



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 03:40 am BST

PDB ID : 5C3I  
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](mailto: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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

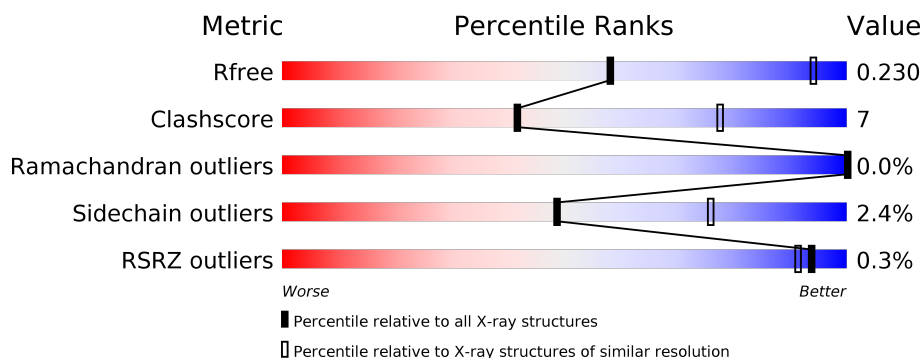
# 1 Overall quality at a glance

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.






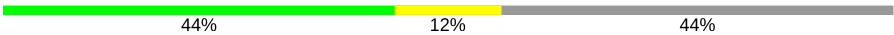
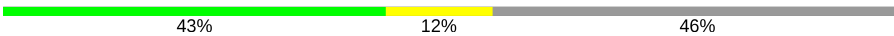
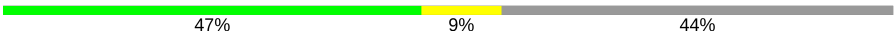












Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>67%</div> <div>13%</div> <div>•</div> <div>19%</div> </div>
1	E	188	<div> <div>69%</div> <div>11%</div> <div>•</div> <div>19%</div> </div>
1	I	188	<div> <div>3%</div> <div>65%</div> <div>16%</div> <div>•</div> <div>19%</div> </div>
1	M	188	<div> <div>66%</div> <div>14%</div> <div>•</div> <div>19%</div> </div>
1	Q	188	<div> <div>61%</div> <div>20%</div> <div>•</div> <div>18%</div> </div>
1	U	188	<div> <div>3%</div> <div>64%</div> <div>15%</div> <div>•</div> <div>20%</div> </div>

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Mol	Chain	Length	Quality of chain
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.

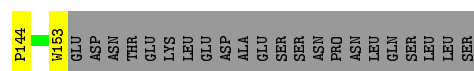
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	63	Total	C	N	O	S	0	0	0
			481	284	86	109	2			
4	H	56	Total	C	N	O	S	0	0	0
			446	263	79	102	2			
4	L	56	Total	C	N	O	S	0	0	0
			446	263	79	102	2			
4	P	48	Total	C	N	O	S	0	0	0
			365	219	58	87	1			
4	T	56	Total	C	N	O	S	0	0	0
			443	262	79	100	2			
4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

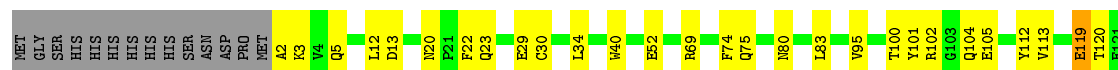
Chain	Residue	Modelled	Actual	Comment	Reference
D	62	SER	-	expression tag	UNP P49736
H	62	SER	-	expression tag	UNP P49736
L	62	SER	-	expression tag	UNP P49736
P	62	SER	-	expression tag	UNP P49736
T	62	SER	-	expression tag	UNP P49736
X	62	SER	-	expression tag	UNP P49736



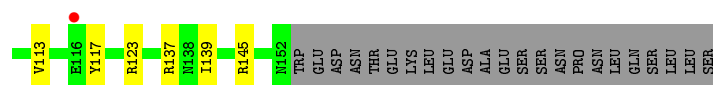




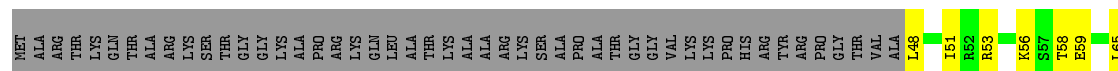
- Molecule 1: Histone chaperone ASF1A



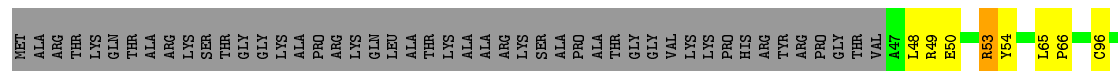
- Molecule 1: Histone chaperone ASF1A



- Molecule 2: Histone H3.1



- Molecule 2: Histone H3.1



- Molecule 2: Histone H3.1





Met	Ser	Gly	Arg	Gly	Lys	Gly	Lys	Lys	Leu	Gly	Lys	Gly	Gly	Ala	Lys	Arg	His	Arg	Arg	Lys	Val	Leu	Arg	Asp	Asn	126	R40	146	L58	A76	G101	Gly
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----

- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|
| MET | SER | GLY | ARG | GLY | LYS | GLY | GLY | LYS | GLY | LEU | LEU | ARG | D24 | D25 | T26 | T29 | T30 | K31 | T46 | R78 | M84 | Y88 | T96 | G101 | GLY |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|

- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
| MET | SER | GLY | ARG | GLY | LYS | GLY | GLY | LYS | GLY | LEU | GLY | LYS | GLY | GLY | ALA | LYS | ARG | HIS | ARG | LYS | VAL | LEU | ARG | LEU | D24 | N25 | I26 | I29 | V57 | L58 | F61 | L62 | V65 | V70 | R78 | M84 | Q93 | L97 | G101 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|

- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|
| MET | SER | GLY | ARG | GLY | LYS | GLY | LVS | GLY | LVS | LEU | GLY | GLY | GLY | GLY | GLY | VAL | LEU | ARG | D94 | D25 | I26 | I29 | T30 | K31 | P32 | R36 | S47 | I50 | L58 | K59 | A76 | K91 | R95 | F100 | GLY | GLY |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|

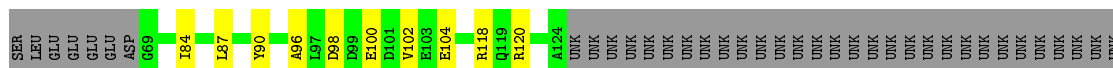
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- WORLD WIDE  
PDB  
PROTEIN DATA BANK

- Molecule 4: DNA replication licensing factor MCM2,MCM2



- Molecule 4: DNA replication licensing factor MCM2,MCM2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.70Å 147.70Å 261.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.99 – 3.50 48.98 – 3.48	Depositor EDS
% Data completeness (in resolution range)	92.8 (48.99-3.50) 92.9 (48.98-3.48)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.20 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.216 , 0.253 0.191 , 0.230	Depositor DCC
$R_{free}$ test set	1987 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.2	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , -4.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	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	0.87	EDS
Total number of atoms	17655	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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 [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	0.42	1/1256 (0.1%)	0.52	0/1719
1	E	0.42	0/1265	0.48	0/1731
1	I	0.42	1/1265 (0.1%)	0.51	0/1731
1	M	0.42	1/1256 (0.1%)	0.50	0/1719
1	Q	0.42	1/1273 (0.1%)	0.52	0/1742
1	U	0.38	1/1235 (0.1%)	0.47	0/1689
2	B	0.33	0/728	0.49	0/974
2	F	0.32	0/733	0.49	0/981
2	J	0.33	0/696	0.51	0/932
2	N	0.33	0/622	0.49	0/834
2	R	0.33	0/606	0.55	0/813
2	V	0.33	0/626	0.50	0/839
3	C	0.32	0/629	0.51	0/843
3	G	0.32	0/625	0.47	0/838
3	K	0.33	0/613	0.49	0/821
3	O	0.33	0/629	0.50	0/843
3	S	0.32	0/629	0.48	0/843
3	W	0.31	0/625	0.47	0/838
4	D	0.28	0/448	0.51	0/600
4	H	0.27	0/448	0.48	0/600
4	L	0.29	0/448	0.51	0/600
4	P	0.31	0/367	0.52	0/495
4	T	0.31	0/445	0.51	0/596
4	X	0.28	0/448	0.51	0/600
All	All	0.36	5/17915 (0.0%)	0.50	0/24221

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	TRP	CD2-CE2	5.04	1.47	1.41
1	U	40	TRP	CD2-CE2	5.03	1.47	1.41
1	Q	40	TRP	CD2-CE2	5.03	1.47	1.41
1	M	153	TRP	CD2-CE2	5.02	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	153	TRP	CD2-CE2	5.01	1.47	1.41

There are no bond angle outliers.

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	16	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	14	0
2	N	615	0	645	14	0
2	R	599	0	630	13	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	14	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	6	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	247	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 247 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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	8	40
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%)	133 (97%)	4 (3%)	42	71
1	E	138/171 (81%)	135 (98%)	3 (2%)	52	78
1	I	138/171 (81%)	136 (99%)	2 (1%)	67	85
1	M	137/171 (80%)	134 (98%)	3 (2%)	52	78
1	Q	139/171 (81%)	131 (94%)	8 (6%)	20	53
1	U	136/171 (80%)	133 (98%)	3 (2%)	52	78
2	B	77/111 (69%)	76 (99%)	1 (1%)	69	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	77/111 (69%)	75 (97%)	2 (3%)	46	74
2	J	73/111 (66%)	72 (99%)	1 (1%)	67	85
2	N	65/111 (59%)	60 (92%)	5 (8%)	13	42
2	R	64/111 (58%)	62 (97%)	2 (3%)	40	70
2	V	66/111 (60%)	66 (100%)	0	100	100
3	C	64/79 (81%)	63 (98%)	1 (2%)	62	83
3	G	64/79 (81%)	63 (98%)	1 (2%)	62	83
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%)	40	70
3	W	64/79 (81%)	64 (100%)	0	100	100
4	D	44/50 (88%)	41 (93%)	3 (7%)	16	48
4	H	44/50 (88%)	43 (98%)	1 (2%)	50	77
4	L	44/50 (88%)	42 (96%)	2 (4%)	27	61
4	P	35/50 (70%)	35 (100%)	0	100	100
4	T	43/50 (86%)	42 (98%)	1 (2%)	50	77
4	X	44/50 (88%)	44 (100%)	0	100	100
All	All	1883/2466 (76%)	1838 (98%)	45 (2%)	49	76

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	98	ASP
2	N	115	LYS
4	T	120	ARG
1	M	74	PHE
2	N	117	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	104	GLN
1	M	143	ASN
1	U	150	HIS
1	M	20	ASN

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Mol	Chain	Res	Type
3	O	25	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 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	152/188 (80%)	-0.11	0 100 100	26, 32, 55, 60	0
1	E	153/188 (81%)	0.14	0 100 100	31, 48, 84, 97	0
1	I	153/188 (81%)	0.05	1 (0%) 87 83	27, 40, 65, 72	0
1	M	152/188 (80%)	-0.04	0 100 100	27, 37, 52, 60	0
1	Q	154/188 (81%)	-0.03	0 100 100	24, 31, 46, 60	0
1	U	150/188 (79%)	0.46	5 (3%) 46 41	49, 83, 117, 132	0
2	B	87/136 (63%)	-0.08	0 100 100	27, 33, 98, 111	0
2	F	88/136 (64%)	-0.16	0 100 100	29, 35, 61, 70	0
2	J	84/136 (61%)	-0.18	0 100 100	27, 39, 59, 69	0
2	N	76/136 (55%)	-0.16	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%)	0.08	0 100 100	40, 51, 66, 72	0
3	C	78/103 (75%)	-0.14	0 100 100	24, 33, 47, 50	0
3	G	77/103 (74%)	-0.13	0 100 100	31, 42, 57, 69	0
3	K	76/103 (73%)	-0.08	0 100 100	27, 38, 56, 66	0
3	O	78/103 (75%)	0.03	0 100 100	34, 50, 72, 76	0
3	S	78/103 (75%)	-0.21	0 100 100	31, 38, 48, 51	0
3	W	77/103 (74%)	-0.06	0 100 100	42, 50, 74, 83	0
4	D	56/93 (60%)	0.05	0 100 100	26, 51, 70, 73	0
4	H	56/93 (60%)	0.18	0 100 100	28, 52, 83, 87	0
4	L	56/93 (60%)	0.17	0 100 100	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%)	0.08	0 100 100	35, 54, 72, 74	0
4	X	56/93 (60%)	0.42	1 (1%) 68 62	41, 70, 93, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	2191/3120 (70%)	0.01	7 (0%) 94 91	24, 42, 83, 132	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	35	SER	2.8
1	U	30	CYS	2.6
4	X	120	ARG	2.1
1	U	31	ILE	2.1
1	U	65	VAL	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 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.