



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:10 PM UTC

PDB ID : 5NL0 / pdb_00005nl0
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 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

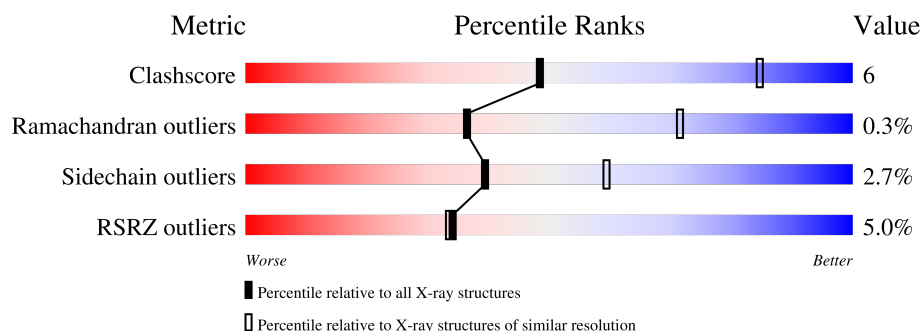
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



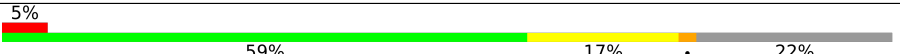
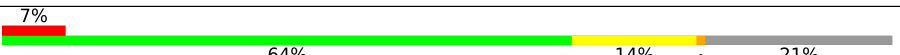
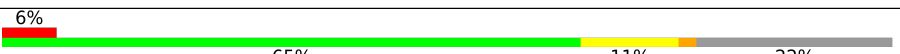
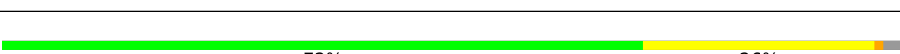
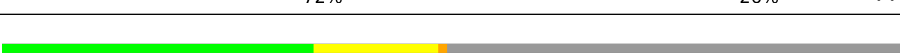
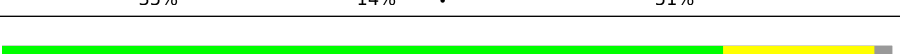
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1117 (6.80-4.00)
Ramachandran outliers	187476	1020 (6.80-3.96)
Sidechain outliers	187428	1019 (6.86-3.94)
RSRZ outliers	180081	1053 (6.80-4.00)

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	135	3% 64% 9% 27%
1	E	135	4% 55% 16% 28%
1	K	135	8% 61% 11% 27%
2	B	102	4% 72% 10% 19%
2	F	102	11% 72% 10% 19%
2	L	102	8% 75% 6% 19%

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Mol	Chain	Length	Quality of chain
3	C	129	
3	G	129	
3	M	129	
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			

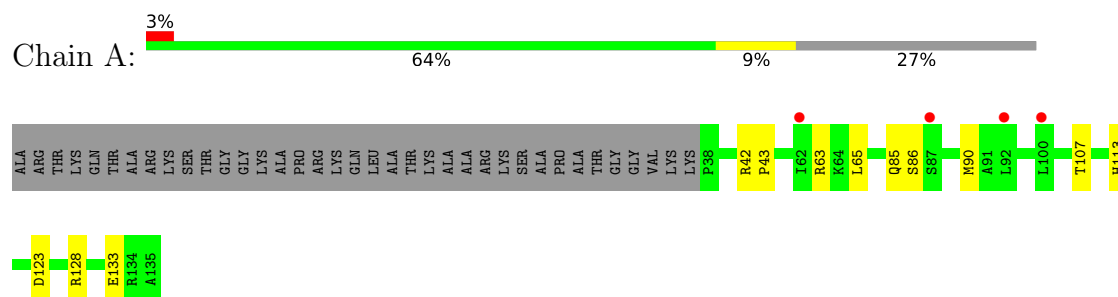
- Molecule 7 is a protein called Histone H1.0-B.

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

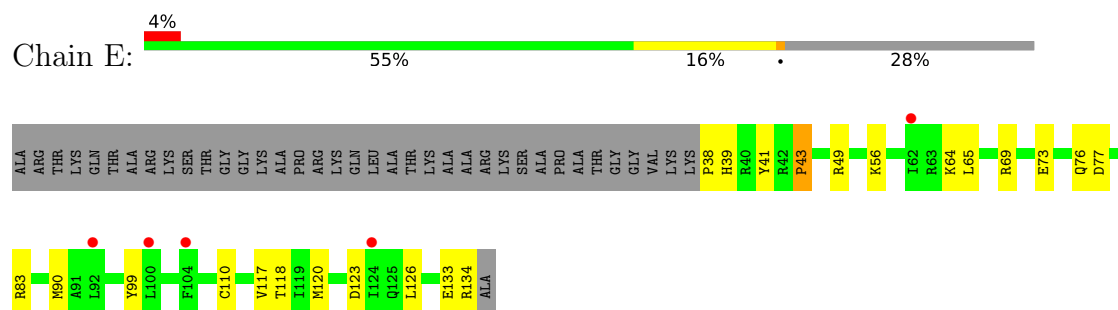
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

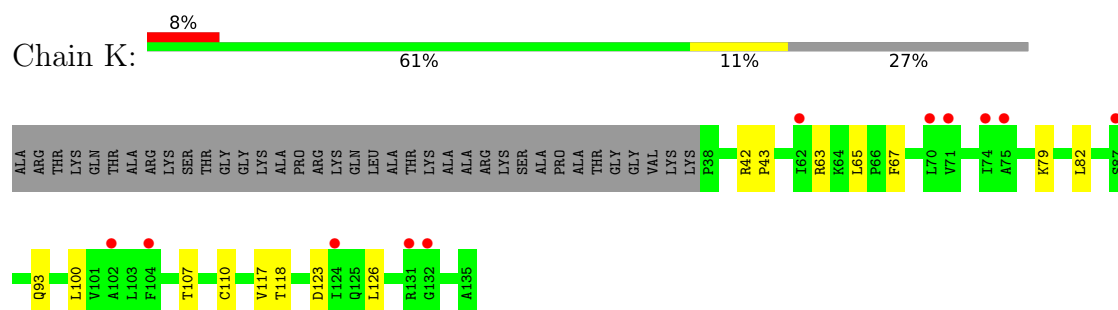
- Molecule 1: Histone H3.2



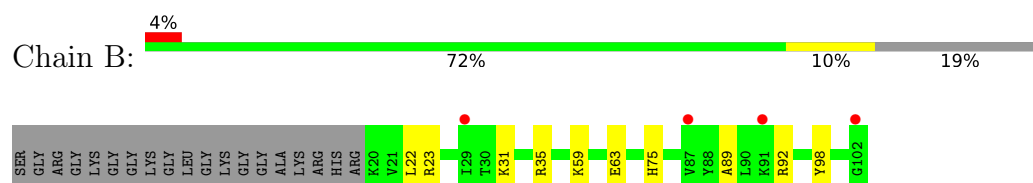
- Molecule 1: Histone H3.2



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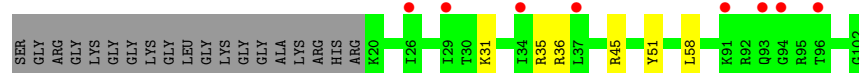
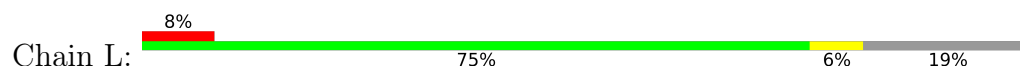
- Molecule 2: Histone H4



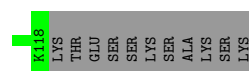
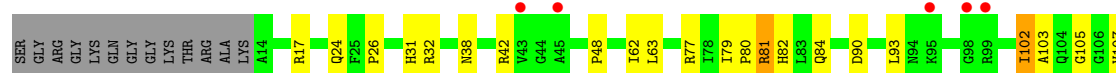
- Molecule 2: Histone H4



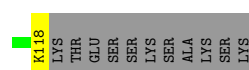
- Molecule 2: Histone H4



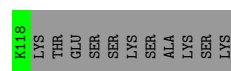
- Molecule 3: Histone H2A type 1



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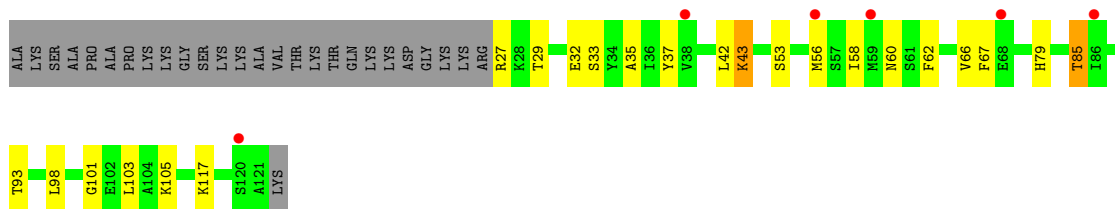


- Molecule 3: Histone H2A type 1

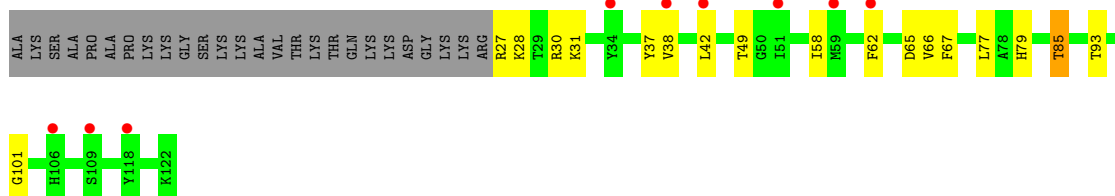


- Molecule 4: Histone H2B 1.1

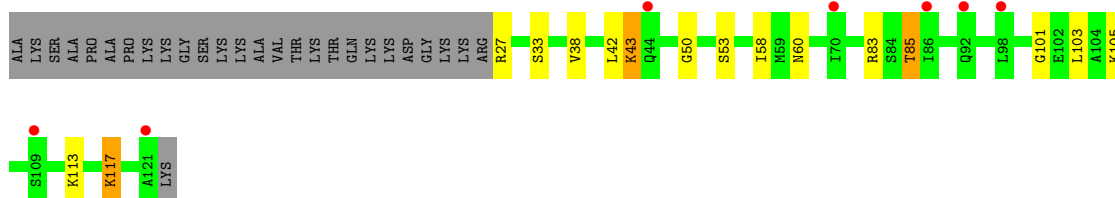




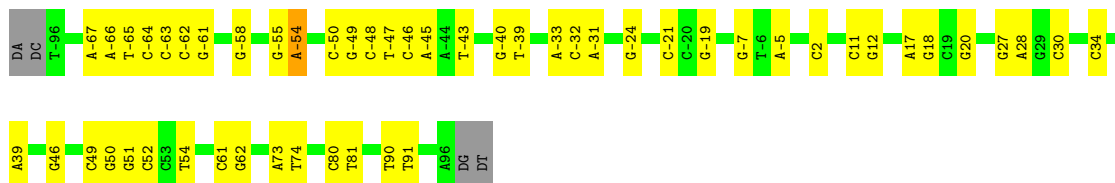
- Molecule 4: Histone H2B 1.1



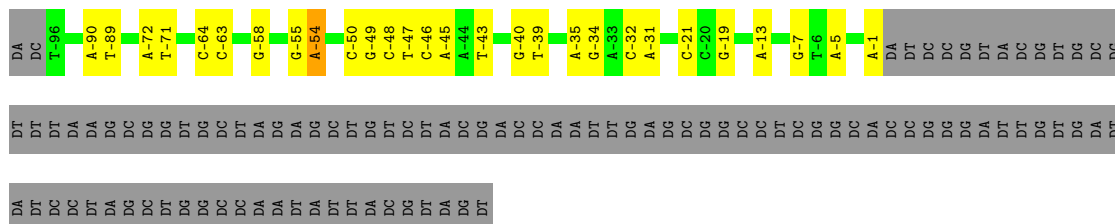
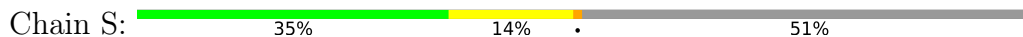
- Molecule 4: Histone H2B 1.1



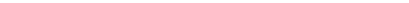
- Molecule 5: DNA (197-MER)

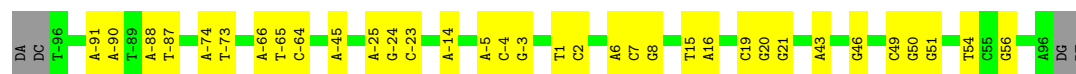


- Molecule 5: DNA (197-MER)

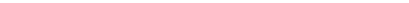


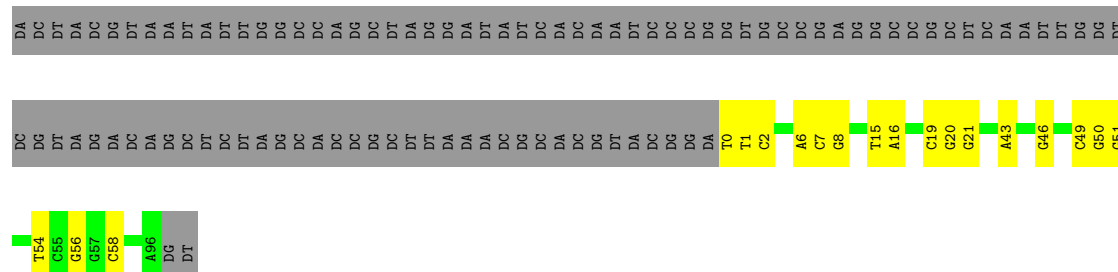
- Molecule 6: DNA (197-MER)

Chain J:  81% 17% .



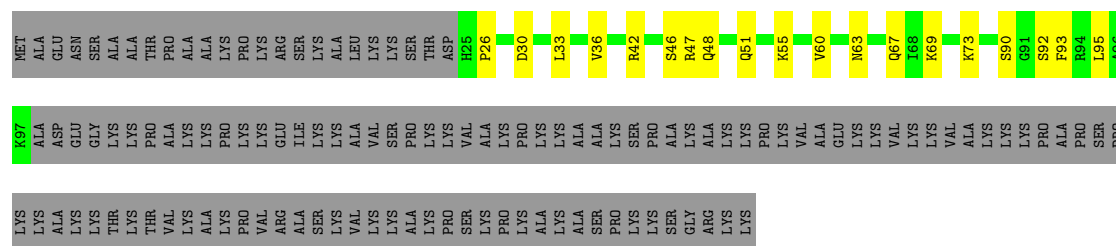
- Molecule 6: DNA (197-MER)

Chain T:  40% 10% 51%



- Molecule 7: Histone H1.0-B

Chain Z: 28% 10% 63%



4 Data and refinement statistics

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) 99.1 (49.13-5.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.25 , 184.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.19	0/820	0.44	0/1099
1	E	0.56	0/814	0.98	2/1092 (0.2%)
1	K	0.32	0/820	0.55	0/1099
2	B	0.34	0/669	0.63	0/894
2	F	0.41	0/669	0.79	0/894
2	L	0.34	0/669	0.65	0/894
3	C	0.39	1/819 (0.1%)	0.67	0/1106
3	G	0.47	0/805	0.96	2/1088 (0.2%)
3	M	0.34	0/819	0.68	0/1106
4	D	0.40	0/757	0.74	1/1018 (0.1%)
4	H	0.58	0/767	0.97	1/1029 (0.1%)
4	N	0.32	0/757	0.68	0/1018
5	I	0.40	0/4439	0.90	6/6849 (0.1%)
5	S	0.29	0/2206	0.86	2/3401 (0.1%)
6	J	0.37	0/4437	0.86	3/6846 (0.0%)
6	T	0.28	0/2230	0.83	2/3441 (0.1%)
7	Z	0.38	0/564	0.79	0/750
All	All	0.37	1/23061 (0.0%)	0.83	19/33624 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	24	GLN	C-N	5.47	1.44	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	30	ARG	N-CA-C	7.43	120.37	108.41
6	J	54	DT	P-O3'-C3'	6.04	129.26	120.20
6	T	54	DT	P-O3'-C3'	5.98	129.17	120.20
4	D	98	LEU	N-CA-C	5.93	118.63	111.40
5	I	-58	DG	P-O3'-C3'	5.76	128.83	120.20
5	I	54	DT	P-O3'-C3'	5.72	128.77	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	-58	DG	P-O3'-C3'	5.69	128.73	120.20
1	E	69	ARG	CD-NE-CZ	5.59	132.23	124.40
1	E	43	PRO	CB-CA-C	5.55	118.92	111.71
3	G	97	LEU	CD1-CG-CD2	-5.55	98.60	110.80
5	S	-54	DA	C4'-C3'-O3'	-5.50	101.75	110.00
5	I	-54	DA	C4'-C3'-O3'	-5.50	101.75	110.00
5	I	20	DG	P-O3'-C3'	5.44	128.36	120.20
6	J	-14	DA	C4'-C3'-O3'	-5.20	102.20	110.00
5	I	34	DC	P-O3'-C3'	5.19	127.98	120.20
6	T	43	DA	P-O3'-C3'	5.12	127.87	120.20
6	J	43	DA	P-O3'-C3'	5.11	127.86	120.20
5	I	-33	DA	P-O3'-C3'	5.05	127.78	120.20
3	G	118	LYS	CG-CD-CE	-5.04	99.71	111.30

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	25	0
1	K	808	0	846	9	0
2	B	662	0	709	7	0
2	F	662	0	709	10	0
2	L	662	0	709	6	0
3	C	809	0	864	18	0
3	G	795	0	846	21	1
3	M	809	0	864	28	0
4	D	746	0	773	18	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	14	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	Z	558	0	587	13	0
All	All	21492	0	16663	211	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 6.

All (211) 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:M:21:ALA:C	4:N:117:LYS:HE3	1.96	0.88
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
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
3:M:21:ALA:C	4:N:117:LYS:CE	2.65	0.69
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
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
6:T:49:DC:H2'	6:T:50:DG:C8	2.32	0.64
7:Z:42:ARG:HD2	7:Z:42:ARG:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:56:LYS:NZ	5:I:-64:DC:OP1	2.23	0.60
2:F:35:ARG:NH2	2:F:51:TYR:OH	2.34	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
1:E:64:LYS:HD2	1:E:90:MET:HE1	1.88	0.55
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
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
3:M:31:HIS:HD1	3:M:48:PRO:HG3	1.74	0.52
5:S:-50:DC:H2''	5:S:-49:DG:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:E:99:TYR:OH	1:E:133:GLU:OE1	2.28	0.49
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
3:C:31:HIS:HD1	3:C:48:PRO:HG3	1.78	0.48
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:H:67:PHE:C	4:H:67:PHE:CD2	2.93	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:O	3:G:81:ARG:HG3	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
3:G:76:THR:C	4:H:49:THR:HG23	2.41	0.45
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
3:G:102:ILE:O	3:G:103:ALA:C	2.59	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
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:HE3	4:N:105:LYS:HB2	1.81	0.44
5:S:-64:DC:H2''	5:S:-63:DC:C6	2.52	0.44
1:E:120:MET:C	2:F:50:ILE:HD11	2.43	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:17:ARG:HG3	5:S:-43:DT:P	2.59	0.43
3:M:22:GLY:N	4:N:117:LYS:HE2	2.32	0.43
1:A:86:SER:O	1:A:90:MET:HG2	2.18	0.43
5:I:2:DC:C5'	7:Z:90:SER:HB3	2.43	0.43
5:I:27:DG:N2	5:I:28:DA:C2	2.87	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:-90:DA:H2''	5:S:-89:DT:H72	2.01	0.42
5:S:-45:DA:C2	6:T:46:DG:N2	2.87	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:HA	1:K:63:ARG:HD3	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
1:A:85:GLN:HA	5:I:-24:DG:O5'	2.20	0.41
4:D:105:LYS:HE3	4:D:105:LYS:HB2	1.81	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
4:D:67:PHE:CD2	4:D:67:PHE:C	2.98	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
3:C:17:ARG:NE	5:I:-43:DT:OP2	2.47	0.41
1:E:118:THR:HA	2:F:45:ARG:HB3	2.03	0.41
5:I:-62:DC:H2'	5:I:-61:DG:C8	2.56	0.41
2:B:75:HIS:ND1	4:D:93:THR:OG1	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:102:ILE:O	3:C:103:ALA:C	2.64	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:17:ARG:NE	5:S:-43:DT:OP2	2.46	0.41
7:Z:46:SER:HA	7:Z:92:SER:HA	2.03	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
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
1:A:113:HIS:CE1	1:E:123:ASP:OD1	2.74	0.40
3:C:90:ASP:HB3	3:C:93:LEU:HB2	2.02	0.40
3:G:63:LEU:HD11	4:H:38:VAL:HG13	2.04	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	11	45
4	H	94/122 (77%)	90 (96%)	3 (3%)	1 (1%)	11	45
4	N	93/122 (76%)	88 (95%)	4 (4%)	1 (1%)	11	45
7	Z	71/196 (36%)	68 (96%)	3 (4%)	0	100	100
All	All	1188/1660 (72%)	1133 (95%)	52 (4%)	3 (0%)	36	71

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 ⓘ

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%)	84 (99%)	1 (1%)	63	74
1	E	85/110 (77%)	84 (99%)	1 (1%)	63	74
1	K	85/110 (77%)	83 (98%)	2 (2%)	43	62
2	B	68/78 (87%)	68 (100%)	0	100	100
2	F	68/78 (87%)	68 (100%)	0	100	100
2	L	68/78 (87%)	68 (100%)	0	100	100
3	C	83/101 (82%)	80 (96%)	3 (4%)	31	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	82/101 (81%)	79 (96%)	3 (4%)	30	51
3	M	83/101 (82%)	80 (96%)	3 (4%)	31	52
4	D	81/102 (79%)	77 (95%)	4 (5%)	22	43
4	H	82/102 (80%)	79 (96%)	3 (4%)	30	51
4	N	81/102 (79%)	76 (94%)	5 (6%)	16	37
7	Z	60/158 (38%)	58 (97%)	2 (3%)	33	54
All	All	1011/1331 (76%)	984 (97%)	27 (3%)	39	59

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
3	C	62	ILE
3	C	81	ARG
3	C	102	ILE
4	D	43	LYS
4	D	53	SER
4	D	85	THR
4	D	103	LEU
1	E	117	VAL
3	G	62	ILE
3	G	81	ARG
3	G	102	ILE
4	H	27	ARG
4	H	31	LYS
4	H	85	THR
1	K	65	LEU
1	K	117	VAL
3	M	62	ILE
3	M	81	ARG
3	M	102	ILE
4	N	43	LYS
4	N	53	SER
4	N	85	THR
4	N	103	LEU
4	N	117	LYS
7	Z	60	VAL
7	Z	93	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10)

such sidechains are listed below:

Mol	Chain	Res	Type
3	C	89	ASN
4	D	60	ASN
4	D	64	ASN
4	H	46	HIS
4	H	81	ASN
3	M	24	GLN
4	N	60	ASN
4	N	64	ASN
4	N	92	GLN
7	Z	57	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	A	98/135 (72%)	0.33	4 (4%) 41 38	203, 236, 286, 306	0
1	E	97/135 (71%)	0.22	5 (5%) 33 32	212, 247, 301, 328	0
1	K	98/135 (72%)	0.58	11 (11%) 10 16	210, 248, 298, 341	0
2	B	83/102 (81%)	0.33	4 (4%) 35 34	199, 221, 253, 264	0
2	F	83/102 (81%)	0.45	11 (13%) 7 13	199, 235, 273, 302	0
2	L	83/102 (81%)	0.52	8 (9%) 13 19	203, 236, 274, 291	0
3	C	105/129 (81%)	0.31	5 (4%) 35 34	186, 240, 285, 317	0
3	G	103/129 (79%)	0.62	9 (8%) 16 21	198, 230, 263, 282	0
3	M	105/129 (81%)	0.51	11 (10%) 11 17	202, 244, 286, 303	0
4	D	95/122 (77%)	0.50	6 (6%) 26 29	197, 225, 291, 325	0
4	H	96/122 (78%)	0.57	9 (9%) 14 19	198, 224, 280, 316	0
4	N	95/122 (77%)	0.52	7 (7%) 20 25	200, 244, 290, 340	0
5	I	193/197 (97%)	0.16	0 100 100	281, 339, 444, 470	0
5	S	96/197 (48%)	0.16	0 100 100	289, 357, 437, 447	0
6	J	193/197 (97%)	0.14	0 100 100	266, 338, 448, 469	0
6	T	97/197 (49%)	0.12	0 100 100	289, 354, 441, 450	0
7	Z	73/196 (37%)	0.15	0 100 100	326, 402, 441, 449	0
All	All	1793/2448 (73%)	0.34	90 (5%) 34 33	186, 258, 422, 470	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	29	ILE	5.2
3	G	63	LEU	4.7
1	A	100	LEU	4.4
3	G	62	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
2	L	94	GLY	3.9
4	H	59	MET	3.9
3	M	58	LEU	3.8
2	F	57	VAL	3.8
4	D	59	MET	3.8
4	N	70	ILE	3.8
1	K	104	PHE	3.8
4	N	86	ILE	3.7
1	E	104	PHE	3.7
3	M	99	ARG	3.6
4	H	62	PHE	3.5
4	N	98	LEU	3.5
2	F	91	LYS	3.4
2	F	94	GLY	3.4
2	F	29	ILE	3.3
3	M	55	LEU	3.2
1	K	62	ILE	3.2
2	L	96	THR	3.2
2	F	58	LEU	3.2
2	F	54	THR	3.1
3	M	95	LYS	3.1
1	K	70	LEU	3.1
1	E	124	ILE	3.0
2	F	93	GLN	3.0
2	L	91	LYS	3.0
3	M	34	LEU	3.0
4	H	34	TYR	3.0
2	L	37	LEU	3.0
4	D	38	VAL	3.0
4	D	86	ILE	2.9
2	F	37	LEU	2.9
1	K	132	GLY	2.9
1	A	62	ILE	2.9
1	K	87	SER	2.9
1	K	74	ILE	2.9
4	H	38	VAL	2.9
1	A	92	LEU	2.8
2	F	96	THR	2.8
2	L	34	ILE	2.8
4	N	92	GLN	2.7
4	N	44	GLN	2.7
3	C	99	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
3	G	45	ALA	2.7
3	G	78	ILE	2.7
3	G	49	VAL	2.6
1	K	124	ILE	2.6
2	B	87	VAL	2.6
4	H	51	ILE	2.5
1	K	71	VAL	2.5
3	G	99	ARG	2.5
4	H	42	LEU	2.5
4	N	109	SER	2.5
2	L	26	ILE	2.5
4	D	68	GLU	2.5
3	M	62	ILE	2.5
2	B	29	ILE	2.4
3	C	98	GLY	2.4
1	A	87	SER	2.4
3	C	95	LYS	2.4
1	E	92	LEU	2.4
2	L	93	GLN	2.4
3	G	19	SER	2.4
4	H	118	TYR	2.4
1	E	100	LEU	2.3
3	M	111	ILE	2.3
1	E	62	ILE	2.3
2	B	102	GLY	2.3
1	K	102	ALA	2.3
3	M	98	GLY	2.3
1	K	75	ALA	2.3
4	H	109	SER	2.3
4	N	121	ALA	2.3
3	G	83	LEU	2.2
4	H	106	HIS	2.2
3	C	45	ALA	2.2
3	M	91	GLU	2.2
3	G	44	GLY	2.1
3	C	43	VAL	2.1
4	D	120	SER	2.1
3	M	96	LEU	2.1
2	F	46	ILE	2.1
1	K	131	ARG	2.0
2	F	43	VAL	2.0
2	B	91	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
3	M	51	LEU	2.0
4	D	56	MET	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.