



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 12:31 AM UTC

PDB ID : 3VD0 / pdb_00003vd0
Title : structure of p73 DNA binding domain tetramer modulates p73 transactivation
Authors : Ethayathulla, A.S.; Tse, P.W.; Nguyen, S.; Viadiu, H.
Deposited on : 2012-01-04
Resolution : 2.95 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

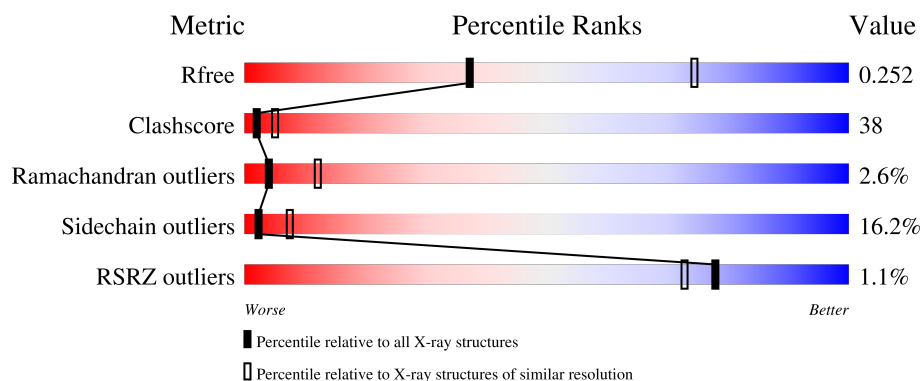
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	210	 3% 32% 43% 19% • •
1	B	210	 31% 48% 16% • •
1	C	210	 2% 37% 49% 10% • •
1	D	210	 36% 44% 14% • 5%
1	I	210	 42% 41% 10% • 5%

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14734 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	202	Total	C	N	O	S	0	0	0
			1596	999	288	298	11			
1	B	201	Total	C	N	O	S	0	0	0
			1580	987	285	297	11			
1	C	202	Total	C	N	O	S	0	0	0
			1596	999	288	298	11			
1	D	200	Total	C	N	O	S	2	0	0
			1572	985	282	294	11			
1	I	199	Total	C	N	O	S	0	0	0
			1567	982	281	293	11			
1	J	199	Total	C	N	O	S	1	0	0
			1561	976	281	293	11			
1	K	206	Total	C	N	O	S	0	0	0
			1631	1020	298	302	11			
1	L	201	Total	C	N	O	S	1	0	0
			1586	993	285	297	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 O15350
B	105	HIS	-	expression tag	UNP O15350
B	106	HIS	-	expression tag	UNP O15350
B	107	HIS	-	expression tag	UNP O15350
B	108	HIS	-	expression tag	UNP O15350
B	109	HIS	-	expression tag	UNP O15350
B	110	HIS	-	expression tag	UNP O15350
B	111	HIS	-	expression tag	UNP O15350
B	112	HIS	-	expression tag	UNP O15350
B	113	GLU	-	expression tag	UNP O15350
B	114	PHE	-	expression tag	UNP O15350
C	103	MET	-	initiating methionine	UNP O15350
C	104	GLY	-	expression tag	UNP O15350
C	105	HIS	-	expression tag	UNP O15350
C	106	HIS	-	expression tag	UNP O15350
C	107	HIS	-	expression tag	UNP O15350
C	108	HIS	-	expression tag	UNP O15350
C	109	HIS	-	expression tag	UNP O15350
C	110	HIS	-	expression tag	UNP O15350
C	111	HIS	-	expression tag	UNP O15350
C	112	HIS	-	expression tag	UNP O15350
C	113	GLU	-	expression tag	UNP O15350
C	114	PHE	-	expression tag	UNP O15350
D	103	MET	-	initiating methionine	UNP O15350
D	104	GLY	-	expression tag	UNP O15350
D	105	HIS	-	expression tag	UNP O15350
D	106	HIS	-	expression tag	UNP O15350
D	107	HIS	-	expression tag	UNP O15350
D	108	HIS	-	expression tag	UNP O15350
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
I	103	MET	-	initiating methionine	UNP O15350
I	104	GLY	-	expression tag	UNP O15350
I	105	HIS	-	expression tag	UNP O15350
I	106	HIS	-	expression tag	UNP O15350
I	107	HIS	-	expression tag	UNP O15350
I	108	HIS	-	expression tag	UNP O15350
I	109	HIS	-	expression tag	UNP O15350

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Chain	Residue	Modelled	Actual	Comment	Reference
I	110	HIS	-	expression tag	UNP O15350
I	111	HIS	-	expression tag	UNP O15350
I	112	HIS	-	expression tag	UNP O15350
I	113	GLU	-	expression tag	UNP O15350
I	114	PHE	-	expression tag	UNP O15350
J	103	MET	-	initiating methionine	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
K	103	MET	-	initiating methionine	UNP O15350
K	104	GLY	-	expression tag	UNP O15350
K	105	HIS	-	expression tag	UNP O15350
K	106	HIS	-	expression tag	UNP O15350
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
L	103	MET	-	initiating methionine	UNP O15350
L	104	GLY	-	expression tag	UNP O15350
L	105	HIS	-	expression tag	UNP O15350
L	106	HIS	-	expression tag	UNP O15350
L	107	HIS	-	expression tag	UNP O15350
L	108	HIS	-	expression tag	UNP O15350
L	109	HIS	-	expression tag	UNP O15350
L	110	HIS	-	expression tag	UNP O15350
L	111	HIS	-	expression tag	UNP O15350
L	112	HIS	-	expression tag	UNP O15350
L	113	GLU	-	expression tag	UNP O15350
L	114	PHE	-	expression tag	UNP O15350

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

TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	11	Total	C	N	O	P	0	0	0
			221	106	41	64	10			
2	F	11	Total	C	N	O	P	0	0	0
			227	107	43	66	11			
2	G	11	Total	C	N	O	P	0	0	0
			227	107	43	66	11			
2	H	11	Total	C	N	O	P	0	0	0
			221	106	41	64	10			
2	M	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
2	N	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
2	O	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
2	P	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is water.

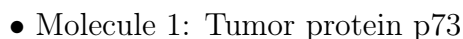
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		

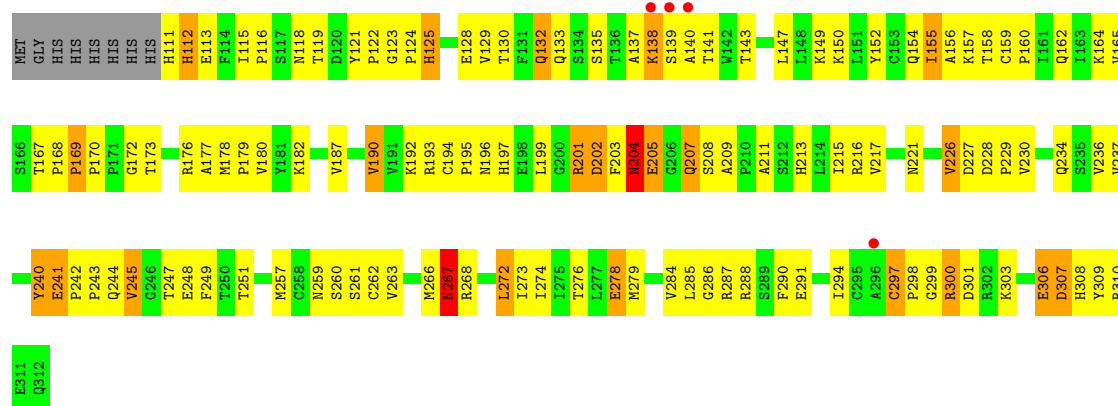
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	19	Total 19	O 19	0	0
4	C	19	Total 19	O 19	0	0
4	D	13	Total 13	O 13	0	0
4	I	19	Total 19	O 19	0	0
4	J	14	Total 14	O 14	0	0
4	K	34	Total 34	O 34	0	0
4	L	30	Total 30	O 30	0	0
4	E	1	Total 1	O 1	0	0
4	N	1	Total 1	O 1	0	0
4	O	1	Total 1	O 1	0	0

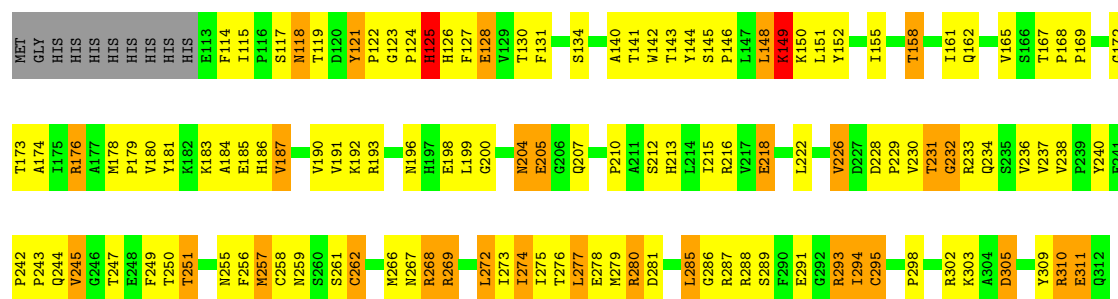
- Molecule 1: Tumor protein p73





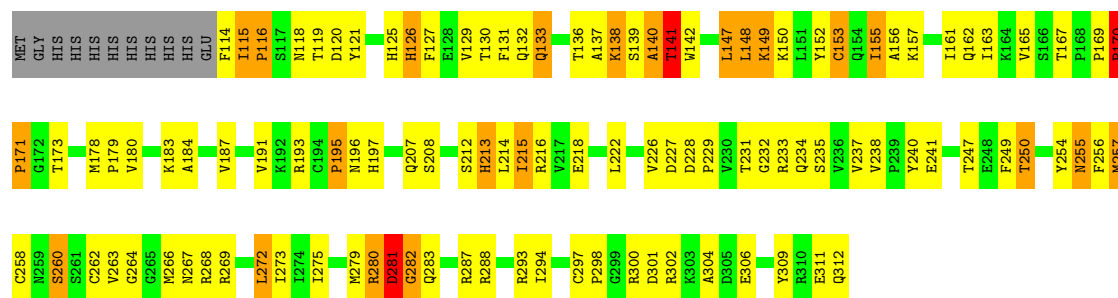
• Molecule 1: Tumor protein p73

Chain D: 36% 44% 14% • 5%



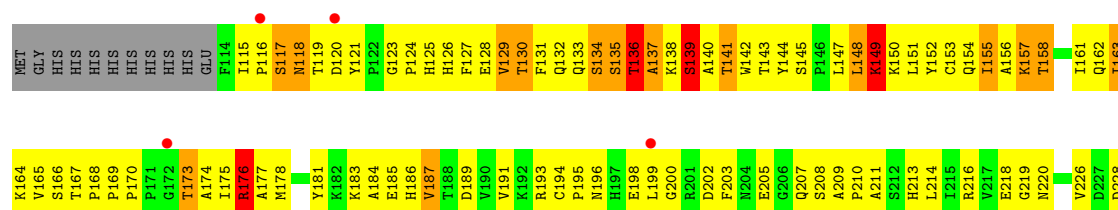
• Molecule 1: Tumor protein p73

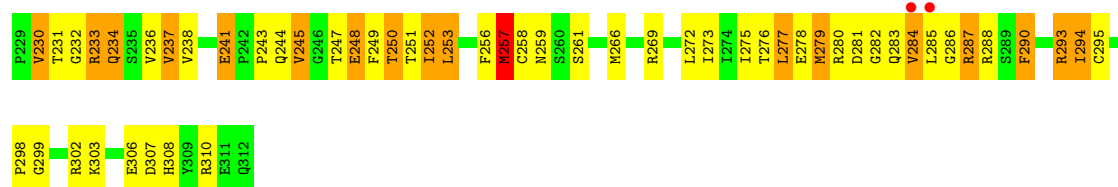
Chain I: 42% 41% 10% • 5%



• Molecule 1: Tumor protein p73

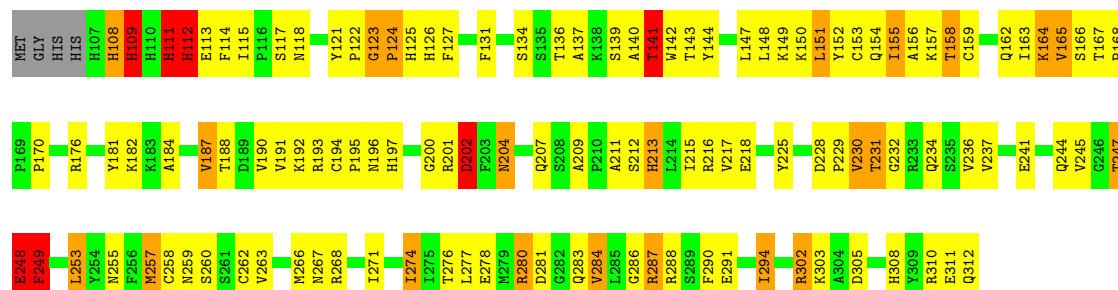
Chain J: 3% 27% 50% 15% • 5%





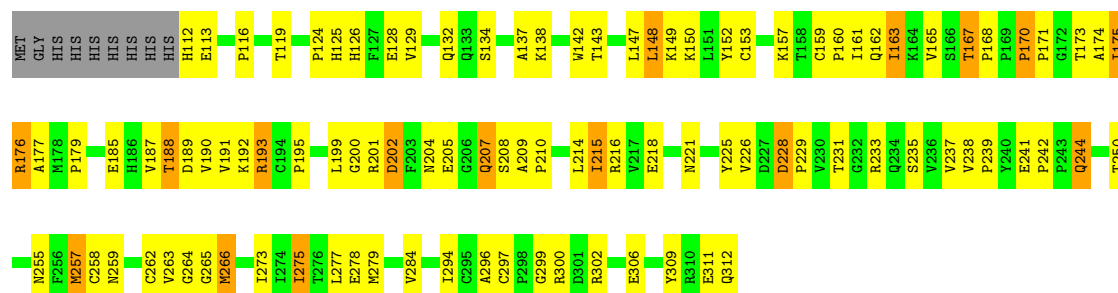
- Molecule 1: Tumor protein p73

Chain K: 40% 44% 10% . .



- Molecule 1: Tumor protein p73

Chain L: 48% 40% 8% .



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

Chain E: 42% 50% 8%

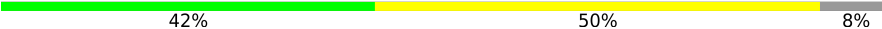


- Molecule 2: DNA (5'-D(*CP*AP*GP*GP*CP*AP*TP*GP*CP*CP*TP*G)-3')

Chain F: 50% 42% 8%

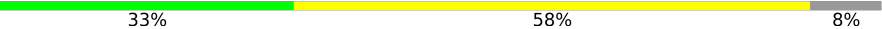


- Molecule 2: DNA (5'-D(*CP*AP*GP*GP*CP*AP*TP*GP*CP*CP*TP*G)-3')

Chain G:  42% 50% 8%

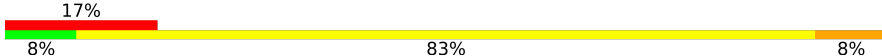


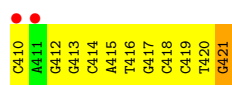
- Molecule 2: DNA (5'-D(*CP*AP*GP*GP*CP*AP*TP*GP*CP*CP*TP*G)-3')

Chain H:  33% 58% 8%

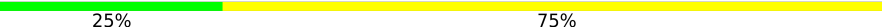


- Molecule 2: DNA (5'-D(*CP*AP*GP*GP*CP*AP*TP*GP*CP*CP*TP*G)-3')

Chain M:  17% 8% 83% 8%



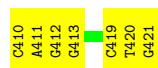
- Molecule 2: DNA (5'-D(*CP*AP*GP*GP*CP*AP*TP*GP*CP*CP*TP*G)-3')

Chain N:  25% 75%



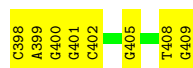
- Molecule 2: DNA (5'-D(*CP*AP*GP*GP*CP*AP*TP*GP*CP*CP*TP*G)-3')

Chain O:  42% 58%



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

Chain P:  33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.09Å 104.52Å 122.99Å 90.00° 96.18° 90.00°	Depositor
Resolution (Å)	19.92 – 2.95 19.92 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.92-2.95) 99.3 (19.92-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 2.93Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.235 , 0.254 0.234 , 0.252	Depositor DCC
R_{free} test set	877 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	69.5	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14734	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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

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	0.56	0/1638	1.19	18/2225 (0.8%)
1	B	0.55	0/1620	1.19	18/2201 (0.8%)
1	C	0.59	0/1638	1.22	20/2225 (0.9%)
1	D	0.52	0/1612	1.12	13/2190 (0.6%)
1	I	0.62	1/1607 (0.1%)	1.22	20/2183 (0.9%)
1	J	0.53	0/1600	1.13	15/2174 (0.7%)
1	K	0.55	0/1676	1.18	16/2277 (0.7%)
1	L	0.64	1/1627 (0.1%)	1.21	17/2210 (0.8%)
2	E	0.36	0/247	0.79	0/379
2	F	0.47	0/254	0.93	0/390
2	G	0.48	0/254	0.77	0/390
2	H	0.48	0/247	0.92	0/379
2	M	0.46	0/272	0.86	1/418 (0.2%)
2	N	0.43	0/272	1.02	0/418
2	O	0.36	0/272	0.83	0/418
2	P	0.37	0/272	0.75	0/418
All	All	0.55	2/15108 (0.0%)	1.14	138/20895 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	148	LEU	C-O	-5.19	1.17	1.24
1	L	275	ILE	CA-CB	5.14	1.60	1.54

The worst 5 of 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	208	SER	N-CA-C	11.43	123.82	111.36
1	D	200	GLY	N-CA-C	-9.85	101.50	112.33
1	A	257	MET	N-CA-C	9.52	122.87	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	257	MET	N-CA-C	9.46	124.37	113.01
1	K	200	GLY	N-CA-C	-9.27	102.13	112.33

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	1596	0	1558	163	0
1	B	1580	0	1544	157	0
1	C	1596	0	1558	120	0
1	D	1572	0	1540	141	0
1	I	1567	0	1538	111	0
1	J	1561	0	1531	159	0
1	K	1631	0	1581	130	0
1	L	1586	0	1551	67	0
2	E	221	0	125	8	0
2	F	227	0	124	8	0
2	G	227	0	124	5	0
2	H	221	0	125	6	0
2	M	243	0	136	11	0
2	N	243	0	136	14	0
2	O	243	0	136	10	0
2	P	243	0	136	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	18	0	0	2	0
4	B	19	0	0	1	0
4	C	19	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	13	0	0	0	0
4	E	1	0	0	0	0
4	I	19	0	0	3	0
4	J	14	0	0	2	0
4	K	34	0	0	0	0
4	L	30	0	0	3	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
All	All	14734	0	13443	1067	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 38.

The worst 5 of 1067 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:K:280:ARG:HG2	1:K:280:ARG:HH11	1.02	1.13
1:I:231:THR:CG2	1:I:233:ARG:HG2	1.83	1.08
2:N:401:DG:H2''	2:N:402:DC:H5''	1.33	1.08
1:C:240:TYR:C	1:C:240:TYR:CD2	2.30	1.05
1:B:169:PRO:HG2	1:B:170:PRO:HD3	1.43	1.00

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	200/210 (95%)	168 (84%)	23 (12%)	9 (4%)	2	4
1	B	199/210 (95%)	173 (87%)	20 (10%)	6 (3%)	3	9
1	C	200/210 (95%)	180 (90%)	18 (9%)	2 (1%)	12	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	198/210 (94%)	177 (89%)	20 (10%)	1 (0%)	24	49
1	I	197/210 (94%)	172 (87%)	18 (9%)	7 (4%)	2	6
1	J	197/210 (94%)	164 (83%)	26 (13%)	7 (4%)	2	6
1	K	204/210 (97%)	180 (88%)	16 (8%)	8 (4%)	2	5
1	L	199/210 (95%)	174 (87%)	24 (12%)	1 (0%)	24	49
All	All	1594/1680 (95%)	1388 (87%)	165 (10%)	41 (3%)	4	12

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	PRO
1	A	207	GLN
1	B	169	PRO
1	C	202	ASP
1	I	282	GLY

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	179/186 (96%)	146 (82%)	33 (18%)	1	4
1	B	177/186 (95%)	144 (81%)	33 (19%)	1	4
1	C	179/186 (96%)	154 (86%)	25 (14%)	3	10
1	D	176/186 (95%)	148 (84%)	28 (16%)	2	8
1	I	176/186 (95%)	157 (89%)	19 (11%)	6	18
1	J	175/186 (94%)	133 (76%)	42 (24%)	1	1
1	K	182/186 (98%)	151 (83%)	31 (17%)	2	5
1	L	178/186 (96%)	158 (89%)	20 (11%)	6	17
All	All	1422/1488 (96%)	1191 (84%)	231 (16%)	2	7

5 of 231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	295	CYS
1	L	189	ASP
1	J	139	SER
1	L	187	VAL
1	K	231	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	308	HIS
1	J	267	ASN
1	I	312	GLN
1	J	220	ASN
1	K	111	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	202/210 (96%)	0.35	6 (2%) 52 45	22, 89, 123, 127	3 (1%)
1	B	201/210 (95%)	0.05	1 (0%) 87 83	24, 75, 108, 136	1 (0%)
1	C	202/210 (96%)	-0.10	4 (1%) 65 57	41, 71, 108, 135	0
1	D	200/210 (95%)	0.09	0 100 100	49, 82, 112, 144	2 (1%)
1	I	199/210 (94%)	-0.11	0 100 100	44, 70, 105, 114	1 (0%)
1	J	199/210 (94%)	0.34	6 (3%) 52 45	52, 88, 121, 129	1 (0%)
1	K	206/210 (98%)	-0.17	0 100 100	32, 60, 108, 128	0
1	L	201/210 (95%)	-0.49	0 100 100	26, 49, 80, 95	1 (0%)
2	E	11/12 (91%)	0.05	0 100 100	59, 76, 97, 100	0
2	F	11/12 (91%)	0.10	0 100 100	50, 80, 122, 133	0
2	G	11/12 (91%)	0.87	0 100 100	91, 117, 128, 148	0
2	H	11/12 (91%)	0.49	0 100 100	76, 98, 129, 130	0
2	M	12/12 (100%)	0.27	2 (16%) 4 4	43, 75, 126, 136	0
2	N	12/12 (100%)	0.01	0 100 100	50, 80, 93, 94	0
2	O	12/12 (100%)	-0.07	0 100 100	53, 66, 132, 133	0
2	P	12/12 (100%)	-0.05	0 100 100	49, 65, 121, 124	0
All	All	1702/1776 (95%)	0.00	19 (1%) 78 73	22, 73, 117, 148	9 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	159	CYS	7.6
1	A	216	ARG	5.5
1	C	140	ALA	4.8
1	A	139	SER	4.0
2	M	410	DC	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 oligosaccharides 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, 95th 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
3	ZN	I	401	1/1	0.96	0.04	74,74,74,74	0
3	ZN	C	401	1/1	0.99	0.05	50,50,50,50	0
3	ZN	D	401	1/1	0.99	0.03	62,62,62,62	0
3	ZN	A	401	1/1	0.99	0.03	72,72,72,72	0
3	ZN	L	401	1/1	0.99	0.06	50,50,50,50	0
3	ZN	J	401	1/1	1.00	0.02	70,70,70,70	0
3	ZN	K	401	1/1	1.00	0.01	48,48,48,48	0
3	ZN	B	401	1/1	1.00	0.03	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.