

wwPDB X-ray Structure Validation Summary Report (i)

Nov 21, 2023 – 06:23 AM JST

PDB ID	:	7EZJ
Title	:	Crystal structure of p73 DNA binding domain complex bound with 1 bp and
		2 bp spacer DNA response elements.
Authors	:	Koley, T.; Roy Chowdhury, S.; Kumar, M.; Kaur, P.; Singh, T.P.; Viadiu, H.;
		Ethayathulla, A.S.
Deposited on	:	2021-06-01
Resolution	:	2.90 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.90 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	$1957 \ (2.90-2.90)$
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	А	210	% 95%	•••
1	В	210	3% 94%	• •
1	С	210	2% 9 5%	• •
1	D	210	2% 9 4%	5%
1	Ι	210	2% 9 5%	5%
1	J	210	92%	• 6%
1	К	210	2% 9 5%	•



Mol	Chain	Length	Quality of chain	
1	L	210	95%	5%
1	a	210	% 94%	5%
1	h	210	% • •	. 5%
1	0	210	% •	5.0
1		210	.% •	5%
	d	210	93% 3%	• 6%
1	i	210	96%	•
1	j	210	91%	• 7%
1	k	210	98%	•
1	1	210	95%	5%
2	Ε	12	92%	8%
2	F	12	92%	8%
2	G	12	100%	
2	Н	12	100%	
2	М	19	100%	
2	N	12	100%	
	N	12	100%	
2	0	12	8%	
2	Р	12	100%	
2	е	12	92%	8%
2	f	12	92%	8%
2	g	12	100%	
2	h	12	8%	
2	m	12	100%	
2	n	12	100%	
2	0	19	100%	
		10	100 %	
	h h	12	100%	



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 29062 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	202	Total	С	Ν	0	S	0	0	0
	A	202	1591	996	286	298	11	0	0	0
1	В	201	Total	С	Ν	0	S	0	0	0
	D	201	1580	987	285	297	11	0	0	0
1	C	201	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	0	201	1586	993	285	297	11	0	0	0
1	О	199	Total	С	Ν	Ο	\mathbf{S}	0	0	0
-		100	1558	978	280	289	11	0	· · · · · · · · · · · · · · · · · · ·	
1	T	199	Total	С	Ν	Ο	S	0	0	0
	-	100	1559	979	280	289	11	Ŭ		
1	J	197	Total	С	Ν	Ο	S	0	0	0
	, in the second	101	1542	966	278	287	11	Ŭ		Ŭ
1	K	201	Total	С	Ν	0	S	0	0	0
		-01	1586	993	285	297	11	Ŭ		
1	L	200	Total	С	N	0	S	0	0	0
			1576	988	283	294	11	_	_	
1	a	199	Total	C	N	0	S	0	0	0
			1566	982	280	293	<u> </u>			
1	b	199	Total	C	N	0	S	0	0	0
			1561	977	282	291	<u> </u>			
1	с	200	Total	C	N OOT	0	S 11	0	0	0
				989	285	292	<u></u>			
1	d	198		075	N 070	0	5 11	0	0	0
			1553 Tet d	975	279 N	288	<u></u>			
1	i	201	10tal 1577	000	N 1022	0 205	5 11	0	0	0
			Total	900	200 N	295	C			
1	j	196	1526	080	1N 977	0 200	い 11	0	0	0
			Total	900	211 N	200	11 C			
1	k	206	1626	1018	1N 207	300	い 11	0	0	0
			Total	<u> </u>	N	0	<u>S</u>			
1	1	200	1576	088	-1N -283	204	11	0	0	0
			1010	900	200	294	11			

• Molecule 1 is a protein called Tumor protein p73.



7EZJ	
11110	

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	MET	-	expression tag	UNP 015350
A	104	GLY	-	expression tag	UNP 015350
A	105	HIS	-	expression tag	UNP 015350
A	106	HIS	-	expression tag	UNP 015350
A	107	HIS	-	expression tag	UNP 015350
A	108	HIS	-	expression tag	UNP 015350
A	109	HIS	-	expression tag	UNP 015350
A	110	HIS	-	expression tag	UNP 015350
А	111	HIS	-	expression tag	UNP 015350
A	112	HIS	-	expression tag	UNP 015350
A	113	GLU	-	expression tag	UNP 015350
А	114	PHE	-	expression tag	UNP 015350
В	103	MET	-	expression tag	UNP 015350
В	104	GLY	-	expression tag	UNP 015350
В	105	HIS	-	expression tag	UNP 015350
В	106	HIS	-	expression tag	UNP 015350
В	107	HIS	-	expression tag	UNP 015350
В	108	HIS	-	expression tag	UNP 015350
В	109	HIS	-	expression tag	UNP 015350
В	110	HIS	-	expression tag	UNP 015350
В	111	HIS	-	expression tag	UNP 015350
В	112	HIS	-	expression tag	UNP 015350
В	113	GLU	-	expression tag	UNP 015350
В	114	PHE	-	expression tag	UNP 015350
С	103	MET	-	expression tag	UNP 015350
С	104	GLY	-	expression tag	UNP 015350
С	105	HIS	-	expression tag	UNP 015350
С	106	HIS	-	expression tag	UNP 015350
С	107	HIS	-	expression tag	UNP 015350
С	108	HIS	-	expression tag	UNP 015350
С	109	HIS	-	expression tag	UNP 015350
С	110	HIS	_	expression tag	UNP 015350
С	111	HIS	-	expression tag	UNP 015350
C	112	HIS	_	expression tag	UNP 015350
С	113	GLU	_	expression tag	UNP 015350
С	114	PHE	-	expression tag	UNP 015350
D	103	MET	-	expression tag	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
	100	1110		prossion tug	0111 010000

There are 192 discrepancies between the modelled and reference sequences:



Continu	cu jioni pre	tious puge			
Chain	Residue	Modelled	Actual	Comment	Reference
D	109	HIS	-	expression tag	UNP O15350
D	110	HIS	-	expression tag	UNP O15350
D	111	HIS	-	expression tag	UNP O15350
D	112	HIS	-	expression tag	UNP O15350
D	113	GLU	-	expression tag	UNP O15350
D	114	PHE	-	expression tag	UNP O15350
Ι	103	MET	-	expression tag	UNP O15350
Ι	104	GLY	-	expression tag	UNP O15350
Ι	105	HIS	-	expression tag	UNP O15350
Ι	106	HIS	-	expression tag	UNP O15350
Ι	107	HIS	-	expression tag	UNP O15350
Ι	108	HIS	-	expression tag	UNP O15350
Ι	109	HIS	-	expression tag	UNP O15350
Ι	110	HIS	-	expression tag	UNP O15350
Ι	111	HIS	-	expression tag	UNP O15350
Ι	112	HIS	-	expression tag	UNP O15350
Ι	113	GLU	-	expression tag	UNP O15350
Ι	114	PHE	-	expression tag	UNP O15350
J	103	MET	-	expression tag	UNP O15350
J	104	GLY	-	expression tag	UNP O15350
J	105	HIS	-	expression tag	UNP O15350
J	106	HIS	-	expression tag	UNP O15350
J	107	HIS	_	expression tag	UNP O15350
J	108	HIS	-	expression tag	UNP O15350
J	109	HIS	-	expression tag	UNP O15350
J	110	HIS	-	expression tag	UNP O15350
J	111	HIS	-	expression tag	UNP O15350
J	112	HIS	-	expression tag	UNP O15350
J	113	GLU	-	expression tag	UNP O15350
J	114	PHE	-	expression tag	UNP O15350
Κ	103	MET	-	expression tag	UNP O15350
Κ	104	GLY	-	expression tag	UNP O15350
Κ	105	HIS	-	expression tag	UNP O15350
Κ	106	HIS	-	expression tag	UNP O15350
К	107	HIS	_	expression tag	UNP O15350
К	108	HIS	-	expression tag	UNP O15350
К	109	HIS	-	expression tag	UNP 015350
K	110	HIS	-	expression tag	UNP 015350
К	111	HIS	-	expression tag	UNP O15350
K	112	HIS	-	expression tag	UNP 015350
K	113	GLU	-	expression tag	UNP 015350
K	114	PHE	-	expression tag	UNP 015350
			1		1

Continued from previous page...



Chain	Residue	Modelled	Actual	Comment	Reference
L	103	MET	-	expression tag	UNP 015350
L	104	GLY	-	expression tag	UNP 015350
L	105	HIS	-	expression tag	UNP O15350
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 O15350
L	113	GLU	-	expression tag	UNP 015350
L	114	PHE	-	expression tag	UNP 015350
a	103	MET	-	expression tag	UNP 015350
a	104	GLY	-	expression tag	UNP 015350
a	105	HIS	-	expression tag	UNP 015350
a	106	HIS	-	expression tag	UNP 015350
a	107	HIS	-	expression tag	UNP 015350
a	108	HIS	-	expression tag	UNP 015350
a	109	HIS	-	expression tag	UNP 015350
a	110	HIS	-	expression tag	UNP 015350
a	111	HIS	-	expression tag	UNP 015350
a	112	HIS	-	expression tag	UNP 015350
a	113	GLU	-	expression tag	UNP 015350
a	114	PHE	-	expression tag	UNP 015350
b	103	MET	-	expression tag	UNP 015350
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
с	103	MET	-	expression tag	UNP 015350
c	104	GLY	-	expression tag	UNP 015350
c	105	HIS	-	expression tag	UNP 015350
с	106	HIS	-	expression tag	UNP 015350
c	107	HIS	-	expression tag	UNP 015350
с	108	HIS	-	expression tag	UNP 015350



	Residue	Modelled	Actual	Comment	Reference
chain	109	HIS	-	expression tag	UNP 015350
С С	105	HIS	_	expression tag	UNP 015350
С С	110	HIS	-	expression tag	UNP 015350
0	111	HIS	-	expression tag	UNP 015350
С С	112	GLU	-	expression tag	UNP 015350
С С	110	DHE	-	expression tag	UNP 015350
d d	114	MET	-	expression tag	000000000000000000000000000000000000
d	105		-	expression tag	$\frac{\text{UNP O15550}}{\text{UND O15250}}$
d	104		-	expression tag	UNP 015550
d	105	HIS	-	expression tag	$\frac{\text{UNP O15350}}{\text{UND O15250}}$
<u>a</u>	100	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	-	expression tag	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
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	-	expression tag	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
i	112	HIS	-	expression tag	UNP 015350
i	113	GLU	_	expression tag	UNP 015350
j	114	PHE	-	expression tag	UNP 015350
	1	1		· · 0	1



Chain	Residue	Modelled	Actual	Comment	Reference
k	103	MET	-	expression tag	UNP O15350
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 O15350
k	108	HIS	-	expression tag	UNP O15350
k	109	HIS	-	expression tag	UNP O15350
k	110	HIS	-	expression tag	UNP O15350
k	111	HIS	-	expression tag	UNP O15350
k	112	HIS	-	expression tag	UNP O15350
k	113	GLU	-	expression tag	UNP O15350
k	114	PHE	-	expression tag	UNP O15350
1	103	MET	-	expression tag	UNP O15350
1	104	GLY	-	expression tag	UNP O15350
1	105	HIS	-	expression tag	UNP O15350
1	106	HIS	-	expression tag	UNP O15350
1	107	HIS	-	expression tag	UNP O15350
1	108	HIS	-	expression tag	UNP O15350
1	109	HIS	-	expression tag	UNP O15350
1	110	HIS	-	expression tag	UNP O15350
1	111	HIS	-	expression tag	UNP O15350
1	112	HIS	-	expression tag	UNP 015350
1	113	GLU	-	expression tag	UNP 015350
1	114	PHE	-	expression tag	UNP 015350

• Molecule 2 is a DNA chain called 12-mer DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
0		11	Total	С	Ν	0	Р	0	0	0
	Ľ	11	221	106	41	64	10	0	0	0
0	Б	11	Total	С	Ν	0	Р	0	0	0
	Г	11	227	107	43	66	11	0	0	U
2	С	19	Total	С	Ν	Ο	Р	0	0 0	0
	G	12	243	116	46	70	11	0		0
2	н	12	Total	С	Ν	Ο	Р	0	0	0
	11		243	116	46	70	11			
2	М	19	Total	С	Ν	N O	Р	0	0	0
2	101	12	243	116	46	70	11	0	0	0
2	N	19	Total	С	Ν	Ο	Р	0	0	0
	2 IN	12	243	116	46	70	11	0	0	0
2	0	19	Total	С	Ν	Ο	Р	0	0	0
	U	0 12	243	116	46	70	11		U	0



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
0	D	10	Total	С	Ν	0	Р	0	0	0
	Г	12	243	116	46	70	11	0	0	0
0	0	11	Total	С	Ν	Ο	Р	0	0	0
	е	11	221	106	41	64	10	0	0	0
9	f	11	Total	С	Ν	Ο	Р	0	0	0
	1	11	227	107	43	66	11	0	0	U
9	ď	19	Total	С	Ν	Ο	Р	0	0	0
	g	12	243	116	46	70	11	0	0	0
2	h	19	Total	С	Ν	Ο	Р	0	0	0
2	11	12	243	116	46	70	11	0	0	0
2	m	19	Total	С	Ν	Ο	Р	0	0	0
2	111	12	243	116	46	70	11	0	0	
2	n	19	Total	С	Ν	Ο	Р	0	0	0
2	11	12	243	116	46	70	11	0	0	0
2	2 o	19	Total	С	Ν	Ο	Р	0	0	0
2			243	116	46	70	11	0	0	0
2	n	19	Total	C	N	Ō	Р	0	0	
2 p		243	116	46	70	11		0		

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Zn 1 1	0	0
3	В	1	Total Zn 1 1	0	0
3	С	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	Ι	1	Total Zn 1 1	0	0
3	J	1	Total Zn 1 1	0	0
3	K	1	Total Zn 1 1	0	0
3	L	1	Total Zn 1 1	0	0
3	a	1	Total Zn 1 1	0	0
3	b	1	Total Zn 1 1	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	с	1	Total Zn 1 1	0	0
3	d	1	Total Zn 1 1	0	0
3	i	1	Total Zn 1 1	0	0
3	j	1	Total Zn 1 1	0	0
3	k	1	Total Zn 1 1	0	0
3	1	1	Total Zn 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	4	Total O 4 4	0	0
4	В	5	Total O 5 5	0	0
4	С	5	Total O 5 5	0	0
4	D	2	Total O 2 2	0	0
4	Ι	3	Total O 3 3	0	0
4	J	2	Total O 2 2	0	0
4	К	1	Total O 1 1	0	0
4	${ m L}$	14	Total O 14 14	0	0
4	a	2	Total O 2 2	0	0
4	b	4	Total O 4 4	0	0
4	с	6	Total O 6 6	0	0
4	d	5	$\begin{array}{cc} \text{Total} & \text{O} \\ 5 & 5 \end{array}$	0	0
4	i	9	Total O 9 9	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	j	1	Total O 1 1	0	0
4	k	11	Total O 11 11	0	0
4	1	7	Total O 7 7	0	0
4	Н	1	Total O 1 1	0	0
4	h	1	Total O 1 1	0	0
4	О	1	Total O 1 1	0	0



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: Tumor protein p73







• Molecule 1: Tumor protein p73		
Chain i:	96%	·
MET GLY HIS HIS HIS HIS HIS HIS F114 F114 F113 F113 F113 F113 F113 F113		
• Molecule 1: Tumor protein p73		
Chain j:	91%	• 7%
MET GLY HIS HIS HIS HIS HIS HIS CLU PII6 P124 P126 H126 H126 H126 H126 H126 H126 G172 G172	H173 H174 H186 H186 V196 V196 V196 C194 C194 C194 C194 C22 C286 C286 C286 C286 C286 C286 C286	
• Molecule 1: Tumor protein p73		
Chain k:	98%	
MET GLY HIS HI07 H107 H107 C268 C268 C268 C268 C268 C268		
• Molecule 1: Tumor protein p73		
Chain l:	95%	5%
MET GLY HIS HIS HIS HIS HIS HIS HIS BII CLN GLN		
• Molecule 2: 12-mer DNA		
Chain E:	92%	8%
D G G G G G G G G G G G G G G G G G G G		
• Molecule 2: 12-mer DNA		
Chain F:	92%	8%
bc A411 6421		
• Molecule 2: 12-mer DNA		
Chain G:	100%	
There are no outlier residues record	led for this chain.	
• Molecule 2: 12-mer DNA		



Chain H:	100%	
There are no outlier resid	dues recorded for this chain	
• Molecule 2: 12-mer DN	NA	
Chain M:		
I here are no outlier resid	dues recorded for this chain.	
• Molecule 2: 12-mer Dr	NA	
Chain N:	100%	
There are no outlier resid	dues recorded for this chain.	
• Molecule 2: 12-mer DN	NA	
Chain O:	100%	
There are no outlier resid	dues recorded for this chain.	
• Molecule 2: 12-mer DN	NA	
Chain P:	100%	
. _		
0338 047 03		
• Molecule 2: 12-mer DN	NA	
Chain a		
Cham e:	92%	8%
DG C339 DG DG C339		
• Molecule 2: 12-mer DN	JA	
	111	
Chain f:	92%	8%
DC A411 6421		
• Molecule 2: 12-mer DN	NA	
Chain g:	100%	
There are no outlier resid	dues recorded for this chain.	
• Molecule 2: 12-mer DN	NA	

Chain h:

8%

100%

C512 6523

• Molecule 2: 12-mer D	NA	
Chain m:	100%	
There are no outlier res	sidues recorded for this chain.	
• Molecule 2: 12-mer E	NA	
Chain n:	100%	
There are no outlier res	sidues recorded for this chain.	
• Molecule 2: 12-mer D	NA	
Chain o:	100%	
There are no outlier res	sidues recorded for this chain.	
• Molecule 2: 12-mer D	NA	
Chain p:	100%	

There are no outlier residues recorded for this chain.



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	139.70Å 105.50Å 155.50Å	Depositor
a, b, c, α , β , γ	90.00° 112.36° 90.00°	Depositor
Bosolution(Å)	40.93 - 2.90	Depositor
Resolution (A)	46.64 - 2.90	EDS
% Data completeness	95.0 (40.93-2.90)	Depositor
(in resolution range)	$95.4 \ (46.64 - 2.90)$	EDS
R _{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.31 (at 2.91 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
P. P.	0.241 , 0.306	Depositor
Λ, Λ_{free}	0.256 , 0.305	DCC
R_{free} test set	4387 reflections $(4.98%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	78.8	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.26 , 43.0	EDS
L-test for $twinning^2$	$ < L >=0.53, < L^2>=0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29062	wwPDB-VP
Average B, all atoms $(Å^2)$	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 86.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.5269e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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).

Mal	Chain	Bo	nd lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.54	0/1632	0.70	0/2217	
1	В	0.57	0/1620	0.71	0/2201	
1	С	0.56	0/1627	0.73	0/2210	
1	D	0.58	1/1598~(0.1%)	0.70	0/2173	
1	Ι	0.52	0/1599	0.71	0/2174	
1	J	0.49	0/1581	0.68	0/2150	
1	Κ	0.50	0/1627	0.67	0/2210	
1	L	0.59	0/1617	0.75	0/2198	
1	a	0.54	0/1606	0.75	0/2183	
1	b	0.53	0/1601	0.70	0/2177	
1	с	0.55	0/1619	0.70	0/2201	
1	d	0.54	0/1593	0.69	0/2166	
1	i	0.52	0/1617	0.71	0/2197	
1	j	0.57	0/1574	0.77	1/2139~(0.0%)	
1	k	0.56	0/1671	0.76	0/2272	
1	1	0.60	0/1617	0.74	0/2198	
2	Ε	0.63	0/247	0.79	0/379	
2	\mathbf{F}	0.57	0/254	0.79	0/390	
2	G	0.54	0/272	0.74	0/418	
2	Н	0.66	0/272	0.73	0/418	
2	М	0.70	0/272	0.80	0/418	
2	Ν	0.49	0/272	0.76	0/418	
2	Ο	0.70	0/272	0.82	0/418	
2	Р	0.61	0/272	0.78	0/418	
2	е	0.72	0/247	0.78	0/379	
2	f	0.64	0/254	0.82	0/390	
2	g	0.63	0/272	0.77	0/418	
2	h	0.56	0/272	0.79	0/418	
2	m	0.38	0/272	0.76	0/418	
2	n	0.63	0/272	0.76	0/418	
2	0	0.36	$0/\overline{272}$	0.73	0/418	
2	р	0.54	0/272	0.75	0/418	



Mol	Chain	Bond lengths		Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
All	All	0.55	1/30065~(0.0%)	0.73	1/41620 (0.0%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	D	169	PRO	C-N	8.51	1.50	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	j	116	PRO	N-CA-CB	5.63	110.06	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	Perce	entiles
1	А	200/210~(95%)	189 (94%)	11 (6%)	0	100	100
1	В	199/210~(95%)	186 (94%)	12 (6%)	1 (0%)	29	61
1	С	199/210~(95%)	190 (96%)	9~(4%)	0	100	100
1	D	197/210~(94%)	188 (95%)	9~(5%)	0	100	100
1	Ι	197/210~(94%)	184 (93%)	13 (7%)	0	100	100
1	J	195/210~(93%)	188 (96%)	6 (3%)	1 (0%)	29	61
1	К	199/210~(95%)	195 (98%)	4 (2%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	L	198/210~(94%)	186 (94%)	12 (6%)	0	100	100
1	a	197/210~(94%)	193~(98%)	4 (2%)	0	100	100
1	b	197/210~(94%)	188~(95%)	8 (4%)	1 (0%)	29	61
1	с	198/210~(94%)	194 (98%)	4 (2%)	0	100	100
1	d	196/210~(93%)	188 (96%)	8 (4%)	0	100	100
1	i	199/210~(95%)	192 (96%)	7 (4%)	0	100	100
1	j	194/210~(92%)	182 (94%)	12 (6%)	0	100	100
1	k	204/210~(97%)	200~(98%)	4 (2%)	0	100	100
1	1	198/210 (94%)	185~(93%)	13 (7%)	0	100	100
All	All	3167/3360~(94%)	3028 (96%)	136 (4%)	3~(0%)	51	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	124	PRO
1	b	179	PRO
1	В	232	GLY

5.3.2 Protein sidechains (i)

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	Perce	ntiles
1	А	178/186~(96%)	176~(99%)	2(1%)	73	92
1	В	177/186~(95%)	175~(99%)	2(1%)	73	92
1	С	178/186~(96%)	176~(99%)	2(1%)	73	92
1	D	174/186~(94%)	174 (100%)	0	100	100
1	Ι	174/186~(94%)	174 (100%)	0	100	100
1	J	173/186~(93%)	171~(99%)	2(1%)	71	91
1	Κ	178/186~(96%)	177~(99%)	1 (1%)	86	96
1	L	177/186~(95%)	176 (99%)	1 (1%)	86	96





Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	a	176/186~(95%)	175~(99%)	1 (1%)	86	96
1	b	175/186~(94%)	171~(98%)	4 (2%)	50	80
1	с	177/186~(95%)	177~(100%)	0	100	100
1	d	174/186~(94%)	172~(99%)	2(1%)	73	92
1	i	176/186~(95%)	176~(100%)	0	100	100
1	j	172/186~(92%)	168~(98%)	4 (2%)	50	80
1	k	181/186~(97%)	180~(99%)	1 (1%)	86	96
1	1	177/186~(95%)	176 (99%)	1 (1%)	86	96
All	All	2817/2976~(95%)	2794 (99%)	23 (1%)	81	94

5 of 23 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	b	276	THR
1	j	127	PHE
1	d	248	GLU
1	j	193	ARG
1	J	132	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	132	GLN
1	a	255	ASN
1	k	255	ASN
1	L	213	HIS
1	a	259	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 16 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 (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} 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>	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	А	202/210~(96%)	0.04	3 (1%) 73 73	54, 86, 126, 174	0
1	В	201/210~(95%)	0.04	7 (3%) 44 38	53, 84, 120, 150	0
1	С	201/210~(95%)	-0.11	4 (1%) 65 63	53, 76, 109, 155	0
1	D	199/210~(94%)	-0.05	5 (2%) 57 55	57, 80, 120, 201	0
1	Ι	199/210~(94%)	-0.01	4 (2%) 65 63	56, 76, 120, 144	0
1	J	197/210~(93%)	0.29	14 (7%) 16 12	63, 105, 167, 196	0
1	K	201/210~(95%)	0.31	4 (1%) 65 63	80, 110, 151, 210	0
1	L	200/210~(95%)	-0.27	0 100 100	45, 63, 94, 120	0
1	a	199/210~(94%)	0.06	3 (1%) 73 73	61, 95, 141, 163	0
1	b	199/210~(94%)	0.01	3 (1%) 73 73	59, 92, 131, 169	0
1	с	200/210~(95%)	-0.02	3 (1%) 73 73	58, 81, 119, 144	0
1	d	198/210~(94%)	0.04	3 (1%) 73 73	68, 93, 133, 157	0
1	i	201/210~(95%)	0.06	6 (2%) 50 45	56, 78, 119, 150	0
1	j	196/210~(93%)	0.20	14 (7%) 16 12	62, 93, 143, 179	0
1	k	206/210~(98%)	-0.05	4 (1%) 66 65	52, 72, 123, 170	0
1	1	200/210~(95%)	-0.17	0 100 100	49, 71, 98, 128	0
2	Е	11/12~(91%)	-0.07	1 (9%) 9 6	81, 92, 103, 117	0
2	F	11/12~(91%)	-0.37	0 100 100	72, 94, 115, 119	0
2	G	12/12~(100%)	-0.01	0 100 100	78, 97, 120, 121	0
2	Н	12/12~(100%)	-0.12	0 100 100	72, 101, 113, 120	0
2	М	12/12~(100%)	-0.40	0 100 100	70, 95, 109, 110	0
2	N	12/12~(100%)	-0.24	0 100 100	77, 95, 112, 119	0
2	Ο	$\overline{12/12}\ (100\%)$	-0.15	0 100 100	93, 113, 165, 165	0
2	Р	12/12~(100%)	0.22	1 (8%) 11 8	87, 101, 171, 178	0



Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
2	e	11/12~(91%)	-0.34	0 100 100	81, 96, 113, 148	0
2	f	$11/12 \ (91\%)$	-0.34	0 100 100	79, 103, 124, 129	0
2	g	12/12~(100%)	-0.06	0 100 100	87, 107, 148, 152	0
2	h	12/12~(100%)	0.39	1 (8%) 11 8	44, 88, 143, 156	0
2	m	12/12~(100%)	-0.22	0 100 100	67, 86, 109, 109	0
2	n	12/12~(100%)	-0.21	0 100 100	74, 97, 114, 121	0
2	О	12/12~(100%)	-0.10	0 100 100	74, 86, 108, 110	0
2	р	12/12~(100%)	0.21	0 100 100	69, 89, 114, 124	0
All	All	3387/3552~(95%)	0.01	80 (2%) 59 56	44, 85, 134, 210	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	i	139	SER	7.0
1	b	112	HIS	6.4
1	Ι	135	SER	5.8
2	h	523	DG	5.5
1	k	107	HIS	5.1

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 monosaccharides 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^{th} 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	$B-factors(Å^2)$	Q<0.9
3	ZN	L	401	1/1	0.90	0.15	$63,\!63,\!63,\!63$	0
3	ZN	В	401	1/1	0.94	0.19	59, 59, 59, 59, 59	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\operatorname{\AA}^2)$	Q<0.9
3	ZN	a	401	1/1	0.94	0.14	85,85,85,85	0
3	ZN	i	401	1/1	0.94	0.18	86,86,86,86	0
3	ZN	d	401	1/1	0.95	0.17	76, 76, 76, 76, 76	0
3	ZN	K	401	1/1	0.96	0.15	101,101,101,101	0
3	ZN	1	401	1/1	0.97	0.14	$68,\!68,\!68,\!68$	0
3	ZN	Ι	401	1/1	0.98	0.14	76, 76, 76, 76, 76	0
3	ZN	b	401	1/1	0.98	0.12	$59,\!59,\!59,\!59$	0
3	ZN	J	401	1/1	0.98	0.18	81,81,81,81	0
3	ZN	А	401	1/1	0.98	0.11	84,84,84,84	0
3	ZN	j	401	1/1	0.98	0.13	$79,\!79,\!79,\!79$	0
3	ZN	k	401	1/1	0.98	0.17	$69,\!69,\!69,\!69$	0
3	ZN	D	401	1/1	0.98	0.13	63,63,63,63	0
3	ZN	с	401	1/1	0.99	0.21	$65,\!65,\!65,\!65$	0
3	ZN	С	401	1/1	0.99	0.20	63,63,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.

