



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2022 – 06:09 PM JST

PDB ID : 7VP3  
Title : Structure of a transcription factor and DNA complex  
Authors : Zhang, Y.; Xu, Y.P.; Wang, B.; Su, X.D.  
Deposited on : 2021-10-15  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

The types of validation reports are described at

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

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

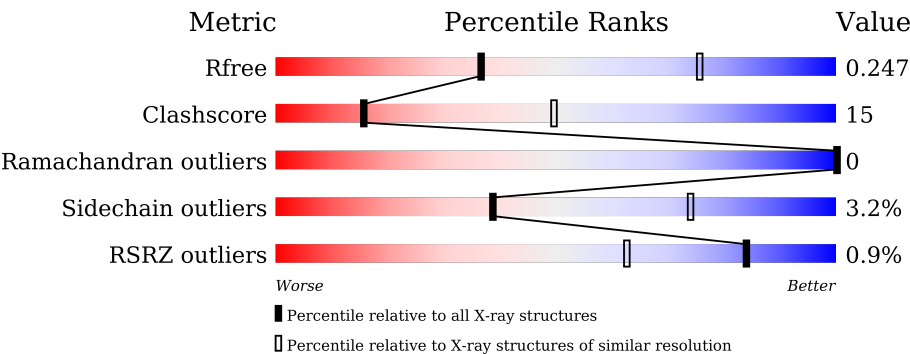
MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.









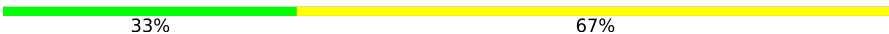
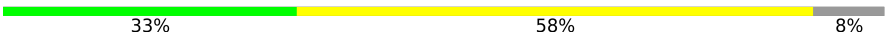


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	12	<div><div></div><div>75%17%8%</div></div>
1	B	12	<div><div>8%</div><div>25%67%8%</div></div>
1	H	12	<div><div></div><div>67%25%8%</div></div>
1	O	12	<div><div></div><div>17%67%17%</div></div>
2	C	72	<div><div>%</div><div>57%28%14%</div></div>
2	D	72	<div><div>%</div><div>64%17%19%</div></div>

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Mol	Chain	Length	Quality of chain
2	G	72	
2	I	72	
2	J	72	
2	L	72	
2	N	72	
2	P	72	
3	E	12	
3	F	12	
3	K	12	
3	M	12	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5399 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 DNA chain called DNA (5'-D(\*TP\*GP\*GP\*GP\*GP\*AP\*CP\*CP\*CP\*AP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	11	Total	C	N	O	P	0	0	0
			223	106	44	63	10			
1	A	11	Total	C	N	O	P	0	0	0
			223	106	44	63	10			
1	H	11	Total	C	N	O	P	0	0	0
			223	106	44	63	10			
1	O	10	Total	C	N	O	P	0	0	0
			206	96	42	58	10			

- Molecule 2 is a protein called Transcription factor TCP15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	58	Total	C	N	O	S	0	0	0
			447	274	89	81	3			
2	J	58	Total	C	N	O	S	0	0	0
			443	272	86	82	3			
2	C	62	Total	C	N	O	S	0	0	0
			452	279	86	85	2			
2	G	56	Total	C	N	O	S	0	0	0
			414	256	80	76	2			
2	I	59	Total	C	N	O	S	0	0	0
			444	271	89	82	2			
2	L	59	Total	C	N	O	S	0	0	0
			454	278	89	84	3			
2	N	62	Total	C	N	O	S	0	0	0
			464	285	92	85	2			
2	P	61	Total	C	N	O	S	0	0	0
			456	278	88	87	3			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	50	MET	-	initiating methionine	UNP Q9C9L2
D	114	LEU	-	expression tag	UNP Q9C9L2
D	115	GLU	-	expression tag	UNP Q9C9L2
D	116	HIS	-	expression tag	UNP Q9C9L2
D	117	HIS	-	expression tag	UNP Q9C9L2
D	118	HIS	-	expression tag	UNP Q9C9L2
D	119	HIS	-	expression tag	UNP Q9C9L2
D	120	HIS	-	expression tag	UNP Q9C9L2
D	121	HIS	-	expression tag	UNP Q9C9L2
J	50	MET	-	initiating methionine	UNP Q9C9L2
J	114	LEU	-	expression tag	UNP Q9C9L2
J	115	GLU	-	expression tag	UNP Q9C9L2
J	116	HIS	-	expression tag	UNP Q9C9L2
J	117	HIS	-	expression tag	UNP Q9C9L2
J	118	HIS	-	expression tag	UNP Q9C9L2
J	119	HIS	-	expression tag	UNP Q9C9L2
J	120	HIS	-	expression tag	UNP Q9C9L2
J	121	HIS	-	expression tag	UNP Q9C9L2
C	50	MET	-	initiating methionine	UNP Q9C9L2
C	114	LEU	-	expression tag	UNP Q9C9L2
C	115	GLU	-	expression tag	UNP Q9C9L2
C	116	HIS	-	expression tag	UNP Q9C9L2
C	117	HIS	-	expression tag	UNP Q9C9L2
C	118	HIS	-	expression tag	UNP Q9C9L2
C	119	HIS	-	expression tag	UNP Q9C9L2
C	120	HIS	-	expression tag	UNP Q9C9L2
C	121	HIS	-	expression tag	UNP Q9C9L2
G	50	MET	-	initiating methionine	UNP Q9C9L2
G	114	LEU	-	expression tag	UNP Q9C9L2
G	115	GLU	-	expression tag	UNP Q9C9L2
G	116	HIS	-	expression tag	UNP Q9C9L2
G	117	HIS	-	expression tag	UNP Q9C9L2
G	118	HIS	-	expression tag	UNP Q9C9L2
G	119	HIS	-	expression tag	UNP Q9C9L2
G	120	HIS	-	expression tag	UNP Q9C9L2
G	121	HIS	-	expression tag	UNP Q9C9L2
I	50	MET	-	initiating methionine	UNP Q9C9L2
I	114	LEU	-	expression tag	UNP Q9C9L2
I	115	GLU	-	expression tag	UNP Q9C9L2
I	116	HIS	-	expression tag	UNP Q9C9L2
I	117	HIS	-	expression tag	UNP Q9C9L2
I	118	HIS	-	expression tag	UNP Q9C9L2
I	119	HIS	-	expression tag	UNP Q9C9L2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	120	HIS	-	expression tag	UNP Q9C9L2
I	121	HIS	-	expression tag	UNP Q9C9L2
L	50	MET	-	initiating methionine	UNP Q9C9L2
L	114	LEU	-	expression tag	UNP Q9C9L2
L	115	GLU	-	expression tag	UNP Q9C9L2
L	116	HIS	-	expression tag	UNP Q9C9L2
L	117	HIS	-	expression tag	UNP Q9C9L2
L	118	HIS	-	expression tag	UNP Q9C9L2
L	119	HIS	-	expression tag	UNP Q9C9L2
L	120	HIS	-	expression tag	UNP Q9C9L2
L	121	HIS	-	expression tag	UNP Q9C9L2
N	50	MET	-	initiating methionine	UNP Q9C9L2
N	114	LEU	-	expression tag	UNP Q9C9L2
N	115	GLU	-	expression tag	UNP Q9C9L2
N	116	HIS	-	expression tag	UNP Q9C9L2
N	117	HIS	-	expression tag	UNP Q9C9L2
N	118	HIS	-	expression tag	UNP Q9C9L2
N	119	HIS	-	expression tag	UNP Q9C9L2
N	120	HIS	-	expression tag	UNP Q9C9L2
N	121	HIS	-	expression tag	UNP Q9C9L2
P	50	MET	-	initiating methionine	UNP Q9C9L2
P	114	LEU	-	expression tag	UNP Q9C9L2
P	115	GLU	-	expression tag	UNP Q9C9L2
P	116	HIS	-	expression tag	UNP Q9C9L2
P	117	HIS	-	expression tag	UNP Q9C9L2
P	118	HIS	-	expression tag	UNP Q9C9L2
P	119	HIS	-	expression tag	UNP Q9C9L2
P	120	HIS	-	expression tag	UNP Q9C9L2
P	121	HIS	-	expression tag	UNP Q9C9L2

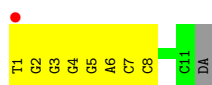
- Molecule 3 is a DNA chain called DNA (5'-D(\*AP\*TP\*GP\*TP\*GP\*GP\*GP\*TP\*CP\*CP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	12	Total	C	N	O	P	0	0	0
			242	116	43	72	11			
3	F	11	Total	C	N	O	P	0	0	0
			224	106	38	69	11			
3	K	12	Total	C	N	O	P	0	0	0
			242	116	43	72	11			
3	M	12	Total	C	N	O	P	0	0	0
			242	116	43	72	11			

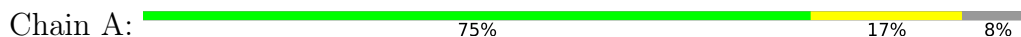
### 3 Residue-property plots [i](#)

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: DNA (5'-D(\*TP\*GP\*GP\*GP\*GP\*AP\*CP\*CP\*CP\*AP\*C)-3')



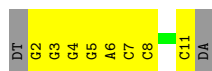
- Molecule 1: DNA (5'-D(\*TP\*GP\*GP\*GP\*GP\*AP\*CP\*CP\*CP\*AP\*C)-3')



- Molecule 1: DNA (5'-D(\*TP\*GP\*GP\*GP\*GP\*AP\*CP\*CP\*CP\*AP\*C)-3')



- Molecule 1: DNA (5'-D(\*TP\*GP\*GP\*GP\*GP\*AP\*CP\*CP\*CP\*AP\*C)-3')



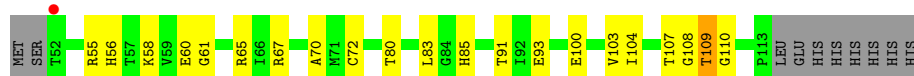
- Molecule 2: Transcription factor TCP15



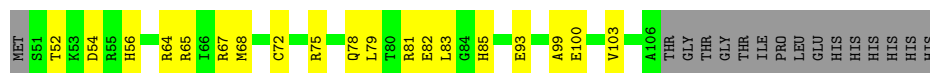
- Molecule 2: Transcription factor TCP15



- Molecule 2: Transcription factor TCP15



- Molecule 2: Transcription factor TCP15



- Molecule 2: Transcription factor TCP15



- Molecule 2: Transcription factor TCP15



- Molecule 2: Transcription factor TCP15




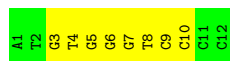
- Molecule 2: Transcription factor TCP15



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



Chain E:  33% 67%



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

Chain F:  33% 58% 8%



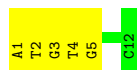
- Molecule 3: DNA (5'-D(\*AP\*TP\*GP\*TP\*GP\*GP\*GP\*TP\*CP\*CP\*CP\*C)-3')

Chain K:  50% 50%



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

Chain M:  58% 42%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.22Å 112.78Å 156.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.17 – 3.00 18.28 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.8 (18.17-3.00) 93.8 (18.28-3.00)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.75 (at 3.03Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.198 , 0.246 0.197 , 0.247	Depositor DCC
$R_{free}$ test set	1210 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.3	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 58.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5399	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.97	0/250	0.88	0/384
1	B	0.80	0/250	0.72	0/384
1	H	0.98	0/250	1.02	0/384
1	O	1.01	0/231	0.87	0/354
2	C	0.67	0/459	0.68	0/624
2	D	0.60	0/453	0.66	0/609
2	G	0.42	0/420	0.61	0/568
2	I	0.63	0/450	0.71	0/608
2	J	0.52	0/449	0.73	0/605
2	L	0.73	0/460	0.69	0/618
2	N	0.53	0/471	0.64	0/638
2	P	0.87	0/462	0.73	0/624
3	E	0.78	0/270	0.77	0/415
3	F	0.76	0/249	0.72	0/382
3	K	1.06	0/270	1.12	0/415
3	M	0.91	0/270	0.86	0/415
All	All	0.75	0/5664	0.77	0/8027

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	223	0	124	3	0
1	B	223	0	124	12	0
1	H	223	0	124	2	0
1	O	206	0	111	8	0
2	C	452	0	435	24	0
2	D	447	0	446	13	0
2	G	414	0	400	19	0
2	I	444	0	434	14	0
2	J	443	0	440	15	0
2	L	454	0	454	15	0
2	N	464	0	457	14	0
2	P	456	0	444	16	0
3	E	242	0	137	14	0
3	F	224	0	125	7	0
3	K	242	0	137	10	0
3	M	242	0	137	11	0
All	All	5399	0	4529	146	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 15.

All (146) 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:B:7:DC:H5	3:E:7:DG:H1	1.02	0.92
2:I:67:ARG:HG2	2:L:65:ARG:HD3	1.55	0.89
2:C:107:THR:HG23	2:C:109:THR:H	1.41	0.85
2:C:67:ARG:HG2	2:G:65:ARG:HD3	1.57	0.84
3:K:2:DT:H3	3:M:1:DA:H2	1.22	0.81
3:M:3:DG:H1	1:O:11:DC:H5	1.31	0.79
2:L:85:HIS:ND1	2:L:91:THR:HG22	1.98	0.78
2:D:67:ARG:HG2	2:J:65:ARG:HD3	1.65	0.78
1:B:7:DC:H5	3:E:7:DG:N1	1.81	0.77
2:J:85:HIS:ND1	2:J:91:THR:HG22	2.04	0.73
3:M:2:DT:H2''	3:M:3:DG:H5''	1.70	0.72
2:C:83:LEU:HB2	2:C:85:HIS:CD2	2.24	0.71
2:C:104:ILE:HG12	2:C:110:GLY:HA2	1.73	0.71
2:N:85:HIS:ND1	2:N:91:THR:HG22	2.06	0.71
2:N:65:ARG:HG3	2:P:67:ARG:HG3	1.72	0.70
3:E:8:DT:H2'	3:E:9:DC:C6	2.29	0.67
2:I:106:ALA:HB1	2:L:83:LEU:HD11	1.76	0.67
2:I:66:ILE:HD13	2:L:88:ASP:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:4:DT:H2'	3:E:5:DG:C8	2.31	0.66
2:G:100:GLU:HA	2:G:103:VAL:HG22	1.79	0.63
2:P:100:GLU:O	2:P:104:ILE:HG22	1.98	0.63
1:B:5:DG:H2'	1:B:6:DA:C8	2.33	0.63
2:G:78:GLN:HG3	2:G:79:LEU:N	2.15	0.62
1:A:4:DG:OP2	2:C:67:ARG:HG3	2.00	0.62
2:C:65:ARG:HG3	2:G:67:ARG:HG2	1.82	0.62
2:P:80:THR:HA	2:P:91:THR:HG21	1.82	0.62
3:E:6:DG:H2''	3:E:7:DG:H8	1.64	0.61
3:K:1:DA:H2	3:M:2:DT:H3	1.47	0.61
1:A:3:DG:OP2	2:G:64:ARG:NH2	2.33	0.61
2:D:65:ARG:HG3	2:J:67:ARG:HG3	1.83	0.60
2:N:92:ILE:HD12	2:P:92:ILE:HD12	1.83	0.60
2:I:85:HIS:ND1	2:I:91:THR:HG22	2.17	0.60
3:K:1:DA:H2''	3:K:2:DT:H5'	1.84	0.59
2:I:100:GLU:O	2:I:104:ILE:HG12	2.02	0.59
1:A:4:DG:N7	2:C:67:ARG:NH1	2.48	0.59
2:D:85:HIS:ND1	2:D:91:THR:HG22	2.18	0.58
3:K:2:DT:N3	3:M:1:DA:H2	1.98	0.57
2:D:82:GLU:OE2	2:J:107:THR:HA	2.05	0.56
3:F:4:DT:H2'	3:F:5:DG:C8	2.40	0.56
3:K:1:DA:H5''	3:K:1:DA:H8	1.70	0.56
2:P:54:ASP:CG	2:P:56:HIS:HD1	2.08	0.56
1:O:4:DG:N7	2:N:67:ARG:NH1	2.54	0.56
2:C:83:LEU:HB2	2:C:85:HIS:HD2	1.71	0.55
1:B:4:DG:N7	2:D:67:ARG:NH1	2.54	0.55
3:E:9:DC:H5''	3:E:9:DC:H6	1.72	0.55
1:B:6:DA:H2'	1:B:7:DC:O2	2.07	0.55
1:B:3:DG:H2'	1:B:4:DG:C8	2.42	0.54
2:N:112:ILE:HD12	2:N:113:PRO:HD2	1.90	0.54
2:P:85:HIS:ND1	2:P:91:THR:HG22	2.23	0.54
2:C:107:THR:HA	2:G:82:GLU:HG2	1.89	0.53
2:I:65:ARG:HG3	2:L:67:ARG:HG2	1.91	0.53
2:C:93:GLU:HG2	2:G:72:CYS:HB2	1.89	0.53
2:G:79:LEU:O	2:G:83:LEU:HB2	2.08	0.53
1:B:6:DA:H2'	1:B:7:DC:C2	2.44	0.53
2:C:70:ALA:HA	2:G:64:ARG:HD2	1.90	0.53
3:M:4:DT:H2'	3:M:5:DG:C8	2.43	0.53
1:B:7:DC:H2''	1:B:8:DC:H5'	1.91	0.52
2:C:103:VAL:O	2:C:107:THR:HG22	2.10	0.52
2:J:94:TRP:O	2:J:98:GLN:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:9:DC:H2'	3:E:10:DC:C6	2.46	0.51
2:J:54:ASP:OD2	2:J:56:HIS:ND1	2.44	0.51
2:C:56:HIS:NE2	3:F:5:DG:N7	2.59	0.51
3:F:7:DG:H2'	3:F:8:DT:C6	2.46	0.50
2:L:62:ARG:HG2	2:L:62:ARG:HH11	1.76	0.50
2:L:99:ALA:O	2:L:103:VAL:HG13	2.12	0.50
2:C:60:GLU:OE1	2:G:81:ARG:NH2	2.37	0.49
1:B:3:DG:OP2	2:J:64:ARG:NH2	2.46	0.49
3:K:1:DA:H5''	3:K:1:DA:C8	2.48	0.49
2:N:94:TRP:HZ3	2:P:103:VAL:HG12	1.77	0.49
2:D:54:ASP:OD2	2:D:56:HIS:ND1	2.46	0.49
3:E:9:DC:C6	3:E:9:DC:H5''	2.48	0.48
1:O:7:DC:H2'	1:O:8:DC:C6	2.48	0.48
1:B:5:DG:H2'	1:B:6:DA:H8	1.77	0.48
2:C:80:THR:HA	2:C:91:THR:HG21	1.95	0.48
3:E:9:DC:H2'	3:E:10:DC:H6	1.79	0.48
2:G:54:ASP:OD2	2:G:56:HIS:ND1	2.46	0.47
3:K:1:DA:C2	3:M:2:DT:N3	2.74	0.47
3:M:2:DT:H2''	3:M:3:DG:C5'	2.43	0.47
2:C:107:THR:HG23	2:C:108:GLY:N	2.29	0.47
3:E:8:DT:H2'	3:E:9:DC:H6	1.78	0.47
2:P:79:LEU:HD21	2:P:94:TRP:CZ3	2.50	0.47
2:C:107:THR:CG2	2:C:108:GLY:N	2.78	0.46
3:K:6:DG:H2''	3:K:7:DG:H8	1.79	0.46
3:E:6:DG:H2''	3:E:7:DG:C8	2.48	0.46
2:J:53:LYS:HE3	2:J:53:LYS:HB3	1.42	0.46
2:D:53:LYS:HG2	2:D:54:ASP:N	2.30	0.46
2:G:75:ARG:O	2:G:78:GLN:HG2	2.16	0.46
2:I:83:LEU:HD13	2:I:85:HIS:HE1	1.80	0.46
2:C:85:HIS:CG	2:C:91:THR:HG22	2.49	0.46
3:F:10:DC:OP2	2:G:52:THR:HG22	2.16	0.46
3:M:3:DG:N1	1:O:11:DC:H5	2.07	0.46
3:K:1:DA:H2	3:M:2:DT:N3	2.13	0.45
2:N:78:GLN:O	2:N:82:GLU:HG2	2.15	0.45
2:N:82:GLU:OE1	2:P:107:THR:HB	2.16	0.45
2:C:65:ARG:HG3	2:G:67:ARG:CG	2.46	0.45
2:C:55:ARG:NH2	3:F:3:DG:O6	2.49	0.45
2:N:94:TRP:O	2:N:98:GLN:HG2	2.17	0.45
3:M:2:DT:C2'	3:M:3:DG:H5''	2.44	0.45
2:D:103:VAL:HG13	2:J:79:LEU:HD11	1.99	0.45
2:L:80:THR:HA	2:L:91:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:78:GLN:O	2:D:82:GLU:HG3	2.16	0.44
1:H:4:DG:N7	2:I:67:ARG:NH1	2.63	0.44
2:N:107:THR:HB	2:P:82:GLU:OE1	2.17	0.44
1:B:1:DT:H4'	1:B:2:DG:OP1	2.17	0.44
2:C:100:GLU:O	2:C:104:ILE:HG13	2.17	0.44
3:K:4:DT:H2'	3:K:5:DG:C8	2.53	0.44
1:O:5:DG:H2''	1:O:6:DA:O5'	2.17	0.44
2:J:68:MET:HE3	2:J:68:MET:HB2	1.65	0.44
1:B:4:DG:OP2	2:D:67:ARG:HG3	2.18	0.44
1:H:6:DA:H2'	1:H:7:DC:C6	2.52	0.44
2:P:52:THR:O	2:P:53:LYS:C	2.56	0.44
2:D:62:ARG:NH2	2:J:88:ASP:OD2	2.52	0.43
1:O:2:DG:OP2	2:P:56:HIS:HA	2.18	0.43
2:C:58:LYS:HD3	2:C:61:GLY:O	2.18	0.43
2:L:83:LEU:HD23	2:L:85:HIS:CE1	2.54	0.43
2:I:92:ILE:HG22	2:L:72:CYS:SG	2.59	0.43
2:P:58:LYS:HB3	2:P:62:ARG:O	2.19	0.43
2:C:72:CYS:HB2	2:G:93:GLU:HG2	2.00	0.42
2:C:107:THR:CG2	2:C:108:GLY:H	2.32	0.42
2:L:68:MET:HE3	2:L:68:MET:HB2	1.85	0.42
3:E:9:DC:OP1	2:J:53:LYS:HG2	2.20	0.42
2:G:99:ALA:O	2:G:103:VAL:HG13	2.19	0.42
2:G:83:LEU:HB3	2:G:85:HIS:CD2	2.54	0.42
1:O:8:DC:OP2	2:N:52:THR:HG22	2.19	0.42
2:J:103:VAL:O	2:J:107:THR:HG23	2.19	0.42
2:D:70:ALA:HA	2:J:64:ARG:HD2	2.01	0.42
2:D:56:HIS:NE2	3:E:5:DG:N7	2.57	0.42
3:F:2:DT:H2''	3:F:3:DG:O5'	2.20	0.41
2:N:104:ILE:HG12	2:N:109:THR:O	2.20	0.41
2:N:66:ILE:HD12	2:P:68:MET:CE	2.51	0.41
2:G:78:GLN:CG	2:G:79:LEU:N	2.83	0.41
2:N:96:LEU:HD23	2:N:96:LEU:HA	1.93	0.41
2:P:99:ALA:O	2:P:103:VAL:HG13	2.21	0.41
2:L:87:SER:O	2:L:90:GLU:HB2	2.20	0.41
2:J:62:ARG:HH11	2:J:62:ARG:HD2	1.72	0.41
2:I:58:LYS:HB3	2:I:62:ARG:O	2.20	0.41
2:I:93:GLU:HG2	2:L:72:CYS:HB2	2.03	0.41
2:L:68:MET:HE3	2:L:73:ALA:HB2	2.02	0.41
1:O:2:DG:H2'	1:O:3:DG:C8	2.56	0.41
3:E:3:DG:C8	3:E:4:DT:H72	2.56	0.41
2:P:85:HIS:CG	2:P:91:THR:HG22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3:DG:H2'	3:F:4:DT:C6	2.57	0.40
2:G:68:MET:HE3	2:G:68:MET:HB2	1.79	0.40
2:I:59:VAL:HG23	2:L:77:PHE:HE2	1.86	0.40
2:I:80:THR:HA	2:I:91:THR:HG21	2.03	0.40
2:I:83:LEU:HD13	2:I:85:HIS:CE1	2.56	0.40

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	
2	C	60/72 (83%)	57 (95%)	3 (5%)	0	100	100
2	D	56/72 (78%)	55 (98%)	1 (2%)	0	100	100
2	G	54/72 (75%)	51 (94%)	3 (6%)	0	100	100
2	I	57/72 (79%)	52 (91%)	5 (9%)	0	100	100
2	J	56/72 (78%)	55 (98%)	1 (2%)	0	100	100
2	L	57/72 (79%)	56 (98%)	1 (2%)	0	100	100
2	N	60/72 (83%)	58 (97%)	2 (3%)	0	100	100
2	P	59/72 (82%)	50 (85%)	9 (15%)	0	100	100
All	All	459/576 (80%)	434 (95%)	25 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	Percentiles	
2	C	43/59 (73%)	42 (98%)	1 (2%)	50	80
2	D	44/59 (75%)	44 (100%)	0	100	100
2	G	39/59 (66%)	39 (100%)	0	100	100
2	I	43/59 (73%)	42 (98%)	1 (2%)	50	80
2	J	44/59 (75%)	42 (96%)	2 (4%)	27	64
2	L	46/59 (78%)	43 (94%)	3 (6%)	17	50
2	N	45/59 (76%)	45 (100%)	0	100	100
2	P	45/59 (76%)	41 (91%)	4 (9%)	9	35
All	All	349/472 (74%)	338 (97%)	11 (3%)	39	74

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	52	THR
2	J	53	LYS
2	C	109	THR
2	I	75	ARG
2	L	51	SER
2	L	75	ARG
2	L	97	GLN
2	P	51	SER
2	P	64	ARG
2	P	65	ARG
2	P	67	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	11/12 (91%)	-0.43	0 <span>100</span> <span>100</span>	44, 53, 60, 108	0
1	B	11/12 (91%)	-0.19	1 (9%) <span>9</span> <span>3</span>	48, 60, 74, 105	0
1	H	11/12 (91%)	-0.52	0 <span>100</span> <span>100</span>	44, 49, 63, 100	0
1	O	10/12 (83%)	-0.23	0 <span>100</span> <span>100</span>	61, 71, 82, 87	0
2	C	62/72 (86%)	-0.49	1 (1%) <span>72</span> <span>44</span>	45, 60, 100, 119	0
2	D	58/72 (80%)	-0.52	1 (1%) <span>70</span> <span>41</span>	41, 54, 77, 97	0
2	G	56/72 (77%)	-0.52	0 <span>100</span> <span>100</span>	42, 57, 79, 89	0
2	I	59/72 (81%)	-0.57	0 <span>100</span> <span>100</span>	43, 53, 76, 106	0
2	J	58/72 (80%)	-0.58	1 (1%) <span>70</span> <span>41</span>	42, 53, 77, 86	0
2	L	59/72 (81%)	-0.54	0 <span>100</span> <span>100</span>	40, 54, 76, 82	0
2	N	62/72 (86%)	-0.44	0 <span>100</span> <span>100</span>	51, 68, 93, 100	0
2	P	61/72 (84%)	-0.32	1 (1%) <span>72</span> <span>44</span>	49, 68, 106, 130	0
3	E	12/12 (100%)	-0.44	0 <span>100</span> <span>100</span>	20, 55, 73, 76	0
3	F	11/12 (91%)	-0.67	0 <span>100</span> <span>100</span>	42, 46, 65, 74	0
3	K	12/12 (100%)	-0.45	0 <span>100</span> <span>100</span>	41, 50, 68, 82	0
3	M	12/12 (100%)	-0.48	0 <span>100</span> <span>100</span>	51, 63, 83, 91	0
All	All	565/672 (84%)	-0.48	5 (0%) <span>84</span> <span>63</span>	20, 59, 89, 130	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	51	SER	3.3
2	P	51	SER	3.1
2	J	52	THR	3.0
1	B	1	DT	2.7
2	C	52	THR	2.6

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.