



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 04:54 am BST

PDB ID : 4GUO  
Title : structure of p73 DNA binding domain complex with 12 bp DNA  
Authors : Ethayathulla, A.S.; Viadiu, H.  
Deposited on : 2012-08-29  
Resolution : 3.19 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

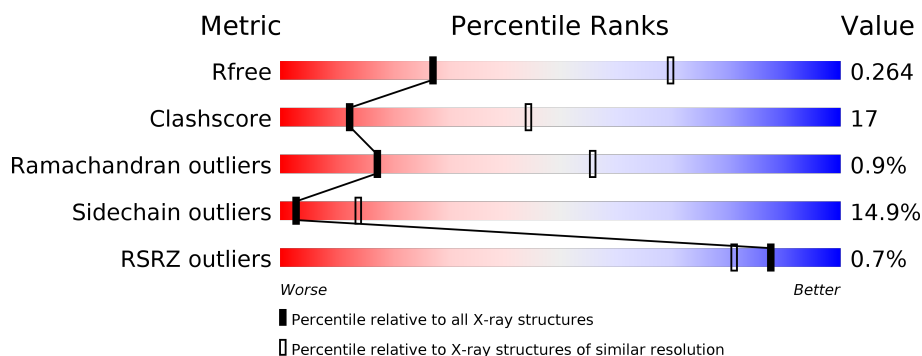
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.19 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	210	<div> <div>60%</div> <div>31%</div> <div>• • •</div> </div>
1	B	210	<div> <div>55%</div> <div>36%</div> <div>• 6%</div> </div>
1	C	210	<div> <div>63%</div> <div>28%</div> <div>5% •</div> </div>
1	D	210	<div> <div>60%</div> <div>29%</div> <div>5% 6%</div> </div>
1	I	210	<div> <div>59%</div> <div>30%</div> <div>5% 6%</div> </div>
1	J	210	<div> <div>57%</div> <div>31%</div> <div>7% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	210	
1	L	210	
2	E	12	
2	G	12	
2	M	12	
2	O	12	
3	F	12	
3	H	12	
3	N	12	
3	P	12	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14607 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 Tumor protein p73.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1571	982	283	295	11			
1	B	198	Total	C	N	O	S	0	0	0
			1553	975	279	288	11			
1	C	201	Total	C	N	O	S	0	0	0
			1586	993	285	297	11			
1	D	198	Total	C	N	O	S	0	0	0
			1551	971	279	290	11			
1	I	198	Total	C	N	O	S	0	0	0
			1556	973	280	292	11			
1	J	199	Total	C	N	O	S	0	0	0
			1561	976	281	293	11			
1	K	201	Total	C	N	O	S	0	0	0
			1576	988	282	295	11			
1	L	201	Total	C	N	O	S	0	0	0
			1581	991	284	295	11			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	MET	-	INITIATING METHIONINE	UNP O15350
A	104	GLY	-	EXPRESSION TAG	UNP O15350
A	105	HIS	-	EXPRESSION TAG	UNP O15350
A	106	HIS	-	EXPRESSION TAG	UNP O15350
A	107	HIS	-	EXPRESSION TAG	UNP O15350
A	108	HIS	-	EXPRESSION TAG	UNP O15350
A	109	HIS	-	EXPRESSION TAG	UNP O15350
A	110	HIS	-	EXPRESSION TAG	UNP O15350
A	111	HIS	-	EXPRESSION TAG	UNP O15350
A	112	HIS	-	EXPRESSION TAG	UNP O15350
A	113	GLU	-	EXPRESSION TAG	UNP O15350
A	114	PHE	-	EXPRESSION TAG	UNP O15350
B	103	MET	-	INITIATING METHIONINE	UNP O15350

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Chain	Residue	Modelled	Actual	Comment	Reference
B	104	GLY	-	EXPRESSION TAG	UNP 015350
B	105	HIS	-	EXPRESSION TAG	UNP 015350
B	106	HIS	-	EXPRESSION TAG	UNP 015350
B	107	HIS	-	EXPRESSION TAG	UNP 015350
B	108	HIS	-	EXPRESSION TAG	UNP 015350
B	109	HIS	-	EXPRESSION TAG	UNP 015350
B	110	HIS	-	EXPRESSION TAG	UNP 015350
B	111	HIS	-	EXPRESSION TAG	UNP 015350
B	112	HIS	-	EXPRESSION TAG	UNP 015350
B	113	GLU	-	EXPRESSION TAG	UNP 015350
B	114	PHE	-	EXPRESSION TAG	UNP 015350
C	103	MET	-	INITIATING METHIONINE	UNP 015350
C	104	GLY	-	EXPRESSION TAG	UNP 015350
C	105	HIS	-	EXPRESSION TAG	UNP 015350
C	106	HIS	-	EXPRESSION TAG	UNP 015350
C	107	HIS	-	EXPRESSION TAG	UNP 015350
C	108	HIS	-	EXPRESSION TAG	UNP 015350
C	109	HIS	-	EXPRESSION TAG	UNP 015350
C	110	HIS	-	EXPRESSION TAG	UNP 015350
C	111	HIS	-	EXPRESSION TAG	UNP 015350
C	112	HIS	-	EXPRESSION TAG	UNP 015350
C	113	GLU	-	EXPRESSION TAG	UNP 015350
C	114	PHE	-	EXPRESSION TAG	UNP 015350
D	103	MET	-	INITIATING METHIONINE	UNP 015350
D	104	GLY	-	EXPRESSION TAG	UNP 015350
D	105	HIS	-	EXPRESSION TAG	UNP 015350
D	106	HIS	-	EXPRESSION TAG	UNP 015350
D	107	HIS	-	EXPRESSION TAG	UNP 015350
D	108	HIS	-	EXPRESSION TAG	UNP 015350
D	109	HIS	-	EXPRESSION TAG	UNP 015350
D	110	HIS	-	EXPRESSION TAG	UNP 015350
D	111	HIS	-	EXPRESSION TAG	UNP 015350
D	112	HIS	-	EXPRESSION TAG	UNP 015350
D	113	GLU	-	EXPRESSION TAG	UNP 015350
D	114	PHE	-	EXPRESSION TAG	UNP 015350
I	103	MET	-	INITIATING METHIONINE	UNP 015350
I	104	GLY	-	EXPRESSION TAG	UNP 015350
I	105	HIS	-	EXPRESSION TAG	UNP 015350
I	106	HIS	-	EXPRESSION TAG	UNP 015350
I	107	HIS	-	EXPRESSION TAG	UNP 015350
I	108	HIS	-	EXPRESSION TAG	UNP 015350
I	109	HIS	-	EXPRESSION TAG	UNP 015350

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Chain	Residue	Modelled	Actual	Comment	Reference
I	110	HIS	-	EXPRESSION TAG	UNP 015350
I	111	HIS	-	EXPRESSION TAG	UNP 015350
I	112	HIS	-	EXPRESSION TAG	UNP 015350
I	113	GLU	-	EXPRESSION TAG	UNP 015350
I	114	PHE	-	EXPRESSION TAG	UNP 015350
J	103	MET	-	INITIATING METHIONINE	UNP 015350
J	104	GLY	-	EXPRESSION TAG	UNP 015350
J	105	HIS	-	EXPRESSION TAG	UNP 015350
J	106	HIS	-	EXPRESSION TAG	UNP 015350
J	107	HIS	-	EXPRESSION TAG	UNP 015350
J	108	HIS	-	EXPRESSION TAG	UNP 015350
J	109	HIS	-	EXPRESSION TAG	UNP 015350
J	110	HIS	-	EXPRESSION TAG	UNP 015350
J	111	HIS	-	EXPRESSION TAG	UNP 015350
J	112	HIS	-	EXPRESSION TAG	UNP 015350
J	113	GLU	-	EXPRESSION TAG	UNP 015350
J	114	PHE	-	EXPRESSION TAG	UNP 015350
K	103	MET	-	INITIATING METHIONINE	UNP 015350
K	104	GLY	-	EXPRESSION TAG	UNP 015350
K	105	HIS	-	EXPRESSION TAG	UNP 015350
K	106	HIS	-	EXPRESSION TAG	UNP 015350
K	107	HIS	-	EXPRESSION TAG	UNP 015350
K	108	HIS	-	EXPRESSION TAG	UNP 015350
K	109	HIS	-	EXPRESSION TAG	UNP 015350
K	110	HIS	-	EXPRESSION TAG	UNP 015350
K	111	HIS	-	EXPRESSION TAG	UNP 015350
K	112	HIS	-	EXPRESSION TAG	UNP 015350
K	113	GLU	-	EXPRESSION TAG	UNP 015350
K	114	PHE	-	EXPRESSION TAG	UNP 015350
L	103	MET	-	INITIATING METHIONINE	UNP 015350
L	104	GLY	-	EXPRESSION TAG	UNP 015350
L	105	HIS	-	EXPRESSION TAG	UNP 015350
L	106	HIS	-	EXPRESSION TAG	UNP 015350
L	107	HIS	-	EXPRESSION TAG	UNP 015350
L	108	HIS	-	EXPRESSION TAG	UNP 015350
L	109	HIS	-	EXPRESSION TAG	UNP 015350
L	110	HIS	-	EXPRESSION TAG	UNP 015350
L	111	HIS	-	EXPRESSION TAG	UNP 015350
L	112	HIS	-	EXPRESSION TAG	UNP 015350
L	113	GLU	-	EXPRESSION TAG	UNP 015350
L	114	PHE	-	EXPRESSION TAG	UNP 015350

- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*GP\*GP\*GP\*CP\*AP\*AP\*GP\*CP\*CP\*

CP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	12	Total	C	N	O	P	0	0	0
			244	115	50	68	11			
2	G	11	Total	C	N	O	P	0	0	0
			228	106	47	64	11			
2	M	12	Total	C	N	O	P	0	0	0
			244	115	50	68	11			
2	O	12	Total	C	N	O	P	0	0	0
			244	115	50	68	11			

- Molecule 3 is a DNA chain called DNA (5'-D(\*CP\*GP\*GP\*GP\*CP\*TP\*TP\*GP\*CP\*CP\*CP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	12	Total	C	N	O	P	0	0	0
			242	115	44	72	11			
3	H	12	Total	C	N	O	P	0	0	0
			242	115	44	72	11			
3	N	12	Total	C	N	O	P	0	0	0
			242	115	44	72	11			
3	P	12	Total	C	N	O	P	0	0	0
			242	115	44	72	11			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	K	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	I	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		

- Molecule 5 is water.

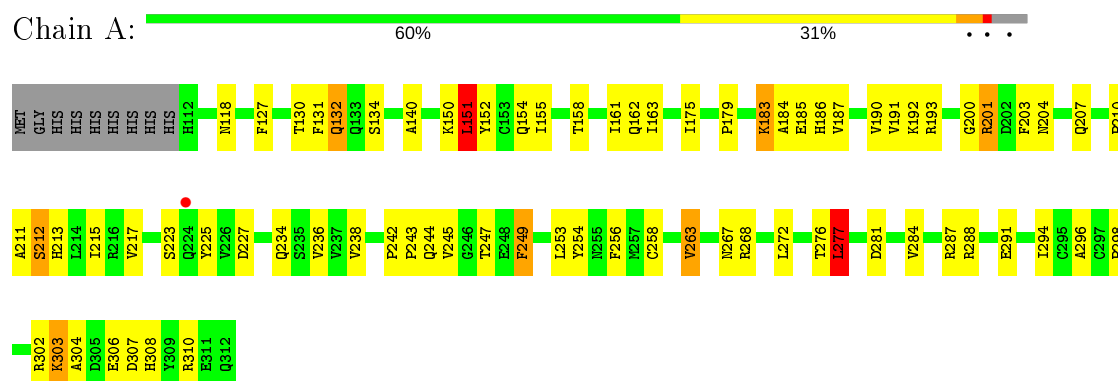
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	16	Total 16	O 16	0	0
5	B	15	Total 15	O 15	0	0
5	C	21	Total 21	O 21	0	0
5	D	18	Total 18	O 18	0	0
5	I	14	Total 14	O 14	0	0
5	J	10	Total 10	O 10	0	0
5	K	18	Total 18	O 18	0	0
5	L	20	Total 20	O 20	0	0
5	E	1	Total 1	O 1	0	0
5	H	1	Total 1	O 1	0	0
5	N	1	Total 1	O 1	0	0
5	P	1	Total 1	O 1	0	0



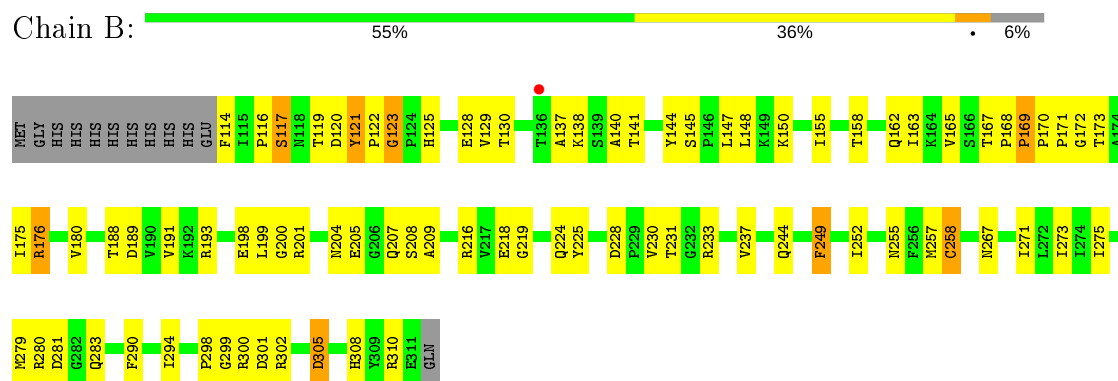
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

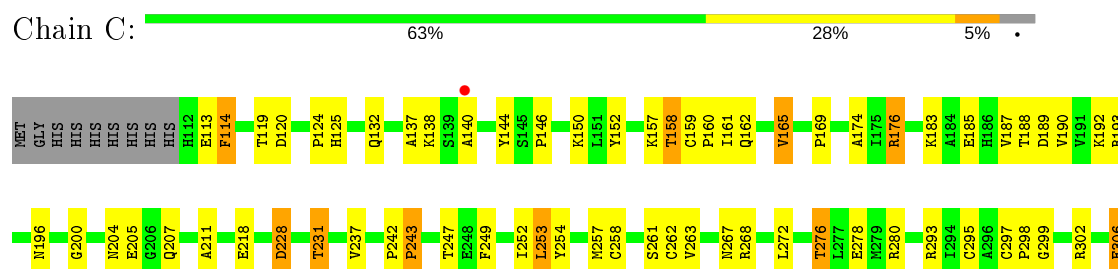
#### • Molecule 1: Tumor protein p73



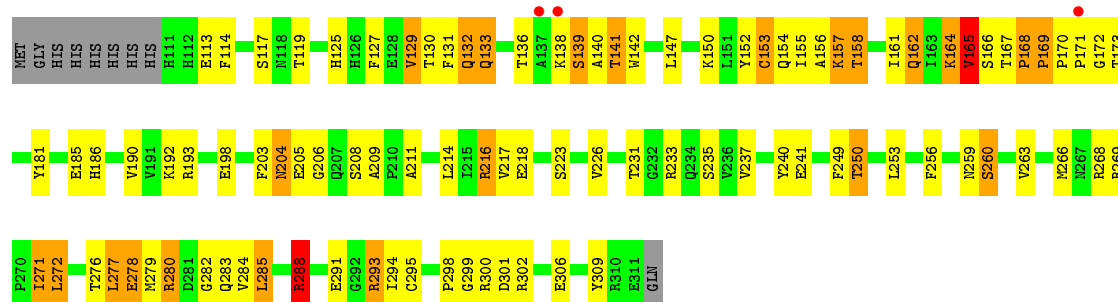
#### • Molecule 1: Tumor protein p73



#### • Molecule 1: Tumor protein p73

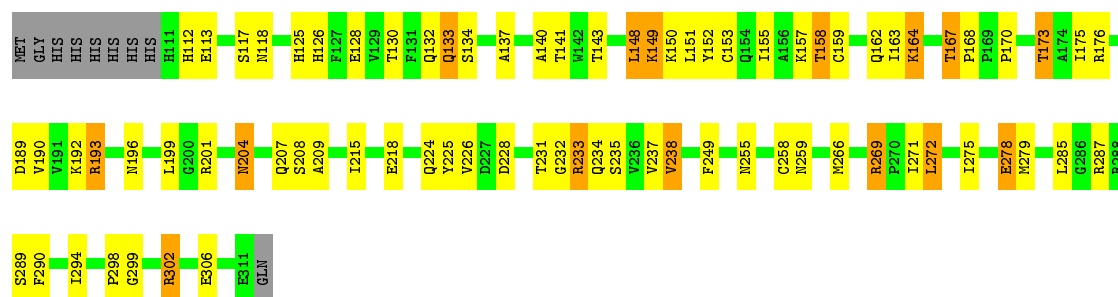






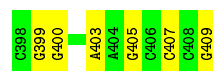
- Molecule 1: Tumor protein p73

Chain L: 59% 30% 7% .



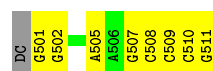
- Molecule 2: DNA (5'-D(\*CP\*GP\*GP\*GP\*CP\*AP\*AP\*GP\*CP\*CP\*CP\*G)-3')

Chain E: 50% 50%



- Molecule 2: DNA (5'-D(\*CP\*GP\*GP\*GP\*CP\*AP\*AP\*GP\*CP\*CP\*CP\*G)-3')

Chain G: 25% 67% 8%



- Molecule 2: DNA (5'-D(\*CP\*GP\*GP\*GP\*CP\*AP\*AP\*GP\*CP\*CP\*CP\*G)-3')

Chain M: 83% 8% 8%



- Molecule 2: DNA (5'-D(\*CP\*GP\*GP\*GP\*CP\*AP\*AP\*GP\*CP\*CP\*CP\*G)-3')

Chain O: 75% 25%



- Molecule 3: DNA (5'-D(\*CP\*GP\*GP\*GP\*CP\*TP\*TP\*GP\*CP\*CP\*CP\*G)-3')



- Molecule 3: DNA (5'-D(\*CP\*GP\*GP\*GP\*CP\*TP\*TP\*GP\*CP\*CP\*CP\*G)-3')



- Molecule 3: DNA (5'-D(\*CP\*GP\*GP\*GP\*CP\*TP\*TP\*GP\*CP\*CP\*CP\*G)-3')



- Molecule 3: DNA (5'-D(\*CP\*GP\*GP\*GP\*CP\*TP\*TP\*GP\*CP\*CP\*CP\*G)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.25Å 104.33Å 123.32Å 90.00° 96.38° 90.00°	Depositor
Resolution (Å)	44.01 – 3.19 43.97 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.01-3.19) 99.1 (43.97-3.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.208 , 0.270 0.202 , 0.264	Depositor DCC
$R_{free}$ test set	1738 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	80.8	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 42.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14607	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.55	0/1610	0.85	2/2188 (0.1%)
1	B	0.57	0/1593	0.93	4/2166 (0.2%)
1	C	0.59	0/1627	0.86	1/2210 (0.0%)
1	D	0.57	0/1590	0.91	5/2162 (0.2%)
1	I	0.57	0/1595	0.90	2/2167 (0.1%)
1	J	0.57	0/1600	0.89	2/2174 (0.1%)
1	K	0.59	0/1616	0.95	5/2197 (0.2%)
1	L	0.59	0/1622	0.89	0/2205
2	E	0.67	1/274 (0.4%)	0.77	0/421
2	G	0.33	0/256	0.66	0/393
2	M	0.76	1/274 (0.4%)	0.87	1/421 (0.2%)
2	O	0.51	0/274	0.82	1/421 (0.2%)
3	F	0.58	0/270	0.88	1/415 (0.2%)
3	H	0.47	0/270	1.00	1/415 (0.2%)
3	N	0.58	0/270	0.92	0/415
3	P	0.61	0/270	1.01	1/415 (0.2%)
All	All	0.57	2/15011 (0.0%)	0.89	26/20785 (0.1%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	600	DC	O3'-P	-6.87	1.52	1.61
2	E	407	DC	O3'-P	-5.18	1.54	1.61

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	216	ARG	NE-CZ-NH2	7.74	124.17	120.30
1	K	288	ARG	NE-CZ-NH2	7.01	123.81	120.30
1	A	277	LEU	CA-CB-CG	6.93	131.25	115.30
1	D	228	ASP	CB-CG-OD2	6.81	124.43	118.30
3	P	716	DC	O5'-P-OP2	-6.29	100.04	105.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	283	GLN	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	1571	0	1535	66	0
1	B	1553	0	1526	54	0
1	C	1586	0	1551	45	0
1	D	1551	0	1523	54	0
1	I	1556	0	1529	51	0
1	J	1561	0	1531	65	0
1	K	1576	0	1540	68	0
1	L	1581	0	1545	58	0
2	E	244	0	134	6	0
2	G	228	0	122	7	0
2	M	244	0	134	1	0
2	O	244	0	134	2	0
3	F	242	0	136	16	0
3	H	242	0	136	4	0
3	N	242	0	136	3	0
3	P	242	0	136	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	16	0	0	2	0
5	B	15	0	0	1	0
5	C	21	0	0	4	0
5	D	18	0	0	0	0
5	E	1	0	0	1	0
5	H	1	0	0	0	0
5	I	14	0	0	5	0
5	J	10	0	0	2	0
5	K	18	0	0	0	0
5	L	20	0	0	2	0
5	N	1	0	0	0	0
5	P	1	0	0	0	0
All	All	14607	0	13348	471	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 17.

The worst 5 of 471 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:L:233:ARG:O	1:L:233:ARG:HD3	1.47	1.14
1:J:255:ASN:HB3	1:J:257:MET:HE1	1.30	1.11
1:L:279:MET:HG3	1:L:285:LEU:HD11	1.32	1.09
1:J:255:ASN:HB3	1:J:257:MET:CE	1.84	1.08
1:K:169:PRO:HB2	1:K:170:PRO:HD2	1.37	1.07

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	199/210 (95%)	189 (95%)	10 (5%)	0	100	100
1	B	196/210 (93%)	179 (91%)	15 (8%)	2 (1%)	15	54
1	C	199/210 (95%)	188 (94%)	9 (4%)	2 (1%)	15	54
1	D	196/210 (93%)	187 (95%)	6 (3%)	3 (2%)	10	44
1	I	196/210 (93%)	188 (96%)	7 (4%)	1 (0%)	29	67
1	J	197/210 (94%)	188 (95%)	8 (4%)	1 (0%)	29	67
1	K	199/210 (95%)	184 (92%)	10 (5%)	5 (2%)	5	32
1	L	199/210 (95%)	187 (94%)	11 (6%)	1 (0%)	29	67
All	All	1581/1680 (94%)	1490 (94%)	76 (5%)	15 (1%)	17	56

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	123	GLY
1	B	169	PRO
1	C	243	PRO
1	D	116	PRO
1	J	122	PRO

### 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	175/186 (94%)	157 (90%)	18 (10%)	7	29
1	B	174/186 (94%)	150 (86%)	24 (14%)	3	16
1	C	178/186 (96%)	155 (87%)	23 (13%)	4	19
1	D	174/186 (94%)	148 (85%)	26 (15%)	3	14
1	I	175/186 (94%)	151 (86%)	24 (14%)	3	17
1	J	175/186 (94%)	144 (82%)	31 (18%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	176/186 (95%)	140 (80%)	36 (20%)	1	6
1	L	177/186 (95%)	150 (85%)	27 (15%)	2	13
All	All	1404/1488 (94%)	1195 (85%)	209 (15%)	3	14

5 of 209 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	147	LEU
1	J	117	SER
1	L	167	THR
1	I	183	LYS
1	I	260	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	255	ASN
1	I	133	GLN
1	L	213	HIS
1	D	267	ASN
1	I	154	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	201/210 (95%)	-0.23	1 (0%) 91 86	59, 98, 147, 172	1 (0%)
1	B	198/210 (94%)	-0.37	1 (0%) 91 86	60, 92, 126, 145	2 (1%)
1	C	201/210 (95%)	-0.41	1 (0%) 91 86	55, 84, 126, 141	0
1	D	198/210 (94%)	-0.39	0 100 100	63, 89, 132, 160	1 (0%)
1	I	198/210 (94%)	-0.33	1 (0%) 91 86	64, 87, 129, 156	0
1	J	199/210 (94%)	-0.02	3 (1%) 73 61	75, 111, 158, 195	0
1	K	201/210 (95%)	-0.26	3 (1%) 73 61	63, 87, 144, 164	0
1	L	201/210 (95%)	-0.49	0 100 100	48, 73, 108, 138	0
2	E	12/12 (100%)	-0.18	0 100 100	73, 100, 152, 178	0
2	G	11/12 (91%)	-0.05	0 100 100	85, 106, 135, 142	0
2	M	12/12 (100%)	-0.58	0 100 100	72, 90, 103, 106	0
2	O	12/12 (100%)	-0.61	0 100 100	92, 106, 140, 146	0
3	F	12/12 (100%)	-0.31	0 100 100	69, 102, 138, 158	0
3	H	12/12 (100%)	0.24	1 (8%) 11 6	79, 115, 157, 170	0
3	N	12/12 (100%)	-0.66	0 100 100	72, 84, 105, 117	0
3	P	12/12 (100%)	-0.35	0 100 100	80, 99, 150, 160	0
All	All	1692/1776 (95%)	-0.32	11 (0%) 87 81	48, 90, 141, 195	4 (0%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	286	GLY	5.2
1	K	137	ALA	4.5
3	H	523	DG	4.4
1	J	137	ALA	4.3
1	I	139	SER	3.8

## 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	I	401	1/1	0.96	0.14	98,98,98,98	0
4	ZN	A	401	1/1	0.98	0.11	87,87,87,87	0
4	ZN	B	401	1/1	0.99	0.16	63,63,63,63	0
4	ZN	C	401	1/1	0.99	0.18	59,59,59,59	0
4	ZN	K	401	1/1	0.99	0.07	89,89,89,89	0
4	ZN	L	401	1/1	0.99	0.11	76,76,76,76	0
4	ZN	D	401	1/1	0.99	0.14	71,71,71,71	0
4	ZN	J	401	1/1	0.99	0.12	84,84,84,84	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.