4:H:79:ARG:NH1	2.48	0.46
6:J:2:DG:H1'	6:J:3:DC:C6	2.50	0.46
1:O:100:LEU:O	1:O:101:VAL:C	2.58	0.46
6:J:101:DT:H2''	6:J:102:DA:C8	2.51	0.46
5:I:108:DC:H2''	5:I:109:DA:C5'	2.46	0.46
1:K:100:LEU:O	1:K:101:VAL:C	2.58	0.46
2:F:31:LYS:N	2:F:32:PRO:HD2	2.31	0.46
5:I:108:DC:H2''	5:I:109:DA:H5'	1.97	0.46
6:J:24:DC:OP2	6:J:24:DC:C6	2.68	0.46
6:J:309:DC:H2''	6:J:310:DG:C8	2.51	0.46
5:I:112:DA:C8	5:I:112:DA:OP2	2.69	0.46
5:I:281:DC:C2'	5:I:282:DC:C6	2.99	0.46
1:K:51:ILE:O	1:K:55:GLN:HG3	2.16	0.46
1:A:126:LEU:HD11	1:A:130:ILE:HD11	1.98	0.46
1:E:51:ILE:O	1:E:55:GLN:HG3	2.16	0.46
5:I:181:DA:OP2	5:I:181:DA:C8	2.69	0.46
5:I:201:DT:H2''	5:I:202:DG:OP2	2.16	0.46
2:B:80:THR:HB	6:J:288:DA:H5''	1.98	0.45
5:I:13:DA:H5''	5:I:13:DA:H8	1.73	0.45
6:J:36:DT:H2''	6:J:37:DG:O5'	2.17	0.45
6:J:57:DT:H2''	6:J:58:DT:OP2	2.16	0.45
2:L:31:LYS:N	2:L:32:PRO:HD2	2.31	0.45
1:O:51:ILE:O	1:O:55:GLN:HG3	2.17	0.45
2:B:31:LYS:N	2:B:32:PRO:HD2	2.32	0.45
5:I:136:DA:H2''	5:I:137:DC:OP2	2.16	0.45
5:I:159:DA:C6	5:I:160:DA:C6	3.05	0.45
4:H:49:HIS:HB3	4:H:52:THR:HG21	1.91	0.45
5:I:143:DA:H2'	5:I:144:DG:C8	2.51	0.45
5:I:173:DC:OP2	5:I:173:DC:C6	2.70	0.45
5:I:212:DC:H2''	5:I:213:DT:OP2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:203:DC:H2''	5:I:204:DC:OP2	2.17	0.45
6:J:11:DT:C6	6:J:12:DT:C7	3.00	0.45
6:J:35:DG:C2'	6:J:36:DT:C7	2.87	0.45
3:M:16:THR:O	3:M:19:SER:OG	2.22	0.45
2:P:31:LYS:N	2:P:32:PRO:HD2	2.31	0.45
6:J:286:DA:H2''	6:J:287:DG:O5'	2.17	0.45
6:J:12:DT:C6	6:J:13:DT:C7	3.00	0.45
1:E:88:ALA:HA	2:F:83:ALA:HA	1.98	0.45
5:I:276:DA:C2	6:J:71:DA:C2	3.05	0.45
6:J:161:DT:H2''	6:J:162:DT:OP2	2.15	0.45
5:I:70:DT:H2''	5:I:71:DA:C8	2.52	0.45
6:J:24:DC:OP2	6:J:24:DC:H6	2.00	0.45
6:J:162:DT:H2''	6:J:163:DT:C4'	2.47	0.45
4:R:70:PHE:CD1	4:R:70:PHE:C	2.95	0.45
5:I:167:DC:H2''	5:I:168:DA:OP2	2.16	0.45
6:J:29:DT:H2''	6:J:30:DC:OP2	2.17	0.45
6:J:185:DT:H2''	6:J:186:DT:OP2	2.17	0.45
6:J:12:DT:C5	6:J:13:DT:H73	2.52	0.45
7:S:46:SER:O	7:S:49:SER:OG	2.28	0.45
5:I:57:DC:H2''	5:I:58:DT:OP2	2.16	0.44
5:I:197:DC:H2''	5:I:198:DC:H5'	1.98	0.44
6:J:15:DT:C2'	6:J:16:DT:O5'	2.51	0.44
6:J:12:DT:C6	6:J:13:DT:H71	2.52	0.44
4:R:65:PHE:CE1	4:R:69:ILE:HD11	2.53	0.44
2:B:88:TYR:CD1	4:D:83:TYR:CZ	3.06	0.44
4:D:70:PHE:CD1	4:D:70:PHE:C	2.96	0.44
1:E:126:LEU:HD11	1:E:130:ILE:HD11	2.00	0.44
5:I:108:DC:H2''	5:I:109:DA:O5'	2.18	0.44
5:I:144:DG:H1'	5:I:145:DA:C8	2.52	0.44
5:I:338:DA:C2	6:J:9:DT:O2	2.70	0.44
6:J:263:DC:C4	6:J:264:DG:O6	2.71	0.44
1:K:119:ILE:C	2:L:50:ILE:HD11	2.41	0.44
1:O:126:LEU:HD11	1:O:130:ILE:HD11	1.99	0.44
5:I:86:DC:H2''	5:I:87:DT:OP2	2.17	0.44
5:I:262:DG:C2'	5:I:263:DT:OP2	2.44	0.44
6:J:93:DC:H2'	6:J:94:DG:C8	2.52	0.44
6:J:324:DG:H2''	6:J:325:DA:OP2	2.17	0.44
5:I:12:DA:H2''	5:I:13:DA:O5'	2.17	0.44
5:I:91:DT:H4'	5:I:92:DA:OP1	2.17	0.44
4:H:70:PHE:CD1	4:H:70:PHE:C	2.96	0.44
4:N:65:PHE:CE1	4:N:69:ILE:HD11	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:261:DC:H2''	6:J:262:DG:OP2	2.17	0.44
1:E:108:ASN:ND2	2:F:42:GLY:O	2.50	0.43
5:I:150:DC:H2''	5:I:151:DA:OP2	2.18	0.43
5:I:310:DA:H2''	5:I:311:DC:OP2	2.17	0.43
3:M:71:ARG:HB3	3:M:71:ARG:NH1	2.33	0.43
3:G:62:ILE:HD11	4:H:65:PHE:CE1	2.52	0.43
6:J:11:DT:H1'	6:J:12:DT:C6	2.54	0.43
4:N:70:PHE:CD1	4:N:70:PHE:C	2.96	0.43
5:I:101:DT:C2'	5:I:102:DA:C8	3.00	0.43
5:I:284:DC:H2''	5:I:285:DT:OP2	2.18	0.43
6:J:247:DA:C4	6:J:248:DA:C8	3.06	0.43
1:E:37:LYS:HG3	1:E:38:PRO:HD2	2.00	0.43
2:F:56:GLY:O	2:F:60:VAL:HG23	2.19	0.43
5:I:17:DC:O2	5:I:18:DG:O4'	2.37	0.43
5:I:175:DA:H1'	5:I:176:DG:O5'	2.18	0.43
5:I:332:DA:C2	6:J:15:DT:C2	3.06	0.43
6:J:110:DC:H2''	6:J:111:DT:OP2	2.19	0.43
6:J:188:DT:C1'	6:J:189:DT:H5'	2.45	0.43
3:M:111:ILE:HG12	1:O:51:ILE:HG21	2.00	0.43
7:S:28:TYR:HA	7:S:31:MET:HB2	2.00	0.43
2:F:66:ILE:O	2:F:67:ARG:C	2.62	0.43
5:I:197:DC:H2'	5:I:198:DC:C6	2.54	0.43
5:I:6:DG:C2	5:I:7:DA:C2	3.07	0.43
5:I:161:DA:N6	6:J:184:DT:O4	2.52	0.43
6:J:39:DC:H2''	6:J:40:DT:C6	2.54	0.43
6:J:212:DC:H2''	6:J:213:DC:OP2	2.18	0.43
3:C:50:TYR:OH	4:D:95:GLN:NE2	2.40	0.43
5:I:281:DC:H2'	5:I:282:DC:C5	2.54	0.43
5:I:309:DC:H2''	5:I:310:DA:O5'	2.19	0.43
6:J:193:DT:H3'	6:J:194:DG:H8	1.84	0.43
6:J:210:DT:C4	6:J:211:DG:C6	3.07	0.43
2:L:56:GLY:O	2:L:60:VAL:HG23	2.19	0.43
1:A:41:TYR:OH	6:J:193:DT:H2''	2.18	0.42
5:I:2:DG:O6	6:J:343:DG:O6	2.36	0.42
6:J:44:DG:OP2	3:Q:20:ARG:NH2	2.51	0.42
6:J:205:DA:H1'	6:J:206:DC:C6	2.53	0.42
3:M:57:TYR:CZ	4:N:109:HIS:HB3	2.54	0.42
1:A:63:ARG:NH1	5:I:72:DA:H4'	2.34	0.42
3:C:16:THR:O	3:C:19:SER:OG	2.22	0.42
4:D:65:PHE:CZ	4:D:69:ILE:CD1	3.03	0.42
5:I:89:DT:H1'	5:I:90:DC:H5'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:123:DC:H2''	5:I:124:DT:H72	2.01	0.42
5:I:337:DA:H2'	5:I:337:DA:O5'	2.19	0.42
6:J:108:DT:H2''	6:J:109:DG:OP2	2.18	0.42
5:I:41:DA:C2	5:I:42:DA:C2	3.06	0.42
6:J:11:DT:O4'	6:J:12:DT:H5'	2.19	0.42
6:J:40:DT:H2''	6:J:41:DG:OP2	2.18	0.42
6:J:59:DC:H4'	6:J:60:DT:H5'	2.01	0.42
6:J:315:DC:OP2	6:J:315:DC:C6	2.69	0.42
1:K:113:HIS:CG	1:O:126:LEU:HD22	2.54	0.42
5:I:142:DG:H1'	5:I:143:DA:C8	2.54	0.42
6:J:14:DT:C5	6:J:15:DT:H73	2.54	0.42
6:J:107:DG:H2''	6:J:108:DT:OP2	2.20	0.42
1:K:131:ARG:HD3	1:K:133:GLU:OE2	2.19	0.42
4:H:30:LYS:O	4:H:30:LYS:HG2	2.19	0.42
4:H:65:PHE:CE1	4:H:69:ILE:HD11	2.54	0.42
5:I:327:DA:C2	6:J:20:DG:N2	2.87	0.42
1:K:126:LEU:HD11	1:K:130:ILE:HD11	2.02	0.42
4:N:80:LEU:HD13	4:N:96:THR:HB	2.02	0.42
1:A:119:ILE:CG1	2:B:50:ILE:CD1	2.98	0.42
5:I:107:DC:H2''	5:I:108:DC:O5'	2.19	0.42
5:I:142:DG:N2	6:J:205:DA:C2	2.87	0.42
5:I:165:DA:C2'	5:I:166:DG:OP2	2.62	0.42
5:I:187:DA:H1'	5:I:188:DA:O5'	2.19	0.42
6:J:210:DT:H2''	6:J:211:DG:OP2	2.19	0.42
6:J:312:DC:H2''	6:J:313:DC:OP2	2.20	0.42
2:B:66:ILE:O	2:B:67:ARG:C	2.62	0.42
5:I:316:DG:C2	5:I:317:DA:C2	3.07	0.42
5:I:320:DC:C4	5:I:321:DC:N4	2.88	0.42
6:J:248:DA:H2''	6:J:249:DC:C6	2.55	0.42
1:K:120:MET:O	1:K:121:PRO:C	2.63	0.42
3:M:67:GLY:HA3	4:N:49:HIS:CD2	2.55	0.42
2:P:56:GLY:O	2:P:60:VAL:HG23	2.20	0.42
6:J:14:DT:C2	6:J:15:DT:C6	3.08	0.42
6:J:314:DT:H2''	6:J:315:DC:C5	2.54	0.42
6:J:335:DT:H2''	6:J:336:DT:C7	2.50	0.42
7:S:95:LEU:N	7:S:95:LEU:CD2	2.81	0.42
2:B:56:GLY:O	2:B:60:VAL:HG23	2.20	0.42
3:C:42:ARG:O	4:D:88:THR:HA	2.19	0.42
5:I:206:DA:H4'	3:M:77:ARG:CZ	2.49	0.42
6:J:51:DA:C5	6:J:52:DA:C6	3.08	0.42
5:I:30:DC:C2'	5:I:31:DG:OP2	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:33:DG:C6	5:I:34:DG:C6	3.08	0.41
5:I:186:DA:H2''	5:I:187:DA:OP2	2.19	0.41
5:I:302:DC:H2''	5:I:303:DT:OP2	2.19	0.41
6:J:193:DT:H2'	6:J:194:DG:C1'	2.50	0.41
6:J:203:DT:C2'	6:J:204:DC:OP2	2.68	0.41
6:J:307:DA:C5	6:J:308:DG:C6	3.08	0.41
5:I:171:DC:C2'	5:I:172:DT:O5'	2.53	0.41
5:I:181:DA:H2''	5:I:182:DA:OP2	2.19	0.41
5:I:184:DA:H2''	5:I:185:DA:OP2	2.20	0.41
7:S:46:SER:O	7:S:50:ILE:HG23	2.20	0.41
5:I:210:DC:H2''	5:I:211:DG:OP2	2.21	0.41
7:S:36:ILE:HD12	7:S:95:LEU:HD21	2.01	0.41
1:E:120:MET:O	1:E:121:PRO:C	2.64	0.41
5:I:308:DG:H2''	5:I:309:DC:C5	2.55	0.41
4:R:65:PHE:CZ	4:R:69:ILE:CD1	3.04	0.41
7:S:24:ASP:N	7:S:59:LYS:HG2	2.35	0.41
5:I:60:DT:H2''	5:I:61:DA:C8	2.56	0.41
6:J:150:DG:H2''	6:J:151:DA:H5'	2.02	0.41
2:B:75:HIS:HB2	4:D:96:THR:HG21	2.02	0.41
5:I:325:DA:C4	5:I:326:DC:C6	3.09	0.41
6:J:34:DC:H2''	6:J:35:DG:O4'	2.21	0.41
6:J:81:DA:O5'	6:J:81:DA:H2'	2.21	0.41
2:L:66:ILE:O	2:L:67:ARG:C	2.62	0.41
4:H:65:PHE:CZ	4:H:69:ILE:CD1	3.03	0.41
5:I:23:DC:O2	6:J:324:DG:N2	2.54	0.41
6:J:199:DG:H2''	6:J:200:DG:O5'	2.19	0.41
6:J:273:DT:C6	6:J:274:DT:H72	2.55	0.41
5:I:189:DA:H2''	5:I:190:DA:OP2	2.20	0.41
5:I:337:DA:O5'	5:I:337:DA:C2'	2.69	0.41
6:J:289:DG:H2''	6:J:290:DC:H6	1.86	0.41
2:P:66:ILE:O	2:P:67:ARG:C	2.62	0.41
1:A:131:ARG:HD3	1:A:133:GLU:OE2	2.20	0.41
1:E:131:ARG:HD3	1:E:133:GLU:OE2	2.21	0.41
6:J:11:DT:H1'	6:J:12:DT:O5'	2.21	0.41
6:J:47:DT:H2''	6:J:48:DA:H5'	2.03	0.41
6:J:136:DG:C5	6:J:137:DG:C5	3.09	0.41
6:J:147:DC:H2''	6:J:148:DG:C8	2.56	0.41
6:J:336:DT:H1'	6:J:337:DT:H5'	2.02	0.41
5:I:152:DC:H2''	5:I:153:DA:C5'	2.50	0.41
5:I:195:DT:H2''	5:I:196:DC:OP2	2.21	0.41
4:N:65:PHE:CZ	4:N:69:ILE:CD1	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:197:DC:H42	6:J:149:DG:H1	1.68	0.40
5:I:219:DG:H2''	5:I:220:DG:OP2	2.21	0.40
6:J:14:DT:H1'	6:J:15:DT:O5'	2.21	0.40
6:J:183:DT:O2	6:J:184:DT:O4'	2.38	0.40
6:J:201:DT:H2''	6:J:202:DC:OP2	2.21	0.40
7:S:32:ILE:CD1	7:S:68:ILE:HG23	2.51	0.40
5:I:50:DT:H2''	5:I:51:DA:N7	2.36	0.40
5:I:345:DG:C2'	5:I:346:DG:C8	3.04	0.40
6:J:11:DT:H6	6:J:11:DT:H2'	1.77	0.40
7:S:25:HIS:HB2	7:S:31:MET:CE	2.51	0.40
5:I:31:DG:OP2	5:I:31:DG:H8	2.04	0.40
6:J:32:DC:H4'	3:Q:77:ARG:NE	2.36	0.40
6:J:262:DG:H2''	6:J:263:DC:OP2	2.21	0.40
2:F:88:TYR:CE1	4:H:83:TYR:CE1	3.09	0.40
5:I:8:DA:C2	6:J:339:DT:O2	2.74	0.40
5:I:335:DA:C6	5:I:336:DA:C6	3.08	0.40
6:J:14:DT:C6	6:J:15:DT:C7	3.04	0.40
6:J:68:DG:H2''	6:J:69:DT:OP2	2.20	0.40
6:J:225:DA:C6	6:J:226:DA:C6	3.09	0.40
1:O:120:MET:O	1:O:121:PRO:C	2.63	0.40
1:A:83:ARG:O	2:B:81:VAL:N	2.47	0.40
5:I:6:DG:N1	5:I:7:DA:C2	2.90	0.40
5:I:10:DA:N6	6:J:335:DT:O4	2.54	0.40
5:I:17:DC:H1'	5:I:18:DG:H5'	2.03	0.40
5:I:45:DG:N2	6:J:302:DA:C2	2.90	0.40
5:I:161:DA:OP2	5:I:161:DA:H2'	2.21	0.40
2:L:88:TYR:CE1	4:N:83:TYR:CE1	3.09	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:1:DC:O5'	5:I:349:DC:O3'[4_446]	1.84	0.36
6:J:112:DA:OP1	7:S:52:LYS:NZ[3_555]	2.09	0.11

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	
1	A	87/111 (78%)	84 (97%)	3 (3%)	32	57
1	E	86/111 (78%)	82 (95%)	4 (5%)	23	50
1	K	86/111 (78%)	84 (98%)	2 (2%)	44	63
1	O	85/111 (77%)	82 (96%)	3 (4%)	32	56
2	B	66/79 (84%)	65 (98%)	1 (2%)	57	69
2	F	67/79 (85%)	65 (97%)	2 (3%)	36	59
2	L	65/79 (82%)	65 (100%)	0	100	100
2	P	65/79 (82%)	64 (98%)	1 (2%)	57	69
3	C	86/100 (86%)	80 (93%)	6 (7%)	14	40
3	G	83/100 (83%)	76 (92%)	7 (8%)	10	34
3	M	84/100 (84%)	78 (93%)	6 (7%)	13	39
3	Q	84/100 (84%)	79 (94%)	5 (6%)	17	43
4	D	82/105 (78%)	73 (89%)	9 (11%)	6	22
4	H	82/105 (78%)	71 (87%)	11 (13%)	4	15
4	N	82/105 (78%)	74 (90%)	8 (10%)	7	27
4	R	82/105 (78%)	72 (88%)	10 (12%)	5	19
7	S	61/158 (39%)	47 (77%)	14 (23%)	1	2
All	All	1333/1738 (77%)	1241 (93%)	92 (7%)	14	40

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	A	129	ARG
1	A	134	ARG
2	B	59	LYS
3	C	13	LYS
3	C	15	LYS
3	C	24	GLN

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Mol	Chain	Res	Type
3	C	74	LYS
3	C	81	ARG
3	C	99	ARG
4	D	31	ARG
4	D	34	LYS
4	D	38	SER
4	D	46	LYS
4	D	55	SER
4	D	85	LYS
4	D	101	LEU
4	D	106	LEU
4	D	122	THR
1	E	48	LEU
1	E	65	LEU
1	E	129	ARG
1	E	134	ARG
2	F	35	ARG
2	F	63	GLU
3	G	15	LYS
3	G	24	GLN
3	G	29	ARG
3	G	71	ARG
3	G	74	LYS
3	G	80	PRO
3	G	81	ARG
4	H	31	ARG
4	H	38	SER
4	H	46	LYS
4	H	52	THR
4	H	55	SER
4	H	80	LEU
4	H	85	LYS
4	H	101	LEU
4	H	106	LEU
4	H	108	LYS
4	H	122	THR
1	K	63	ARG
1	K	129	ARG
3	M	24	GLN
3	M	36	LYS
3	M	71	ARG
3	M	74	LYS

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Mol	Chain	Res	Type
3	M	81	ARG
3	M	118	LYS
4	N	31	ARG
4	N	38	SER
4	N	46	LYS
4	N	55	SER
4	N	85	LYS
4	N	101	LEU
4	N	106	LEU
4	N	122	THR
1	O	48	LEU
1	O	129	ARG
1	O	134	ARG
2	P	35	ARG
3	Q	24	GLN
3	Q	29	ARG
3	Q	74	LYS
3	Q	81	ARG
3	Q	99	ARG
4	R	33	ARG
4	R	38	SER
4	R	46	LYS
4	R	52	THR
4	R	55	SER
4	R	80	LEU
4	R	85	LYS
4	R	101	LEU
4	R	106	LEU
4	R	122	THR
7	S	24	ASP
7	S	25	HIS
7	S	33	VAL
7	S	36	ILE
7	S	40	LYS
7	S	47	ARG
7	S	48	GLN
7	S	50	ILE
7	S	54	ILE
7	S	59	LYS
7	S	63	ASN
7	S	65	ASP
7	S	82	LYS

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Mol	Chain	Res	Type
7	S	97	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
3	C	24	GLN
3	C	38	ASN
3	C	68	ASN
4	D	47	GLN
1	E	76	GLN
3	G	24	GLN
3	G	31	HIS
3	G	104	GLN
4	H	47	GLN
4	H	84	ASN
3	M	24	GLN
3	M	38	ASN
3	M	68	ASN
3	M	104	GLN
4	N	47	GLN
4	N	49	HIS
4	N	95	GLN
4	N	109	HIS
1	O	108	ASN
3	Q	24	GLN
3	Q	31	HIS
3	Q	38	ASN
4	R	47	GLN
4	R	49	HIS
7	S	51	GLN
7	S	63	ASN
7	S	83	GLN

5.3.3 RNA ⓘ

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](#)

Of 30 ligands modelled in this entry, 30 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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(Å²)	Q<0.9
1	A	100/136 (73%)	-0.88	0	100	100	94, 119, 167, 210	0
1	E	99/136 (72%)	-0.65	0	100	100	94, 123, 168, 190	0
1	K	99/136 (72%)	-0.62	0	100	100	91, 116, 160, 215	0
1	O	98/136 (72%)	-0.63	0	100	100	97, 131, 179, 216	0
2	B	81/103 (78%)	-0.77	0	100	100	90, 114, 143, 190	0
2	F	82/103 (79%)	-0.65	0	100	100	91, 117, 153, 221	0
2	L	80/103 (77%)	-0.76	0	100	100	87, 111, 148, 220	0
2	P	80/103 (77%)	-0.48	0	100	100	100, 126, 155, 211	0
3	C	110/130 (84%)	-0.64	0	100	100	101, 129, 198, 251	0
3	G	105/130 (80%)	-0.44	0	100	100	96, 127, 183, 202	0
3	M	106/130 (81%)	-0.34	2 (1%)	66	51	95, 127, 173, 227	0
3	Q	105/130 (80%)	-0.55	0	100	100	90, 127, 177, 196	0
4	D	96/126 (76%)	-0.67	0	100	100	93, 129, 182, 225	0
4	H	96/126 (76%)	-0.54	0	100	100	98, 135, 185, 245	0
4	N	96/126 (76%)	-0.43	2 (2%)	63	48	99, 130, 196, 241	0
4	R	96/126 (76%)	-0.64	0	100	100	96, 132, 190, 231	0
5	I	349/349 (100%)	-1.02	0	100	100	115, 177, 263, 321	0
6	J	349/349 (100%)	-0.99	0	100	100	112, 179, 267, 315	0
7	S	74/194 (38%)	-0.67	0	100	100	155, 197, 234, 256	1 (1%)
All	All	2301/2872 (80%)	-0.73	4 (0%)	91	87	87, 139, 221, 321	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	50	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
4	N	44	VAL	2.2
4	N	65	PHE	2.1
3	M	63	LEU	2.1

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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	CA	J	410	1/1	0.69	0.06	181,181,181,181	0
8	CA	I	409	1/1	0.78	0.05	190,190,190,190	0
8	CA	I	406	1/1	0.78	0.15	175,175,175,175	0
8	CA	I	405	1/1	0.79	0.08	174,174,174,174	0
9	K	I	413	1/1	0.82	0.08	130,130,130,130	0
8	CA	J	404	1/1	0.84	0.15	177,177,177,177	0
9	K	J	413	1/1	0.84	0.17	154,154,154,154	0
8	CA	J	409	1/1	0.87	0.05	173,173,173,173	0
9	K	J	415	1/1	0.88	0.12	156,156,156,156	0
8	CA	J	408	1/1	0.89	0.05	160,160,160,160	0
8	CA	I	407	1/1	0.89	0.07	145,145,145,145	0
8	CA	I	408	1/1	0.89	0.10	191,191,191,191	0
9	K	I	412	1/1	0.90	0.18	153,153,153,153	0
8	CA	J	401	1/1	0.90	0.09	126,126,126,126	0
8	CA	I	402	1/1	0.90	0.09	126,126,126,126	0
9	K	J	414	1/1	0.90	0.07	157,157,157,157	0
8	CA	J	407	1/1	0.90	0.04	150,150,150,150	0
8	CA	J	405	1/1	0.92	0.04	145,145,145,145	0
8	CA	I	401	1/1	0.92	0.14	148,148,148,148	0
8	CA	M	201	1/1	0.93	0.04	155,155,155,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	CA	I	403	1/1	0.94	0.04	124,124,124,124	0
9	K	J	411	1/1	0.94	0.16	146,146,146,146	0
9	K	J	412	1/1	0.94	0.07	147,147,147,147	0
8	CA	J	406	1/1	0.94	0.06	159,159,159,159	0
8	CA	J	403	1/1	0.94	0.09	135,135,135,135	0
8	CA	G	201	1/1	0.94	0.06	140,140,140,140	0
8	CA	I	410	1/1	0.95	0.06	151,151,151,151	0
8	CA	J	402	1/1	0.95	0.09	137,137,137,137	0
8	CA	I	411	1/1	0.95	0.03	153,153,153,153	0
8	CA	I	404	1/1	0.96	0.12	139,139,139,139	0

6.5 Other polymers [i](#)

There are no such residues in this entry.