



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:09 AM UTC

PDB ID : 8YTI / pdb_00008yti
Title : Crystal Structure of Nucleosome-H1x Linker Histone Assembly (sticky-169a DNA fragment)
Authors : Adhireksan, Z.; Qiuye, B.; Padavattan, S.; Davey, C.A.
Deposited on : 2024-03-26
Resolution : 2.70 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

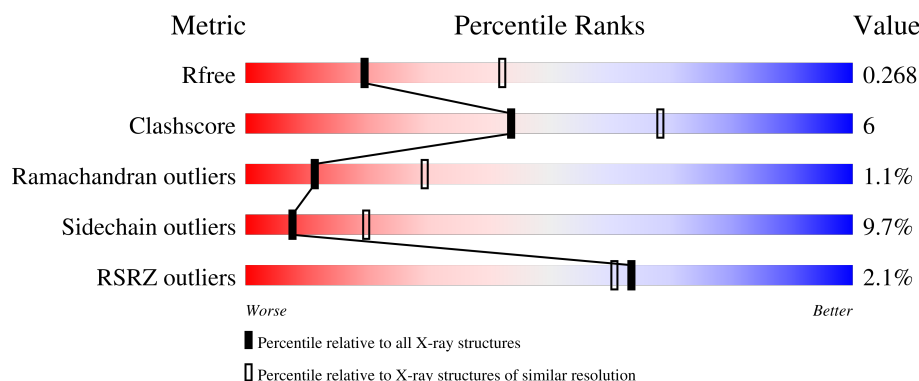
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	3% 64% 7% 26%
1	E	136	% 66% 7% 24%
1	K	136	4% 68% 7% 22%
1	O	136	63% 9% 26%
2	B	103	4% 68% 11% 20%

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Mol	Chain	Length	Quality of chain
2	F	103	
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	169	
5	S	169	
6	J	169	
6	T	169	
7	U	213	
7	V	213	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28083 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	103	Total	C	N	O	S	0	0	0
			840	529	163	144	4			
1	K	106	Total	C	N	O	S	0	0	0
			859	541	166	148	4			
1	O	100	Total	C	N	O	S	0	0	0
			825	520	160	141	4			

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	82	Total	C	N	O	S	0	0	0
			653	412	127	113	1			
2	F	83	Total	C	N	O	S	0	0	0
			662	418	129	114	1			
2	L	84	Total	C	N	O	S	0	0	0
			673	424	133	115	1			
2	P	102	Total	C	N	O	S	0	0	0
			792	494	163	134	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	109	Total	C	N	O	0	0	0
			844	532	167	145			
3	G	104	Total	C	N	O	0	0	0
			805	508	157	140			
3	M	109	Total	C	N	O	0	0	0
			844	532	167	145			
3	Q	105	Total	C	N	O	0	0	0
			814	514	159	141			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	97	Total	C	N	O	S	0	0	0
			766	480	142	142	2			
4	H	102	Total	C	N	O	S	0	0	0
			805	504	150	149	2			
4	N	98	Total	C	N	O	S	0	0	0
			775	486	144	143	2			
4	R	98	Total	C	N	O	S	0	0	0
			775	486	144	143	2			

- Molecule 5 is a DNA chain called DNA (169-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	169	Total	C	N	O	P	0	0	0
			3462	1646	637	1011	168			
5	S	169	Total	C	N	O	P	0	0	0
			3462	1646	637	1011	168			

- Molecule 6 is a DNA chain called DNA (169-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	169	Total	C	N	O	P	0	0	0
			3461	1646	634	1013	168			
6	T	169	Total	C	N	O	P	0	0	0
			3461	1646	634	1013	168			

- Molecule 7 is a protein called Histone H1x.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	U	87	Total	C	N	O	0	0	0
			703	443	135	125			
7	V	94	Total	C	N	O	0	0	0
			752	471	145	136			

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total 1 Cl 1	0	0
8	C	1	Total 1 Cl 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total Cl 1 1	0	0
8	G	1	Total Cl 1 1	0	0
8	K	1	Total Cl 1 1	0	0
8	M	1	Total Cl 1 1	0	0
8	O	1	Total Cl 1 1	0	0
8	R	1	Total Cl 1 1	0	0

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	3	Total Ca 3 3	0	0
9	G	3	Total Ca 3 3	0	0
9	I	8	Total Ca 8 8	0	0
9	J	9	Total Ca 9 9	0	0
9	N	1	Total Ca 1 1	0	0
9	Q	3	Total Ca 3 3	0	0
9	R	1	Total Ca 1 1	0	0
9	S	18	Total Ca 18 18	0	0
9	T	6	Total Ca 6 6	0	0

- Molecule 10 is POTASSIUM ION (CCD ID: K) (formula: K).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	J	1	Total K 1 1	0	0
10	M	1	Total K 1 1	0	0
10	S	2	Total K 2 2	0	0
10	T	1	Total K 1 1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total O 1 1	0	0
11	B	5	Total O 5 5	0	0
11	C	4	Total O 4 4	0	0
11	D	3	Total O 3 3	0	0
11	E	4	Total O 4 4	0	0
11	F	3	Total O 3 3	0	0
11	G	4	Total O 4 4	0	0
11	H	3	Total O 3 3	0	0
11	I	3	Total O 3 3	0	0
11	J	7	Total O 7 7	0	0
11	K	11	Total O 11 11	0	0
11	L	12	Total O 12 12	0	0
11	M	11	Total O 11 11	0	0
11	N	10	Total O 10 10	0	0
11	O	14	Total O 14 14	0	0

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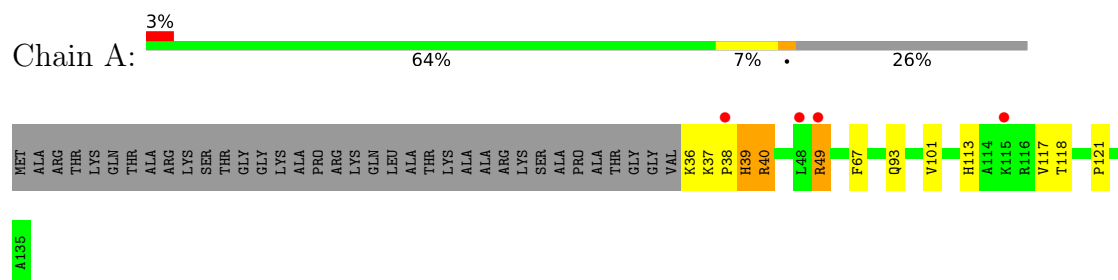
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	P	12	Total 12	O 12	0	0
11	Q	9	Total 9	O 9	0	0
11	R	8	Total 8	O 8	0	0
11	S	13	Total 13	O 13	0	0
11	T	20	Total 20	O 20	0	0

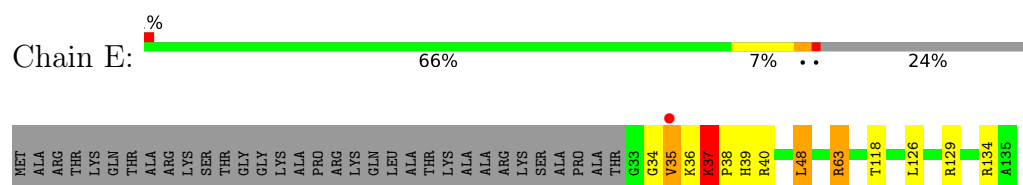
3 Residue-property plots

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.

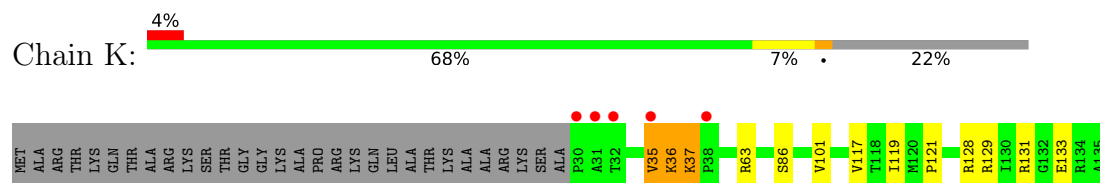
• Molecule 1: Histone H3.1



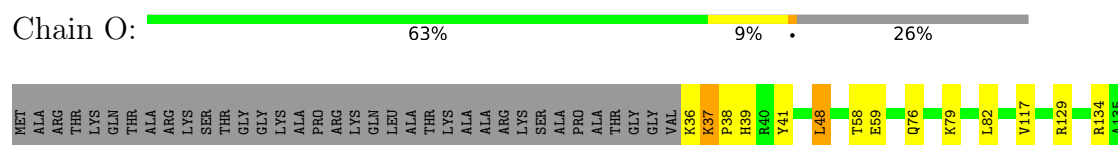
• Molecule 1: Histone H3.1



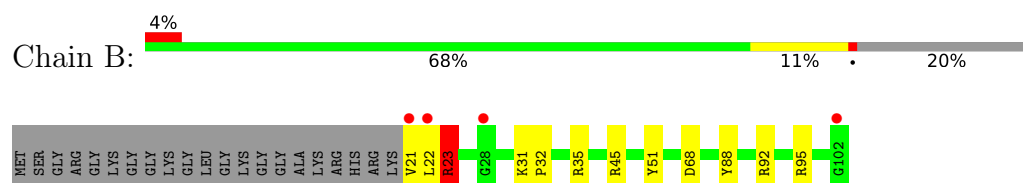
• Molecule 1: Histone H3.1



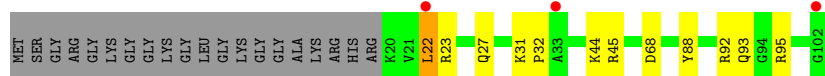
• Molecule 1: Histone H3.1



• Molecule 2: Histone H4



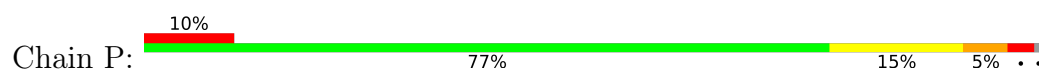
- Molecule 2: Histone H4



- Molecule 2: Histone H4



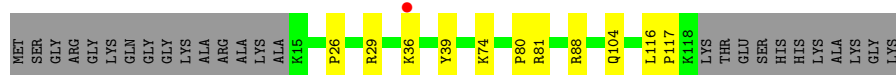
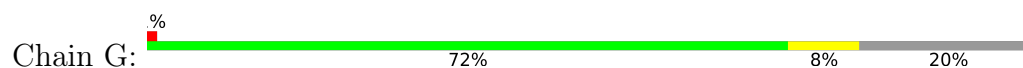
- Molecule 2: Histone H4



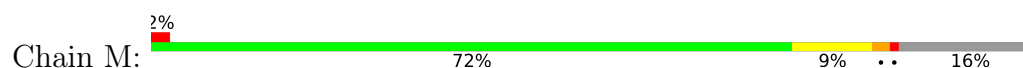
- Molecule 3: Histone H2A type 1-B/E



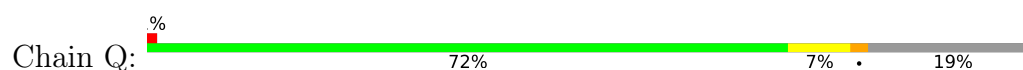
- Molecule 3: Histone H2A type 1-B/E



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

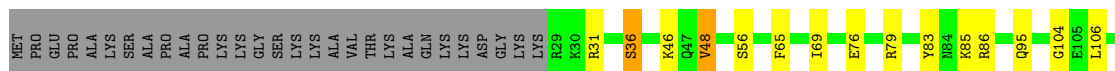


- Molecule 3: Histone H2A type 1-B/E





- Molecule 4: Histone H2B type 1-J



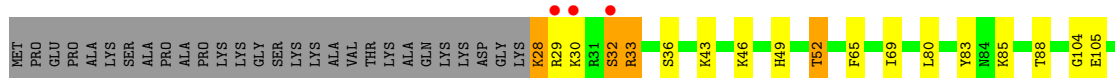
- Molecule 4: Histone H2B type 1-J



- Molecule 4: Histone H2B type 1-J

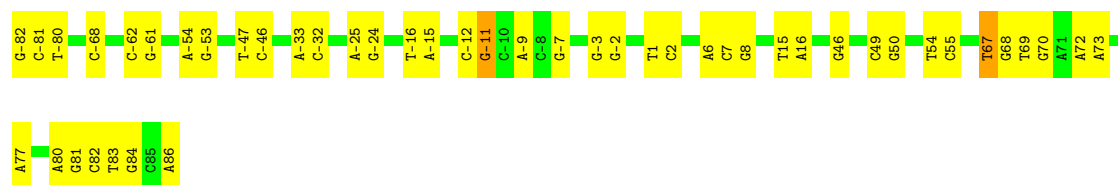


- Molecule 4: Histone H2B type 1-J

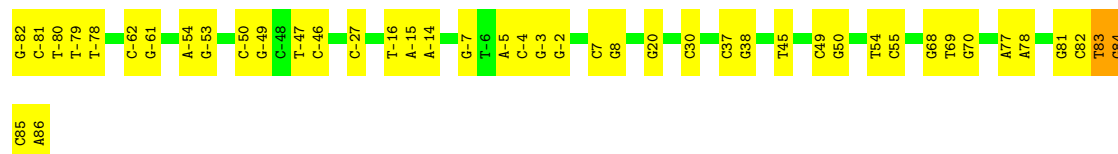


- Molecule 5: DNA (169-MER)

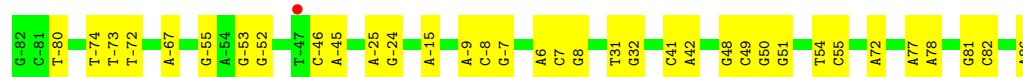
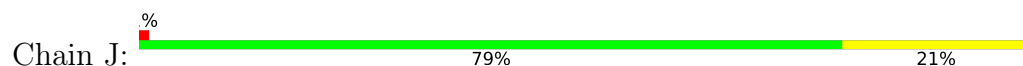




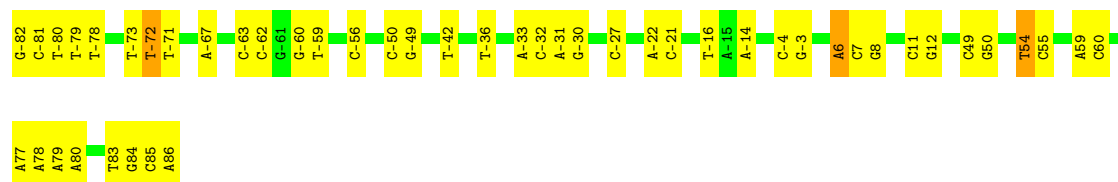
• Molecule 5: DNA (169-MER)



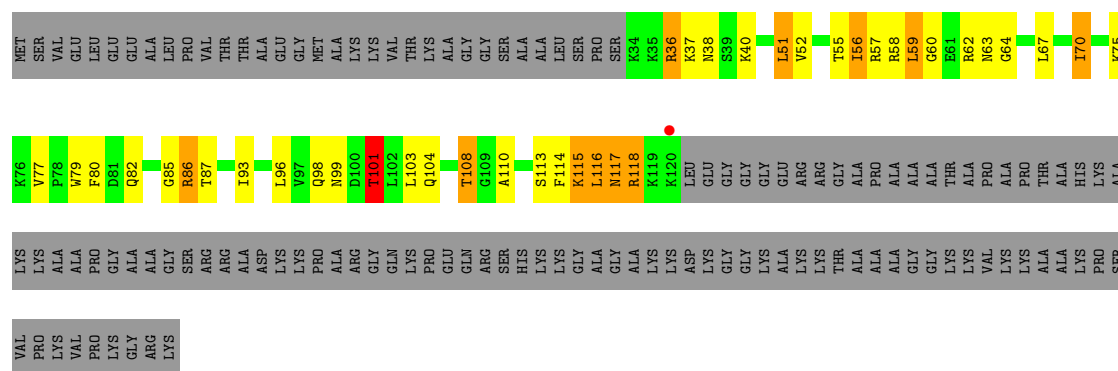
• Molecule 6: DNA (169-MER)



• Molecule 6: DNA (169-MER)



• Molecule 7: Histone H1x



• Molecule 7: Histone H1x



PRO	LYS	GLY	ARG	LYS	GLY	VAL	GLY	LEU	GLU	ALA	LEU	PRO	VAL	THR	THR	ALA	GLY	GLY	MET	ALA	LYS	LYS	VAL	THR	LYS	ALA	GLY	GLY	SER	ALA	ALA	LEU	SER	PRO	SER	K34	K35	R36	K37	K40	K41	K42	N43	L51	V52	V53	E54	T55	I56	L59	G60	E61	R62	H63	G64	L67	A68	K69
I70	T71	T72	E73	A74	K75	K76	V77	F80	D81	Q82	G85	I93	L96	V97	L102	L103	Q104	G107	T108	G109	A110	N111	G112	S113	F114	K115	L116	N117	R118	K119	R127	ARG	GLY	ALA	ALA	PRO	ALA	ALA	ALA	ALA	ALA	THR	ALA	ALA	ALA	THR	ALA	ALA	LYS	LYS	VAL	PRO	LYS	LYS	ALA	ALA		
PRO	GLY	ALA	GLY	SER	ARG	ARG	ALA	ASP	LYS	PRO	ALA	ARG	GLN	PRO	GLU	GLN	ARG	SER	HIS	LYS	GLY	GLY	ALA	LYS	LYS	ASP	LYS	GLY	GLY	LYS	ALA	LYS	LYS	THR	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA			
PRO	LYS	GLY	ARG	LYS																																																						

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.85Å 102.11Å 216.18Å 90.00° 96.34° 90.00°	Depositor
Resolution (Å)	92.22 – 2.70 92.22 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (92.22-2.70) 99.6 (92.22-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.210 , 0.267 0.212 , 0.268	Depositor DCC
R_{free} test set	2402 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å ²)	67.9	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28083	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.5434e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CA, K, CL

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	0.95	0/837	1.53	5/1120 (0.4%)
1	E	0.96	0/852	1.50	0/1140
1	K	1.00	0/872	1.50	2/1168 (0.2%)
1	O	0.96	0/837	1.50	1/1120 (0.1%)
2	B	0.97	0/660	1.52	1/883 (0.1%)
2	F	1.00	0/669	1.55	0/894
2	L	0.93	0/680	1.48	0/908
2	P	1.04	1/800 (0.1%)	1.54	3/1061 (0.3%)
3	C	0.99	0/854	1.55	0/1150
3	G	0.97	0/815	1.54	0/1100
3	M	0.97	0/854	1.52	3/1150 (0.3%)
3	Q	0.95	0/824	1.49	0/1111
4	D	0.98	0/777	1.56	0/1040
4	H	1.00	0/816	1.59	0/1089
4	N	0.99	0/786	1.57	0/1051
4	R	0.95	0/786	1.55	0/1051
5	I	0.36	0/3884	0.77	4/5993 (0.1%)
5	S	0.40	0/3884	0.82	7/5993 (0.1%)
6	J	0.37	0/3882	0.77	1/5990 (0.0%)
6	T	0.41	0/3882	0.84	6/5990 (0.1%)
7	U	1.06	0/712	1.62	3/947 (0.3%)
7	V	1.08	0/761	1.65	2/1011 (0.2%)
All	All	0.74	1/29724 (0.0%)	1.19	38/42960 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	2
7	U	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	101	GLY	C-O	5.71	1.28	1.23

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	-11	DG	C2'-C3'-O3'	7.30	122.46	111.50
5	I	-9	DA	C2'-C3'-O3'	7.28	122.42	111.50
5	S	20	DG	C2'-C3'-O3'	6.92	121.88	111.50
6	J	-55	DG	C2'-C3'-O3'	-6.86	101.21	111.50
5	I	67	DT	C4'-C3'-O3'	6.81	120.21	110.00
5	S	83	DT	C4'-C3'-O3'	6.57	119.85	110.00
6	T	-72	DT	C4'-C3'-O3'	6.44	119.66	110.00
2	B	23	ARG	N-CA-C	-6.16	105.77	113.28
5	S	-2	DG	C2'-C3'-O3'	-6.11	102.33	111.50
5	S	84	DG	C2'-C3'-O3'	5.95	120.43	111.50
2	P	35	ARG	CB-CA-C	5.93	120.93	110.85
6	T	-36	DT	C2'-C3'-O3'	-5.81	102.79	111.50
7	U	60	GLY	CA-C-O	-5.74	117.98	122.52
3	M	13	LYS	CB-CA-C	5.73	119.54	111.86
6	T	54	DT	C4'-C3'-O3'	5.71	118.57	110.00
5	I	77	DA	C2'-C3'-O3'	5.69	120.04	111.50
6	T	-16	DT	C2'-C3'-O3'	-5.59	103.11	111.50
5	S	-5	DA	C4'-C3'-O3'	-5.53	101.70	110.00
1	A	38	PRO	CA-C-N	5.52	132.08	121.54
1	A	38	PRO	C-N-CA	5.52	132.08	121.54
7	V	40	LYS	CA-C-N	5.48	129.04	120.82
7	V	40	LYS	C-N-CA	5.48	129.04	120.82
5	S	83	DT	C2'-C3'-O3'	-5.41	103.38	111.50
1	A	117	VAL	N-CA-C	-5.24	108.18	113.47
6	T	-14	DA	C4'-C3'-O3'	-5.21	102.19	110.00
1	A	101	VAL	CA-C-N	5.19	125.74	119.98
1	A	101	VAL	C-N-CA	5.19	125.74	119.98
7	U	70	ILE	CA-C-N	5.14	127.12	120.44
7	U	70	ILE	C-N-CA	5.14	127.12	120.44
1	K	101	VAL	CA-C-N	5.10	125.64	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	101	VAL	C-N-CA	5.10	125.64	119.98
2	P	4	GLY	CA-C-N	5.10	127.07	120.44
2	P	4	GLY	C-N-CA	5.10	127.07	120.44
3	M	15	LYS	CA-C-N	5.09	128.31	120.82
3	M	15	LYS	C-N-CA	5.09	128.31	120.82
6	T	6	DA	C4'-C3'-O3'	-5.09	102.37	110.00
1	O	117	VAL	N-CA-C	-5.05	108.37	113.47
5	S	-14	DA	C2'-C3'-O3'	5.01	119.01	111.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	36	LYS	Peptide
2	P	18	HIS	Peptide
2	P	21	VAL	Peptide
7	U	101	THR	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	6	0
1	E	840	0	884	13	0
1	K	859	0	904	9	0
1	O	825	0	869	6	0
2	B	653	0	696	9	0
2	F	662	0	709	9	0
2	L	673	0	722	14	0
2	P	792	0	855	17	0
3	C	844	0	910	10	0
3	G	805	0	861	5	0
3	M	844	0	910	12	0
3	Q	814	0	874	6	0
4	D	766	0	797	12	0
4	H	805	0	843	11	0
4	N	775	0	810	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	775	0	810	18	0
5	I	3462	0	1901	38	0
5	S	3462	0	1901	33	0
6	J	3461	0	1902	31	0
6	T	3461	0	1902	35	0
7	U	703	0	751	28	0
7	V	752	0	796	27	0
8	A	1	0	0	1	0
8	C	1	0	0	0	0
8	E	1	0	0	0	0
8	G	1	0	0	0	0
8	K	1	0	0	1	0
8	M	1	0	0	0	0
8	O	1	0	0	0	0
8	R	1	0	0	0	0
9	C	3	0	0	0	0
9	G	3	0	0	0	0
9	I	8	0	0	0	0
9	J	9	0	0	0	0
9	N	1	0	0	0	0
9	Q	3	0	0	0	0
9	R	1	0	0	0	0
9	S	18	0	0	0	0
9	T	6	0	0	0	0
10	C	1	0	0	0	0
10	I	2	0	0	0	0
10	J	1	0	0	0	0
10	M	1	0	0	0	0
10	S	2	0	0	0	0
10	T	1	0	0	0	0
11	A	1	0	0	0	0
11	B	5	0	0	1	0
11	C	4	0	0	0	0
11	D	3	0	0	0	0
11	E	4	0	0	0	0
11	F	3	0	0	0	0
11	G	4	0	0	0	0
11	H	3	0	0	0	0
11	I	3	0	0	0	0
11	J	7	0	0	1	0
11	K	11	0	0	0	0
11	L	12	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	M	11	0	0	0	0
11	N	10	0	0	0	0
11	O	14	0	0	0	0
11	P	12	0	0	0	0
11	Q	9	0	0	0	0
11	R	8	0	0	0	0
11	S	13	0	0	1	0
11	T	20	0	0	2	0
All	All	28083	0	22476	304	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 6.

All (304) 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)
4:H:49:HIS:HB3	4:H:52:THR:HG23	1.42	0.99
6:J:-74:DT:H2''	6:J:-73:DT:O5'	1.61	0.99
7:V:37:LYS:HE2	7:V:127:ARG:HD3	1.45	0.96
4:R:49:HIS:HB3	4:R:52:THR:HG23	1.47	0.95
4:H:49:HIS:HB3	4:H:52:THR:CG2	1.99	0.93
4:R:49:HIS:HB3	4:R:52:THR:CG2	1.98	0.91
5:I:67:DT:H4'	5:I:68:DG:OP1	1.70	0.89
7:V:75:LYS:HB2	7:V:82:GLN:HE22	1.40	0.86
5:S:83:DT:H4'	5:S:84:DG:OP1	1.76	0.86
5:I:81:DG:C2'	5:I:82:DC:H5'	2.08	0.82
5:S:-16:DT:H2''	5:S:-15:DA:C8	2.16	0.80
6:T:85:DC:OP1	7:U:117:ASN:ND2	2.17	0.78
5:I:81:DG:H2''	5:I:82:DC:H5'	1.65	0.77
1:E:36:LYS:C	1:E:38:PRO:HD2	2.10	0.77
4:R:65:PHE:CE1	4:R:69:ILE:CD1	2.68	0.76
4:R:65:PHE:CE1	4:R:69:ILE:HD11	2.22	0.74
1:E:37:LYS:N	1:E:38:PRO:HD2	2.04	0.73
6:T:-72:DT:H4'	6:T:-71:DT:OP1	1.88	0.73
5:I:81:DG:N2	6:J:-80:DT:O2	2.21	0.73
6:J:-46:DC:H2''	6:J:-45:DA:C8	2.25	0.71
4:R:28:LYS:N	5:S:-27:DC:OP1	2.23	0.71
2:F:68:ASP:OD2	2:F:92:ARG:NH1	2.23	0.70
5:S:45:DT:OP2	11:S:201:HOH:O	2.09	0.70
3:Q:15:LYS:HE3	6:T:-42:DT:OP1	1.93	0.68
6:J:7:DC:H2''	6:J:8:DG:C8	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:13:LYS:HA	3:M:13:LYS:CE	2.23	0.68
4:D:65:PHE:CE1	4:D:69:ILE:CD1	2.77	0.68
6:J:-74:DT:C2'	6:J:-73:DT:O5'	2.40	0.68
4:D:31:ARG:HG2	6:J:51:DG:OP1	1.95	0.67
6:T:-56:DC:OP1	11:T:201:HOH:O	2.13	0.67
6:T:54:DT:H2''	6:T:55:DC:C6	2.29	0.67
2:L:68:ASP:OD2	2:L:92:ARG:NH1	2.27	0.66
6:T:7:DC:H2''	6:T:8:DG:C8	2.30	0.66
3:M:81:ARG:NH2	3:M:107:VAL:O	2.27	0.66
4:N:65:PHE:CE1	4:N:69:ILE:CD1	2.78	0.66
4:H:65:PHE:CE1	4:H:69:ILE:CD1	2.80	0.65
7:U:36:ARG:HG2	7:U:36:ARG:HH11	1.61	0.65
1:E:36:LYS:C	1:E:38:PRO:CD	2.69	0.65
4:H:49:HIS:CB	4:H:52:THR:HG23	2.23	0.65
7:V:64:GLY:H	7:V:115:LYS:HD3	1.62	0.64
6:J:86:DA:H2''	5:S:-82:DG:O4'	1.98	0.64
2:L:23:ARG:HE	2:L:23:ARG:HA	1.64	0.63
4:N:65:PHE:CE1	4:N:69:ILE:HD11	2.34	0.63
3:M:13:LYS:HA	3:M:13:LYS:NZ	2.14	0.63
3:M:62:ILE:HD11	4:N:65:PHE:CZ	2.34	0.63
4:R:65:PHE:CZ	4:R:69:ILE:HD13	2.34	0.62
4:N:28:LYS:HA	6:T:-27:DC:OP1	1.98	0.62
6:T:79:DA:H2''	6:T:80:DA:O5'	2.00	0.62
5:I:7:DC:H2''	5:I:8:DG:C8	2.35	0.61
3:Q:24:GLN:HG3	4:R:43:LYS:HB3	1.82	0.61
4:R:65:PHE:CZ	4:R:69:ILE:CD1	2.84	0.61
4:R:124:ALA:O	4:R:125:LYS:HB2	2.00	0.60
7:U:101:THR:HG22	7:U:103:LEU:HD22	1.83	0.60
2:P:19:ARG:HG3	6:T:-21:DC:OP1	2.01	0.60
3:Q:15:LYS:O	3:Q:15:LYS:HD3	2.01	0.60
5:S:84:DG:H2''	5:S:85:DC:OP2	2.02	0.59
7:V:107:GLY:HA2	7:V:112:GLY:HA2	1.84	0.59
1:E:34:GLY:HA2	6:J:72:DA:OP1	2.02	0.59
6:J:-73:DT:H2''	6:J:-72:DT:O5'	2.03	0.59
2:P:88:TYR:CE1	4:R:83:TYR:CE1	2.89	0.59
1:K:119:ILE:HD12	2:L:50:ILE:HD13	1.84	0.59
5:I:86:DA:HO3'	6:T:-82:DG:HO5'	1.51	0.59
3:C:81:ARG:NH2	3:C:107:VAL:O	2.35	0.59
2:P:10:LEU:HB2	2:P:12:LYS:HG3	1.83	0.58
7:V:34:LYS:HE3	7:V:34:LYS:HA	1.86	0.58
7:V:70:ILE:O	7:V:74:ALA:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:64:GLY:N	7:V:115:LYS:HD3	2.18	0.58
5:I:83:DT:H2''	5:I:84:DG:C8	2.39	0.57
5:I:69:DT:H1'	5:I:70:DG:H5''	1.87	0.57
5:S:7:DC:H2''	5:S:8:DG:C8	2.40	0.56
1:K:35:VAL:HG12	1:K:35:VAL:O	2.06	0.56
3:C:118:LYS:H	3:C:118:LYS:HD2	1.70	0.56
2:L:23:ARG:HA	2:L:23:ARG:NE	2.20	0.56
5:S:-47:DT:H2''	5:S:-46:DC:C6	2.40	0.56
6:T:-73:DT:H2''	6:T:-72:DT:O5'	2.06	0.56
7:V:70:ILE:CD1	7:V:93:ILE:HD11	2.36	0.56
1:E:37:LYS:N	1:E:38:PRO:CD	2.68	0.56
7:V:104:GLN:HB2	7:V:107:GLY:HA3	1.86	0.56
1:E:39:HIS:CG	1:E:39:HIS:O	2.59	0.56
7:U:55:THR:O	7:U:59:LEU:HB2	2.06	0.56
7:U:55:THR:HA	7:U:58:ARG:HG2	1.87	0.55
7:U:75:LYS:HG2	7:U:82:GLN:HE22	1.72	0.55
7:U:103:LEU:CD2	7:U:117:ASN:HB3	2.37	0.55
2:F:88:TYR:CE1	4:H:83:TYR:CE1	2.94	0.55
5:S:49:DC:H2'	5:S:50:DG:C8	2.41	0.55
4:R:32:SER:O	4:R:33:ARG:HB3	2.06	0.55
7:V:67:LEU:C	7:V:67:LEU:HD23	2.32	0.55
7:V:70:ILE:HD11	7:V:93:ILE:HD11	1.89	0.54
6:J:-74:DT:H2'	6:J:-73:DT:C6	2.42	0.54
6:J:49:DC:H2'	6:J:50:DG:C8	2.42	0.54
2:P:19:ARG:HG3	6:T:-21:DC:P	2.47	0.54
6:J:-46:DC:C2'	6:J:-45:DA:C8	2.90	0.53
7:V:103:LEU:HB2	7:V:117:ASN:HB2	1.89	0.53
6:T:-79:DT:H2''	6:T:-78:DT:H5''	1.90	0.53
5:I:69:DT:C2'	5:I:70:DG:H5''	2.39	0.53
5:S:-4:DC:H2''	5:S:-3:DG:C8	2.43	0.52
5:S:81:DG:H2''	5:S:82:DC:OP2	2.09	0.52
7:V:40:LYS:HD2	7:V:41:LYS:H	1.74	0.52
5:I:72:DA:H2'	5:I:73:DA:C8	2.44	0.52
3:C:113:ALA:HA	3:C:116:LEU:CD1	2.40	0.51
7:V:67:LEU:O	7:V:70:ILE:HG12	2.11	0.51
1:O:59:GLU:OE1	1:O:59:GLU:N	2.43	0.51
6:T:-31:DA:H2''	6:T:-30:DG:OP2	2.09	0.51
6:T:49:DC:H2'	6:T:50:DG:C8	2.44	0.51
1:A:40:ARG:HH11	1:A:40:ARG:HB2	1.75	0.51
5:I:-81:DC:H2''	5:I:-80:DT:O4'	2.10	0.51
7:V:96:LEU:HB3	7:V:102:LEU:HD13	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:-50:DC:H2''	5:S:-49:DG:C8	2.46	0.51
6:T:-50:DC:H2''	6:T:-49:DG:C8	2.46	0.51
5:S:54:DT:H4'	5:S:55:DC:OP1	2.09	0.51
2:P:68:ASP:OD2	2:P:92:ARG:NH1	2.43	0.50
7:V:60:GLY:O	7:V:115:LYS:NZ	2.24	0.50
2:P:88:TYR:CD1	4:R:83:TYR:CZ	2.98	0.50
5:S:85:DC:H2''	5:S:86:DA:C8	2.46	0.50
5:I:81:DG:H2'	5:I:82:DC:H5'	1.93	0.50
2:B:21:VAL:HG12	2:B:22:LEU:HG	1.94	0.50
1:K:119:ILE:HG13	2:L:50:ILE:CD1	2.42	0.50
2:L:35:ARG:NH1	11:L:202:HOH:O	2.45	0.50
7:V:103:LEU:HB2	7:V:117:ASN:CB	2.41	0.49
1:A:49:ARG:HH21	6:J:-67:DA:H4'	1.76	0.49
1:O:37:LYS:HB3	1:O:38:PRO:HD2	1.94	0.49
7:U:80:PHE:CE1	7:U:85:GLY:HA3	2.48	0.49
3:M:32:ARG:NH1	4:N:35:GLU:OE2	2.43	0.49
5:I:69:DT:H2''	5:I:70:DG:C5'	2.41	0.49
7:U:80:PHE:CZ	7:U:85:GLY:HA3	2.47	0.49
6:J:-73:DT:H2'	6:J:-72:DT:C6	2.47	0.49
3:C:31:HIS:CD2	3:C:48:PRO:HG3	2.48	0.49
5:S:-62:DC:H2'	5:S:-61:DG:C8	2.48	0.49
5:S:54:DT:H2''	5:S:55:DC:C6	2.47	0.49
2:B:31:LYS:N	2:B:32:PRO:HD2	2.27	0.49
4:H:65:PHE:CE1	4:H:69:ILE:HD11	2.47	0.48
3:Q:118:LYS:N	3:Q:118:LYS:HD2	2.28	0.48
5:I:54:DT:H2''	5:I:55:DC:C6	2.48	0.48
2:B:88:TYR:CE1	4:D:83:TYR:CE1	3.02	0.48
5:I:-47:DT:H2''	5:I:-46:DC:C6	2.48	0.48
2:B:68:ASP:OD2	2:B:92:ARG:NH1	2.45	0.48
4:D:118:VAL:O	4:D:122:THR:OG1	2.32	0.48
5:I:-82:DG:H5'	6:T:86:DA:O3'	2.14	0.48
6:J:54:DT:H4'	6:J:55:DC:OP1	2.14	0.48
2:F:22:LEU:N	2:F:22:LEU:HD23	2.28	0.48
6:T:-56:DC:P	11:T:201:HOH:O	2.71	0.48
3:C:29:ARG:NH1	4:D:36:SER:O	2.45	0.48
7:U:103:LEU:HD22	7:U:103:LEU:N	2.29	0.48
5:I:-82:DG:C6	6:T:86:DA:C6	3.02	0.47
3:M:62:ILE:CD1	4:N:65:PHE:CZ	2.97	0.47
3:M:29:ARG:NH1	4:N:36:SER:O	2.46	0.47
1:E:35:VAL:HG12	1:E:35:VAL:O	2.14	0.47
3:M:118:LYS:HD2	3:M:118:LYS:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:-63:DC:H2''	6:T:-62:DC:O5'	2.14	0.47
4:H:65:PHE:CZ	4:H:69:ILE:HD13	2.49	0.47
6:J:81:DG:H2''	6:J:82:DC:OP2	2.15	0.47
3:M:62:ILE:HD11	4:N:65:PHE:CE1	2.50	0.47
1:A:121:PRO:HD2	8:A:201:CL:CL	2.52	0.47
2:F:45:ARG:CZ	5:I:7:DC:H4'	2.45	0.47
6:T:83:DT:C3'	6:T:84:DG:H5''	2.44	0.47
4:N:28:LYS:CA	6:T:-27:DC:OP1	2.62	0.47
2:P:20:LYS:HG2	6:T:-22:DA:OP1	2.15	0.47
5:I:-62:DC:H2'	5:I:-61:DG:C8	2.50	0.47
5:S:-79:DT:H2''	5:S:-78:DT:H5''	1.96	0.47
7:U:116:LEU:C	7:U:116:LEU:HD23	2.40	0.47
5:I:49:DC:H2'	5:I:50:DG:C8	2.50	0.46
7:V:53:VAL:HG22	7:V:102:LEU:HD11	1.98	0.46
5:I:80:DA:H2''	5:I:81:DG:C8	2.51	0.46
4:D:95:GLN:HE21	4:D:111:VAL:HG13	1.81	0.46
1:E:63:ARG:HG2	1:E:63:ARG:HH11	1.80	0.46
2:F:93:GLN:O	2:F:95:ARG:HG3	2.16	0.46
3:Q:67:GLY:HA3	4:R:49:HIS:CD2	2.50	0.46
2:B:95:ARG:NH1	11:B:202:HOH:O	2.49	0.46
1:A:118:THR:HA	2:B:45:ARG:O	2.16	0.46
5:S:69:DT:C2'	5:S:70:DG:H5''	2.46	0.46
7:U:62:ARG:NH2	7:U:64:GLY:O	2.48	0.46
7:V:55:THR:HG21	7:V:70:ILE:HB	1.97	0.46
1:E:36:LYS:HG3	1:E:38:PRO:HD2	1.98	0.46
5:S:69:DT:H1'	5:S:70:DG:H5''	1.97	0.46
5:I:-33:DA:C5	5:I:-32:DC:C4	3.04	0.46
1:K:121:PRO:HD2	8:K:201:CL:CL	2.53	0.46
4:R:49:HIS:CB	4:R:52:THR:HG23	2.31	0.46
1:A:67:PHE:CZ	1:A:93:GLN:HA	2.51	0.46
7:U:77:VAL:HG22	7:U:80:PHE:HB2	1.98	0.46
6:J:77:DA:H2''	6:J:78:DA:O5'	2.15	0.45
5:I:-16:DT:H2''	5:I:-15:DA:C8	2.52	0.45
5:I:80:DA:H2''	5:I:81:DG:H8	1.80	0.45
2:P:88:TYR:CZ	4:R:83:TYR:CD1	3.03	0.45
3:Q:42:ARG:O	4:R:88:THR:HA	2.15	0.45
6:J:86:DA:C6	5:S:-82:DG:C6	3.05	0.45
1:K:119:ILE:CD1	2:L:50:ILE:HD13	2.45	0.45
2:P:45:ARG:CZ	5:S:7:DC:H4'	2.46	0.45
5:S:69:DT:H2''	5:S:70:DG:C5'	2.45	0.45
5:I:-3:DG:C6	5:I:-2:DG:C6	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:88:TYR:CD1	4:N:83:TYR:CZ	3.04	0.45
5:S:77:DA:H2''	5:S:78:DA:O5'	2.16	0.45
2:L:88:TYR:CE1	4:N:83:TYR:CE1	3.04	0.45
4:N:80:LEU:CD1	4:N:96:THR:HB	2.47	0.45
7:U:56:ILE:HD11	7:U:70:ILE:CD1	2.47	0.45
6:J:31:DT:H2''	6:J:32:DG:C8	2.52	0.45
4:D:31:ARG:HG2	6:J:51:DG:P	2.56	0.45
4:D:65:PHE:CE1	4:D:69:ILE:HD11	2.50	0.45
1:E:37:LYS:HE2	5:I:68:DC:OP1	2.17	0.45
5:I:54:DT:H4'	5:I:55:DC:OP1	2.16	0.45
5:I:69:DT:H2''	5:I:70:DG:H5''	1.99	0.45
4:N:68:ASP:OD2	2:P:98:TYR:OH	2.27	0.45
7:U:52:VAL:O	7:U:56:ILE:HG12	2.17	0.45
1:A:113:HIS:CG	1:E:126:LEU:HD22	2.52	0.45
6:J:7:DC:H2''	6:J:8:DG:H8	1.81	0.44
2:L:31:LYS:N	2:L:32:PRO:HD2	2.33	0.44
7:U:36:ARG:HH11	7:U:36:ARG:CG	2.26	0.44
5:I:46:DG:N2	6:J:-45:DA:C2	2.85	0.44
3:M:47:ALA:N	3:M:48:PRO:HD2	2.32	0.44
1:O:39:HIS:HE1	1:O:41:TYR:CE1	2.35	0.44
5:S:-54:DA:C6	5:S:-53:DG:C6	3.06	0.44
7:U:103:LEU:N	7:U:115:LYS:O	2.49	0.44
1:O:48:LEU:HD22	2:P:44:LYS:HE3	2.00	0.44
6:T:77:DA:H2''	6:T:78:DA:O5'	2.18	0.44
2:L:19:ARG:HG3	2:L:22:LEU:HB2	1.99	0.44
3:M:77:ARG:CZ	5:S:-54:DA:H4'	2.48	0.44
2:P:35:ARG:O	2:P:39:ARG:HG2	2.18	0.44
4:N:80:LEU:HD13	4:N:96:THR:HB	2.00	0.44
6:T:-81:DC:H2''	6:T:-80:DT:O4'	2.18	0.43
6:T:59:DA:C5	6:T:60:DC:C4	3.06	0.43
1:K:119:ILE:HG13	2:L:50:ILE:HD12	2.00	0.43
6:T:-32:DC:H2''	6:T:-31:DA:OP2	2.18	0.43
2:B:31:LYS:HG3	2:B:51:TYR:CE1	2.53	0.43
2:P:3:ARG:HG2	2:P:4:GLY:N	2.33	0.43
6:T:11:DC:H2'	6:T:12:DG:C8	2.53	0.43
7:U:86:ARG:HH11	7:U:87:THR:HG23	1.83	0.43
2:B:88:TYR:CD1	4:D:83:TYR:CZ	3.07	0.43
6:T:-72:DT:C4'	6:T:-71:DT:OP1	2.63	0.43
6:T:-33:DA:C5	6:T:-32:DC:C4	3.07	0.43
7:V:110:ALA:O	7:V:112:GLY:N	2.52	0.43
3:C:113:ALA:O	3:C:116:LEU:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:26:PRO:HG3	4:H:40:TYR:CE2	2.54	0.43
4:R:33:ARG:HG2	4:R:33:ARG:HH11	1.81	0.43
4:D:76:GLU:OE2	4:D:79:ARG:NH1	2.51	0.43
2:F:88:TYR:CD1	4:H:83:TYR:CZ	3.06	0.43
3:G:88:ARG:HA	3:G:88:ARG:HD3	1.82	0.43
7:U:101:THR:HG22	7:U:103:LEU:CD2	2.48	0.43
3:G:80:PRO:HB2	3:G:104:GLN:O	2.19	0.43
5:I:-54:DA:C6	5:I:-53:DG:C6	3.07	0.43
1:K:128:ARG:HD2	1:K:133:GLU:OE1	2.19	0.43
1:E:48:LEU:HD22	2:F:44:LYS:HE3	2.01	0.42
2:B:23:ARG:H	2:B:23:ARG:HD3	1.84	0.42
6:J:-15:DA:H2''	11:J:203:HOH:O	2.18	0.42
7:V:69:LYS:HD2	7:V:69:LYS:C	2.44	0.42
5:I:15:DT:H2''	5:I:16:DA:C8	2.54	0.42
7:U:108:THR:HG22	7:U:110:ALA:HB3	2.01	0.42
7:V:37:LYS:CE	7:V:127:ARG:HD3	2.34	0.42
2:F:31:LYS:N	2:F:32:PRO:HD2	2.34	0.42
7:V:80:PHE:CZ	7:V:85:GLY:HA3	2.54	0.42
7:U:77:VAL:CG2	7:U:80:PHE:HB2	2.50	0.42
1:K:131:ARG:HD3	1:K:133:GLU:OE2	2.19	0.42
2:P:21:VAL:HG12	2:P:21:VAL:O	2.20	0.42
7:V:37:LYS:HE2	7:V:127:ARG:CD	2.33	0.42
2:P:22:LEU:HD13	2:P:22:LEU:HA	1.94	0.42
1:E:118:THR:HA	2:F:45:ARG:O	2.19	0.42
6:T:85:DC:H2''	6:T:86:DA:C8	2.55	0.42
7:U:51:LEU:HD22	7:U:55:THR:HG23	2.01	0.42
3:C:64:GLU:OE1	4:D:48:VAL:HG13	2.20	0.42
3:C:113:ALA:HA	3:C:116:LEU:HD12	2.01	0.42
6:J:7:DC:C2'	6:J:8:DG:C8	3.00	0.42
3:M:104:GLN:NE2	1:O:58:THR:O	2.53	0.42
3:G:116:LEU:HB3	3:G:117:PRO:HD2	2.02	0.42
4:N:68:ASP:O	4:N:71:GLU:HB2	2.20	0.42
5:I:6:DA:N6	6:J:-7:DG:C6	2.88	0.41
6:J:48:DG:H1'	6:J:49:DC:C6	2.55	0.41
4:R:29:ARG:HA	4:R:29:ARG:HD2	1.75	0.41
5:S:-81:DC:H2''	5:S:-80:DT:C6	2.55	0.41
5:I:-7:DG:C6	6:J:6:DA:N6	2.88	0.41
2:L:89:ALA:O	2:L:93:GLN:HG2	2.20	0.41
4:N:29:ARG:CZ	5:S:30:DC:H4'	2.50	0.41
7:U:79:TRP:CD1	7:U:79:TRP:C	2.98	0.41
6:J:-25:DA:H1'	6:J:-24:DG:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:20:LYS:C	2:P:21:VAL:HG23	2.45	0.41
7:U:103:LEU:O	7:U:115:LYS:HD2	2.19	0.41
3:C:77:ARG:CZ	5:I:-54:DA:H4'	2.51	0.41
5:I:-25:DA:H1'	5:I:-24:DG:C8	2.56	0.41
7:U:57:ARG:HD2	7:U:57:ARG:O	2.20	0.41
7:V:64:GLY:CA	7:V:115:LYS:HD3	2.51	0.41
2:P:89:ALA:O	2:P:93:GLN:HG2	2.21	0.41
5:S:37:DC:H2''	5:S:38:DG:C8	2.56	0.41
5:S:83:DT:C2'	5:S:84:DG:C8	3.02	0.41
7:V:93:ILE:O	7:V:97:VAL:HG23	2.20	0.41
3:C:37:GLY:HA3	3:C:39:TYR:CE2	2.56	0.41
4:H:46:LYS:HA	4:H:46:LYS:HD3	1.82	0.41
5:I:-12:DC:H2''	5:I:-11:DG:C8	2.56	0.41
7:U:56:ILE:N	7:U:56:ILE:HD13	2.35	0.41
7:U:63:ASN:O	7:U:115:LYS:NZ	2.48	0.41
7:U:96:LEU:O	7:U:101:THR:N	2.36	0.41
4:D:95:GLN:NE2	4:D:111:VAL:HG13	2.36	0.41
3:G:39:TYR:OH	4:H:71:GLU:OE1	2.30	0.41
6:J:-9:DA:C5	6:J:-8:DC:C4	3.09	0.41
1:K:35:VAL:O	1:K:35:VAL:CG1	2.69	0.41
5:S:68:DG:C2	6:T:-67:DA:C2	3.09	0.41
5:I:1:DT:H2''	5:I:2:DC:OP2	2.20	0.40
5:I:69:DT:C1'	5:I:70:DG:H5''	2.51	0.40
5:S:83:DT:H2'	5:S:84:DG:C8	2.56	0.40
6:J:-53:DG:C6	6:J:-52:DG:C6	3.09	0.40
5:S:-7:DG:C6	6:T:6:DA:N6	2.89	0.40
5:S:83:DT:C4'	5:S:84:DG:OP1	2.56	0.40
6:T:-60:DG:H2''	6:T:-59:DT:H5'	2.02	0.40
6:J:41:DC:H2''	6:J:42:DA:C8	2.56	0.40
2:L:31:LYS:HG3	2:L:51:TYR:CE1	2.57	0.40
7:V:56:ILE:CD1	7:V:102:LEU:HD21	2.52	0.40
1:O:79:LYS:HB3	1:O:82:LEU:HD11	2.04	0.40
6:T:-4:DC:H2''	6:T:-3:DG:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	98/136 (72%)	95 (97%)	2 (2%)	1 (1%)	12	32
1	E	101/136 (74%)	98 (97%)	1 (1%)	2 (2%)	6	16
1	K	104/136 (76%)	101 (97%)	1 (1%)	2 (2%)	6	17
1	O	98/136 (72%)	97 (99%)	1 (1%)	0	100	100
2	B	80/103 (78%)	75 (94%)	5 (6%)	0	100	100
2	F	81/103 (79%)	76 (94%)	5 (6%)	0	100	100
2	L	82/103 (80%)	80 (98%)	2 (2%)	0	100	100
2	P	100/103 (97%)	90 (90%)	7 (7%)	3 (3%)	3	8
3	C	107/130 (82%)	104 (97%)	3 (3%)	0	100	100
3	G	102/130 (78%)	97 (95%)	5 (5%)	0	100	100
3	M	107/130 (82%)	103 (96%)	4 (4%)	0	100	100
3	Q	103/130 (79%)	101 (98%)	2 (2%)	0	100	100
4	D	95/126 (75%)	93 (98%)	1 (1%)	1 (1%)	11	29
4	H	100/126 (79%)	97 (97%)	2 (2%)	1 (1%)	12	32
4	N	96/126 (76%)	93 (97%)	2 (2%)	1 (1%)	12	32
4	R	96/126 (76%)	90 (94%)	3 (3%)	3 (3%)	3	8
7	U	85/213 (40%)	72 (85%)	10 (12%)	3 (4%)	3	6
7	V	92/213 (43%)	79 (86%)	11 (12%)	2 (2%)	5	14
All	All	1727/2406 (72%)	1641 (95%)	67 (4%)	19 (1%)	11	29

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	E	37	LYS
1	K	35	VAL
1	K	37	LYS

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Mol	Chain	Res	Type
2	P	21	VAL
2	P	22	LEU
7	U	118	ARG
4	D	104	GLY
4	N	104	GLY
2	P	19	ARG
4	R	104	GLY
7	U	37	LYS
7	U	101	THR
7	V	111	ASN
7	V	113	SER
4	R	30	LYS
4	R	33	ARG
1	E	35	VAL
4	H	104	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	87/111 (78%)	82 (94%)	5 (6%)	18	43
1	E	88/111 (79%)	82 (93%)	6 (7%)	14	35
1	K	90/111 (81%)	84 (93%)	6 (7%)	15	36
1	O	87/111 (78%)	81 (93%)	6 (7%)	14	34
2	B	67/79 (85%)	65 (97%)	2 (3%)	36	66
2	F	68/79 (86%)	65 (96%)	3 (4%)	25	53
2	L	69/79 (87%)	62 (90%)	7 (10%)	7	18
2	P	78/79 (99%)	70 (90%)	8 (10%)	7	18
3	C	86/100 (86%)	83 (96%)	3 (4%)	32	61
3	G	83/100 (83%)	79 (95%)	4 (5%)	23	50
3	M	86/100 (86%)	78 (91%)	8 (9%)	8	21
3	Q	84/100 (84%)	76 (90%)	8 (10%)	8	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	83/105 (79%)	74 (89%)	9 (11%)	6	16
4	H	87/105 (83%)	75 (86%)	12 (14%)	3	9
4	N	84/105 (80%)	77 (92%)	7 (8%)	10	26
4	R	84/105 (80%)	76 (90%)	8 (10%)	8	20
7	U	76/157 (48%)	57 (75%)	19 (25%)	0	2
7	V	80/157 (51%)	59 (74%)	21 (26%)	0	2
All	All	1467/1894 (78%)	1325 (90%)	142 (10%)	8	20

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	37	LYS
1	A	39	HIS
1	A	40	ARG
1	A	49	ARG
2	B	23	ARG
2	B	35	ARG
3	C	81	ARG
3	C	91	GLU
3	C	110	ASN
4	D	36	SER
4	D	46	LYS
4	D	48	VAL
4	D	56	SER
4	D	85	LYS
4	D	86	ARG
4	D	106	LEU
4	D	122	THR
4	D	125	LYS
1	E	37	LYS
1	E	40	ARG
1	E	48	LEU
1	E	63	ARG
1	E	129	ARG
1	E	134	ARG
2	F	22	LEU
2	F	23	ARG
2	F	27	GLN
3	G	29	ARG

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Mol	Chain	Res	Type
3	G	36	LYS
3	G	74	LYS
3	G	81	ARG
4	H	24	LYS
4	H	28	LYS
4	H	30	LYS
4	H	31	ARG
4	H	33	ARG
4	H	48	VAL
4	H	52	THR
4	H	80	LEU
4	H	86	ARG
4	H	105	GLU
4	H	106	LEU
4	H	125	LYS
1	K	36	LYS
1	K	37	LYS
1	K	63	ARG
1	K	86	SER
1	K	117	VAL
1	K	129	ARG
2	L	19	ARG
2	L	22	LEU
2	L	23	ARG
2	L	47	SER
2	L	50	ILE
2	L	52	GLU
2	L	59	LYS
3	M	13	LYS
3	M	15	LYS
3	M	36	LYS
3	M	73	ASN
3	M	74	LYS
3	M	77	ARG
3	M	81	ARG
3	M	91	GLU
4	N	32	SER
4	N	34	LYS
4	N	36	SER
4	N	46	LYS
4	N	85	LYS
4	N	106	LEU

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Mol	Chain	Res	Type
4	N	122	THR
1	O	36	LYS
1	O	37	LYS
1	O	48	LEU
1	O	76	GLN
1	O	129	ARG
1	O	134	ARG
2	P	3	ARG
2	P	5	LYS
2	P	10	LEU
2	P	19	ARG
2	P	20	LYS
2	P	22	LEU
2	P	27	GLN
2	P	91	LYS
3	Q	15	LYS
3	Q	24	GLN
3	Q	29	ARG
3	Q	64	GLU
3	Q	71	ARG
3	Q	74	LYS
3	Q	76	THR
3	Q	81	ARG
4	R	28	LYS
4	R	32	SER
4	R	36	SER
4	R	46	LYS
4	R	52	THR
4	R	80	LEU
4	R	85	LYS
4	R	105	GLU
7	U	36	ARG
7	U	38	ASN
7	U	40	LYS
7	U	51	LEU
7	U	56	ILE
7	U	59	LEU
7	U	67	LEU
7	U	86	ARG
7	U	93	ILE
7	U	98	GLN
7	U	99	ASN

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Mol	Chain	Res	Type
7	U	104	GLN
7	U	108	THR
7	U	113	SER
7	U	114	PHE
7	U	115	LYS
7	U	116	LEU
7	U	117	ASN
7	U	118	ARG
7	V	34	LYS
7	V	35	LYS
7	V	37	LYS
7	V	40	LYS
7	V	41	LYS
7	V	43	ASN
7	V	51	LEU
7	V	55	THR
7	V	59	LEU
7	V	62	ARG
7	V	72	THR
7	V	73	GLU
7	V	75	LYS
7	V	76	LYS
7	V	77	VAL
7	V	108	THR
7	V	111	ASN
7	V	113	SER
7	V	116	LEU
7	V	118	ARG
7	V	119	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	68	GLN
1	A	76	GLN
3	C	31	HIS
3	C	38	ASN
3	C	73	ASN
4	D	95	GLN
1	E	68	GLN
2	F	25	ASN
3	G	24	GLN

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Mol	Chain	Res	Type
3	G	31	HIS
3	G	38	ASN
3	G	73	ASN
4	H	47	GLN
1	K	68	GLN
3	M	24	GLN
3	M	104	GLN
4	N	95	GLN
1	O	39	HIS
4	R	47	GLN
7	U	43	ASN
7	U	82	GLN
7	U	104	GLN
7	U	117	ASN
7	V	38	ASN
7	V	82	GLN
7	V	99	ASN
7	V	104	GLN
7	V	111	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 68 ligands modelled in this entry, 68 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	100/136 (73%)	0.22	4 (4%) 42 38	55, 76, 115, 146	0
1	E	103/136 (75%)	0.10	1 (0%) 79 78	54, 69, 132, 159	0
1	K	106/136 (77%)	-0.11	5 (4%) 36 33	38, 52, 137, 162	0
1	O	100/136 (73%)	-0.24	0 100 100	36, 51, 91, 138	0
2	B	82/103 (79%)	0.18	4 (4%) 35 31	55, 71, 100, 148	0
2	F	83/103 (80%)	0.06	3 (3%) 46 42	52, 68, 91, 152	0
2	L	84/103 (81%)	-0.11	3 (3%) 46 42	38, 50, 109, 154	0
2	P	102/103 (99%)	0.29	10 (9%) 13 11	39, 53, 162, 184	0
3	C	109/130 (83%)	0.11	1 (0%) 81 80	57, 75, 110, 135	0
3	G	104/130 (80%)	0.01	1 (0%) 79 78	53, 74, 104, 110	0
3	M	109/130 (83%)	-0.01	2 (1%) 67 65	43, 55, 94, 128	0
3	Q	105/130 (80%)	-0.14	1 (0%) 79 78	41, 55, 85, 123	0
4	D	97/126 (76%)	0.21	2 (2%) 63 61	55, 77, 112, 149	0
4	H	102/126 (80%)	0.10	3 (2%) 53 50	57, 74, 138, 161	0
4	N	98/126 (77%)	-0.15	0 100 100	40, 57, 103, 138	0
4	R	98/126 (77%)	0.02	4 (4%) 41 37	42, 55, 117, 145	0
5	I	169/169 (100%)	-0.13	0 100 100	76, 121, 190, 219	0
5	S	169/169 (100%)	-0.36	0 100 100	58, 93, 181, 205	0
6	J	169/169 (100%)	-0.12	1 (0%) 85 85	80, 121, 190, 226	0
6	T	169/169 (100%)	-0.37	0 100 100	59, 93, 182, 216	0
7	U	87/213 (40%)	0.49	1 (1%) 78 76	115, 145, 170, 202	0
7	V	94/213 (44%)	0.54	4 (4%) 40 36	88, 120, 158, 164	0
All	All	2439/3082 (79%)	-0.01	50 (2%) 63 61	36, 77, 158, 226	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	22	LEU	4.7
2	B	102	GLY	4.7
2	L	102	GLY	4.5
2	F	22	LEU	4.4
2	L	21	VAL	3.9
2	B	22	LEU	3.8
4	D	123	SER	3.8
1	K	30	PRO	3.7
3	C	45	ALA	3.6
2	B	21	VAL	3.3
2	P	15	ALA	3.2
2	P	10	LEU	3.1
4	H	63	ASN	3.1
3	G	36	LYS	3.1
3	M	13	LYS	3.1
1	E	35	VAL	3.1
4	H	35	GLU	3.0
1	A	115	LYS	2.9
2	P	18	HIS	2.9
1	K	35	VAL	2.8
1	A	38	PRO	2.7
2	P	12	LYS	2.7
1	K	31	ALA	2.7
2	P	21	VAL	2.7
2	F	102	GLY	2.7
1	K	38	PRO	2.7
7	V	116	LEU	2.6
4	R	30	LYS	2.6
4	R	29	ARG	2.6
4	H	31	ARG	2.5
4	R	32	SER	2.5
6	J	-47	DT	2.5
2	F	33	ALA	2.5
3	M	12	ALA	2.5
7	V	114	PHE	2.5
1	K	32	THR	2.4
2	B	28	GLY	2.4
2	P	9	GLY	2.4
4	D	122	THR	2.4
2	P	2	GLY	2.4
2	P	51	TYR	2.3
7	V	103	LEU	2.3
3	Q	15	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	49	ARG	2.3
4	R	124	ALA	2.2
7	U	120	LYS	2.2
2	P	22	LEU	2.2
7	V	108	THR	2.1
2	P	6	GLY	2.1
1	A	48	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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
9	CA	I	105	1/1	0.70	0.08	133,133,133,133	0
9	CA	S	118	1/1	0.70	0.12	121,121,121,121	0
9	CA	J	105	1/1	0.71	0.22	125,125,125,125	0
9	CA	I	107	1/1	0.74	0.10	123,123,123,123	0
9	CA	G	203	1/1	0.75	0.20	132,132,132,132	0
9	CA	S	112	1/1	0.80	0.10	118,118,118,118	0
10	K	I	110	1/1	0.80	0.19	113,113,113,113	0
9	CA	J	107	1/1	0.82	0.11	123,123,123,123	0
9	CA	S	115	1/1	0.83	0.09	114,114,114,114	0
9	CA	S	104	1/1	0.84	0.13	120,120,120,120	0
10	K	S	119	1/1	0.84	0.12	100,100,100,100	0
9	CA	G	201	1/1	0.85	0.07	121,121,121,121	0
9	CA	T	102	1/1	0.85	0.15	113,113,113,113	0
9	CA	T	103	1/1	0.85	0.06	122,122,122,122	0
9	CA	I	104	1/1	0.85	0.06	123,123,123,123	0
9	CA	J	108	1/1	0.85	0.08	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CA	S	116	1/1	0.87	0.09	106,106,106,106	0
9	CA	R	201	1/1	0.87	0.11	117,117,117,117	0
9	CA	Q	202	1/1	0.88	0.20	101,101,101,101	0
9	CA	Q	203	1/1	0.88	0.10	103,103,103,103	0
8	CL	A	201	1/1	0.88	0.12	98,98,98,98	0
9	CA	I	103	1/1	0.88	0.07	121,121,121,121	0
9	CA	S	109	1/1	0.89	0.17	114,114,114,114	0
9	CA	T	104	1/1	0.89	0.10	110,110,110,110	0
9	CA	C	202	1/1	0.89	0.10	114,114,114,114	0
9	CA	S	106	1/1	0.89	0.06	110,110,110,110	0
8	CL	C	204	1/1	0.90	0.14	91,91,91,91	0
9	CA	Q	201	1/1	0.90	0.14	114,114,114,114	0
9	CA	S	110	1/1	0.90	0.08	114,114,114,114	0
10	K	J	110	1/1	0.90	0.10	99,99,99,99	0
9	CA	J	104	1/1	0.90	0.19	114,114,114,114	0
10	K	M	202	1/1	0.91	0.08	92,92,92,92	0
9	CA	S	117	1/1	0.91	0.10	114,114,114,114	0
9	CA	S	105	1/1	0.92	0.08	110,110,110,110	0
8	CL	E	201	1/1	0.92	0.22	82,82,82,82	0
9	CA	I	101	1/1	0.92	0.08	89,89,89,89	0
9	CA	C	201	1/1	0.92	0.15	103,103,103,103	0
9	CA	T	106	1/1	0.93	0.13	107,107,107,107	0
9	CA	J	106	1/1	0.93	0.05	122,122,122,122	0
9	CA	S	107	1/1	0.93	0.19	98,98,98,98	0
9	CA	J	101	1/1	0.93	0.07	106,106,106,106	0
9	CA	J	103	1/1	0.93	0.10	102,102,102,102	0
10	K	S	120	1/1	0.93	0.07	106,106,106,106	0
10	K	T	107	1/1	0.93	0.10	95,95,95,95	0
9	CA	S	103	1/1	0.94	0.05	99,99,99,99	0
9	CA	S	113	1/1	0.94	0.10	113,113,113,113	0
9	CA	J	102	1/1	0.95	0.14	118,118,118,118	0
9	CA	J	109	1/1	0.95	0.05	111,111,111,111	0
8	CL	O	201	1/1	0.95	0.17	71,71,71,71	0
8	CL	K	201	1/1	0.95	0.08	76,76,76,76	0
9	CA	I	106	1/1	0.95	0.09	93,93,93,93	0
9	CA	T	101	1/1	0.95	0.14	100,100,100,100	0
9	CA	I	102	1/1	0.95	0.05	94,94,94,94	0
9	CA	G	202	1/1	0.95	0.09	107,107,107,107	0
9	CA	S	111	1/1	0.96	0.14	102,102,102,102	0
9	CA	S	108	1/1	0.96	0.06	85,85,85,85	0
8	CL	R	202	1/1	0.96	0.07	65,65,65,65	0
9	CA	T	105	1/1	0.96	0.09	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CA	I	108	1/1	0.96	0.11	102,102,102,102	0
10	K	I	109	1/1	0.96	0.07	91,91,91,91	0
9	CA	N	201	1/1	0.97	0.06	94,94,94,94	0
9	CA	S	101	1/1	0.97	0.05	81,81,81,81	0
9	CA	S	114	1/1	0.97	0.10	91,91,91,91	0
9	CA	S	102	1/1	0.97	0.07	75,75,75,75	0
8	CL	G	204	1/1	0.97	0.04	75,75,75,75	0
8	CL	M	201	1/1	0.98	0.21	63,63,63,63	0
10	K	C	205	1/1	0.98	0.05	105,105,105,105	0
9	CA	C	203	1/1	0.98	0.05	115,115,115,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.