



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 24, 2017 – 02:03 PM EST

PDB ID : 5JXT  
Title : Crystal structure of MtISWI bound with histone H4 tail  
Authors : Chen, Z.; Yan, L.  
Deposited on : 2016-05-13  
Resolution : 3.01 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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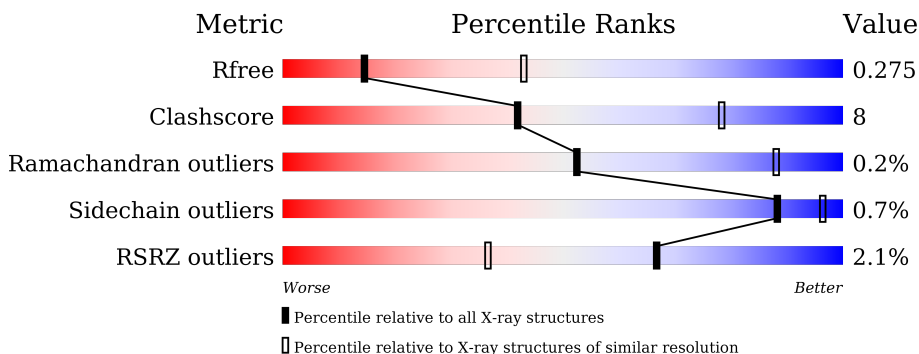
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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## X-RAY DIFFRACTION

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.



<b>Metric</b>	<b>Whole archive (#Entries)</b>	<b>Similar resolution (#Entries, resolution range(Å))</b>
R <sub>free</sub>	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	349	<p>71% 21% 6%</p>
1	B	349	<p>74% 20% 6%</p>
1	C	349	<p>71% 21% 7%</p>
1	D	349	<p>64% 19% 16%</p>
1	E	349	<p>74% 16% 10%</p>
1	F	349	<p>71% 22% 7%</p>

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Mol	Chain	Length	Quality of chain
1	G	349	
1	H	349	
1	I	349	
1	J	349	
1	K	349	
1	L	349	
1	M	349	
1	N	349	
1	O	349	
1	P	349	
2	Q	21	
2	R	21	
2	S	21	
2	T	21	
2	U	21	
2	V	21	
2	W	21	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 40399 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.

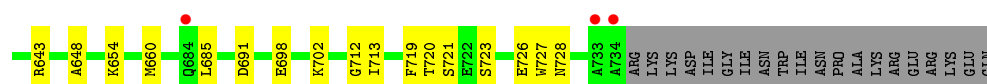
- Molecule 1 is a protein called Chromatin-remodeling complex ATPase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	328	Total	C	N	O	S	0	0	0
			2599	1636	454	497	12			
1	E	313	Total	C	N	O	S	0	0	0
			2484	1566	437	469	12			
1	F	324	Total	C	N	O	S	0	0	0
			2578	1623	450	493	12			
1	G	308	Total	C	N	O	S	0	0	0
			2439	1536	430	461	12			
1	J	317	Total	C	N	O	S	0	0	0
			2515	1583	439	481	12			
1	N	319	Total	C	N	O	S	0	0	0
			2536	1596	442	486	12			
1	O	322	Total	C	N	O	S	0	0	0
			2563	1613	447	491	12			
1	P	316	Total	C	N	O	S	0	0	0
			2517	1585	439	481	12			
1	C	324	Total	C	N	O	S	0	0	0
			2574	1623	446	493	12			
1	H	321	Total	C	N	O	S	0	0	0
			2549	1602	446	489	12			
1	K	306	Total	C	N	O	S	0	0	0
			2427	1529	426	460	12			
1	L	311	Total	C	N	O	S	0	0	0
			2464	1551	434	467	12			
1	A	327	Total	C	N	O	S	0	0	0
			2597	1636	453	496	12			
1	I	301	Total	C	N	O	S	0	0	0
			2388	1506	420	450	12			
1	D	292	Total	C	N	O	S	0	0	0
			2326	1467	411	437	11			
1	M	324	Total	C	N	O	S	0	0	0
			2574	1622	448	492	12			

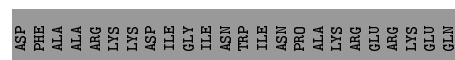
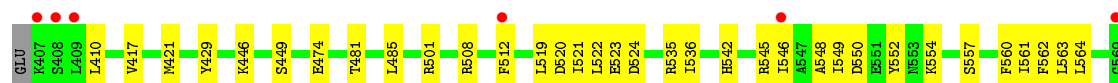
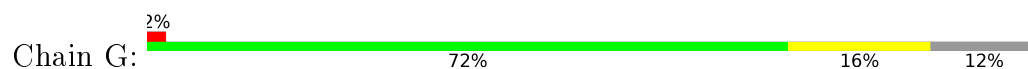
- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	R	5	Total	C	N	O	0	0	0
			39	23	11	5			
2	S	5	Total	C	N	O	0	0	0
			39	23	11	5			
2	U	5	Total	C	N	O	0	0	0
			39	23	11	5			
2	Q	5	Total	C	N	O	0	0	0
			39	23	11	5			
2	T	5	Total	C	N	O	0	0	0
			39	23	11	5			
2	V	5	Total	C	N	O	0	0	0
			39	23	11	5			
2	W	4	Total	C	N	O	0	0	0
			35	21	10	4			

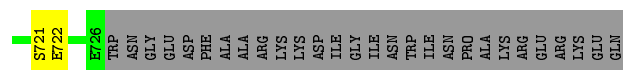
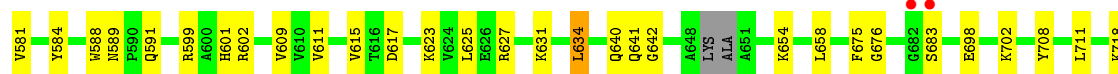
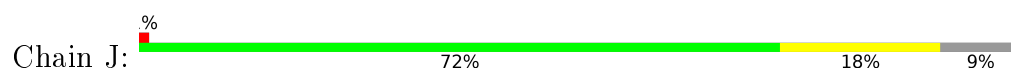




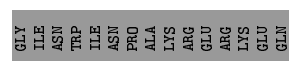
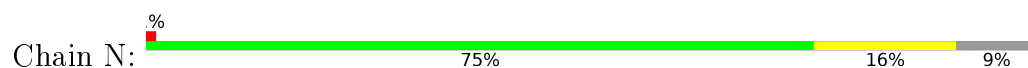
- Molecule 1: Chromatin-remodeling complex ATPase-like protein



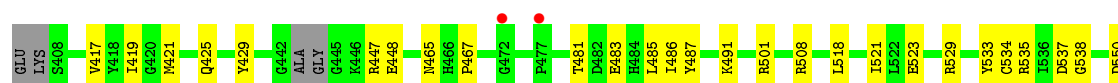
- Molecule 1: Chromatin-remodeling complex ATPase-like protein

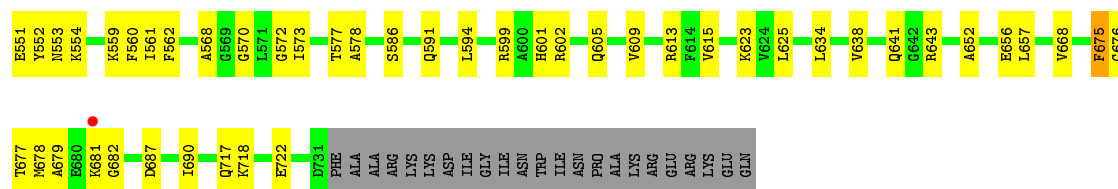


- Molecule 1: Chromatin-remodeling complex ATPase-like protein

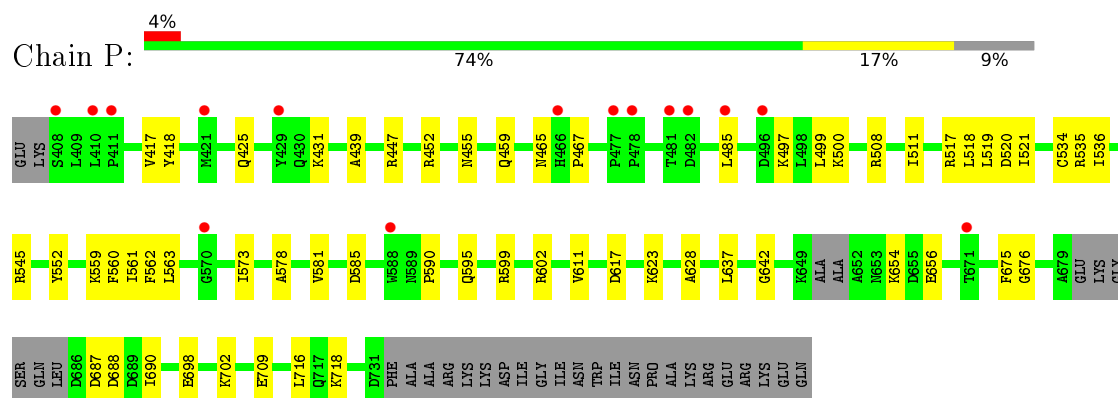


- Molecule 1: Chromatin-remodeling complex ATPase-like protein

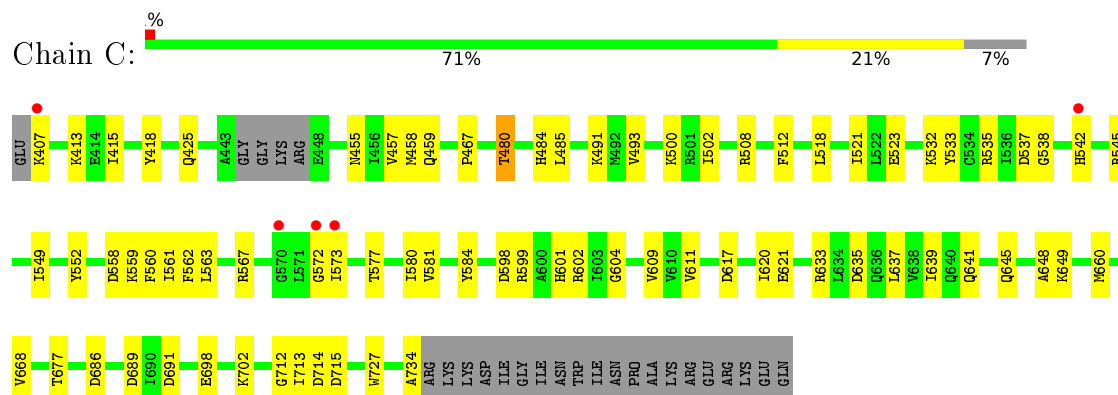




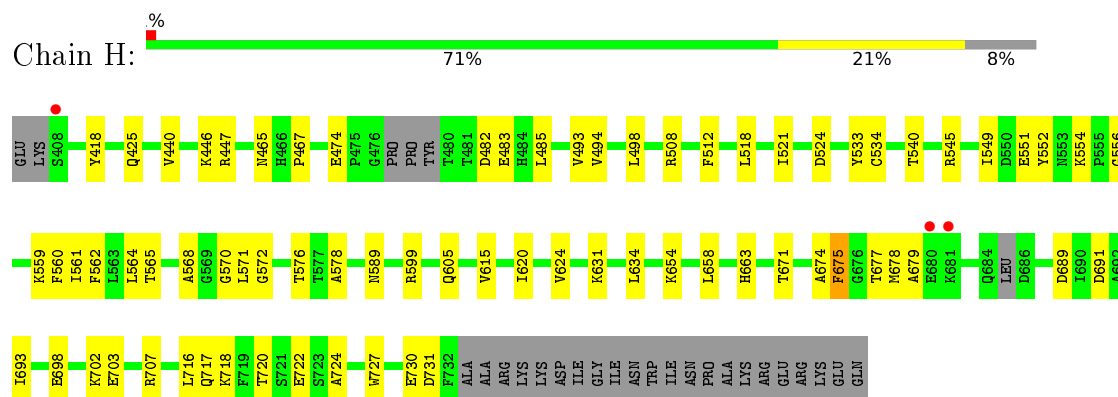
• Molecule 1: Chromatin-remodeling complex ATPase-like protein



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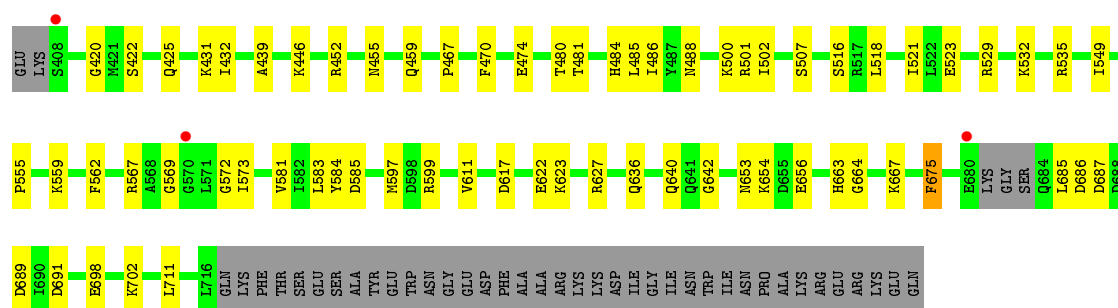


• Molecule 1: Chromatin-remodeling complex ATPase-like protein

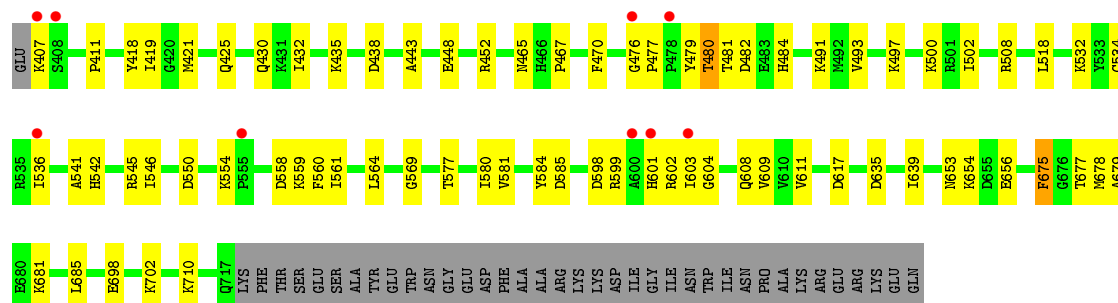


• Molecule 1: Chromatin-remodeling complex ATPase-like protein

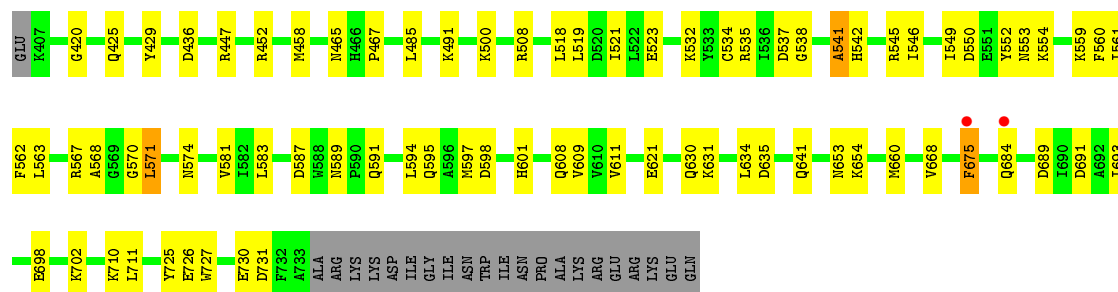
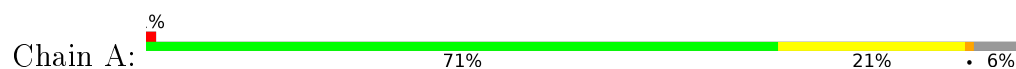




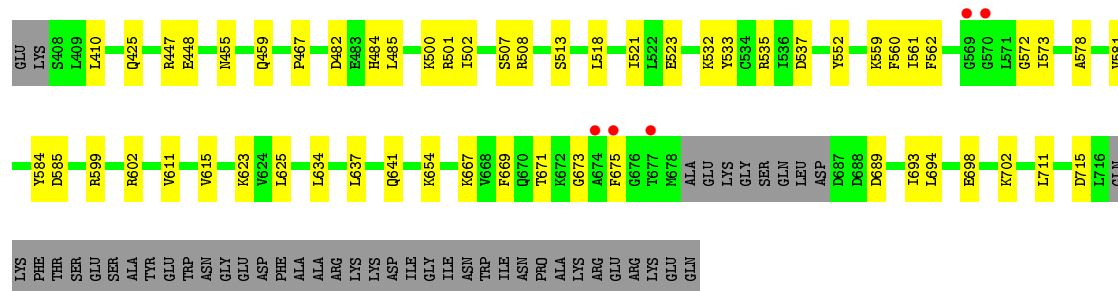
- Molecule 1: Chromatin-remodeling complex ATPase-like protein



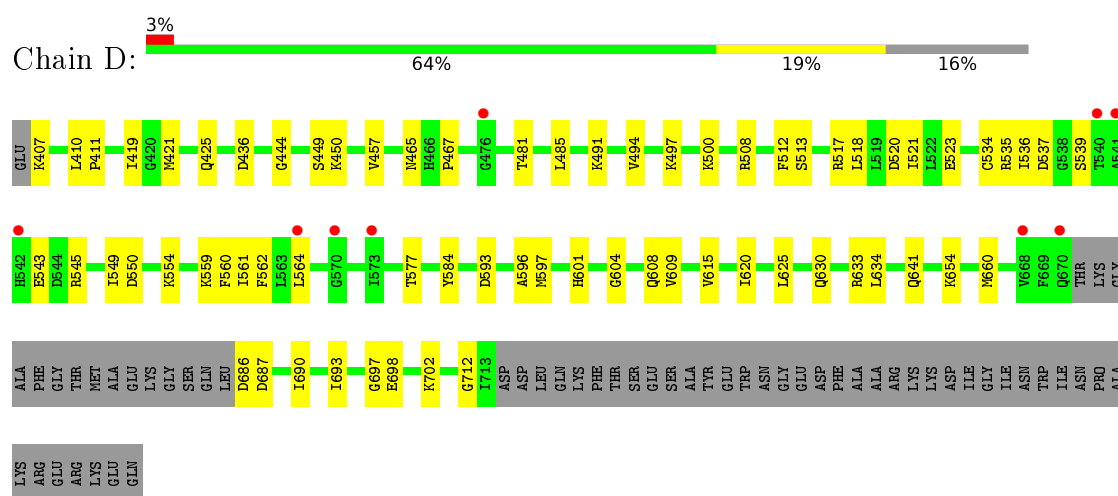
- Molecule 1: Chromatin-remodeling complex ATPase-like protein



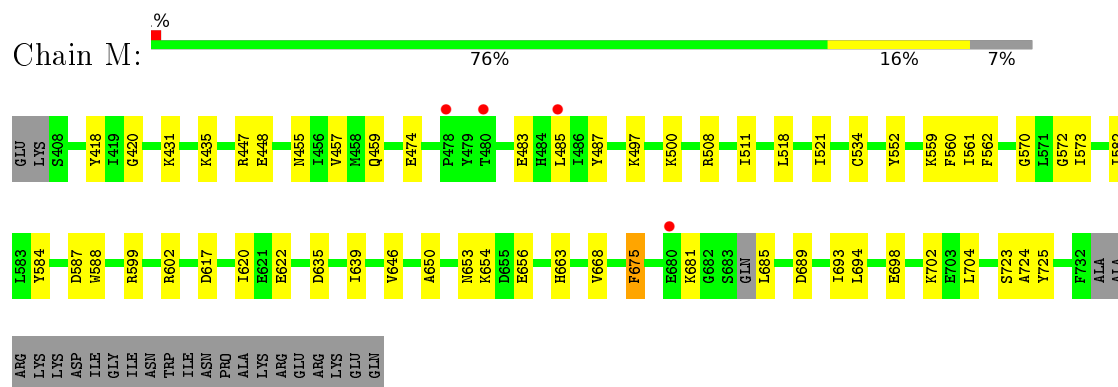
- Molecule 1: Chromatin-remodeling complex ATPase-like protein



- Molecule 1: Chromatin-remodeling complex ATPase-like protein



- Molecule 1: Chromatin-remodeling complex ATPase-like protein



- Molecule 2: Histone H4



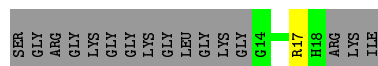
- Molecule 2: Histone H4



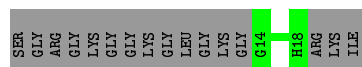
- Molecule 2: Histone H4



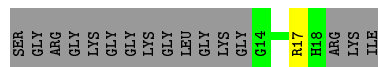
- Molecule 2: Histone H4



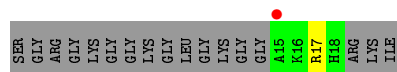
- Molecule 2: Histone H4



- Molecule 2: Histone H4



- Molecule 2: Histone H4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.24Å 119.32Å 132.50Å 89.59° 105.96° 93.08°	Depositor
Resolution (Å)	42.00 – 3.01 45.37 – 3.01	Depositor EDS
% Data completeness (in resolution range)	94.2 (42.00-3.01) 94.3 (45.37-3.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.218 , 0.276 0.217 , 0.275	Depositor DCC
$R_{free}$ test set	5659 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.6	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	40399	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/2637	0.48	1/3549 (0.0%)
1	B	0.26	0/2639	0.43	0/3552
1	C	0.25	0/2613	0.44	0/3518
1	D	0.27	0/2359	0.48	1/3174 (0.0%)
1	E	0.25	0/2520	0.44	0/3389
1	F	0.25	0/2617	0.42	0/3521
1	G	0.25	0/2474	0.43	0/3328
1	H	0.26	0/2584	0.42	0/3472
1	I	0.24	0/2422	0.39	0/3259
1	J	0.24	0/2551	0.39	0/3432
1	K	0.24	0/2461	0.40	0/3312
1	L	0.25	0/2499	0.45	0/3362
1	M	0.24	0/2613	0.40	0/3516
1	N	0.24	0/2574	0.40	0/3465
1	O	0.24	0/2601	0.40	0/3500
1	P	0.23	0/2554	0.39	0/3436
2	Q	0.21	0/39	0.46	0/49
2	R	0.21	0/39	0.32	0/49
2	S	0.21	0/39	0.40	0/49
2	T	0.20	0/39	0.48	0/49
2	U	0.22	0/39	0.40	0/49
2	V	0.22	0/39	0.47	0/49
2	W	0.17	0/35	0.36	0/44
All	All	0.25	0/40987	0.42	2/55123 (0.0%)

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	A	0	1
1	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	O	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	571	LEU	CA-CB-CG	-5.89	101.75	115.30
1	D	436	ASP	CB-CG-OD2	5.30	123.07	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	570	GLY	Peptide
1	H	675	PHE	Peptide
1	O	681	LYS	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	2597	0	2607	66	0
1	B	2599	0	2603	55	0
1	C	2574	0	2579	54	0
1	D	2326	0	2364	49	0
1	E	2484	0	2521	45	0
1	F	2578	0	2580	61	0
1	G	2439	0	2476	54	0
1	H	2549	0	2553	57	0
1	I	2388	0	2422	40	0
1	J	2515	0	2532	44	0
1	K	2427	0	2456	54	0
1	L	2464	0	2499	54	0
1	M	2574	0	2580	42	0
1	N	2536	0	2539	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	2563	0	2571	56	0
1	P	2517	0	2522	43	0
2	Q	39	0	40	4	0
2	R	39	0	40	2	0
2	S	39	0	40	1	0
2	T	39	0	40	0	0
2	U	39	0	40	1	0
2	V	39	0	40	1	0
2	W	35	0	37	4	0
All	All	40399	0	40681	684	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 8.

The worst 5 of 684 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:F:532:LYS:NZ	1:F:558:ASP:OD2	1.84	1.10
1:D:481:THR:HG22	1:M:447:ARG:HH12	1.19	1.04
1:M:681:LYS:NZ	1:M:689:ASP:OD2	1.91	1.03
1:N:481:THR:HG22	2:R:17:ARG:HH12	1.21	1.02
1:E:523:GLU:OE1	1:E:535:ARG:NH1	1.92	1.02

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	325/349 (93%)	309 (95%)	14 (4%)	2 (1%)	30	72
1	B	326/349 (93%)	309 (95%)	17 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	320/349 (92%)	307 (96%)	13 (4%)	0	100	100
1	D	288/349 (82%)	279 (97%)	9 (3%)	0	100	100
1	E	311/349 (89%)	294 (94%)	17 (6%)	0	100	100
1	F	320/349 (92%)	310 (97%)	10 (3%)	0	100	100
1	G	306/349 (88%)	297 (97%)	9 (3%)	0	100	100
1	H	315/349 (90%)	307 (98%)	6 (2%)	2 (1%)	30	72
1	I	297/349 (85%)	287 (97%)	10 (3%)	0	100	100
1	J	313/349 (90%)	302 (96%)	10 (3%)	1 (0%)	46	84
1	K	302/349 (86%)	293 (97%)	8 (3%)	1 (0%)	46	84
1	L	309/349 (88%)	297 (96%)	12 (4%)	0	100	100
1	M	320/349 (92%)	311 (97%)	9 (3%)	0	100	100
1	N	315/349 (90%)	307 (98%)	8 (2%)	0	100	100
1	O	318/349 (91%)	307 (96%)	10 (3%)	1 (0%)	46	84
1	P	310/349 (89%)	298 (96%)	11 (4%)	1 (0%)	46	84
2	Q	3/21 (14%)	2 (67%)	1 (33%)	0	100	100
2	R	3/21 (14%)	2 (67%)	1 (33%)	0	100	100
2	S	3/21 (14%)	2 (67%)	1 (33%)	0	100	100
2	T	3/21 (14%)	2 (67%)	1 (33%)	0	100	100
2	U	3/21 (14%)	2 (67%)	1 (33%)	0	100	100
2	V	3/21 (14%)	2 (67%)	1 (33%)	0	100	100
2	W	2/21 (10%)	2 (100%)	0	0	100	100
All	All	5015/5731 (88%)	4828 (96%)	179 (4%)	8 (0%)	52	88

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	731	ASP
1	O	676	GLY
1	J	676	GLY
1	A	541	ALA
1	H	540	THR

### 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	275/294 (94%)	273 (99%)	2 (1%)	88	96
1	B	274/294 (93%)	273 (100%)	1 (0%)	93	98
1	C	273/294 (93%)	271 (99%)	2 (1%)	88	96
1	D	248/294 (84%)	248 (100%)	0	100	100
1	E	264/294 (90%)	263 (100%)	1 (0%)	93	98
1	F	273/294 (93%)	271 (99%)	2 (1%)	88	96
1	G	259/294 (88%)	259 (100%)	0	100	100
1	H	270/294 (92%)	268 (99%)	2 (1%)	88	96
1	I	254/294 (86%)	252 (99%)	2 (1%)	86	96
1	J	268/294 (91%)	264 (98%)	4 (2%)	72	92
1	K	258/294 (88%)	256 (99%)	2 (1%)	86	96
1	L	262/294 (89%)	260 (99%)	2 (1%)	86	96
1	M	273/294 (93%)	271 (99%)	2 (1%)	88	96
1	N	269/294 (92%)	267 (99%)	2 (1%)	88	96
1	O	273/294 (93%)	270 (99%)	3 (1%)	80	94
1	P	268/294 (91%)	267 (100%)	1 (0%)	93	98
2	Q	3/12 (25%)	3 (100%)	0	100	100
2	R	3/12 (25%)	3 (100%)	0	100	100
2	S	3/12 (25%)	3 (100%)	0	100	100
2	T	3/12 (25%)	3 (100%)	0	100	100
2	U	3/12 (25%)	3 (100%)	0	100	100
2	V	3/12 (25%)	3 (100%)	0	100	100
2	W	3/12 (25%)	3 (100%)	0	100	100
All	All	4282/4788 (89%)	4254 (99%)	28 (1%)	88	96

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	675	PHE
1	C	562	PHE
1	I	675	PHE
1	P	562	PHE
1	C	480	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	542	HIS
1	O	589	ASN
1	L	641	GLN
1	F	591	GLN
1	H	484	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	327/349 (93%)	-0.07	2 (0%) 90 73	40, 74, 108, 133	0
1	B	328/349 (93%)	0.03	12 (3%) 45 19	38, 68, 111, 145	0
1	C	324/349 (92%)	-0.20	5 (1%) 76 49	38, 61, 90, 139	0
1	D	292/349 (83%)	0.12	9 (3%) 52 24	38, 76, 125, 169	0
1	E	313/349 (89%)	-0.11	3 (0%) 84 60	40, 71, 104, 132	0
1	F	324/349 (92%)	0.25	19 (5%) 26 10	42, 80, 128, 177	0
1	G	308/349 (88%)	-0.03	7 (2%) 64 33	45, 75, 107, 142	0
1	H	321/349 (91%)	-0.10	3 (0%) 85 64	41, 64, 97, 121	0
1	I	301/349 (86%)	-0.18	5 (1%) 73 45	35, 58, 109, 145	0
1	J	317/349 (90%)	-0.28	2 (0%) 90 73	36, 55, 91, 124	0
1	K	306/349 (87%)	-0.15	3 (0%) 84 60	42, 63, 99, 137	0
1	L	311/349 (89%)	-0.00	9 (2%) 55 26	46, 69, 105, 139	0
1	M	324/349 (92%)	-0.13	4 (1%) 81 55	38, 65, 98, 132	0
1	N	319/349 (91%)	-0.25	2 (0%) 90 73	39, 63, 92, 132	0
1	O	322/349 (92%)	-0.04	3 (0%) 85 64	45, 75, 101, 128	0
1	P	316/349 (90%)	0.23	15 (4%) 35 14	46, 92, 125, 151	0
2	Q	5/21 (23%)	-0.12	0 100 100	58, 66, 78, 80	0
2	R	5/21 (23%)	0.44	0 100 100	63, 71, 74, 88	0
2	S	5/21 (23%)	0.57	1 (20%) 1 1	76, 77, 81, 113	0
2	T	5/21 (23%)	0.47	0 100 100	53, 56, 85, 87	0
2	U	5/21 (23%)	-0.05	1 (20%) 1 1	58, 65, 72, 91	0
2	V	5/21 (23%)	0.47	0 100 100	64, 66, 79, 79	0
2	W	4/21 (19%)	1.59	1 (25%) 1 1	79, 81, 81, 85	0
All	All	5087/5731 (88%)	-0.05	106 (2%) 67 36	35, 69, 109, 177	0

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	444	GLY	15.3
1	F	445	GLY	11.9
1	P	478	PRO	6.9
1	K	680	GLU	6.4
1	D	542	HIS	6.3

## 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 carbohydrates 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.