



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 29, 2020 – 02:11 PM JST

PDB ID : 6LA9
Title : 349 bp di-nucleosome harboring cohesive DNA termini assembled with linker histone H1.0 (high cryoprotectant)
Authors : Adhireksan, Z.; Sharma, D.; Lee, P.L.; Davey, C.A.
Deposited on : 2019-11-12
Resolution : 3.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	2.14.6
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)	:	2.14.6

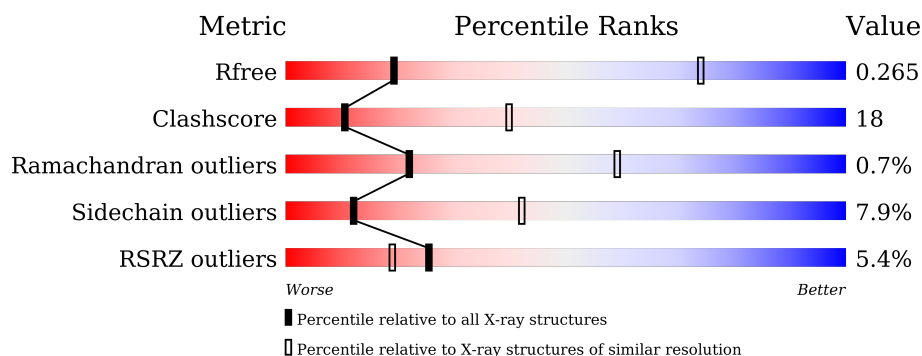
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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 $\leq 5\%$. 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	<div> <div></div> <div>61% 11% 27%</div> </div>
1	E	136	<div> <div>%</div> <div>63% 8% 28%</div> </div>
1	K	136	<div> <div>%</div> <div>64% 8% 27%</div> </div>
1	O	136	<div> <div></div> <div>61% 11% 28%</div> </div>
2	B	103	<div> <div></div> <div>69% 9% 22%</div> </div>
2	F	103	<div> <div>2%</div> <div>68% 11% 20%</div> </div>

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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	
7	T	194	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	CA	O	204	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 27560 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	99	Total	C	N	O	S	0	0	0
			816	514	158	140	4			
1	E	98	Total	C	N	O	S	0	0	0
			807	508	156	139	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	80	Total	C	N	O	S	0	0	0
			638	401	125	111	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	106	Total	C	N	O	0	0	0
			819	517	160	142			
3	G	106	Total	C	N	O	0	0	0
			819	517	160	142			
3	M	106	Total	C	N	O	0	0	0
			819	517	160	142			
3	Q	106	Total	C	N	O	0	0	0
			821	518	160	143			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	95	Total	C	N	O	S	0	0	0
			746	468	136	140	2			
4	H	95	Total	C	N	O	S	0	0	0
			746	468	136	140	2			
4	N	95	Total	C	N	O	S	0	0	0
			746	468	136	140	2			
4	R	95	Total	C	N	O	S	0	0	0
			746	468	136	140	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	73	Total	C	N	O	S	0	0	0
			560	350	106	103	1			
7	T	74	Total	C	N	O	S	0	0	0
			568	354	107	106	1			

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	2	Total	Ca	0	0
			2	2		
8	J	15	Total	Ca	0	0
			15	15		
8	Q	1	Total	Ca	0	0
			1	1		
8	I	15	Total	Ca	0	0
			15	15		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total 1	Ca 1	0	0
8	A	1	Total 1	Ca 1	0	0
8	O	4	Total 4	Ca 4	0	0
8	F	1	Total 1	Ca 1	0	0

- Molecule 9 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	J	1	Total 1	K 1	0	0
9	I	1	Total 1	K 1	0	0

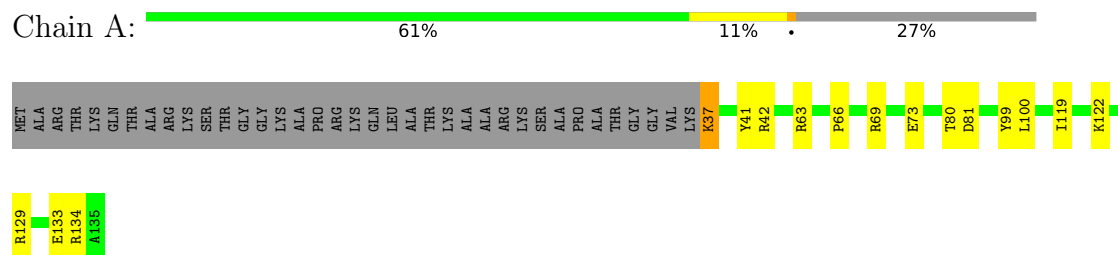
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	1	Total 1	O 1	0	0
10	I	1	Total 1	O 1	0	0
10	J	2	Total 2	O 2	0	0

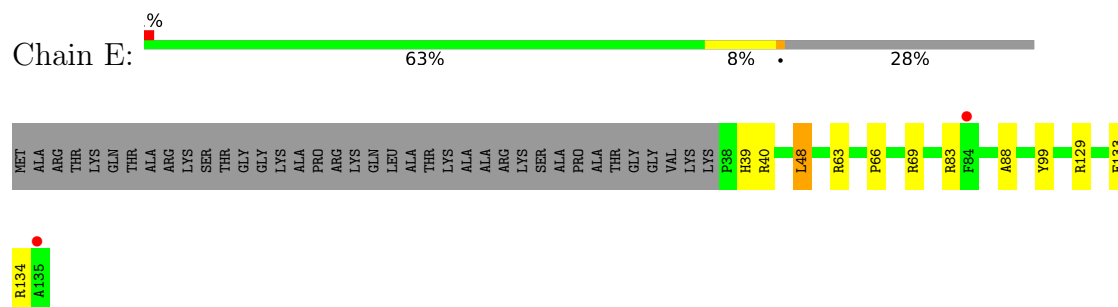
3 Residue-property plots [i](#)

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.

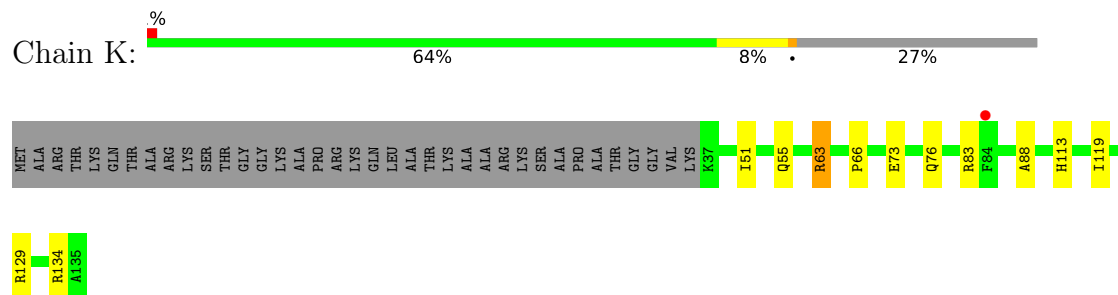
• Molecule 1: Histone H3.1



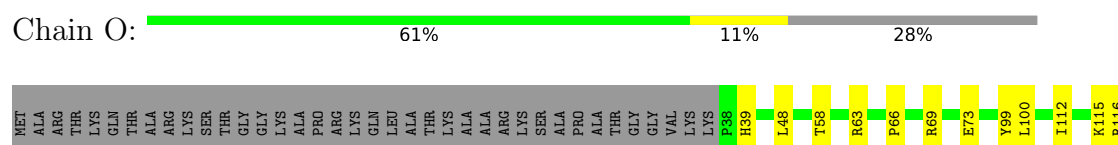
• Molecule 1: Histone H3.1



• Molecule 1: Histone H3.1



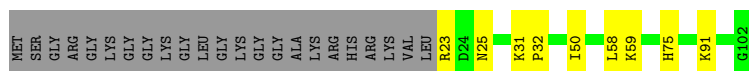
• Molecule 1: Histone H3.1





- Molecule 2: Histone H4

Chain B: 69% 9% 22%



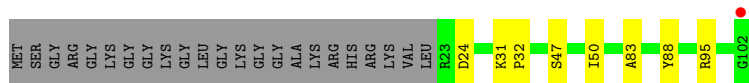
- Molecule 2: Histone H4

Chain F: 2% 68% 11% 20%



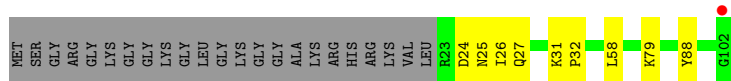
- Molecule 2: Histone H4

Chain L: 70% 8% 22%



- Molecule 2: Histone H4

Chain P: 69% 9% 22%



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

Chain C: 69% 12% 18%



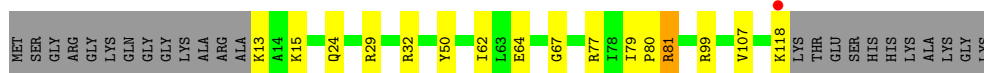
- Molecule 3: Histone H2A type 1-B/E

Chain G: 72% 8% 18%



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

Chain M: 69% 12% 18%



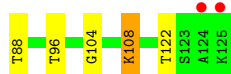
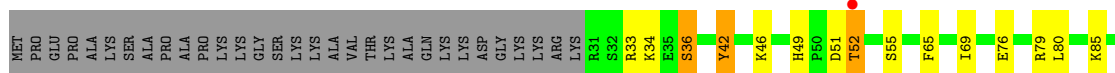
- Molecule 3: Histone H2A type 1-B/E



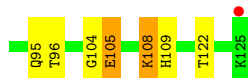
- Molecule 4: Histone H2B type 1-J



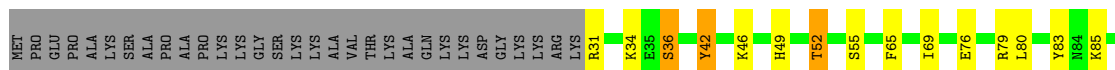
- Molecule 4: Histone H2B type 1-J



- Molecule 4: Histone H2B type 1-J



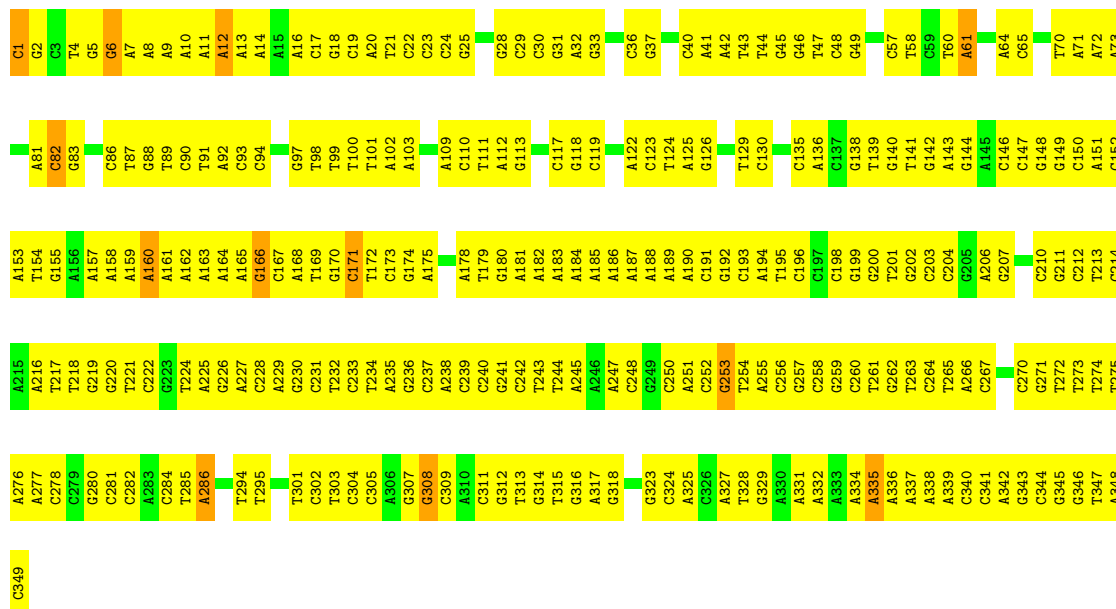
- Molecule 4: Histone H2B type 1-J





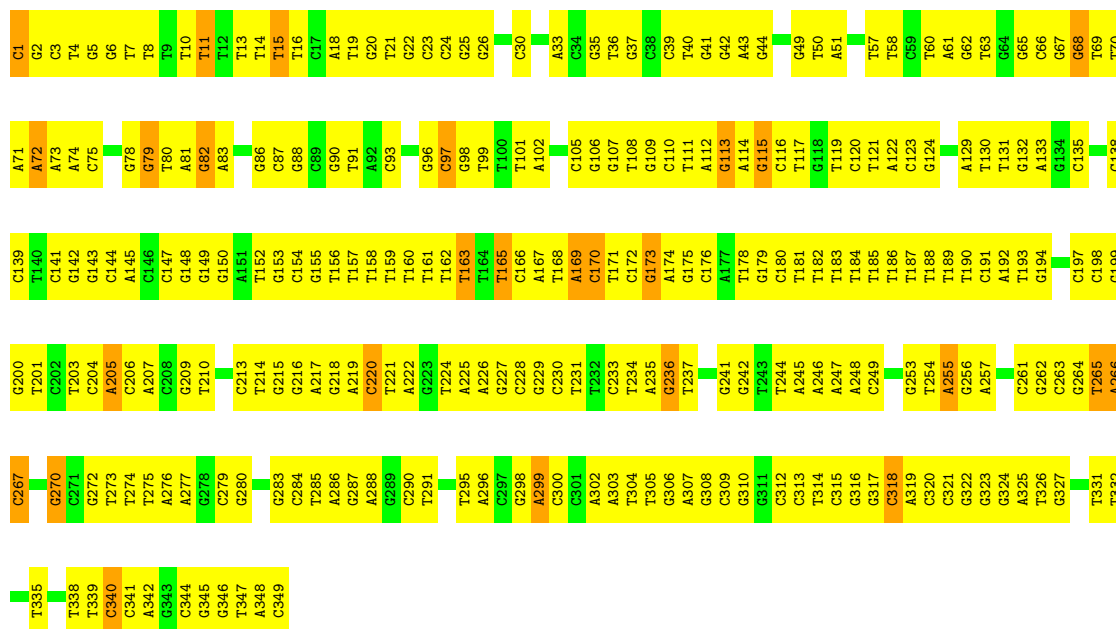
• Molecule 5: DNA (349-MER)

Chain I: 25% 72%

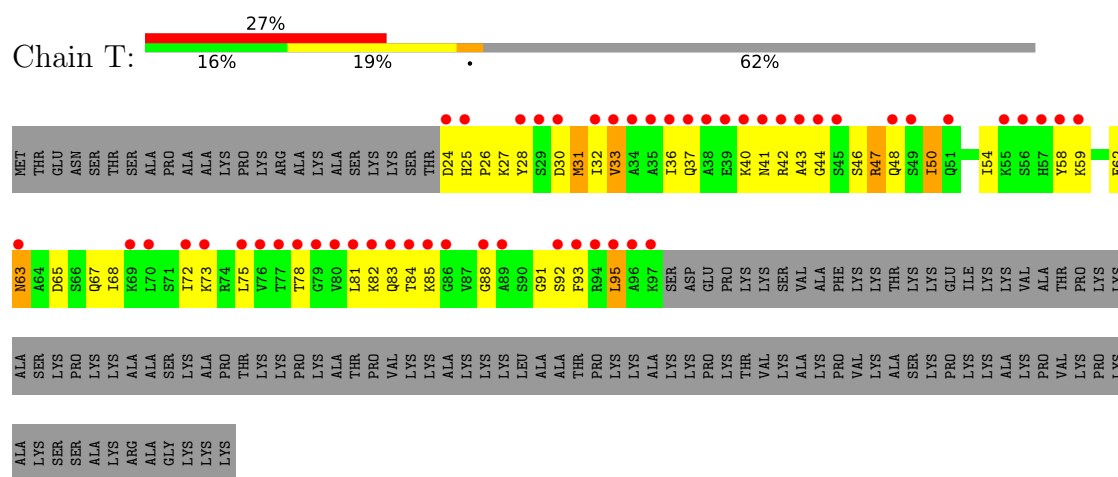
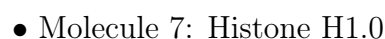


• Molecule 6: DNA (349-MER)

Chain J: 24% 68% 7%



• Molecule 7: Histone H1.0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	120.78Å 172.88Å 216.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.78 – 3.70 91.61 – 3.70	Depositor EDS
% Data completeness (in resolution range)	97.5 (91.78-3.70) 97.5 (91.61-3.70)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.194 , 0.266 0.199 , 0.265	Depositor DCC
R_{free} test set	1001 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å ²)	123.3	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 87.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27560	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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](#)

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	0.61	0/828	0.78	0/1109
1	E	0.61	0/819	0.83	0/1097
1	K	0.62	0/828	0.80	0/1109
1	O	0.62	0/819	0.80	0/1097
2	B	0.64	0/645	0.82	0/862
2	F	0.65	0/660	0.84	0/883
2	L	0.64	0/645	0.78	0/862
2	P	0.63	0/645	0.84	0/862
3	C	0.62	0/829	0.78	0/1118
3	G	0.63	0/829	0.79	0/1118
3	M	0.64	0/829	0.80	0/1118
3	Q	0.62	0/831	0.79	0/1121
4	D	0.66	0/757	0.78	0/1015
4	H	0.67	0/757	0.79	0/1015
4	N	0.66	0/757	0.77	0/1015
4	R	0.67	0/757	0.80	0/1015
5	I	0.56	4/8032 (0.0%)	0.94	10/12384 (0.1%)
6	J	0.63	11/8022 (0.1%)	0.96	22/12387 (0.2%)
7	S	0.76	0/566	0.99	1/754 (0.1%)
7	T	0.72	0/574	0.88	0/765
All	All	0.62	15/29429 (0.1%)	0.89	33/42706 (0.1%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	68	DG	O3'-P	-12.53	1.46	1.61
5	I	1	DC	OP3-P	-10.90	1.48	1.61
6	J	1	DC	OP3-P	-10.65	1.48	1.61
6	J	220	DC	O3'-P	-9.66	1.49	1.61
6	J	97	DC	O3'-P	-7.39	1.52	1.61

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	335	DA	C1'-O4'-C4'	-9.11	100.99	110.10
6	J	267	DC	C1'-O4'-C4'	-6.90	103.20	110.10
6	J	165	DT	C1'-O4'-C4'	-6.86	103.24	110.10
6	J	72	DA	C1'-O4'-C4'	-6.52	103.58	110.10
6	J	86	DG	C1'-O4'-C4'	-6.39	103.71	110.10

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	816	0	856	13	0
1	E	807	0	844	13	0
1	K	816	0	856	12	0
1	O	807	0	844	11	0
2	B	638	0	676	9	0
2	F	653	0	696	7	0
2	L	638	0	676	9	0
2	P	638	0	676	9	0
3	C	819	0	879	10	0
3	G	819	0	879	9	0
3	M	819	0	879	16	0
3	Q	821	0	881	11	0
4	D	746	0	771	11	0
4	H	746	0	771	18	0
4	N	746	0	771	22	0
4	R	746	0	771	22	0
5	I	7149	0	3902	370	0
6	J	7162	0	3943	347	0
7	S	560	0	593	38	0
7	T	568	0	597	44	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
8	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	2	0	0	0	0
8	I	15	0	0	0	0
8	J	15	0	0	0	0
8	O	4	0	0	0	0
8	Q	1	0	0	0	0
9	I	1	0	0	0	0
9	J	1	0	0	0	0
10	C	1	0	0	0	0
10	I	1	0	0	0	0
10	J	2	0	0	0	0
All	All	27560	0	21761	899	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

The worst 5 of 899 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:193:DT:H2'	6:J:194:DG:C8	1.58	1.36
6:J:61:DA:H2''	6:J:62:DG:C8	1.71	1.23
5:I:336:DA:H2''	5:I:337:DA:O5'	1.39	1.17
6:J:80:DT:H2''	6:J:81:DA:N7	1.59	1.16
6:J:15:DT:H2'	6:J:16:DT:H71	1.25	1.14

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	97/136 (71%)	93 (96%)	4 (4%)	0	100	100
1	E	96/136 (71%)	92 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	97/136 (71%)	92 (95%)	5 (5%)	0	100	100
1	O	96/136 (71%)	91 (95%)	5 (5%)	0	100	100
2	B	78/103 (76%)	74 (95%)	4 (5%)	0	100	100
2	F	80/103 (78%)	78 (98%)	1 (1%)	1 (1%)	12	47
2	L	78/103 (76%)	74 (95%)	4 (5%)	0	100	100
2	P	78/103 (76%)	75 (96%)	3 (4%)	0	100	100
3	C	104/130 (80%)	97 (93%)	7 (7%)	0	100	100
3	G	104/130 (80%)	95 (91%)	8 (8%)	1 (1%)	15	51
3	M	104/130 (80%)	97 (93%)	7 (7%)	0	100	100
3	Q	104/130 (80%)	97 (93%)	7 (7%)	0	100	100
4	D	93/126 (74%)	89 (96%)	3 (3%)	1 (1%)	14	50
4	H	93/126 (74%)	88 (95%)	4 (4%)	1 (1%)	14	50
4	N	93/126 (74%)	89 (96%)	3 (3%)	1 (1%)	14	50
4	R	93/126 (74%)	88 (95%)	4 (4%)	1 (1%)	14	50
7	S	71/194 (37%)	61 (86%)	7 (10%)	3 (4%)	3	25
7	T	72/194 (37%)	65 (90%)	5 (7%)	2 (3%)	5	33
All	All	1631/2368 (69%)	1535 (94%)	85 (5%)	11 (1%)	22	59

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	104	GLY
4	H	104	GLY
4	N	104	GLY
4	R	104	GLY
7	S	28	TYR

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	86/111 (78%)	80 (93%)	6 (7%)	15	45
1	E	85/111 (77%)	81 (95%)	4 (5%)	26	56
1	K	86/111 (78%)	83 (96%)	3 (4%)	36	63
1	O	85/111 (77%)	84 (99%)	1 (1%)	71	84
2	B	65/79 (82%)	62 (95%)	3 (5%)	27	57
2	F	67/79 (85%)	64 (96%)	3 (4%)	27	57
2	L	65/79 (82%)	63 (97%)	2 (3%)	40	65
2	P	65/79 (82%)	64 (98%)	1 (2%)	65	81
3	C	84/100 (84%)	79 (94%)	5 (6%)	19	50
3	G	84/100 (84%)	80 (95%)	4 (5%)	25	56
3	M	84/100 (84%)	81 (96%)	3 (4%)	35	63
3	Q	85/100 (85%)	79 (93%)	6 (7%)	14	45
4	D	81/105 (77%)	70 (86%)	11 (14%)	3	21
4	H	81/105 (77%)	71 (88%)	10 (12%)	4	24
4	N	81/105 (77%)	70 (86%)	11 (14%)	3	21
4	R	81/105 (77%)	71 (88%)	10 (12%)	4	24
7	S	60/158 (38%)	46 (77%)	14 (23%)	1	6
7	T	61/158 (39%)	48 (79%)	13 (21%)	1	7
All	All	1386/1896 (73%)	1276 (92%)	110 (8%)	12	42

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	24	ASP
4	N	86	ARG
7	T	47	ARG
3	M	24	GLN
4	N	32	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
4	N	47	GLN
4	N	95	GLN
7	S	83	GLN
1	K	108	ASN

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Mol	Chain	Res	Type
3	M	24	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 42 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(Å ²)	Q<0.9
1	A	99/136 (72%)	-0.09	0 100 100	69, 106, 155, 190	0
1	E	98/136 (72%)	0.05	2 (2%) 65 53	69, 104, 143, 187	0
1	K	99/136 (72%)	0.03	1 (1%) 82 73	74, 98, 141, 156	0
1	O	98/136 (72%)	-0.37	0 100 100	72, 103, 145, 162	0
2	B	80/103 (77%)	-0.16	0 100 100	79, 103, 141, 204	0
2	F	82/103 (79%)	0.10	2 (2%) 59 47	79, 101, 137, 176	0
2	L	80/103 (77%)	0.16	1 (1%) 77 67	72, 97, 132, 172	0
2	P	80/103 (77%)	-0.29	1 (1%) 77 67	71, 98, 142, 178	0
3	C	106/130 (81%)	-0.09	0 100 100	84, 111, 151, 187	0
3	G	106/130 (81%)	0.19	1 (0%) 84 76	83, 113, 157, 185	0
3	M	106/130 (81%)	-0.19	1 (0%) 84 76	65, 109, 147, 178	0
3	Q	106/130 (81%)	-0.05	2 (1%) 66 55	80, 104, 150, 185	0
4	D	95/126 (75%)	-0.10	1 (1%) 80 71	77, 114, 169, 198	0
4	H	95/126 (75%)	0.20	3 (3%) 47 35	88, 117, 173, 195	0
4	N	95/126 (75%)	-0.09	1 (1%) 80 71	80, 106, 153, 231	0
4	R	95/126 (75%)	-0.14	1 (1%) 80 71	77, 104, 165, 197	0
5	I	349/349 (100%)	-0.77	0 100 100	104, 158, 218, 268	0
6	J	349/349 (100%)	-0.78	0 100 100	106, 156, 213, 298	0
7	S	73/194 (37%)	3.32	58 (79%) 0 0	162, 208, 261, 282	1 (1%)
7	T	74/194 (38%)	2.88	52 (70%) 0 0	165, 202, 240, 262	1 (1%)
All	All	2365/3066 (77%)	-0.07	127 (5%) 25 19	65, 122, 207, 298	2 (0%)

The worst 5 of 127 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	41	ASN	8.9
7	S	84	THR	8.1
7	T	93	PHE	7.1
7	S	34	ALA	6.6
7	S	60	VAL	6.5

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 monosaccharides 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(\AA^2)	Q<0.9
8	CA	I	413	1/1	0.52	0.14	140,140,140,140	0
8	CA	J	414	1/1	0.55	0.29	129,129,129,129	0
8	CA	I	411	1/1	0.72	0.18	136,136,136,136	0
9	K	I	416	1/1	0.74	0.23	120,120,120,120	0
8	CA	O	204	1/1	0.74	0.49	149,149,149,149	0
8	CA	J	402	1/1	0.77	0.13	116,116,116,116	0
8	CA	I	408	1/1	0.77	0.09	125,125,125,125	0
8	CA	I	406	1/1	0.78	0.26	123,123,123,123	0
8	CA	I	407	1/1	0.81	0.29	151,151,151,151	0
8	CA	J	407	1/1	0.81	0.16	113,113,113,113	0
8	CA	I	401	1/1	0.81	0.14	109,109,109,109	0
8	CA	I	410	1/1	0.82	0.12	112,112,112,112	0
8	CA	J	409	1/1	0.82	0.15	118,118,118,118	0
8	CA	J	406	1/1	0.82	0.17	100,100,100,100	0
8	CA	J	411	1/1	0.83	0.21	123,123,123,123	0
8	CA	J	415	1/1	0.84	0.30	132,132,132,132	0
8	CA	J	412	1/1	0.84	0.11	127,127,127,127	0
8	CA	A	201	1/1	0.85	0.15	137,137,137,137	0
8	CA	G	201	1/1	0.85	0.19	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	CA	F	201	1/1	0.86	0.17	141,141,141,141	0
8	CA	O	203	1/1	0.86	0.31	123,123,123,123	0
8	CA	J	401	1/1	0.87	0.20	138,138,138,138	0
8	CA	I	404	1/1	0.88	0.24	129,129,129,129	0
8	CA	I	412	1/1	0.88	0.44	162,162,162,162	0
8	CA	J	403	1/1	0.88	0.13	110,110,110,110	0
9	K	J	416	1/1	0.88	0.11	105,105,105,105	0
8	CA	I	409	1/1	0.89	0.50	135,135,135,135	0
8	CA	I	402	1/1	0.90	0.10	117,117,117,117	0
8	CA	O	202	1/1	0.90	0.17	110,110,110,110	0
8	CA	I	405	1/1	0.91	0.22	120,120,120,120	0
8	CA	I	415	1/1	0.91	0.07	116,116,116,116	0
8	CA	C	201	1/1	0.92	0.22	118,118,118,118	0
8	CA	J	404	1/1	0.92	0.22	101,101,101,101	0
8	CA	G	202	1/1	0.93	0.12	121,121,121,121	0
8	CA	Q	201	1/1	0.93	0.17	137,137,137,137	0
8	CA	J	408	1/1	0.93	0.10	119,119,119,119	0
8	CA	J	410	1/1	0.94	0.10	116,116,116,116	0
8	CA	J	405	1/1	0.94	0.13	93,93,93,93	0
8	CA	J	413	1/1	0.94	0.35	121,121,121,121	0
8	CA	I	414	1/1	0.95	0.11	104,104,104,104	0
8	CA	I	403	1/1	0.95	0.13	118,118,118,118	0
8	CA	O	201	1/1	0.97	0.17	102,102,102,102	0

6.5 Other polymers [i](#)

There are no such residues in this entry.