Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:54 pm BST

PDB ID	:	5NL0
Title	:	Crystal structure of a 197-bp palindromic 601L nucleosome in complex with linker histone H1
Authors	:	Garcia-Saez, I.; Petosa, C.; Dimitrov, S.
Deposited on	:	2017-04-03
Resolution	:	5.40 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 following versions of software and data (see references ⓘ) were used in the production of this report:

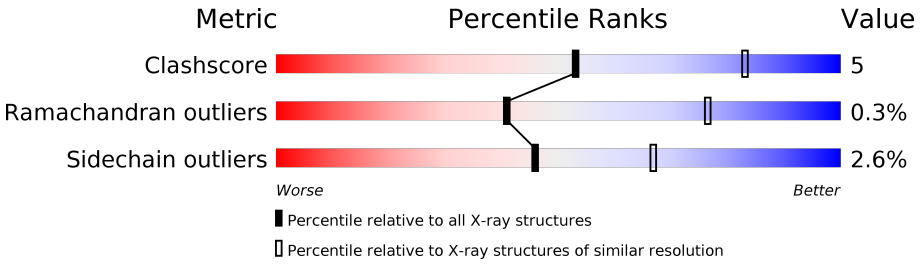
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.40 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))
Clashscore	141614	1016 (6.92-3.86)
Ramachandran outliers	138981	1210 (7.00-3.80)
Sidechain outliers	138945	1181 (7.00-3.80)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	135	64% 8% 27%
1	E	135	56% 16% 28%
1	K	135	63% 10% 27%
2	B	102	72% 10% 19%
2	F	102	72% 10% 19%
2	L	102	75% 7% 19%
3	C	129	66% 15% • 19%
3	G	129	64% 15% • 20%
3	M	129	68% 12% • 19%

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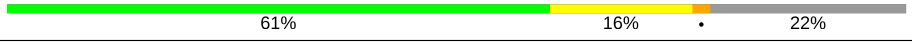
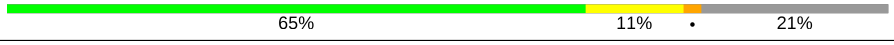
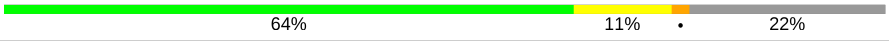
Mol	Chain	Length	Quality of chain
4	D	122	
4	H	122	
4	N	122	
5	I	197	
5	S	197	
6	J	197	
6	T	197	
7	Z	196	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21492 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 H3.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			808	509	156	140	3			
1	E	97	Total	C	N	O	S	0	0	0
			802	506	155	138	3			
1	K	98	Total	C	N	O	S	0	0	0
			808	509	156	140	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	engineered mutation	UNP P84233
E	102	ALA	GLY	engineered mutation	UNP P84233
K	102	ALA	GLY	engineered mutation	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	83	Total	C	N	O	S	0	0	0
			662	418	129	114	1			
2	F	83	Total	C	N	O	S	0	0	0
			662	418	129	114	1			
2	L	83	Total	C	N	O	S	0	0	0
			662	418	129	114	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	105	Total	C	N	O	0	0	0
			809	510	158	141			
3	G	103	Total	C	N	O	0	0	0
			795	501	155	139			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	105	Total	C	N	O	0	0	0
			809	510	158	141			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	conflict	UNP P06897
C	123	SER	ALA	conflict	UNP P06897
G	99	ARG	GLY	conflict	UNP P06897
G	123	SER	ALA	conflict	UNP P06897
M	99	ARG	GLY	conflict	UNP P06897
M	123	SER	ALA	conflict	UNP P06897

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	95	Total	C	N	O	S	0	0	0
			746	469	136	139	2			
4	H	96	Total	C	N	O	S	0	0	0
			756	475	138	141	2			
4	N	95	Total	C	N	O	S	0	0	0
			746	469	136	139	2			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	engineered mutation	UNP P02281
H	29	THR	SER	engineered mutation	UNP P02281
N	29	THR	SER	engineered mutation	UNP P02281

- Molecule 5 is a DNA chain called DNA (197-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	193	Total	C	N	O	P	0	0	0
			3957	1879	728	1157	193			
5	S	96	Total	C	N	O	P	0	0	0
			1966	933	366	571	96			

- Molecule 6 is a DNA chain called DNA (197-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	193	Total	C	N	O	P	0	0	0
			3956	1879	725	1159	193			
6	T	97	Total	C	N	O	P	0	0	0
			1990	946	359	588	97			

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

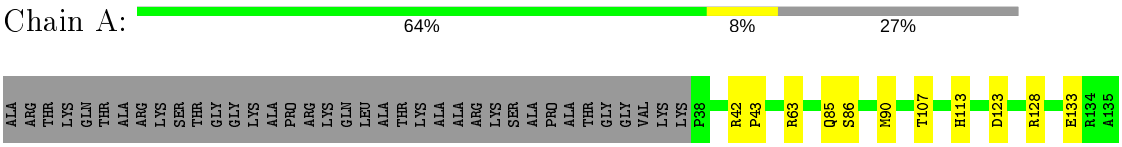
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	Z	73	Total	C	N	O	S	0	0	0
			558	347	106	104	1			

3 Residue-property plots (i)

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

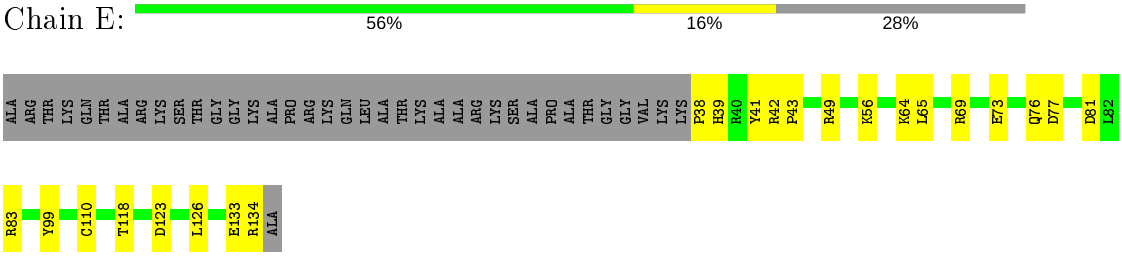
- Molecule 1: Histone H3.2

Chain A:



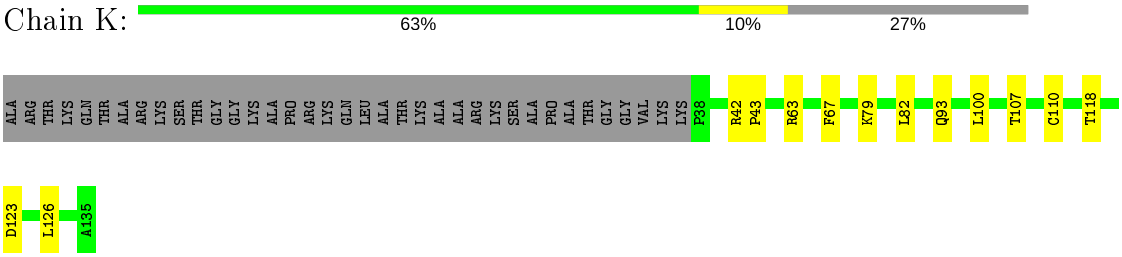
- Molecule 1: Histone H3.2

Chain E:



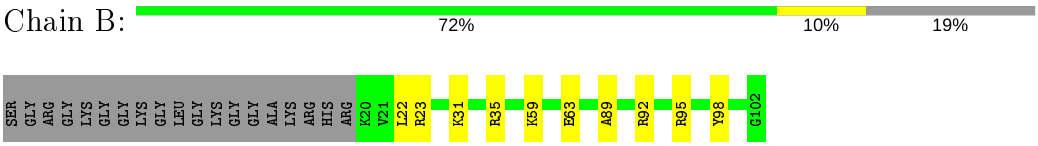
- Molecule 1: Histone H3.2

Chain K:



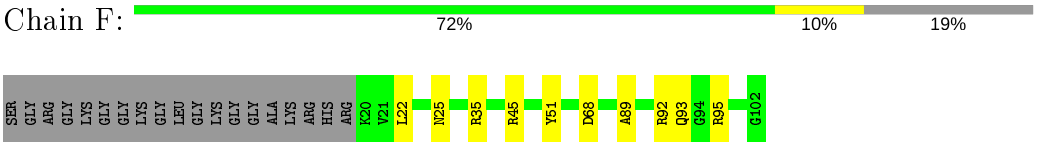
- Molecule 2: Histone H4

Chain B:



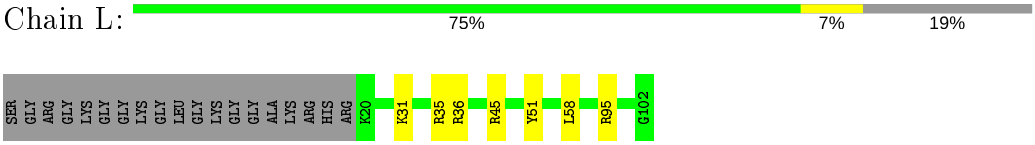
- Molecule 2: Histone H4

Chain F:



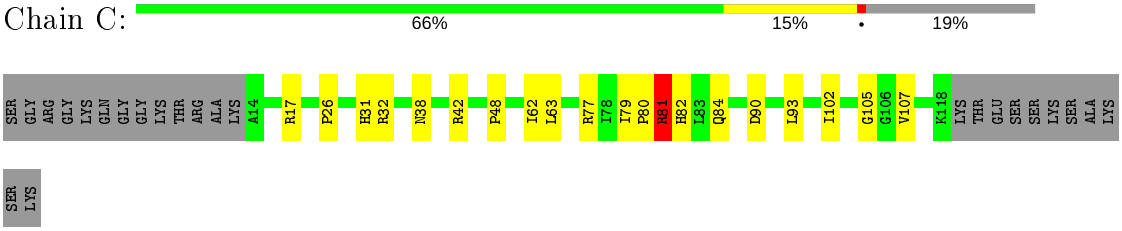
• Molecule 2: Histone H4

Chain L:



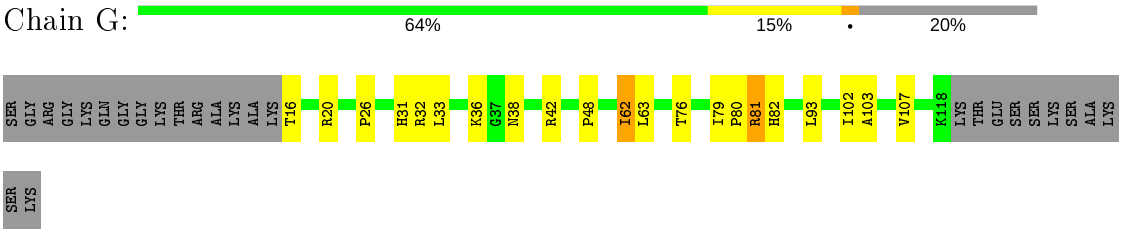
• Molecule 3: Histone H2A type 1

Chain C:



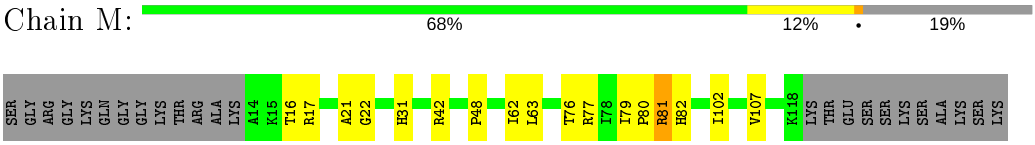
• Molecule 3: Histone H2A type 1

Chain G:



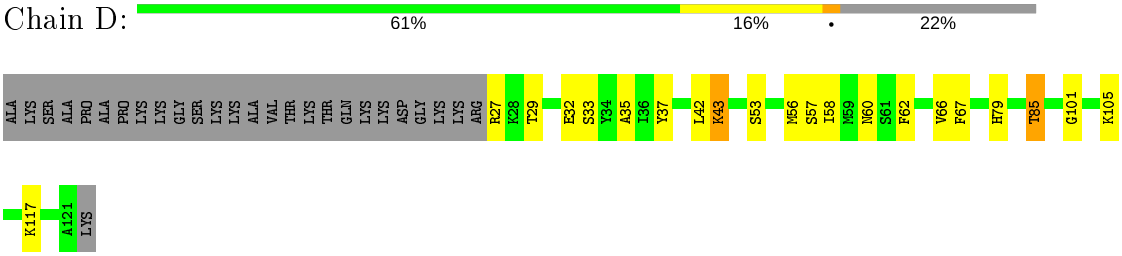
• Molecule 3: Histone H2A type 1

Chain M:



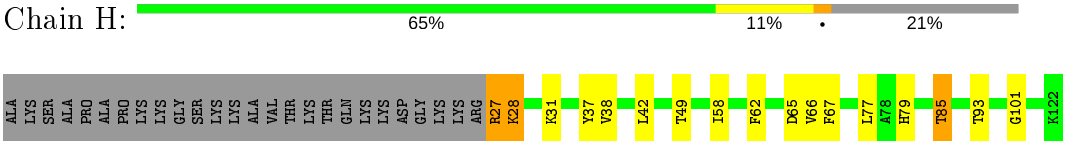
• Molecule 4: Histone H2B 1.1

Chain D:



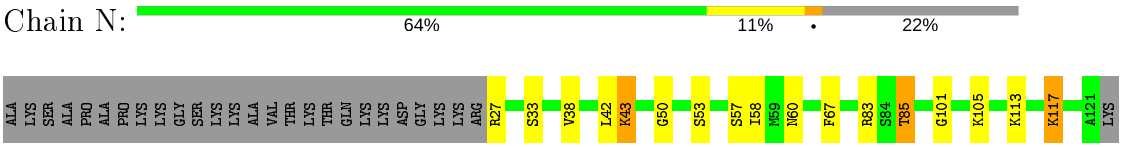
• Molecule 4: Histone H2B 1.1

Chain H:



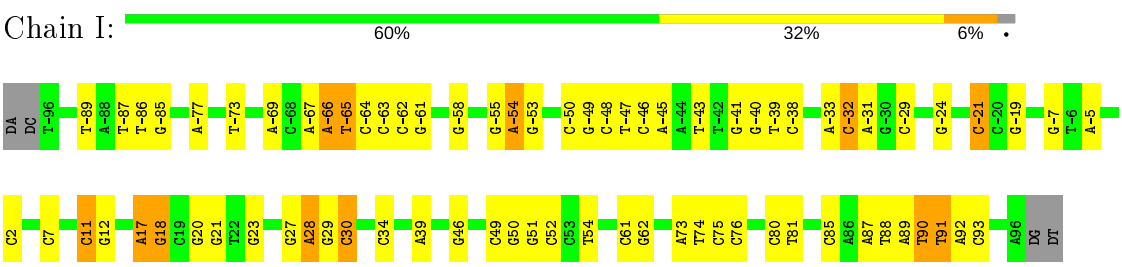
• Molecule 4: Histone H2B 1.1

Chain N:



• Molecule 5: DNA (197-MER)

Chain I:



• Molecule 5: DNA (197-MER)

Chain S:

• Molecule 6: DNA (197-MER)

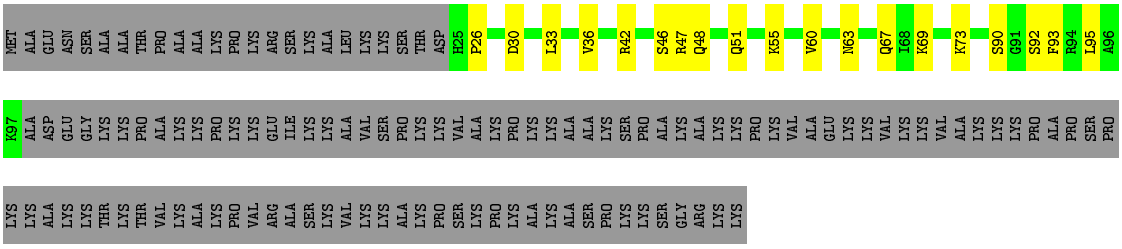
Chain J:

• Molecule 6: DNA (197-MER)

Chain T:

• Molecule 7: Histone H1.0-B

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	61.73Å 405.74Å 348.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.13 – 5.40 49.13 – 5.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.13-5.40) 99.3 (49.13-5.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 5.39Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.240 , 0.265 0.242 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	223.0	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 183.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	21492	wwPDB-VP
Average B, all atoms (Å^2)	308.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

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	A	0.28	0/820	0.43	0/1099
1	E	0.52	0/814	0.96	5/1092 (0.5%)
1	K	0.38	0/820	0.51	0/1099
2	B	0.36	0/669	0.59	0/894
2	F	0.45	0/669	0.73	0/894
2	L	0.35	0/669	0.60	0/894
3	C	0.41	0/819	0.65	1/1106 (0.1%)
3	G	0.48	0/805	0.86	0/1088
3	M	0.36	0/819	0.60	0/1106
4	D	0.44	0/757	0.61	0/1018
4	H	0.47	0/767	0.67	1/1029 (0.1%)
4	N	0.35	0/757	0.57	0/1018
5	I	0.90	16/4439 (0.4%)	1.33	31/6849 (0.5%)
5	S	0.74	0/2206	1.29	10/3401 (0.3%)
6	J	0.86	11/4437 (0.2%)	1.30	29/6846 (0.4%)
6	T	0.70	0/2230	1.28	13/3441 (0.4%)
7	Z	0.38	0/564	0.66	0/750
All	All	0.68	27/23061 (0.1%)	1.10	90/33624 (0.3%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	79	DG	C3'-O3'	-7.21	1.34	1.44
5	I	88	DT	C3'-O3'	-7.19	1.34	1.44
5	I	91	DT	C3'-O3'	-6.82	1.35	1.44
5	I	89	DA	C3'-O3'	6.81	1.52	1.44
6	J	-78	DT	C1'-N1	6.23	1.57	1.49
6	J	-89	DT	C1'-N1	6.20	1.57	1.49
5	I	-69	DA	C3'-O3'	-5.98	1.36	1.44
6	J	-77	DA	C3'-O3'	5.95	1.51	1.44
6	J	82	DG	C3'-O3'	-5.87	1.36	1.44
6	J	-93	DG	C3'-O3'	-5.83	1.36	1.44
6	J	-78	DT	C3'-O3'	5.83	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	90	DT	C5'-C4'	5.81	1.57	1.51
5	I	87	DA	C3'-O3'	-5.80	1.36	1.44
5	I	-85	DG	C3'-O3'	-5.69	1.36	1.44
5	I	75	DC	C1'-N1	-5.54	1.39	1.47
6	J	-94	DC	C3'-O3'	-5.53	1.36	1.44
5	I	92	DA	C3'-O3'	-5.39	1.36	1.44
5	I	-86	DT	C1'-N1	5.34	1.56	1.49
5	I	-77	DA	C3'-O3'	-5.33	1.37	1.44
5	I	85	DC	C3'-O3'	-5.24	1.37	1.44
6	J	88	DT	C1'-N1	5.24	1.56	1.49
5	I	-87	DT	C1'-N1	5.21	1.56	1.49
5	I	-73	DT	C1'-N1	5.14	1.55	1.49
6	J	90	DT	C1'-N1	5.12	1.55	1.49
5	I	-89	DT	C1'-N1	5.07	1.55	1.49
6	J	72	DT	C1'-N1	5.04	1.55	1.49
5	I	90	DT	C1'-N1	-5.03	1.40	1.47

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	21	DG	O4'-C1'-N9	9.66	114.76	108.00
1	E	81	ASP	CB-CG-OD2	8.15	125.64	118.30
6	J	54	DT	P-O3'-C3'	7.97	129.26	119.70
6	T	54	DT	P-O3'-C3'	7.89	129.17	119.70
1	E	81	ASP	CB-CG-OD1	-7.63	111.43	118.30
5	I	-58	DG	P-O3'-C3'	7.61	128.83	119.70
5	I	54	DT	P-O3'-C3'	7.56	128.77	119.70
5	S	-58	DG	P-O3'-C3'	7.53	128.73	119.70
6	J	-2	DG	O4'-C1'-N9	7.44	113.21	108.00
6	J	-10	DC	O4'-C1'-N1	7.33	113.13	108.00
5	I	75	DC	O4'-C1'-N1	7.32	113.12	108.00
5	I	20	DG	P-O3'-C3'	7.22	128.36	119.70
6	J	-77	DA	O5'-P-OP2	-7.19	99.23	105.70
5	S	-32	DC	O4'-C1'-N1	7.11	112.98	108.00
5	I	-32	DC	O4'-C1'-N1	6.99	112.89	108.00
5	I	34	DC	P-O3'-C3'	6.90	127.98	119.70
6	T	43	DA	P-O3'-C3'	6.81	127.87	119.70
6	J	43	DA	P-O3'-C3'	6.80	127.86	119.70
5	I	93	DC	O5'-P-OP1	6.77	118.83	110.70
5	I	29	DG	C3'-C2'-C1'	-6.77	94.38	102.50
5	I	-33	DA	P-O3'-C3'	6.73	127.78	119.70
6	J	42	DA	P-O3'-C3'	6.66	127.70	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	S	-33	DA	P-O3'-C3'	6.65	127.68	119.70
6	T	42	DA	P-O3'-C3'	6.59	127.61	119.70
1	E	69	ARG	NE-CZ-NH1	6.55	123.58	120.30
6	T	57	DG	P-O3'-C3'	6.54	127.55	119.70
6	J	57	DG	P-O3'-C3'	6.53	127.54	119.70
5	S	-38	DC	P-O3'-C3'	6.47	127.46	119.70
5	I	30	DC	O4'-C1'-N1	6.45	112.52	108.00
6	J	23	DG	P-O3'-C3'	6.42	127.40	119.70
6	T	23	DG	P-O3'-C3'	6.41	127.39	119.70
5	I	-38	DC	P-O3'-C3'	6.39	127.37	119.70
6	J	-32	DC	O4'-C1'-N1	6.38	112.47	108.00
6	J	-38	DC	P-O3'-C3'	6.29	127.25	119.70
5	I	-41	DG	P-O3'-C3'	6.21	127.15	119.70
4	H	27	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	E	69	ARG	CD-NE-CZ	6.16	132.23	123.60
6	J	-14	DA	P-O3'-C3'	6.16	127.09	119.70
6	J	16	DA	O4'-C1'-N9	6.15	112.31	108.00
5	S	-41	DG	P-O3'-C3'	6.14	127.07	119.70
6	T	16	DA	O4'-C1'-N9	6.13	112.29	108.00
6	T	72	DT	O4'-C1'-N1	6.13	112.29	108.00
5	I	11	DC	O4'-C1'-N1	6.11	112.28	108.00
6	J	30	DC	O4'-C1'-N1	6.08	112.26	108.00
6	J	-76	DG	O4'-C1'-N9	6.04	112.23	108.00
6	T	30	DC	O4'-C1'-N1	6.04	112.23	108.00
5	S	-29	DC	P-O3'-C3'	5.96	126.85	119.70
5	I	17	DA	O4'-C1'-N9	-5.96	103.83	108.00
5	I	-29	DC	P-O3'-C3'	5.95	126.84	119.70
6	J	-13	DA	P-O3'-C3'	5.95	126.84	119.70
5	I	75	DC	C6-N1-C2	5.86	122.64	120.30
5	I	7	DC	O4'-C1'-N1	5.85	112.09	108.00
5	I	-21	DC	P-O3'-C3'	5.82	126.69	119.70
5	S	-21	DC	P-O3'-C3'	5.77	126.62	119.70
5	I	18	DG	P-O3'-C3'	5.71	126.55	119.70
6	J	-21	DC	O4'-C1'-N1	5.64	111.95	108.00
6	J	-65	DT	N3-C4-O4	5.64	123.28	119.90
6	J	-51	DC	P-O3'-C3'	5.61	126.44	119.70
5	I	23	DG	P-O3'-C3'	5.61	126.43	119.70
6	J	-11	DG	O4'-C1'-N9	5.52	111.86	108.00
5	I	93	DC	O4'-C1'-N1	-5.49	104.15	108.00
5	I	75	DC	C3'-C2'-C1'	-5.37	96.06	102.50
5	I	-66	DA	OP1-P-O3'	5.35	116.97	105.20
6	J	-8	DC	O4'-C1'-N1	5.34	111.74	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	-65	DT	C5-C4-O4	-5.33	121.17	124.90
5	I	-21	DC	O4'-C1'-N1	5.29	111.70	108.00
5	I	-65	DT	P-O3'-C3'	5.28	126.04	119.70
5	S	-21	DC	O4'-C1'-N1	5.28	111.70	108.00
6	J	-49	DG	O4'-C1'-N9	5.27	111.69	108.00
6	J	-91	DA	C3'-C2'-C1'	-5.26	96.19	102.50
1	E	42	ARG	CG-CD-NE	5.23	122.78	111.80
5	I	28	DA	P-O3'-C3'	5.21	125.95	119.70
6	J	-13	DA	O5'-P-OP2	-5.18	101.04	105.70
5	S	-53	DG	C1'-O4'-C4'	-5.17	104.94	110.10
5	I	-53	DG	C1'-O4'-C4'	-5.13	104.97	110.10
6	J	1	DT	P-O3'-C3'	5.10	125.82	119.70
5	S	-54	DA	P-O3'-C3'	5.09	125.81	119.70
5	I	76	DC	O4'-C1'-N1	5.09	111.56	108.00
6	T	1	DT	P-O3'-C3'	5.09	125.81	119.70
6	T	44	DT	O4'-C1'-N1	5.09	111.56	108.00
3	C	81	ARG	NE-CZ-NH2	-5.09	117.76	120.30
5	I	-54	DA	P-O3'-C3'	5.09	125.80	119.70
6	J	44	DT	O4'-C1'-N1	5.07	111.55	108.00
5	I	90	DT	O4'-C1'-N1	5.05	111.54	108.00
6	J	-49	DG	O4'-C1'-C2'	-5.05	101.86	105.90
6	T	29	DG	O4'-C1'-N9	5.04	111.53	108.00
6	J	-23	DC	C1'-O4'-C4'	-5.04	105.06	110.10
6	T	12	DG	O4'-C1'-N9	5.03	111.52	108.00
6	J	29	DG	O4'-C1'-N9	5.01	111.51	108.00
6	T	88	DT	P-O3'-C3'	5.01	125.71	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	808	0	846	10	0
1	E	802	0	841	23	0
1	K	808	0	846	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	662	0	709	6	0
2	F	662	0	709	9	0
2	L	662	0	709	6	0
3	C	809	0	864	16	0
3	G	795	0	846	21	1
3	M	809	0	864	28	0
4	D	746	0	773	16	1
4	H	756	0	786	15	0
4	N	746	0	773	22	1
5	I	3957	0	2169	39	0
5	S	1966	0	1077	24	1
6	J	3956	0	2170	28	0
6	T	1990	0	1094	15	1
7	Z	558	0	587	13	0
All	All	21492	0	16663	206	3

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 5.

All (206) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:PRO:HG2	6:J:-5:DA:H5'	1.41	0.98
3:C:63:LEU:HD13	4:D:42:LEU:HB2	1.57	0.85
1:E:73:GLU:OE1	2:F:25:ASN:HB2	1.75	0.84
3:M:21:ALA:C	4:N:117:LYS:HE3	1.96	0.84
4:N:27:ARG:HE	6:T:51:DG:H5"	1.46	0.81
3:M:63:LEU:HD13	4:N:42:LEU:HB2	1.62	0.80
3:G:76:THR:O	4:H:49:THR:HG23	1.86	0.75
1:E:43:PRO:HG2	6:J:-5:DA:C5'	2.18	0.74
2:L:31:LYS:HE3	2:L:35:ARG:HH21	1.54	0.72
1:E:43:PRO:CG	6:J:-5:DA:H5'	2.18	0.71
2:B:31:LYS:HE3	2:B:35:ARG:HH21	1.55	0.71
3:C:102:ILE:HG23	4:D:58:ILE:HD13	1.72	0.70
4:D:29:THR:OG1	5:I:30:DC:OP1	2.02	0.69
5:I:2:DC:H5"	7:Z:90:SER:HB3	1.75	0.68
3:M:42:ARG:NH1	4:N:85:THR:OG1	2.28	0.67
6:J:-65:DT:H1'	6:J:-64:DC:H5'	1.78	0.66
2:F:68:ASP:OD2	2:F:92:ARG:NH1	2.28	0.66
5:I:11:DC:H2"	5:I:12:DG:C8	2.30	0.66
3:M:21:ALA:CA	4:N:117:LYS:HE3	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:50:DG:H2"	6:J:51:DG:OP2	1.97	0.65
3:G:42:ARG:NH1	4:H:85:THR:OG1	2.29	0.65
3:G:31:HIS:CD2	3:G:48:PRO:HG3	2.32	0.65
3:M:21:ALA:C	4:N:117:LYS:CE	2.65	0.64
6:T:49:DC:H2'	6:T:50:DG:C8	2.32	0.64
7:Z:42:ARG:O	7:Z:42:ARG:HD2	1.97	0.64
6:T:50:DG:H2"	6:T:51:DG:OP2	1.96	0.64
3:C:38:ASN:OD1	4:H:79:HIS:NE2	2.32	0.63
6:J:49:DC:H2'	6:J:50:DG:C8	2.32	0.63
3:M:102:ILE:HG23	4:N:58:ILE:HD13	1.80	0.63
1:E:65:LEU:HD22	5:I:17:DA:H2'	1.80	0.62
7:Z:47:ARG:HH21	7:Z:69:LYS:HB2	1.64	0.62
1:K:42:ARG:HH21	5:S:-5:DA:P	2.23	0.62
3:M:80:PRO:HB3	4:N:58:ILE:CD1	2.30	0.61
3:M:79:ILE:HG12	3:M:82:HIS:CE1	2.34	0.61
3:M:77:ARG:NE	5:S:-54:DA:H4'	2.14	0.61
1:A:113:HIS:NE2	1:E:123:ASP:OD1	2.34	0.61
5:I:61:DC:H2"	5:I:62:DG:C8	2.36	0.61
2:F:35:ARG:NH2	2:F:51:TYR:OH	2.34	0.60
1:E:56:LYS:NZ	5:I:-64:DC:OP1	2.23	0.60
1:K:43:PRO:HG2	5:S:-5:DA:H5'	1.84	0.60
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.37	0.59
3:M:63:LEU:HD11	4:N:38:VAL:HG13	1.84	0.58
3:C:80:PRO:HB3	4:D:58:ILE:HD12	1.85	0.58
3:M:16:THR:HA	5:S:-43:DT:H5"	1.84	0.58
4:N:27:ARG:NE	6:T:51:DG:H5"	2.16	0.58
1:E:64:LYS:HB2	5:I:18:DG:OP2	2.03	0.58
3:G:102:ILE:HG23	4:H:58:ILE:HD13	1.85	0.57
3:G:42:ARG:HG2	5:I:39:DA:H5"	1.86	0.57
3:G:80:PRO:HB3	4:H:58:ILE:CD1	2.35	0.57
2:F:68:ASP:OD2	2:F:93:GLN:NE2	2.37	0.56
2:B:98:TYR:OH	4:H:65:ASP:OD2	2.17	0.56
1:E:77:ASP:OD1	2:F:22:LEU:HD12	2.05	0.56
1:A:43:PRO:HG2	5:I:-5:DA:H5'	1.87	0.56
3:C:81:ARG:NH2	3:C:107:VAL:O	2.33	0.56
5:I:51:DG:H1'	5:I:52:DC:H5'	1.88	0.55
3:M:42:ARG:O	4:N:85:THR:HA	2.07	0.55
3:C:32:ARG:NH2	4:D:32:GLU:OE1	2.30	0.55
1:E:49:ARG:HD2	5:I:-66:DA:H4'	1.89	0.55
1:E:49:ARG:NH1	5:I:-66:DA:H5"	2.22	0.55
3:C:80:PRO:HB3	4:D:58:ILE:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:42:ARG:HB2	4:N:85:THR:HG23	1.91	0.53
1:E:133:GLU:O	1:E:134:ARG:HB2	2.06	0.53
1:A:107:THR:HG23	1:A:123:ASP:HB2	1.90	0.53
3:M:22:GLY:N	4:N:117:LYS:HE3	2.24	0.53
2:L:31:LYS:HE3	2:L:35:ARG:NH2	2.23	0.53
1:E:110:CYS:SG	1:E:126:LEU:HD23	2.49	0.52
3:C:42:ARG:NH1	4:D:85:THR:OG1	2.41	0.52
3:G:81:ARG:NH2	3:G:107:VAL:O	2.41	0.52
5:I:-50:DC:H2"	5:I:-49:DG:C8	2.45	0.52
3:M:22:GLY:N	4:N:117:LYS:CE	2.72	0.52
5:S:-50:DC:H2"	5:S:-49:DG:C8	2.44	0.52
3:M:80:PRO:HB3	4:N:58:ILE:HD12	1.92	0.52
5:I:-64:DC:H2"	5:I:-63:DC:C6	2.45	0.52
3:G:36:LYS:O	3:G:36:LYS:HG2	2.09	0.51
4:N:33:SER:OG	4:N:60:ASN:ND2	2.43	0.51
4:D:33:SER:OG	4:D:60:ASN:ND2	2.43	0.51
1:E:99:TYR:OH	1:E:133:GLU:OE1	2.28	0.51
3:G:32:ARG:HH21	3:G:33:LEU:HD21	1.74	0.51
6:J:-66:DA:H2"	6:J:-65:DT:H72	1.92	0.51
3:M:31:HIS:ND1	3:M:48:PRO:HG3	2.26	0.51
3:G:16:THR:O	3:G:20:ARG:HG3	2.11	0.50
3:M:81:ARG:NH2	3:M:107:VAL:O	2.44	0.50
5:S:-7:DG:C6	6:T:6:DA:N6	2.79	0.50
3:C:81:ARG:O	3:C:81:ARG:HG3	2.09	0.50
6:J:-88:DA:H2"	6:J:-87:DT:H72	1.93	0.50
5:I:-7:DG:C6	6:J:6:DA:N6	2.79	0.50
1:K:79:LYS:HB3	1:K:82:LEU:HD11	1.93	0.50
3:M:77:ARG:HE	5:S:-54:DA:H4'	1.76	0.50
5:I:-47:DT:H2"	5:I:-46:DC:C6	2.47	0.49
6:J:-66:DA:H2"	6:J:-65:DT:C7	2.42	0.49
5:I:-40:DG:H2"	5:I:-39:DT:OP2	2.12	0.49
3:C:26:PRO:HG3	4:D:37:TYR:CZ	2.47	0.49
1:E:49:ARG:CZ	5:I:-66:DA:H5"	2.43	0.49
1:E:83:ARG:HH11	6:J:-23:DC:H5"	1.78	0.49
5:S:-40:DG:H2"	5:S:-39:DT:OP2	2.12	0.49
5:I:90:DT:H2"	5:I:91:DT:H71	1.95	0.49
6:J:15:DT:H2"	6:J:16:DA:C8	2.48	0.48
3:M:76:THR:O	4:N:50:GLY:N	2.30	0.48
5:S:-47:DT:H2"	5:S:-46:DC:C6	2.48	0.48
6:T:15:DT:H2"	6:T:16:DA:C8	2.48	0.48
6:J:-91:DA:C6	6:J:-90:DA:C6	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HH21	5:I:-5:DA:P	2.36	0.48
2:B:31:LYS:HE3	2:B:35:ARG:NH2	2.25	0.48
3:G:80:PRO:HB3	4:H:58:ILE:HD12	1.96	0.48
5:I:-32:DC:H2"	5:I:-31:DA:OP2	2.14	0.47
7:Z:33:LEU:HG	7:Z:95:LEU:HD11	1.96	0.47
3:C:31:HIS:ND1	3:C:48:PRO:HG3	2.29	0.47
5:S:-32:DC:H2"	5:S:-31:DA:OP2	2.14	0.47
6:J:2:DC:H4'	7:Z:48:GLN:HG3	1.97	0.47
4:D:43:LYS:HA	4:D:43:LYS:HD3	1.63	0.46
4:N:43:LYS:HA	4:N:43:LYS:HD3	1.63	0.46
5:S:-55:DG:N2	6:T:56:DG:N2	2.64	0.46
7:Z:36:VAL:HG21	7:Z:95:LEU:HG	1.96	0.46
4:D:27:ARG:HE	6:J:51:DG:H5"	1.80	0.46
2:L:35:ARG:NH2	2:L:51:TYR:OH	2.48	0.46
4:D:79:HIS:NE2	3:G:38:ASN:ND2	2.54	0.46
3:G:63:LEU:HD13	4:H:42:LEU:HB2	1.96	0.46
1:K:107:THR:HG23	1:K:123:ASP:HB2	1.98	0.46
6:T:19:DC:H2"	6:T:20:DG:C8	2.51	0.46
6:J:19:DC:H2"	6:J:20:DG:C8	2.51	0.46
1:A:113:HIS:CG	1:E:126:LEU:HD22	2.51	0.46
3:G:81:ARG:HG3	3:G:81:ARG:O	2.13	0.46
5:I:-19:DG:H1	6:J:19:DC:H42	1.63	0.46
1:E:41:TYR:OH	5:I:-67:DA:H4'	2.15	0.46
7:Z:26:PRO:HB2	7:Z:30:ASP:HB2	1.97	0.46
2:B:22:LEU:O	2:B:23:ARG:HG3	2.16	0.46
5:I:-55:DG:N2	6:J:56:DG:N2	2.64	0.46
5:S:-19:DG:H1	6:T:19:DC:H42	1.64	0.45
4:H:28:LYS:NZ	5:I:51:DG:H5"	2.32	0.45
1:K:100:LEU:HD11	2:L:58:LEU:HD13	1.98	0.45
3:M:76:THR:H	6:T:58:DC:P	2.39	0.45
1:E:49:ARG:HG2	5:I:-65:DT:OP1	2.17	0.45
1:A:63:ARG:HA	1:A:63:ARG:HD3	1.69	0.45
5:I:-21:DC:H42	6:J:21:DG:H1	1.63	0.45
3:M:17:ARG:N	5:S:-43:DT:OP1	2.31	0.45
5:S:-21:DC:H42	6:T:21:DG:H1	1.63	0.45
5:I:80:DC:H2"	5:I:81:DT:C5	2.52	0.45
4:N:113:LYS:O	4:N:117:LYS:HB3	2.16	0.44
2:B:59:LYS:HG2	2:B:63:GLU:OE2	2.17	0.44
3:G:62:ILE:HD13	3:G:93:LEU:HD13	1.99	0.44
4:D:35:ALA:HA	4:D:56:MET:SD	2.57	0.44
3:C:77:ARG:NE	5:I:-54:DA:H4'	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:-66:DA:C2'	6:J:-65:DT:H72	2.48	0.44
2:L:36:ARG:HH12	5:S:-13:DA:P	2.40	0.44
4:N:105:LYS:HB2	4:N:105:LYS:HE3	1.81	0.44
5:S:-64:DC:H2"	5:S:-63:DC:C6	2.52	0.44
6:J:-74:DA:H2"	6:J:-73:DT:H72	1.99	0.43
1:K:110:CYS:SG	1:K:126:LEU:HD23	2.58	0.43
5:I:-45:DA:C2	6:J:46:DG:N2	2.87	0.43
7:Z:63:ASN:O	7:Z:67:GLN:HG3	2.18	0.43
4:D:79:HIS:CE1	3:G:38:ASN:HD22	2.35	0.43
6:J:-25:DA:H1'	6:J:-24:DG:C8	2.53	0.43
3:M:22:GLY:N	4:N:117:LYS:HE2	2.32	0.43
3:M:17:ARG:HG3	5:S:-43:DT:P	2.59	0.43
1:A:86:SER:O	1:A:90:MET:HG2	2.18	0.43
5:I:27:DG:N2	5:I:28:DA:C2	2.87	0.43
5:I:2:DC:C5'	7:Z:90:SER:HB3	2.43	0.43
3:M:42:ARG:NH1	5:S:-35:DA:H4'	2.34	0.43
6:T:7:DC:H2'	6:T:8:DG:C8	2.54	0.43
5:S:-45:DA:C2	6:T:46:DG:N2	2.87	0.42
5:S:-90:DA:H2"	5:S:-89:DT:H72	2.01	0.42
3:C:84:GLN:HG2	3:C:105:GLY:O	2.19	0.42
4:N:83:ARG:HG3	5:S:-34:DG:P	2.60	0.42
1:E:76:GLN:HG2	2:F:22:LEU:HD11	2.01	0.42
3:M:79:ILE:HB	3:M:80:PRO:CD	2.50	0.42
5:I:46:DG:N2	6:J:-45:DA:C2	2.88	0.42
6:J:7:DC:H2'	6:J:8:DG:C8	2.54	0.42
1:K:63:ARG:HD3	1:K:63:ARG:HA	1.78	0.42
2:F:45:ARG:CZ	6:J:-4:DC:H4'	2.50	0.41
5:I:-48:DC:C6	5:I:-47:DT:H72	2.55	0.41
3:G:26:PRO:HG3	4:H:37:TYR:CZ	2.55	0.41
4:H:67:PHE:C	4:H:67:PHE:CD2	2.93	0.41
4:D:105:LYS:HB2	4:D:105:LYS:HE3	1.81	0.41
1:A:85:GLN:HA	5:I:-24:DG:O5'	2.20	0.41
5:I:73:DA:H2"	5:I:74:DT:H72	2.02	0.41
6:J:-4:DC:H2"	6:J:-3:DG:C8	2.55	0.41
1:K:67:PHE:CZ	1:K:93:GLN:HA	2.55	0.41
2:F:89:ALA:O	2:F:92:ARG:HB2	2.19	0.41
4:H:77:LEU:HD21	4:H:93:THR:HG21	2.03	0.41
5:S:-48:DC:C6	5:S:-47:DT:H72	2.55	0.41
1:A:128:ARG:HD2	1:A:133:GLU:OE1	2.20	0.41
1:K:118:THR:HA	2:L:45:ARG:HB3	2.02	0.41
7:Z:69:LYS:O	7:Z:73:LYS:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:THR:HA	2:F:45:ARG:HB3	2.03	0.41
3:C:17:ARG:NE	5:I:-43:DT:OP2	2.47	0.41
5:I:-62:DC:H2'	5:I:-61:DG:C8	2.56	0.41
5:S:-72:DA:H2"	5:S:-71:DT:OP2	2.21	0.41
3:G:79:ILE:HG12	3:G:82:HIS:CE1	2.55	0.41
4:D:62:PHE:O	4:D:66:VAL:HG23	2.21	0.41
6:J:1:DT:H1'	6:J:2:DC:H5'	2.03	0.41
3:M:81:ARG:O	3:M:81:ARG:HG3	2.20	0.41
7:Z:46:SER:HA	7:Z:92:SER:HA	2.03	0.41
3:G:76:THR:C	4:H:49:THR:HG23	2.41	0.41
3:M:17:ARG:NE	5:S:-43:DT:OP2	2.46	0.41
5:I:49:DC:H2'	5:I:50:DG:C8	2.56	0.41
2:B:89:ALA:O	2:B:92:ARG:HB2	2.22	0.40
4:H:62:PHE:O	4:H:66:VAL:HG23	2.21	0.40
1:E:38:PRO:HB2	1:E:39:HIS:H	1.73	0.40
3:G:102:ILE:O	3:G:103:ALA:C	2.59	0.40
6:T:1:DT:H1'	6:T:2:DC:H5'	2.03	0.40
7:Z:47:ARG:O	7:Z:51:GLN:HB2	2.21	0.40
7:Z:51:GLN:O	7:Z:55:LYS:HG3	2.21	0.40
3:C:90:ASP:HB3	3:C:93:LEU:HB2	2.02	0.40
1:A:113:HIS:CE1	1:E:123:ASP:OD1	2.74	0.40
3:G:63:LEU:HD11	4:H:38:VAL:HG13	2.04	0.40
6:T:89:DA:H2"	6:T:90:DT:H71	2.03	0.40

All (3) 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:S:-1:DA:O3'	6:T:0:DT:P[3_554]	1.63	0.57
4:D:117:LYS:NZ	3:G:20:ARG:O[1_455]	2.15	0.05
4:N:117:LYS:NZ	4:N:117:LYS:NZ[3_454]	2.16	0.04

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	96/135 (71%)	93 (97%)	3 (3%)	0	100	100
1	E	95/135 (70%)	91 (96%)	4 (4%)	0	100	100
1	K	96/135 (71%)	91 (95%)	5 (5%)	0	100	100
2	B	81/102 (79%)	79 (98%)	2 (2%)	0	100	100
2	F	81/102 (79%)	79 (98%)	2 (2%)	0	100	100
2	L	81/102 (79%)	81 (100%)	0	0	100	100
3	C	103/129 (80%)	96 (93%)	7 (7%)	0	100	100
3	G	101/129 (78%)	94 (93%)	7 (7%)	0	100	100
3	M	103/129 (80%)	96 (93%)	7 (7%)	0	100	100
4	D	93/122 (76%)	87 (94%)	5 (5%)	1 (1%)	14	52
4	H	94/122 (77%)	90 (96%)	3 (3%)	1 (1%)	14	52
4	N	93/122 (76%)	88 (95%)	4 (4%)	1 (1%)	14	52
7	Z	71/196 (36%)	68 (96%)	3 (4%)	0	100	100
All	All	1188/1660 (72%)	1133 (95%)	52 (4%)	3 (0%)	41	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	101	GLY
4	H	101	GLY
4	N	101	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/110 (77%)	85 (100%)	0	100	100
1	E	85/110 (77%)	85 (100%)	0	100	100
1	K	85/110 (77%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	68/78 (87%)	67 (98%)	1 (2%)	65 80
2	F	68/78 (87%)	67 (98%)	1 (2%)	65 80
2	L	68/78 (87%)	67 (98%)	1 (2%)	65 80
3	C	83/101 (82%)	81 (98%)	2 (2%)	49 69
3	G	82/101 (81%)	80 (98%)	2 (2%)	49 69
3	M	83/101 (82%)	81 (98%)	2 (2%)	49 69
4	D	81/102 (79%)	76 (94%)	5 (6%)	18 45
4	H	82/102 (80%)	78 (95%)	4 (5%)	25 51
4	N	81/102 (79%)	75 (93%)	6 (7%)	13 40
7	Z	60/158 (38%)	58 (97%)	2 (3%)	38 61
All	All	1011/1331 (76%)	985 (97%)	26 (3%)	46 67

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	95	ARG
3	C	62	ILE
3	C	81	ARG
4	D	43	LYS
4	D	53	SER
4	D	57	SER
4	D	67	PHE
4	D	85	THR
2	F	95	ARG
3	G	62	ILE
3	G	81	ARG
4	H	27	ARG
4	H	28	LYS
4	H	31	LYS
4	H	85	THR
2	L	95	ARG
3	M	62	ILE
3	M	81	ARG
4	N	43	LYS
4	N	53	SER
4	N	57	SER
4	N	67	PHE
4	N	85	THR

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Mol	Chain	Res	Type
4	N	117	LYS
7	Z	60	VAL
7	Z	93	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	60	ASN
4	N	60	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.