



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 5, 2022 – 10:11 AM EST

PDB ID : 7MK0
Title : Trypanosoma cruzi Nucleoside Diphosphate Kinase 1 form a quinary multi-hexameric structure
Authors : Gomez, J.A.; Aguilar, C.F.
Deposited on : 2021-04-21
Resolution : 3.50 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	:	2.25
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)	:	2.25

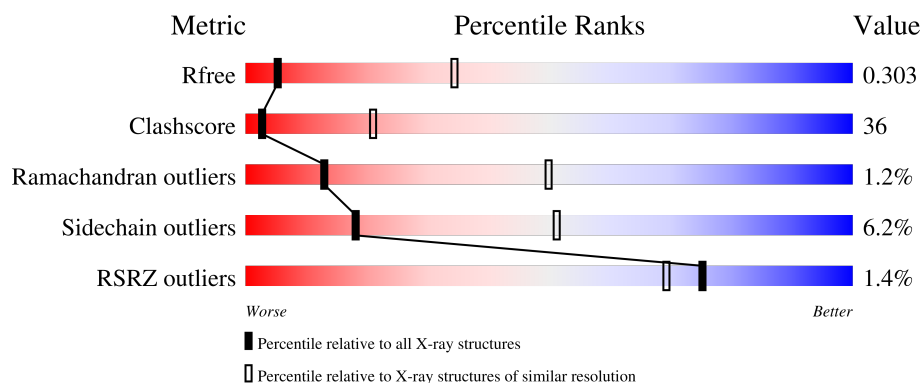
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	151	<div> <div>%</div> <div> <div></div> <div>46%</div> <div>50%</div> <div>..</div> </div> </div>
1	B	151	<div> <div>3%</div> <div> <div></div> <div>46%</div> <div>51%</div> <div>.</div> </div> </div>
1	C	151	<div> <div>5%</div> <div> <div></div> <div>53%</div> <div>42%</div> <div>5%</div> </div> </div>
1	D	151	<div> <div>%</div> <div> <div></div> <div>46%</div> <div>51%</div> <div>..</div> </div> </div>
1	E	151	<div> <div>%</div> <div> <div></div> <div>51%</div> <div>45%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	151	
1	G	151	
1	H	151	
1	I	151	
1	J	151	
1	K	151	
1	L	151	
1	M	151	
1	N	151	
1	O	151	
1	P	151	
1	Q	151	
1	R	151	
1	S	151	
1	T	151	
1	U	151	
1	V	151	
1	W	151	
1	X	151	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 28296 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 Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	B	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	C	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	D	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	E	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	F	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	G	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	H	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	I	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	J	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	K	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	L	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	M	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	N	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	O	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	P	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			

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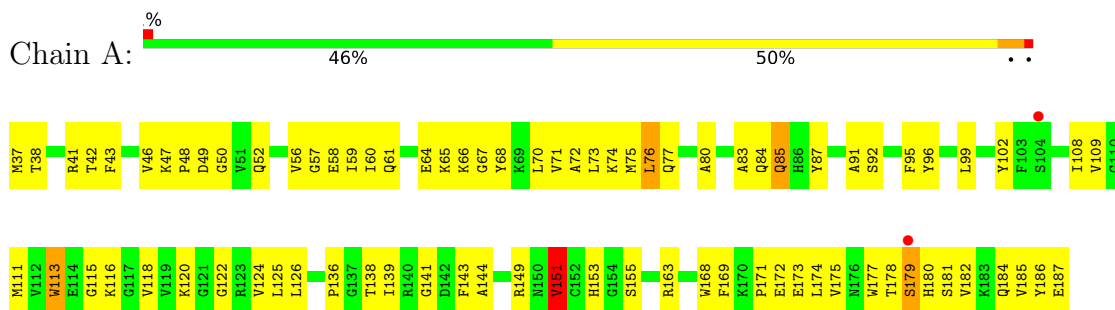
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	R	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	S	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	T	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	U	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	V	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	W	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			
1	X	151	Total	C	N	O	S	0	0	0
			1179	754	203	217	5			

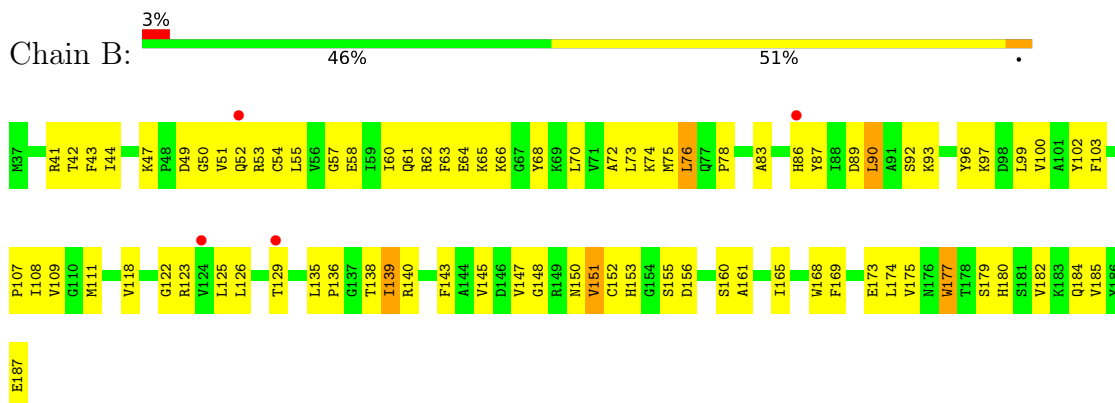
3 Residue-property plots [i](#)

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.

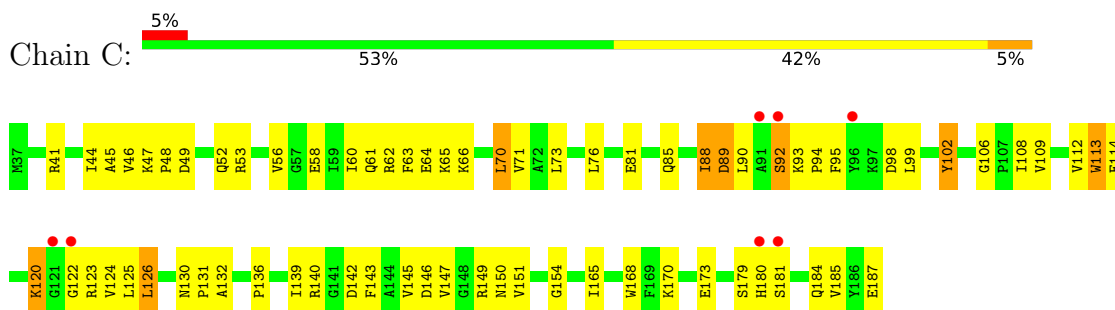
- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase

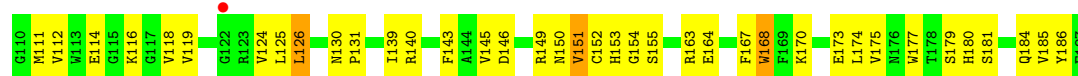


- Molecule 1: Nucleoside diphosphate kinase

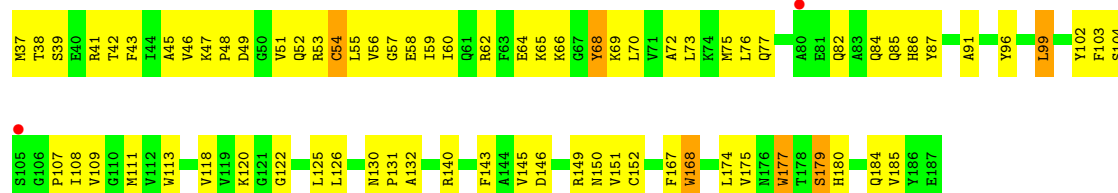


- Molecule 1: Nucleoside diphosphate kinase

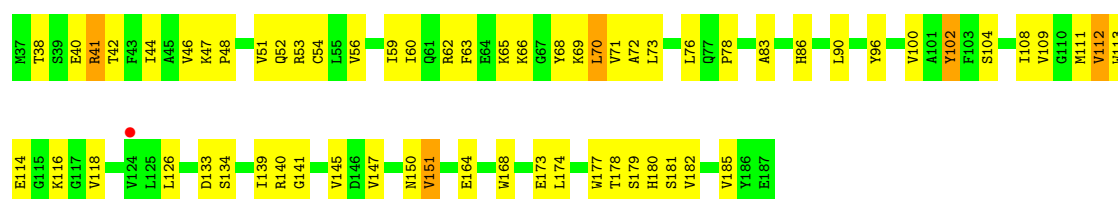




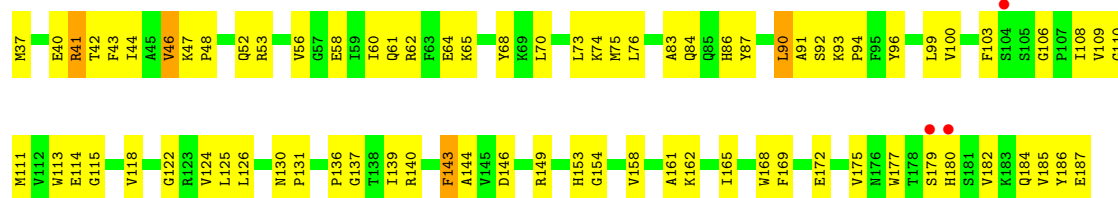
• Molecule 1: Nucleoside diphosphate kinase



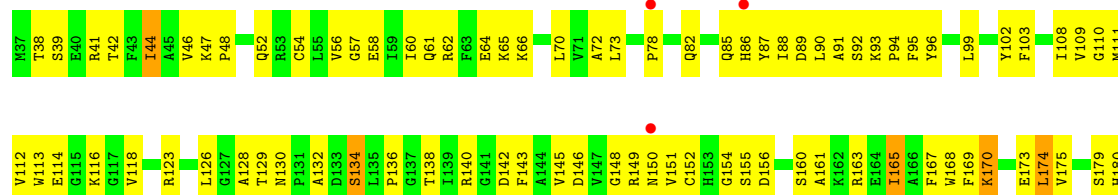
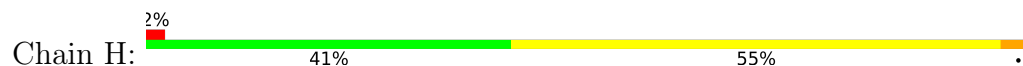
• Molecule 1: Nucleoside diphosphate kinase

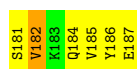


• Molecule 1: Nucleoside diphosphate kinase



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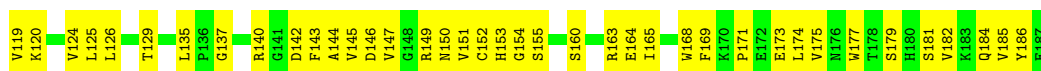




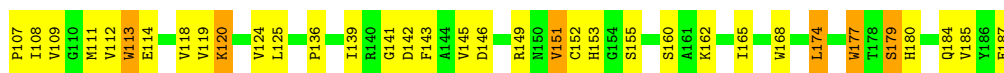
- Molecule 1: Nucleoside diphosphate kinase



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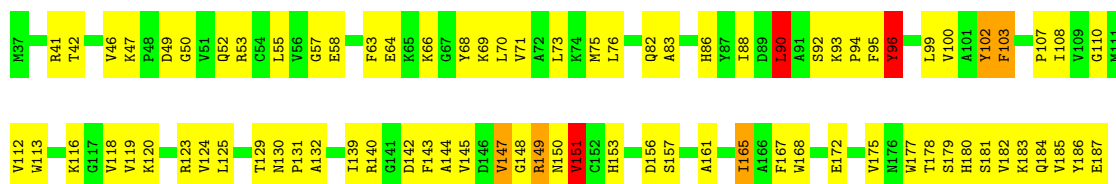


- Molecule 1: Nucleoside diphosphate kinase

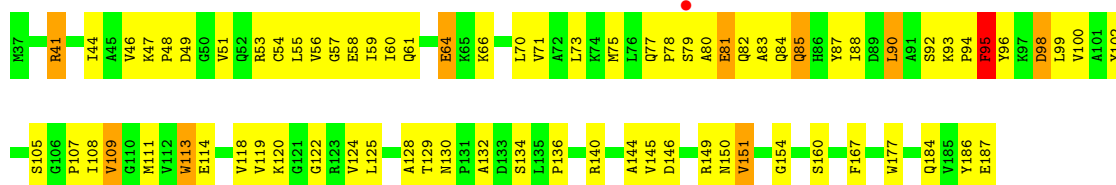




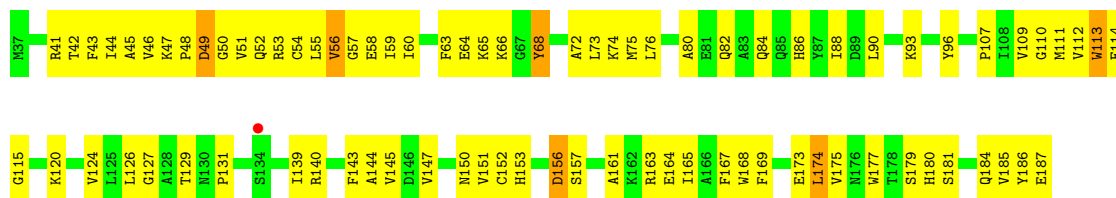
- Molecule 1: Nucleoside diphosphate kinase



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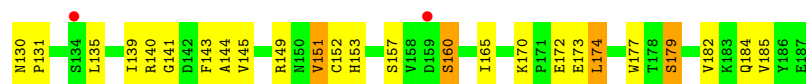


- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase

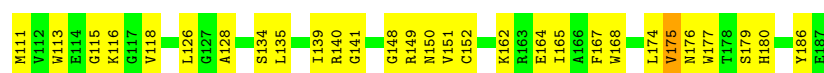




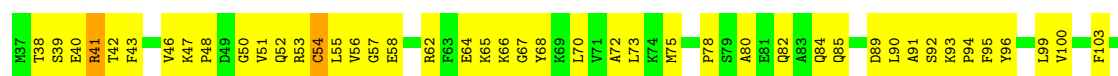
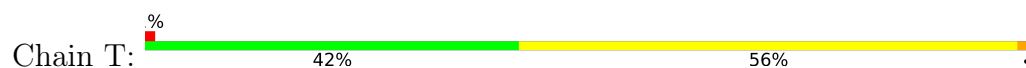
- Molecule 1: Nucleoside diphosphate kinase



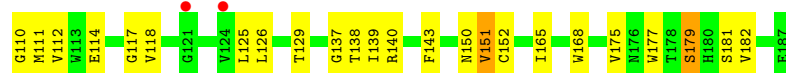
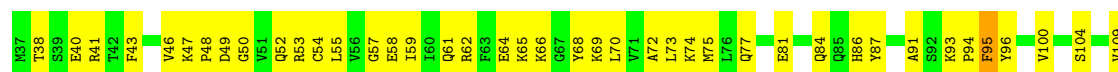
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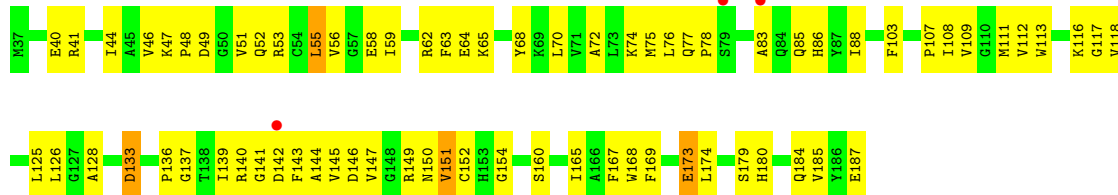
- Molecule 1: Nucleoside diphosphate kinase



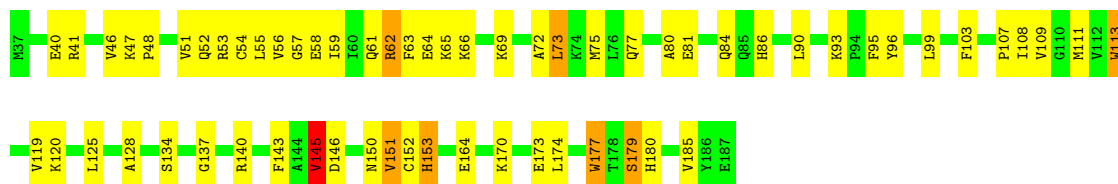
- Molecule 1: Nucleoside diphosphate kinase



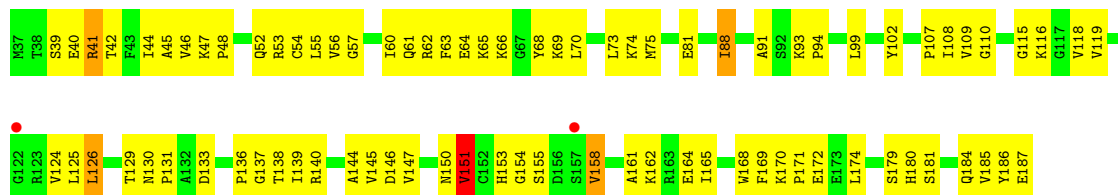
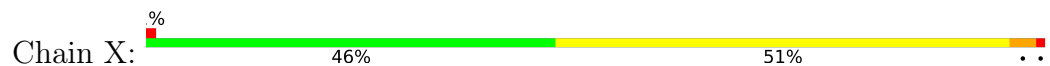
- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	127.84Å 127.84Å 275.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.50 86.30 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (10.00-3.50) 99.3 (86.30-3.50)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.269 , 0.278 0.280 , 0.303	Depositor DCC
R_{free} test set	3152 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.27$, $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	0.309 for -h,-k,l 0.318 for h,-h-k,-l 0.317 for -k,-h,-l	Xtriage
Reported twinning fraction	0.291 for H, K, L 0.237 for -K, -H, -L 0.240 for K, H, -L 0.232 for -h,-k,l	Depositor
Outliers	0 of 63155 reflections	Xtriage
F_o, F_c correlation	0.42	EDS
Total number of atoms	28296	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.58% 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	0.58	2/1206 (0.2%)	0.67	0/1628
1	B	0.57	1/1206 (0.1%)	0.68	1/1628 (0.1%)
1	C	0.57	2/1206 (0.2%)	0.69	1/1628 (0.1%)
1	D	0.57	1/1206 (0.1%)	0.69	1/1628 (0.1%)
1	E	0.56	2/1206 (0.2%)	0.67	0/1628
1	F	0.55	1/1206 (0.1%)	0.68	0/1628
1	G	0.56	0/1206	0.67	0/1628
1	H	0.56	0/1206	0.70	0/1628
1	I	0.55	1/1206 (0.1%)	0.67	0/1628
1	J	0.57	0/1206	0.68	0/1628
1	K	0.55	2/1206 (0.2%)	0.68	0/1628
1	L	0.56	2/1206 (0.2%)	0.68	0/1628
1	M	0.58	2/1206 (0.2%)	0.67	0/1628
1	N	0.57	1/1206 (0.1%)	0.67	1/1628 (0.1%)
1	O	0.57	2/1206 (0.2%)	0.70	0/1628
1	P	0.56	1/1206 (0.1%)	0.69	0/1628
1	Q	0.57	0/1206	0.66	0/1628
1	R	0.58	2/1206 (0.2%)	0.68	0/1628
1	S	0.56	1/1206 (0.1%)	0.65	0/1628
1	T	0.55	0/1206	0.67	0/1628
1	U	0.56	1/1206 (0.1%)	0.69	0/1628
1	V	0.58	1/1206 (0.1%)	0.67	1/1628 (0.1%)
1	W	0.57	2/1206 (0.2%)	0.70	1/1628 (0.1%)
1	X	0.57	0/1206	0.70	1/1628 (0.1%)
All	All	0.57	27/28944 (0.1%)	0.68	7/39072 (0.0%)

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	168	TRP	CD2-CE2	5.50	1.48	1.41
1	C	168	TRP	CD2-CE2	5.34	1.47	1.41
1	I	113	TRP	CD2-CE2	5.31	1.47	1.41
1	A	168	TRP	CD2-CE2	5.30	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	113	TRP	CD2-CE2	5.30	1.47	1.41

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	LEU	CA-CB-CG	5.68	128.37	115.30
1	X	126	LEU	CA-CB-CG	5.47	127.87	115.30
1	V	174	LEU	CA-CB-CG	5.31	127.52	115.30
1	D	54	CYS	CA-CB-SG	5.27	123.48	114.00
1	N	90	LEU	CA-CB-CG	5.19	127.24	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1179	0	1178	206	0
1	B	1179	0	1178	125	0
1	C	1179	0	1178	149	0
1	D	1179	0	1178	151	0
1	E	1179	0	1178	111	0
1	F	1179	0	1178	61	0
1	G	1179	0	1178	125	0
1	H	1179	0	1178	135	0
1	I	1179	0	1178	93	0
1	J	1179	0	1178	118	0
1	K	1179	0	1178	91	0
1	L	1179	0	1178	94	0
1	M	1179	0	1178	158	1
1	N	1179	0	1178	105	0
1	O	1179	0	1178	105	1
1	P	1179	0	1178	126	0
1	Q	1179	0	1178	86	0
1	R	1179	0	1178	80	0
1	S	1179	0	1178	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	1179	0	1178	169	0
1	U	1179	0	1178	86	0
1	V	1179	0	1178	119	0
1	W	1179	0	1178	94	0
1	X	1179	0	1178	114	0
All	All	28296	0	28272	2029	1

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 36.

The worst 5 of 2029 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:N:180:HIS:NE2	1:P:184:GLN:HG3	1.28	1.44
1:C:93:LYS:CA	1:M:92:SER:HB2	1.46	1.42
1:C:93:LYS:HA	1:M:92:SER:CB	1.54	1.38
1:B:92:SER:O	1:N:92:SER:HB3	1.29	1.32
1:G:184:GLN:HG3	1:L:180:HIS:CD2	1.65	1.31

All (1) 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)
1:M:172:GLU:OE1	1:O:78:PRO:O[3_555]	2.07	0.13

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	149/151 (99%)	139 (93%)	8 (5%)	2 (1%)	12 48
1	B	149/151 (99%)	141 (95%)	7 (5%)	1 (1%)	22 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	149/151 (99%)	145 (97%)	3 (2%)	1 (1%)	22	61
1	D	149/151 (99%)	142 (95%)	5 (3%)	2 (1%)	12	48
1	E	149/151 (99%)	141 (95%)	6 (4%)	2 (1%)	12	48
1	F	149/151 (99%)	145 (97%)	3 (2%)	1 (1%)	22	61
1	G	149/151 (99%)	139 (93%)	10 (7%)	0	100	100
1	H	149/151 (99%)	139 (93%)	8 (5%)	2 (1%)	12	48
1	I	149/151 (99%)	142 (95%)	5 (3%)	2 (1%)	12	48
1	J	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
1	K	149/151 (99%)	141 (95%)	7 (5%)	1 (1%)	22	61
1	L	149/151 (99%)	139 (93%)	8 (5%)	2 (1%)	12	48
1	M	149/151 (99%)	138 (93%)	10 (7%)	1 (1%)	22	61
1	N	149/151 (99%)	132 (89%)	13 (9%)	4 (3%)	5	33
1	O	149/151 (99%)	135 (91%)	12 (8%)	2 (1%)	12	48
1	P	149/151 (99%)	139 (93%)	8 (5%)	2 (1%)	12	48
1	Q	149/151 (99%)	138 (93%)	9 (6%)	2 (1%)	12	48
1	R	149/151 (99%)	136 (91%)	10 (7%)	3 (2%)	7	39
1	S	149/151 (99%)	142 (95%)	5 (3%)	2 (1%)	12	48
1	T	149/151 (99%)	137 (92%)	8 (5%)	4 (3%)	5	33
1	U	149/151 (99%)	138 (93%)	8 (5%)	3 (2%)	7	39
1	V	149/151 (99%)	132 (89%)	15 (10%)	2 (1%)	12	48
1	W	149/151 (99%)	143 (96%)	4 (3%)	2 (1%)	12	48
1	X	149/151 (99%)	135 (91%)	13 (9%)	1 (1%)	22	61
All	All	3576/3624 (99%)	3343 (94%)	189 (5%)	44 (1%)	13	50

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	VAL
1	F	151	VAL
1	L	151	VAL
1	R	56	VAL
1	R	151	VAL

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	126/126 (100%)	119 (94%)	7 (6%)	21	54
1	B	126/126 (100%)	121 (96%)	5 (4%)	31	64
1	C	126/126 (100%)	112 (89%)	14 (11%)	6	28
1	D	126/126 (100%)	117 (93%)	9 (7%)	14	46
1	E	126/126 (100%)	119 (94%)	7 (6%)	21	54
1	F	126/126 (100%)	118 (94%)	8 (6%)	18	51
1	G	126/126 (100%)	122 (97%)	4 (3%)	39	69
1	H	126/126 (100%)	114 (90%)	12 (10%)	8	34
1	I	126/126 (100%)	121 (96%)	5 (4%)	31	64
1	J	126/126 (100%)	121 (96%)	5 (4%)	31	64
1	K	126/126 (100%)	114 (90%)	12 (10%)	8	34
1	L	126/126 (100%)	118 (94%)	8 (6%)	18	51
1	M	126/126 (100%)	116 (92%)	10 (8%)	12	41
1	N	126/126 (100%)	116 (92%)	10 (8%)	12	41
1	O	126/126 (100%)	113 (90%)	13 (10%)	7	32
1	P	126/126 (100%)	118 (94%)	8 (6%)	18	51
1	Q	126/126 (100%)	121 (96%)	5 (4%)	31	64
1	R	126/126 (100%)	115 (91%)	11 (9%)	10	38
1	S	126/126 (100%)	120 (95%)	6 (5%)	25	60
1	T	126/126 (100%)	124 (98%)	2 (2%)	62	83
1	U	126/126 (100%)	121 (96%)	5 (4%)	31	64
1	V	126/126 (100%)	120 (95%)	6 (5%)	25	60
1	W	126/126 (100%)	119 (94%)	7 (6%)	21	54
1	X	126/126 (100%)	119 (94%)	7 (6%)	21	54
All	All	3024/3024 (100%)	2838 (94%)	186 (6%)	18	51

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	165	ILE
1	R	41	ARG
1	O	79	SER
1	P	68	TYR
1	R	151	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	52	GLN
1	P	86	HIS
1	W	153	HIS
1	N	85	GLN
1	O	130	ASN

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](#)

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	151/151 (100%)	-0.09	2 (1%) 77 71	4, 7, 57, 141	0
1	B	151/151 (100%)	-0.00	4 (2%) 56 49	4, 7, 48, 105	0
1	C	151/151 (100%)	0.01	7 (4%) 32 28	4, 7, 51, 107	0
1	D	151/151 (100%)	-0.04	1 (0%) 87 83	2, 7, 46, 95	0
1	E	151/151 (100%)	0.02	2 (1%) 77 71	4, 7, 41, 74	0
1	F	151/151 (100%)	-0.19	1 (0%) 87 83	4, 7, 48, 78	0
1	G	151/151 (100%)	-0.03	3 (1%) 65 60	4, 7, 53, 95	0
1	H	151/151 (100%)	0.05	3 (1%) 65 60	4, 7, 54, 97	0
1	I	151/151 (100%)	-0.09	1 (0%) 87 83	4, 7, 54, 105	0
1	J	151/151 (100%)	-0.14	1 (0%) 87 83	4, 7, 54, 91	0
1	K	151/151 (100%)	-0.10	1 (0%) 87 83	4, 7, 46, 84	0
1	L	151/151 (100%)	-0.06	3 (1%) 65 60	4, 7, 43, 79	0
1	M	151/151 (100%)	0.04	2 (1%) 77 71	4, 7, 60, 93	0
1	N	151/151 (100%)	0.01	0 100 100	4, 7, 47, 105	0
1	O	151/151 (100%)	-0.08	1 (0%) 87 83	4, 7, 52, 96	0
1	P	151/151 (100%)	-0.10	1 (0%) 87 83	4, 7, 51, 89	0
1	Q	151/151 (100%)	-0.00	3 (1%) 65 60	4, 7, 42, 73	0
1	R	151/151 (100%)	-0.09	2 (1%) 77 71	4, 7, 45, 90	0
1	S	151/151 (100%)	0.05	5 (3%) 46 41	4, 7, 49, 88	0
1	T	151/151 (100%)	0.02	2 (1%) 77 71	4, 7, 52, 118	0
1	U	151/151 (100%)	-0.01	2 (1%) 77 71	4, 7, 53, 98	0
1	V	151/151 (100%)	0.10	3 (1%) 65 60	4, 7, 47, 98	0
1	W	151/151 (100%)	-0.14	0 100 100	4, 7, 42, 68	0
1	X	151/151 (100%)	-0.14	2 (1%) 77 71	4, 7, 44, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3624/3624 (100%)	-0.04	52 (1%) 75 69	2, 7, 51, 141	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	180	HIS	3.9
1	Q	105	SER	3.5
1	I	180	HIS	3.2
1	J	91	ALA	3.1
1	C	122	GLY	2.9

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.