



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:41 PM UTC

PDB ID : 5C3I / pdb_00005c3i
Title : Crystal structure of the quaternary complex of histone H3-H4 heterodimer with chaperone ASF1 and the replicative helicase subunit MCM2
Authors : Wang, H.; Wang, M.; Yang, N.; Xu, R.M.
Deposited on : 2015-06-17
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 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

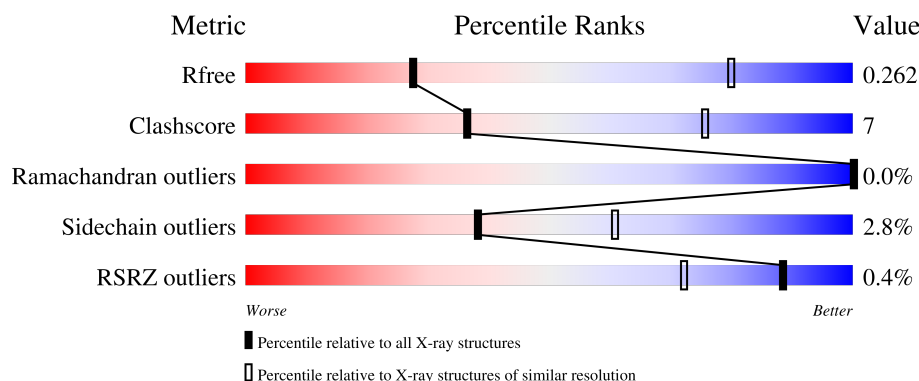
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	188	68%13%19%
1	E	188	68%13%19%
1	I	188	65%16%19%
1	M	188	67%13%19%
1	Q	188	61%20%18%

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Mol	Chain	Length	Quality of chain
1	U	188	
2	B	136	
2	F	136	
2	J	136	
2	N	136	
2	R	136	
2	V	136	
3	C	103	
3	G	103	
3	K	103	
3	O	103	
3	S	103	
3	W	103	
4	D	93	
4	H	93	
4	L	93	
4	P	93	
4	T	93	
4	X	93	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17655 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 chaperone ASF1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1223	786	200	234	3			
1	E	153	Total	C	N	O	S	0	0	0
			1232	791	201	237	3			
1	I	153	Total	C	N	O	S	0	0	0
			1232	791	201	237	3			
1	M	152	Total	C	N	O	S	0	0	0
			1223	786	200	234	3			
1	Q	154	Total	C	N	O	S	0	0	0
			1240	795	202	240	3			
1	U	150	Total	C	N	O	S	0	0	0
			1204	772	197	232	3			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	expression tag	UNP Q9Y294
A	-11	GLY	-	expression tag	UNP Q9Y294
A	-10	SER	-	expression tag	UNP Q9Y294
A	-9	HIS	-	expression tag	UNP Q9Y294
A	-8	HIS	-	expression tag	UNP Q9Y294
A	-7	HIS	-	expression tag	UNP Q9Y294
A	-6	HIS	-	expression tag	UNP Q9Y294
A	-5	HIS	-	expression tag	UNP Q9Y294
A	-4	HIS	-	expression tag	UNP Q9Y294
A	-3	SER	-	expression tag	UNP Q9Y294
A	-2	ASN	-	expression tag	UNP Q9Y294
A	-1	ASP	-	expression tag	UNP Q9Y294
A	0	PRO	-	expression tag	UNP Q9Y294
E	-12	MET	-	expression tag	UNP Q9Y294
E	-11	GLY	-	expression tag	UNP Q9Y294
E	-10	SER	-	expression tag	UNP Q9Y294
E	-9	HIS	-	expression tag	UNP Q9Y294

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	HIS	-	expression tag	UNP Q9Y294
E	-7	HIS	-	expression tag	UNP Q9Y294
E	-6	HIS	-	expression tag	UNP Q9Y294
E	-5	HIS	-	expression tag	UNP Q9Y294
E	-4	HIS	-	expression tag	UNP Q9Y294
E	-3	SER	-	expression tag	UNP Q9Y294
E	-2	ASN	-	expression tag	UNP Q9Y294
E	-1	ASP	-	expression tag	UNP Q9Y294
E	0	PRO	-	expression tag	UNP Q9Y294
I	-12	MET	-	expression tag	UNP Q9Y294
I	-11	GLY	-	expression tag	UNP Q9Y294
I	-10	SER	-	expression tag	UNP Q9Y294
I	-9	HIS	-	expression tag	UNP Q9Y294
I	-8	HIS	-	expression tag	UNP Q9Y294
I	-7	HIS	-	expression tag	UNP Q9Y294
I	-6	HIS	-	expression tag	UNP Q9Y294
I	-5	HIS	-	expression tag	UNP Q9Y294
I	-4	HIS	-	expression tag	UNP Q9Y294
I	-3	SER	-	expression tag	UNP Q9Y294
I	-2	ASN	-	expression tag	UNP Q9Y294
I	-1	ASP	-	expression tag	UNP Q9Y294
I	0	PRO	-	expression tag	UNP Q9Y294
M	-12	MET	-	expression tag	UNP Q9Y294
M	-11	GLY	-	expression tag	UNP Q9Y294
M	-10	SER	-	expression tag	UNP Q9Y294
M	-9	HIS	-	expression tag	UNP Q9Y294
M	-8	HIS	-	expression tag	UNP Q9Y294
M	-7	HIS	-	expression tag	UNP Q9Y294
M	-6	HIS	-	expression tag	UNP Q9Y294
M	-5	HIS	-	expression tag	UNP Q9Y294
M	-4	HIS	-	expression tag	UNP Q9Y294
M	-3	SER	-	expression tag	UNP Q9Y294
M	-2	ASN	-	expression tag	UNP Q9Y294
M	-1	ASP	-	expression tag	UNP Q9Y294
M	0	PRO	-	expression tag	UNP Q9Y294
Q	-12	MET	-	expression tag	UNP Q9Y294
Q	-11	GLY	-	expression tag	UNP Q9Y294
Q	-10	SER	-	expression tag	UNP Q9Y294
Q	-9	HIS	-	expression tag	UNP Q9Y294
Q	-8	HIS	-	expression tag	UNP Q9Y294
Q	-7	HIS	-	expression tag	UNP Q9Y294
Q	-6	HIS	-	expression tag	UNP Q9Y294

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-5	HIS	-	expression tag	UNP Q9Y294
Q	-4	HIS	-	expression tag	UNP Q9Y294
Q	-3	SER	-	expression tag	UNP Q9Y294
Q	-2	ASN	-	expression tag	UNP Q9Y294
Q	-1	ASP	-	expression tag	UNP Q9Y294
Q	0	PRO	-	expression tag	UNP Q9Y294
U	-12	MET	-	expression tag	UNP Q9Y294
U	-11	GLY	-	expression tag	UNP Q9Y294
U	-10	SER	-	expression tag	UNP Q9Y294
U	-9	HIS	-	expression tag	UNP Q9Y294
U	-8	HIS	-	expression tag	UNP Q9Y294
U	-7	HIS	-	expression tag	UNP Q9Y294
U	-6	HIS	-	expression tag	UNP Q9Y294
U	-5	HIS	-	expression tag	UNP Q9Y294
U	-4	HIS	-	expression tag	UNP Q9Y294
U	-3	SER	-	expression tag	UNP Q9Y294
U	-2	ASN	-	expression tag	UNP Q9Y294
U	-1	ASP	-	expression tag	UNP Q9Y294
U	0	PRO	-	expression tag	UNP Q9Y294

- Molecule 2 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	87	Total	C	N	O	S	0	0	0
			720	454	137	125	4			
2	F	88	Total	C	N	O	S	0	0	0
			725	457	138	126	4			
2	J	84	Total	C	N	O	S	0	0	0
			688	435	130	119	4			
2	N	76	Total	C	N	O	S	0	0	0
			615	390	115	106	4			
2	R	74	Total	C	N	O	S	0	0	0
			599	381	110	104	4			
2	V	76	Total	C	N	O	S	0	0	0
			619	392	115	108	4			

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	78	Total	C	N	O	S	0	0	0
			622	393	120	108	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	77	Total	C	N	O	S	0	0	0
			618	391	119	107	1			
3	K	76	Total	C	N	O	S	0	0	0
			606	385	117	103	1			
3	O	78	Total	C	N	O	S	0	0	0
			622	393	120	108	1			
3	S	78	Total	C	N	O	S	0	0	0
			622	393	120	108	1			
3	W	77	Total	C	N	O	S	0	0	0
			618	391	119	107	1			

- Molecule 4 is a protein called DNA replication licensing factor MCM2,MCM2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	63	Total	C	N	O	S	0	0	0
			481	284	86	109	2			
4	H	56	Total	C	N	O	S	0	0	0
			446	263	79	102	2			
4	L	56	Total	C	N	O	S	0	0	0
			446	263	79	102	2			
4	P	48	Total	C	N	O	S	0	0	0
			365	219	58	87	1			
4	T	56	Total	C	N	O	S	0	0	0
			443	262	79	100	2			
4	X	56	Total	C	N	O	S	0	0	0
			446	263	79	102	2			

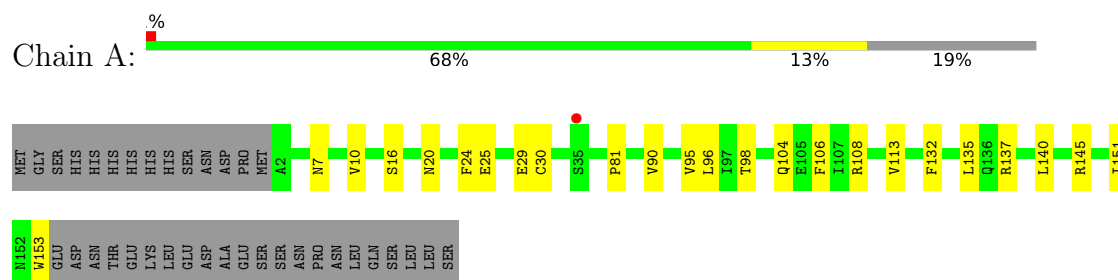
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	62	SER	-	expression tag	UNP P49736
H	62	SER	-	expression tag	UNP P49736
L	62	SER	-	expression tag	UNP P49736
P	62	SER	-	expression tag	UNP P49736
T	62	SER	-	expression tag	UNP P49736
X	62	SER	-	expression tag	UNP P49736

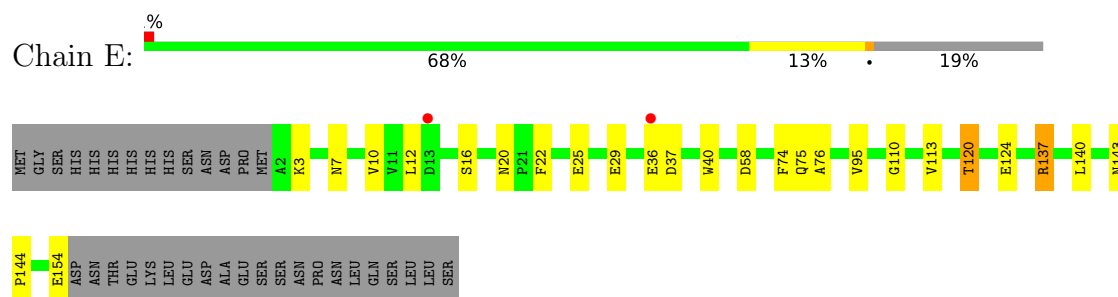
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

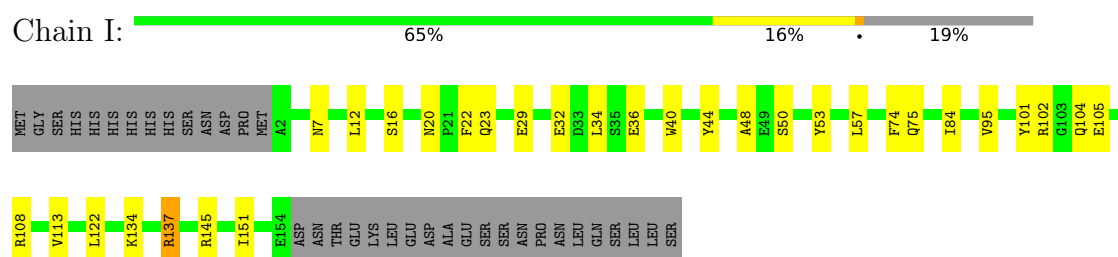
- Molecule 1: Histone chaperone ASF1A



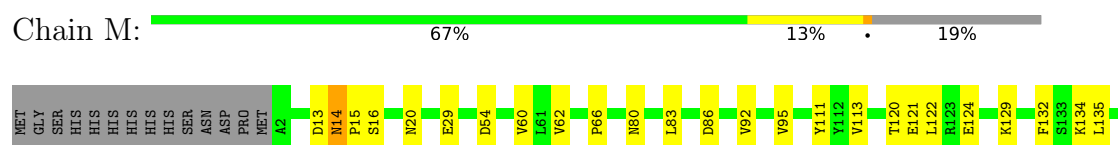
- Molecule 1: Histone chaperone ASF1A

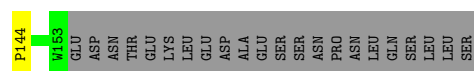


- Molecule 1: Histone chaperone ASF1A



- Molecule 1: Histone chaperone ASF1A

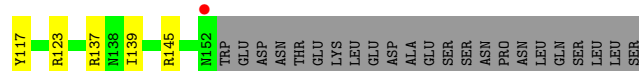




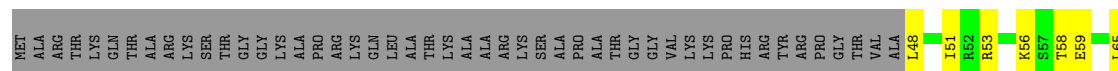
- Molecule 1: Histone chaperone ASF1A



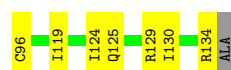
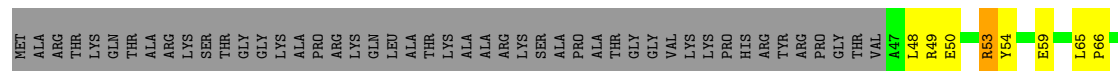
- Molecule 1: Histone chaperone ASF1A



- Molecule 2: Histone H3.1

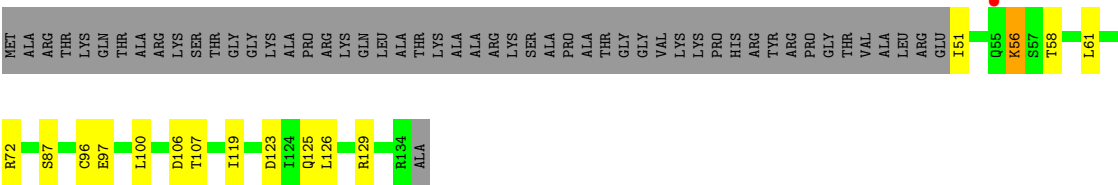


- Molecule 2: Histone H3.1

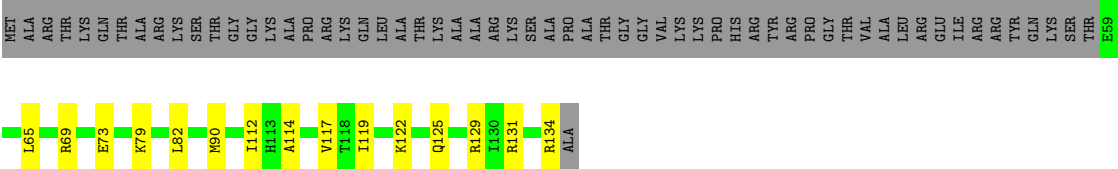


- Molecule 2: Histone H3.1

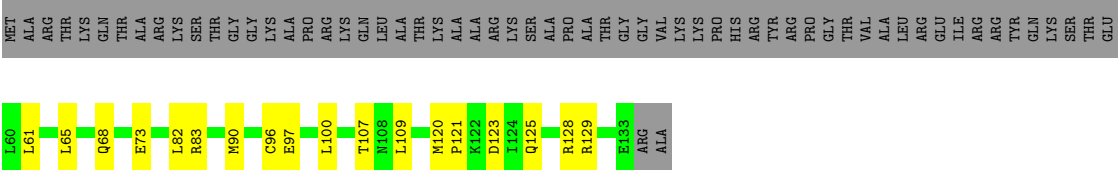




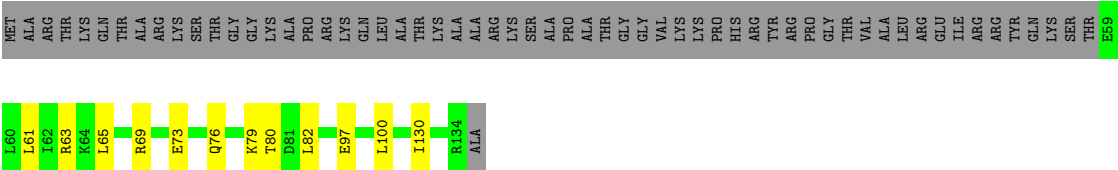
• Molecule 2: Histone H3.1



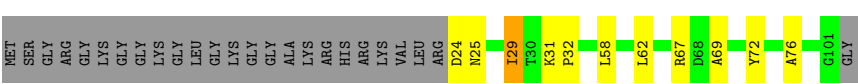
• Molecule 2: Histone H3.1



• Molecule 2: Histone H3.1



• Molecule 3: Histone H4



• Molecule 3: Histone H4



• Molecule 3: Histone H4

MET	SER	GLY	ARG	GLY	LYS	GLY	GLY	LYS	LEU	GLY	LYS	GLY	ALA	LYS	ARG	HTS	ARG	LYS	VAL	LEU	ARG	ASP	ASN	I26	R40	I46	L58	A76	G101	GLY
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- Molecule 3: Histone H4

MET	SER	GLY	ARG	GLY	LYS	GLY	GLY	LYS	GLY	GLY	LEU	GLY	LYS	GLY	GLY	ALA	LYS	ARG	HIS	ARG	LYS	VAL	LEU	ARG	D24	N25	T26	T29	T30	K31	T46	R78	H84	Y88	T96	G101	GLY
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- Molecule 3: Histone H4

MET	GER	LVS	ARG	GLY	LVS	GLY	GLY	LEU	GLY	LVS	GLY	GLY	LVS	ARG	VAL	LVS	ARG	D24	N25	I26	Q27	G28	I29	V57	L58	F61	L62	V65	V70	R78	M84	Q93	L97	G101
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- Molecule 3: Histone H4

MET	GER	GER	ARG	GLY	LVS	GLY	GLY	LVS	LVS	GLY	LEU	GLY	LVS	LVS	GLY	GLY	LVS	ARG	ARG	ARG	LVS	VAL	LEU	LEU	ARG	D24	D25	I26	I29	T30	K31	P32	R36	S47	I50	L58	K59	A76	K91	R95	F100	GLY
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- Molecule 4: DNA replication licensing factor MCM2,MCM2

[illegible]

- Molecule 4: DNA replication licensing factor MCM2,MCM2

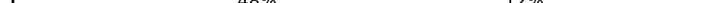
[illegible]

- Molecule 4: DNA replication licensing factor MCM2,MCM2

[illegible]

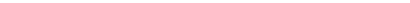
- Molecule 4: DNA replication licensing factor MCM2,MCM2

[illegible]

- Chain T:  48% 12% 40%

[illegible]

UNK	UNK
-----	-----

- Chain X:  49% 11% 40%

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.70Å 147.70Å 261.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.99 – 3.50 48.99 – 3.50	Depositor EDS
% Data completeness (in resolution range)	92.8 (48.99-3.50) 93.4 (48.99-3.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.20 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.216 , 0.253 (Not available) , 0.262	Depositor DCC
R_{free} test set	1987 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 14.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.155 for -h,-k,l	Xtriage
Reported twinning fraction	0.787 for H, K, L 0.213 for -h,-k,l	Depositor
Outliers	0 of 39980 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	17655	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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

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	0.53	0/1256	0.76	0/1719
1	E	0.51	0/1265	0.71	0/1731
1	I	0.52	0/1265	0.75	1/1731 (0.1%)
1	M	0.52	0/1256	0.77	0/1719
1	Q	0.51	0/1273	0.75	0/1742
1	U	0.50	0/1235	0.75	0/1689
2	B	0.47	0/728	0.78	0/974
2	F	0.45	0/733	0.78	0/981
2	J	0.47	0/696	0.83	0/932
2	N	0.47	0/622	0.82	0/834
2	R	0.46	0/606	0.87	0/813
2	V	0.47	0/626	0.85	0/839
3	C	0.48	0/629	0.84	0/843
3	G	0.47	0/625	0.86	0/838
3	K	0.49	0/613	0.85	0/821
3	O	0.49	0/629	0.84	0/843
3	S	0.48	0/629	0.83	0/843
3	W	0.45	0/625	0.84	0/838
4	D	0.38	0/448	0.77	0/600
4	H	0.39	0/448	0.78	0/600
4	L	0.38	0/448	0.76	0/600
4	P	0.41	0/367	0.81	0/495
4	T	0.41	0/445	0.78	0/596
4	X	0.42	0/448	0.79	0/600
All	All	0.48	0/17915	0.79	1/24221 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	84	ILE	N-CA-C	5.07	112.17	107.56

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	1223	0	1176	19	0
1	E	1232	0	1182	17	0
1	I	1232	0	1182	22	0
1	M	1223	0	1176	16	0
1	Q	1240	0	1186	29	0
1	U	1204	0	1161	23	0
2	B	720	0	758	18	0
2	F	725	0	763	11	0
2	J	688	0	722	15	0
2	N	615	0	645	14	0
2	R	599	0	630	15	0
2	V	619	0	649	9	0
3	C	622	0	660	9	0
3	G	618	0	657	11	0
3	K	606	0	650	6	0
3	O	622	0	660	8	0
3	S	622	0	660	15	0
3	W	618	0	657	15	0
4	D	481	0	412	6	0
4	H	446	0	403	7	0
4	L	446	0	403	7	0
4	P	365	0	322	1	0
4	T	443	0	404	11	0
4	X	446	0	403	5	0
All	All	17655	0	17521	252	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 7.

The worst 5 of 252 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)
3:W:29:ILE:CD1	3:W:58:LEU:HD23	1.59	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:29:ILE:HD13	3:W:58:LEU:CD2	1.75	1.17
1:Q:112:TYR:HB2	1:Q:140:LEU:HD12	1.34	1.08
3:W:29:ILE:HD13	3:W:58:LEU:HD23	1.08	1.04
1:I:16:SER:HB2	1:I:20:ASN:HD22	1.25	1.01

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	150/188 (80%)	150 (100%)	0	0	100	100
1	E	151/188 (80%)	149 (99%)	2 (1%)	0	100	100
1	I	151/188 (80%)	149 (99%)	2 (1%)	0	100	100
1	M	150/188 (80%)	145 (97%)	5 (3%)	0	100	100
1	Q	152/188 (81%)	149 (98%)	3 (2%)	0	100	100
1	U	148/188 (79%)	143 (97%)	5 (3%)	0	100	100
2	B	85/136 (62%)	83 (98%)	2 (2%)	0	100	100
2	F	86/136 (63%)	84 (98%)	2 (2%)	0	100	100
2	J	82/136 (60%)	79 (96%)	3 (4%)	0	100	100
2	N	74/136 (54%)	72 (97%)	2 (3%)	0	100	100
2	R	72/136 (53%)	70 (97%)	2 (3%)	0	100	100
2	V	74/136 (54%)	72 (97%)	2 (3%)	0	100	100
3	C	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
3	G	75/103 (73%)	75 (100%)	0	0	100	100
3	K	74/103 (72%)	74 (100%)	0	0	100	100
3	O	76/103 (74%)	73 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	S	76/103 (74%)	74 (97%)	2 (3%)	0	100	100
3	W	75/103 (73%)	75 (100%)	0	0	100	100
4	D	54/93 (58%)	51 (94%)	3 (6%)	0	100	100
4	H	54/93 (58%)	54 (100%)	0	0	100	100
4	L	54/93 (58%)	52 (96%)	1 (2%)	1 (2%)	6	33
4	P	46/93 (50%)	46 (100%)	0	0	100	100
4	T	54/93 (58%)	53 (98%)	1 (2%)	0	100	100
4	X	54/93 (58%)	51 (94%)	3 (6%)	0	100	100
All	All	2143/3120 (69%)	2098 (98%)	44 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	121	ASP

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	137/171 (80%)	135 (98%)	2 (2%)	57	71
1	E	138/171 (81%)	136 (99%)	2 (1%)	59	71
1	I	138/171 (81%)	136 (99%)	2 (1%)	59	71
1	M	137/171 (80%)	134 (98%)	3 (2%)	45	65
1	Q	139/171 (81%)	131 (94%)	8 (6%)	18	44
1	U	136/171 (80%)	134 (98%)	2 (2%)	57	71
2	B	77/111 (69%)	75 (97%)	2 (3%)	40	62
2	F	77/111 (69%)	74 (96%)	3 (4%)	28	54
2	J	73/111 (66%)	70 (96%)	3 (4%)	27	53
2	N	65/111 (59%)	61 (94%)	4 (6%)	16	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	64/111 (58%)	63 (98%)	1 (2%)	55	70
2	V	66/111 (60%)	66 (100%)	0	100	100
3	C	64/79 (81%)	63 (98%)	1 (2%)	55	70
3	G	64/79 (81%)	62 (97%)	2 (3%)	35	59
3	K	62/79 (78%)	62 (100%)	0	100	100
3	O	64/79 (81%)	64 (100%)	0	100	100
3	S	64/79 (81%)	62 (97%)	2 (3%)	35	59
3	W	64/79 (81%)	64 (100%)	0	100	100
4	D	44/50 (88%)	41 (93%)	3 (7%)	14	40
4	H	44/50 (88%)	42 (96%)	2 (4%)	24	50
4	L	44/50 (88%)	40 (91%)	4 (9%)	9	32
4	P	35/50 (70%)	33 (94%)	2 (6%)	18	45
4	T	43/50 (86%)	41 (95%)	2 (5%)	23	49
4	X	44/50 (88%)	41 (93%)	3 (7%)	14	40
All	All	1883/2466 (76%)	1830 (97%)	53 (3%)	38	61

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	121	GLU
1	Q	30	CYS
1	U	145	ARG
2	N	90	MET
2	N	134	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	U	7	ASN
1	U	20	ASN
1	I	20	ASN
1	I	7	ASN
1	U	104	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	152/188 (80%)	-0.18	1 (0%) 84 63	26, 32, 55, 60	0
1	E	153/188 (81%)	0.08	2 (1%) 75 50	31, 48, 84, 97	0
1	I	153/188 (81%)	0.01	0 100 100	27, 40, 65, 72	0
1	M	152/188 (80%)	-0.07	0 100 100	27, 37, 52, 60	0
1	Q	154/188 (81%)	-0.15	0 100 100	24, 31, 46, 60	0
1	U	150/188 (79%)	0.57	3 (2%) 65 39	49, 83, 117, 132	0
2	B	87/136 (63%)	-0.05	0 100 100	27, 33, 98, 111	0
2	F	88/136 (64%)	-0.08	0 100 100	29, 35, 61, 70	0
2	J	84/136 (61%)	-0.14	1 (1%) 76 52	27, 39, 59, 69	0
2	N	76/136 (55%)	-0.08	0 100 100	27, 41, 72, 77	0
2	R	74/136 (54%)	-0.18	0 100 100	29, 34, 49, 50	0
2	V	76/136 (55%)	0.02	0 100 100	40, 51, 66, 72	0
3	C	78/103 (75%)	-0.21	0 100 100	24, 33, 47, 50	0
3	G	77/103 (74%)	-0.11	0 100 100	31, 42, 57, 69	0
3	K	76/103 (73%)	-0.23	0 100 100	27, 38, 56, 66	0
3	O	78/103 (75%)	0.05	0 100 100	34, 50, 72, 76	0
3	S	78/103 (75%)	-0.25	0 100 100	31, 38, 48, 51	0
3	W	77/103 (74%)	-0.05	0 100 100	42, 50, 74, 83	0
4	D	56/93 (60%)	0.06	0 100 100	26, 51, 70, 73	0
4	H	56/93 (60%)	-0.06	1 (1%) 67 42	28, 52, 83, 87	0
4	L	56/93 (60%)	0.15	1 (1%) 67 42	30, 58, 75, 81	0
4	P	48/93 (51%)	0.20	0 100 100	36, 57, 87, 91	0
4	T	56/93 (60%)	0.07	0 100 100	35, 54, 72, 74	0
4	X	56/93 (60%)	0.26	0 100 100	41, 70, 93, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
All	All	2191/3120 (70%)	-0.01	9 (0%)	88 72	24, 42, 83, 132	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	62	VAL	2.6
2	J	55	GLN	2.6
1	E	13	ASP	2.5
1	E	36	GLU	2.4
4	L	111	GLU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.