



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 01:41 PM UTC

PDB ID : 4GUO / pdb_00004guo
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

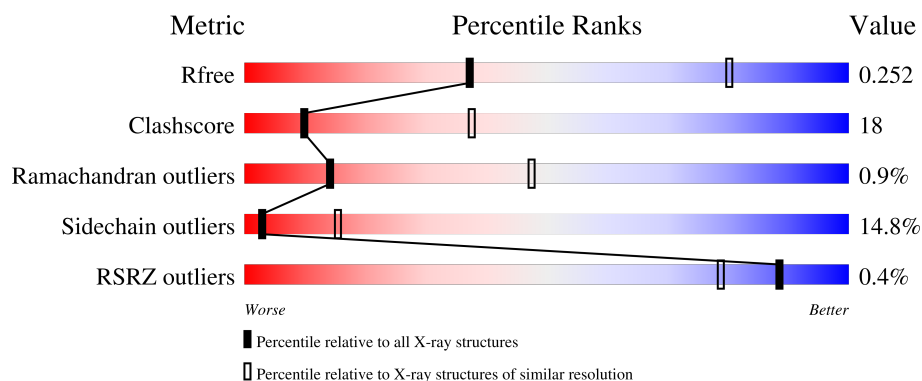
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 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	
1	B	210	
1	C	210	
1	D	210	
1	I	210	

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Mol	Chain	Length	Quality of chain
1	J	210	 % 56% 31% 8% 5%
1	K	210	 % 49% 33% 11% . .
1	L	210	 59% 28% 9% .
2	E	12	 50% 50%
2	G	12	 25% 67% 8%
2	M	12	 83% 8% 8%
2	O	12	 75% 25%
3	F	12	 42% 50% 8%
3	H	12	 58% 42%
3	N	12	 58% 42%
3	P	12	 58% 33% 8%

2 Entry composition

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 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*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 (CCD ID: ZN) (formula: Zn).

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

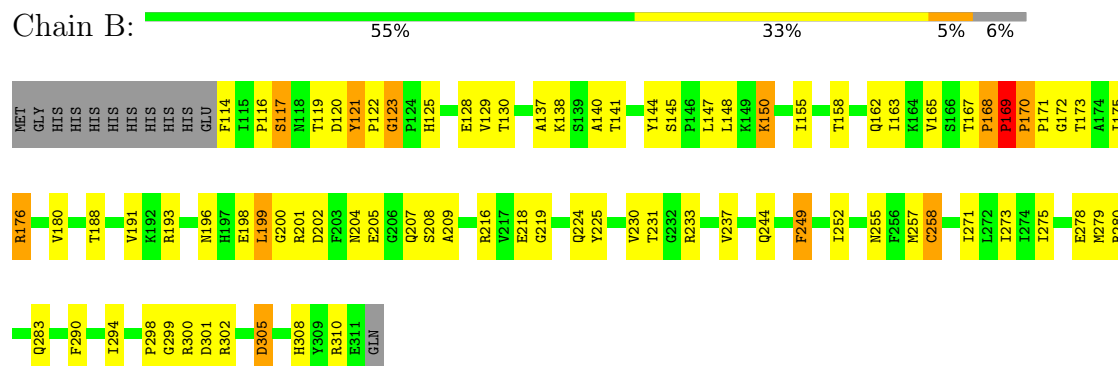
3 Residue-property plots

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.

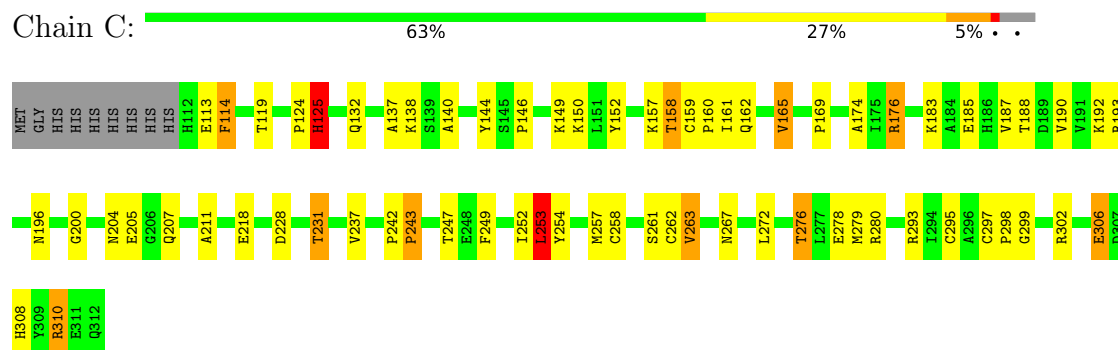
• Molecule 1: Tumor protein p73



• Molecule 1: Tumor protein p73

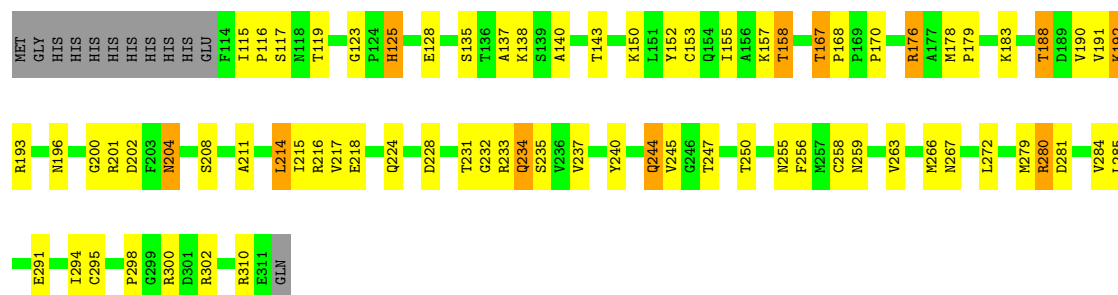


• Molecule 1: Tumor protein p73



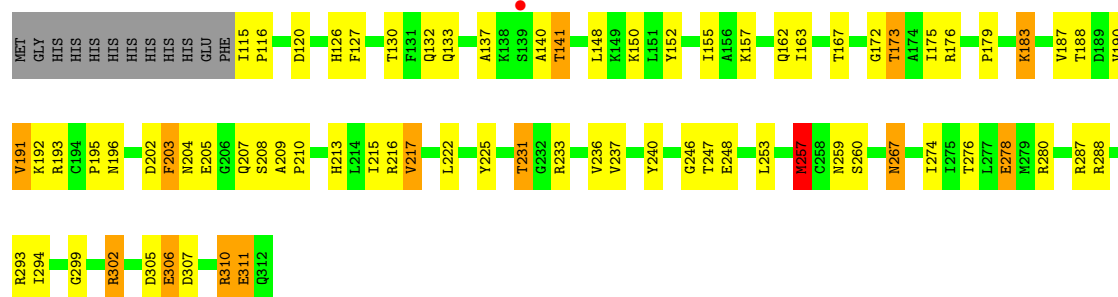
- Molecule 1: Tumor protein p73

Chain D: 



- Molecule 1: Tumor protein p73

Chain I: 



- Molecule 1: Tumor protein p73

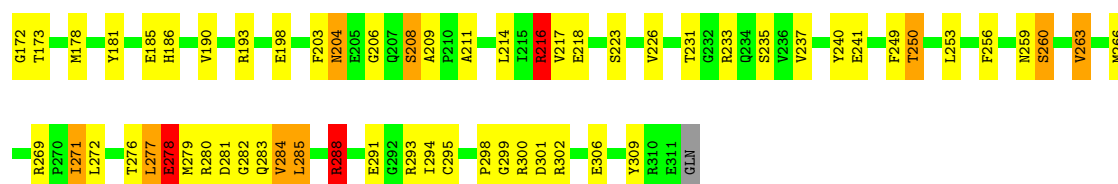
Chain J: 



- Molecule 1: Tumor protein p73

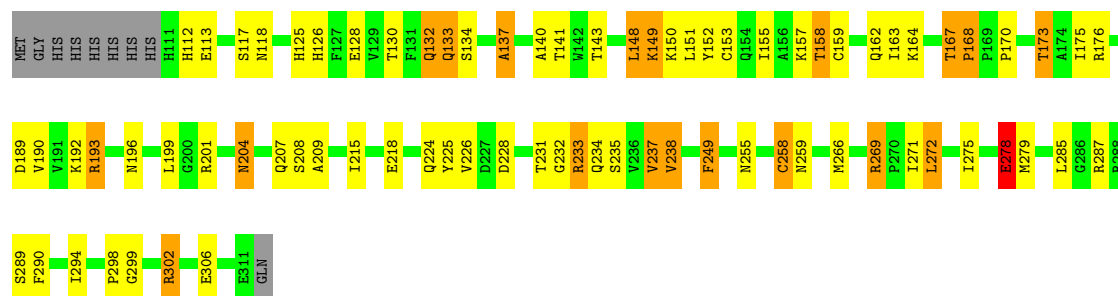
Chain K: 





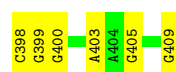
- Molecule 1: Tumor protein p73

Chain L:



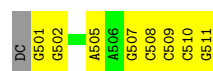
- Molecule 2: DNA (5'-D(*CP*GP*GP*GP*CP*AP*AP*GP*CP*CP*CP*G)-3')

Chain E:



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

Chain G:



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

Chain M:

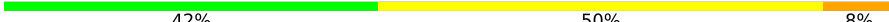


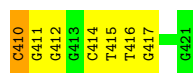
- Molecule 2: DNA (5'-D(*CP*GP*GP*GP*CP*AP*AP*GP*CP*CP*CP*G)-3')

Chain O:



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

Chain F:  42% 50% 8%



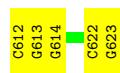
- Molecule 3: DNA (5'-D(*CP*GP*GP*GP*CP*TP*TP*GP*CP*CP*CP*G)-3')

Chain H:  58% 42%



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

Chain N:  58% 42%



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

Chain P:  58% 33% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.25Å 104.33Å 123.32Å 90.00° 96.38° 90.00°	Depositor
Resolution (Å)	44.01 – 3.19 44.01 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.01-3.19) 99.1 (44.01-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.208 , 0.270 (Not available) , 0.252	Depositor DCC
R_{free} test set	1738 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	80.8	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

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	0.78	0/1610	1.06	4/2188 (0.2%)
1	B	0.78	0/1593	1.21	8/2166 (0.4%)
1	C	0.76	0/1627	1.04	2/2210 (0.1%)
1	D	0.76	0/1590	1.16	7/2162 (0.3%)
1	I	0.78	0/1595	1.13	5/2167 (0.2%)
1	J	0.81	1/1600 (0.1%)	1.18	6/2174 (0.3%)
1	K	0.83	2/1616 (0.1%)	1.17	7/2197 (0.3%)
1	L	0.80	0/1622	1.10	5/2205 (0.2%)
2	E	0.55	0/274	0.73	1/421 (0.2%)
2	G	0.34	0/256	0.65	0/393
2	M	0.62	1/274 (0.4%)	0.85	1/421 (0.2%)
2	O	0.45	0/274	0.78	1/421 (0.2%)
3	F	0.47	0/270	0.91	1/415 (0.2%)
3	H	0.41	0/270	0.96	1/415 (0.2%)
3	N	0.49	0/270	0.96	1/415 (0.2%)
3	P	0.50	0/270	0.98	1/415 (0.2%)
All	All	0.75	4/15011 (0.0%)	1.09	51/20785 (0.2%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	168	PRO	CA-C	5.77	1.55	1.51
2	M	600	DC	O3'-P	-5.49	1.52	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	168	PRO	C-O	-5.49	1.18	1.24
1	K	166	SER	CA-C	5.46	1.60	1.52

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	168	PRO	N-CA-C	10.05	120.12	110.47
1	D	208	SER	N-CA-C	9.96	122.21	111.36
1	J	282	GLY	N-CA-C	9.33	127.87	112.85
1	B	168	PRO	N-CA-C	8.66	121.26	110.70
1	B	168	PRO	CA-C-N	8.42	129.06	120.38

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 [i](#)

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	70	0
1	B	1553	0	1526	55	0
1	C	1586	0	1551	45	0
1	D	1551	0	1523	55	0
1	I	1556	0	1529	54	0
1	J	1561	0	1531	69	0
1	K	1576	0	1540	71	0
1	L	1581	0	1545	60	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	487	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 18.

The worst 5 of 487 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: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
3:F:415:DT:H2''	3:F:416:DT:H5''	1.42	0.98

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	12	45
1	C	199/210 (95%)	188 (94%)	9 (4%)	2 (1%)	12	45
1	D	196/210 (93%)	187 (95%)	6 (3%)	3 (2%)	8	37
1	I	196/210 (93%)	188 (96%)	7 (4%)	1 (0%)	24	59
1	J	197/210 (94%)	188 (95%)	8 (4%)	1 (0%)	24	59
1	K	199/210 (95%)	184 (92%)	10 (5%)	5 (2%)	4	27
1	L	199/210 (95%)	187 (94%)	11 (6%)	1 (0%)	24	59
All	All	1581/1680 (94%)	1490 (94%)	76 (5%)	15 (1%)	14	47

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%)	156 (89%)	19 (11%)	6	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	174/186 (94%)	150 (86%)	24 (14%)	3	18
1	C	178/186 (96%)	154 (86%)	24 (14%)	4	19
1	D	174/186 (94%)	149 (86%)	25 (14%)	3	16
1	I	175/186 (94%)	151 (86%)	24 (14%)	3	18
1	J	175/186 (94%)	144 (82%)	31 (18%)	2	10
1	K	176/186 (95%)	143 (81%)	33 (19%)	1	9
1	L	177/186 (95%)	149 (84%)	28 (16%)	2	13
All	All	1404/1488 (94%)	1196 (85%)	208 (15%)	3	15

5 of 208 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	311	GLU
1	J	284	VAL
1	L	233	ARG
1	J	130	THR
1	J	189	ASP

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	267	ASN
1	K	133	GLN
1	J	125	HIS
1	J	186	HIS
1	K	186	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	201/210 (95%)	-0.34	0	100 100	50, 98, 147, 172	1 (0%)
1	B	198/210 (94%)	-0.40	0	100 100	58, 92, 126, 145	2 (1%)
1	C	201/210 (95%)	-0.43	0	100 100	55, 83, 126, 141	0
1	D	198/210 (94%)	-0.42	0	100 100	63, 89, 132, 160	0
1	I	198/210 (94%)	-0.44	1 (0%)	87 76	64, 87, 129, 156	0
1	J	199/210 (94%)	-0.16	2 (1%)	79 63	75, 111, 158, 195	0
1	K	201/210 (95%)	-0.28	3 (1%)	72 52	63, 87, 144, 164	0
1	L	201/210 (95%)	-0.54	0	100 100	48, 73, 108, 138	0
2	E	12/12 (100%)	-0.17	0	100 100	73, 100, 152, 178	0
2	G	11/12 (91%)	-0.36	0	100 100	85, 106, 135, 142	0
2	M	12/12 (100%)	-0.56	0	100 100	72, 90, 103, 106	0
2	O	12/12 (100%)	-0.40	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%)	-0.22	0	100 100	79, 115, 157, 170	0
3	N	12/12 (100%)	-0.45	0	100 100	72, 84, 105, 117	0
3	P	12/12 (100%)	-0.33	0	100 100	80, 99, 150, 160	0
All	All	1692/1776 (95%)	-0.38	6 (0%)	88 79	48, 89, 141, 195	3 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	174	ALA	2.4
1	K	171	PRO	2.4
1	I	139	SER	2.3
1	K	131	PHE	2.1
1	J	285	LEU	2.0

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
4	ZN	A	401	1/1	0.99	0.02	87,87,87,87	0
4	ZN	B	401	1/1	0.99	0.03	63,63,63,63	0
4	ZN	C	401	1/1	0.99	0.05	59,59,59,59	0
4	ZN	I	401	1/1	0.99	0.04	98,98,98,98	0
4	ZN	J	401	1/1	0.99	0.03	84,84,84,84	0
4	ZN	D	401	1/1	1.00	0.02	71,71,71,71	0
4	ZN	K	401	1/1	1.00	0.02	89,89,89,89	0
4	ZN	L	401	1/1	1.00	0.01	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.