



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2024 – 10:55 AM EDT

PDB ID : 4X6A  
Title : Crystal structure of yeast RNA polymerase II encountering oxidative Cyclop-  
urine DNA lesions  
Authors : Wang, L.; Chong, J.; Wang, D.  
Deposited on : 2014-12-07  
Resolution : 3.96 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

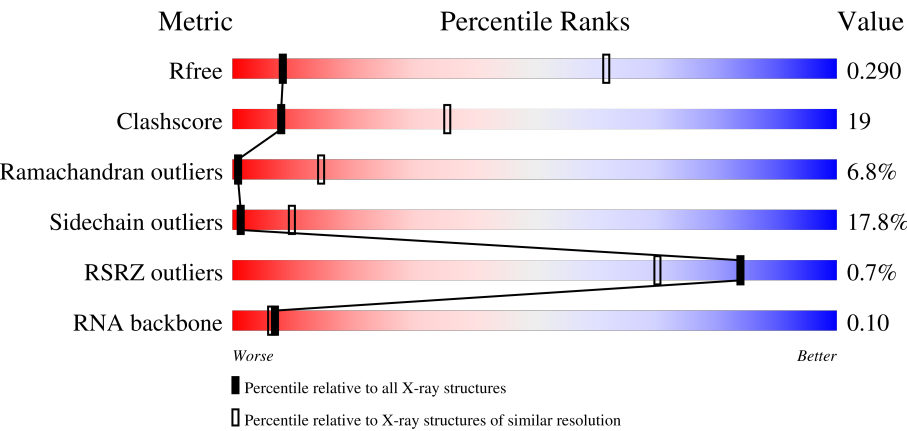
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.96 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.



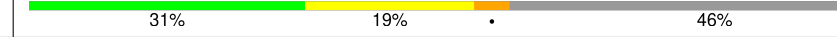

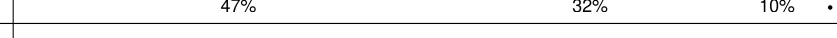

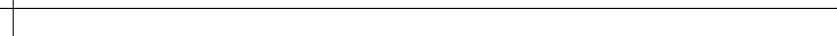


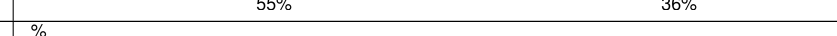
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	164625	1115 (4.20-3.72)
Clashscore	180529	1009 (4.16-3.76)
Ramachandran outliers	177936	1006 (4.18-3.74)
Sidechain outliers	177891	1117 (4.20-3.72)
RSRZ outliers	164620	1116 (4.20-3.72)
RNA backbone	3690	1136 (4.84-3.00)

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	1733	<div><div></div><div><div>44%</div><div>27%</div><div>8%</div><div>•</div><div>20%</div></div></div>
2	B	1224	<div><div></div><div><div>49%</div><div>34%</div><div>6%</div><div>•</div><div>10%</div></div></div>
3	C	318	<div><div></div><div><div>45%</div><div>30%</div><div>8%</div><div>•</div><div>16%</div></div></div>
4	E	215	<div><div></div><div><div>55%</div><div>34%</div><div>10%</div></div></div>

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Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	9	
12	T	29	

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 28548 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1395	Total	C	N	O	S	0	0	0
			10969	6917	1923	2068	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1104	Total	C	N	O	S	0	0	0
			8773	5555	1536	1627	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 11 is a RNA chain called RNA\_9 mer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	9	Total	C	N	O	P	0	0	0
			195	87	37	62	9			

- Molecule 12 is a DNA chain called Template DNA \_29 mer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	11	Total	C	N	O	P	0	0	0
			224	107	40	66	11			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	2	Total	Zn	0	0
			2	2		
13	B	1	Total	Zn	0	0
			1	1		

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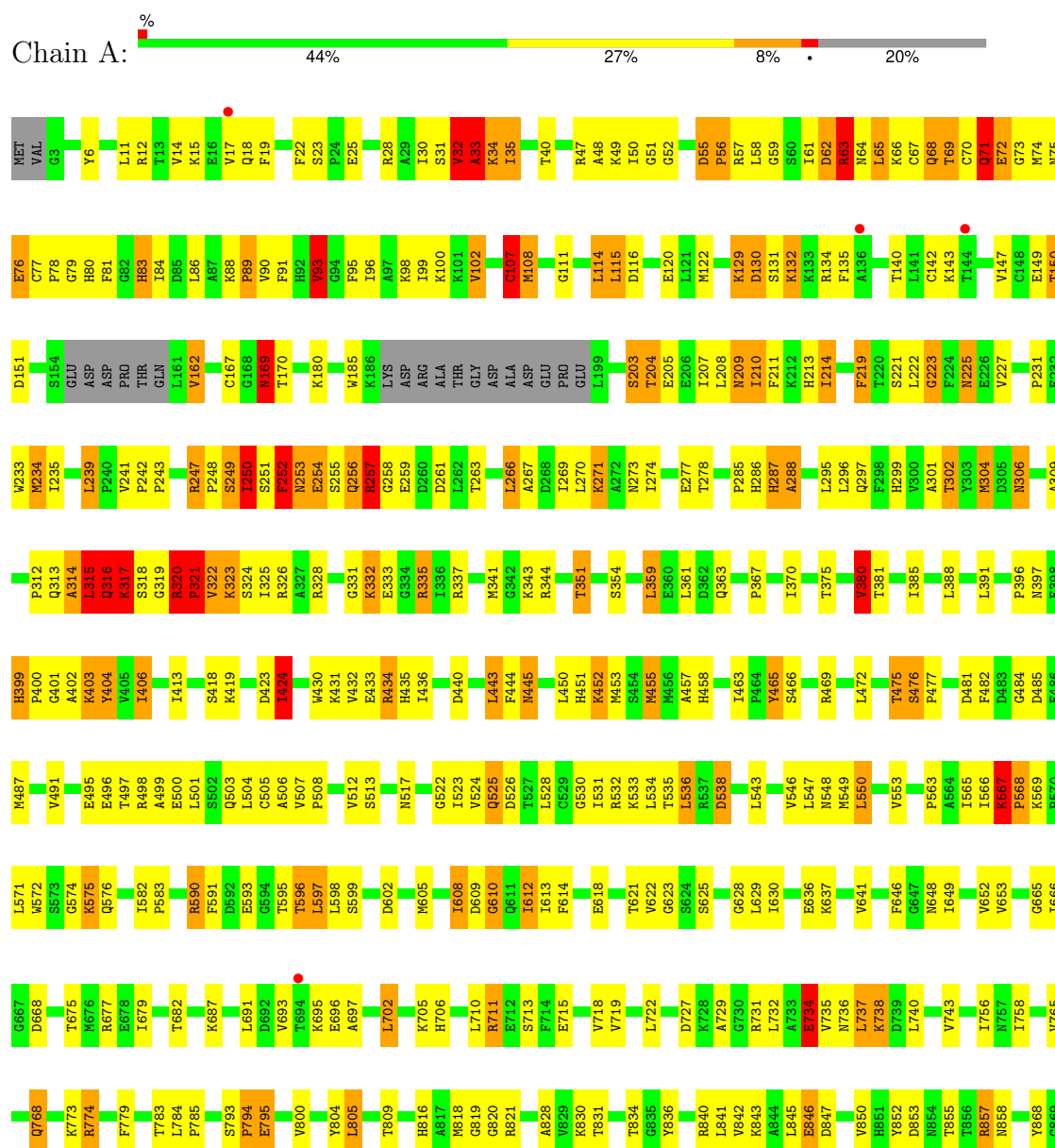
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	1	Total 1	Zn 1	0	0
13	I	2	Total 2	Zn 2	0	0
13	J	1	Total 1	Zn 1	0	0
13	L	1	Total 1	Zn 1	0	0

### 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: DNA-directed RNA polymerase II subunit RPB1

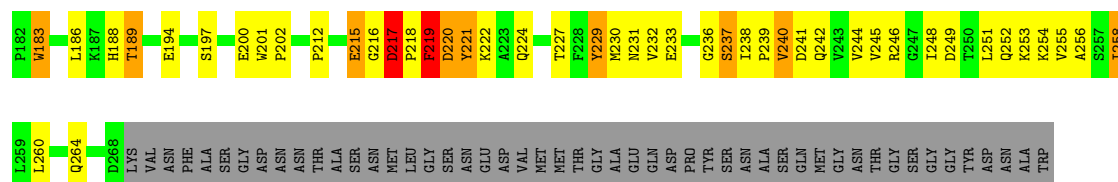




ARG	GLN	MET
LEU	LEU	SER
GLY	ALA	ASP
LYS	GLN	LEU
TYR	HIS	ALA
GLU	THR	ASN
LEU	THR	SER
ILE	GLU	GLU
ALA	SER	LYS
GLU	ASP	TYR
GLY	ASN	TVR
SER	ILE	ASP
GLU	SER	GLU
ASP	ARG	ASP
ASP	LVS	PRA
SER	TVR	TVR
GLY	GLU	GLY
SER	TPO	PHE
K164	K94	D20
F165	I95	E21
F166	Y96	S22
I167	V97	A23
G168	T98	P24
R169		I25
	V102	T26
L174	N103	A27
R175	E104	E28
S176		D29
K177	T109	S30
C178	H110	W31
F179	A111	
L180	L112	I34
L181	Y113	S35
S182	P114	A36
E183	Q115	F37
A184		F38
T185	R118	R39
	R120	E40
L189	N121	K41
Y190	L122	
K191	T123	V44
L192	I124	S45
K193	S125	Q46
E194		Q47
	L128	V55
F197	F129	D56
		Y57
G201	K134	I63
Y202	THR	C64
F203	TVR	E65
I204	GLU	D66
	ILE	S67
G207	ALA	T68
	ASP	L69
V211	VAL	I70
L212		
L213	P80	LEU
P317	GLY	GLU

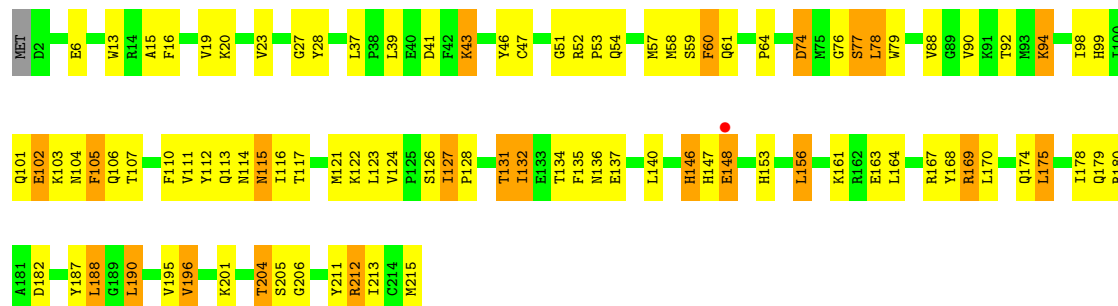







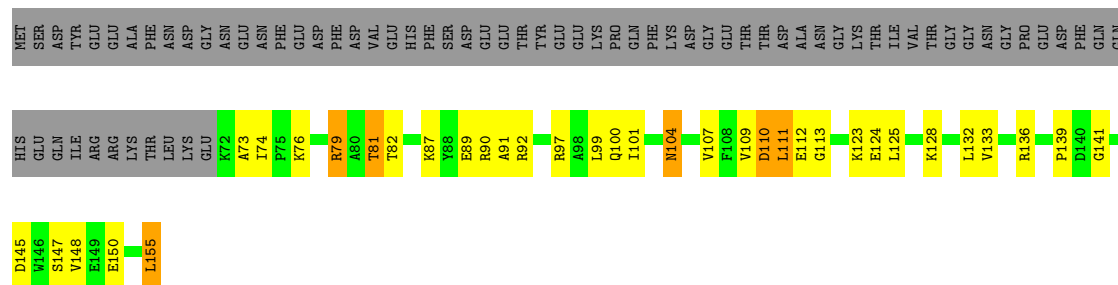
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 



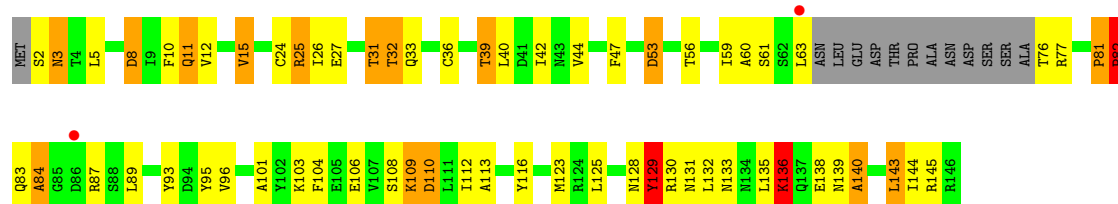
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 



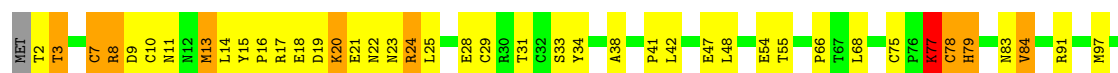
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 



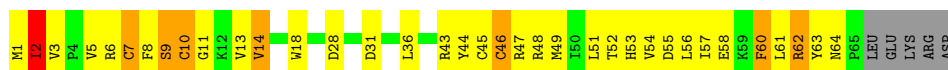
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I: 

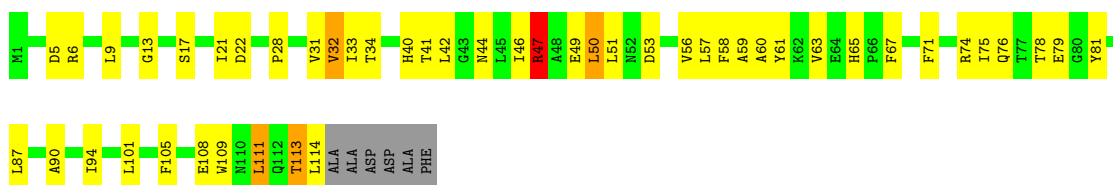




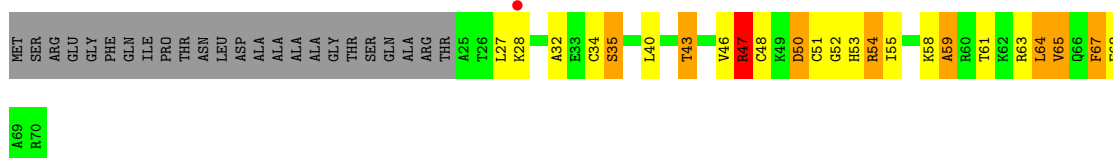
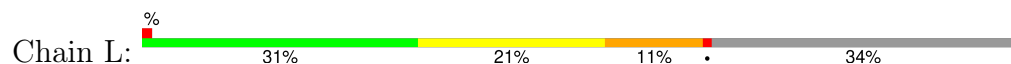
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



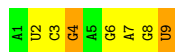
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



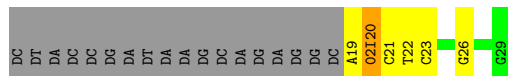
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 11: RNA\_9 mer



- Molecule 12: Template DNA \_29 mer



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.55Å 220.33Å 191.56Å 90.00° 97.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.96 50.00 – 3.96	Depositor EDS
% Data completeness (in resolution range)	89.0 (50.00-3.96) 89.1 (50.00-3.96)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 4.00Å)	Xtriage
Refinement program	REFMAC, PHENIX	Depositor
R, $R_{free}$	0.249 , 0.296 0.243 , 0.290	Depositor DCC
$R_{free}$ test set	2773 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	83.4	Xtriage
Anisotropy	1.330	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 100.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	28548	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 02I, 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	0.42	0/11163	0.76	4/15091 (0.0%)
2	B	0.42	0/8943	0.74	5/12059 (0.0%)
3	C	0.40	0/2133	0.70	0/2891
4	E	0.40	0/1788	0.71	0/2406
5	F	0.41	0/691	0.71	0/933
6	H	0.43	0/1086	0.79	0/1470
7	I	0.44	0/989	0.75	1/1331 (0.1%)
8	J	0.42	0/541	0.75	0/727
9	K	0.40	0/937	0.71	1/1265 (0.1%)
10	L	0.48	0/365	0.93	0/485
11	R	0.31	0/218	0.60	0/338
12	T	0.32	0/225	0.56	0/342
All	All	0.42	0/29079	0.74	11/39338 (0.0%)

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	A	0	13
2	B	0	6
4	E	0	1
6	H	0	5
7	I	0	1
10	L	0	1
All	All	0	27

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	637	LEU	CA-CB-CG	9.57	137.31	115.30
7	I	77	LYS	CB-CA-C	-7.66	95.08	110.40
2	B	485	ARG	NE-CZ-NH1	6.82	123.71	120.30
9	K	47	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	315	LEU	CA-CB-CG	6.06	129.24	115.30

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	CYS	Peptide
1	A	169	ASN	Peptide
1	A	203	SER	Peptide
1	A	209	ASN	Peptide
1	A	33	ALA	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10969	0	11069	432	0
2	B	8773	0	8811	387	0
3	C	2095	0	2051	104	0
4	E	1752	0	1776	64	0
5	F	679	0	701	20	0
6	H	1068	0	1040	46	0
7	I	971	0	927	43	0
8	J	532	0	542	35	0
9	K	919	0	929	44	0
10	L	363	0	387	20	0
11	R	195	0	98	6	0
12	T	224	0	123	15	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	28548	0	28454	1095	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 19.

The worst 5 of 1095 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)
3:C:38:ILE:HD11	3:C:176:ILE:CD1	1.39	1.51
3:C:38:ILE:CD1	3:C:176:ILE:HD11	1.72	1.19
7:I:7:CYS:HB3	7:I:14:LEU:HD21	1.23	1.14
3:C:38:ILE:CD1	3:C:176:ILE:CD1	2.27	1.10
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.37	1.07

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1383/1733 (80%)	1057 (76%)	217 (16%)	109 (8%)	1	12
2	B	1086/1224 (89%)	858 (79%)	162 (15%)	66 (6%)	1	16
3	C	264/318 (83%)	206 (78%)	45 (17%)	13 (5%)	2	19
4	E	212/215 (99%)	174 (82%)	29 (14%)	9 (4%)	2	21
5	F	82/155 (53%)	62 (76%)	15 (18%)	5 (6%)	1	16
6	H	129/146 (88%)	97 (75%)	23 (18%)	9 (7%)	1	14
7	I	117/122 (96%)	85 (73%)	20 (17%)	12 (10%)	0	7
8	J	63/70 (90%)	48 (76%)	11 (18%)	4 (6%)	1	16
9	K	112/120 (93%)	95 (85%)	14 (12%)	3 (3%)	4	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	L	44/70 (63%)	26 (59%)	10 (23%)	8 (18%)	0	2
All	All	3492/4173 (84%)	2708 (78%)	546 (16%)	238 (7%)	1	15

5 of 238 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	55	ASP
1	A	62	ASP
1	A	63	ARG
1	A	68	GLN

### 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	1218/1520 (80%)	984 (81%)	234 (19%)	1	8
2	B	958/1061 (90%)	802 (84%)	156 (16%)	2	12
3	C	234/274 (85%)	194 (83%)	40 (17%)	1	11
4	E	196/197 (100%)	162 (83%)	34 (17%)	1	10
5	F	74/137 (54%)	61 (82%)	13 (18%)	1	10
6	H	117/128 (91%)	98 (84%)	19 (16%)	2	12
7	I	113/116 (97%)	95 (84%)	18 (16%)	2	13
8	J	60/65 (92%)	44 (73%)	16 (27%)	0	3
9	K	99/102 (97%)	86 (87%)	13 (13%)	3	17
10	L	40/57 (70%)	31 (78%)	9 (22%)	1	5
All	All	3109/3657 (85%)	2557 (82%)	552 (18%)	1	10

5 of 552 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	215	MET

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Mol	Chain	Res	Type
5	F	155	LEU
4	E	212	ARG
8	J	14	VAL
1	A	1189	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	518	HIS
2	B	878	GLN
7	I	11	ASN
2	B	590	HIS
2	B	740	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	8/9 (88%)	4 (50%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	2	U
11	R	3	C
11	R	4	G
11	R	9	U

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	02I	T	20	12	15,24,25	3.45	6 (40%)	15,37,40	4.17	6 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	02I	T	20	12	-	0/0/28/29	0/3/4/4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	20	02I	O4'-C1'	-7.69	1.25	1.42
12	T	20	02I	O4'-C4'	-7.47	1.33	1.44
12	T	20	02I	C2-N3	4.10	1.38	1.32
12	T	20	02I	C4'-C5'	-4.08	1.45	1.52
12	T	20	02I	O3'-C3'	-3.75	1.35	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	20	02I	C5-C6-N6	11.29	137.50	120.31
12	T	20	02I	N6-C6-N1	-7.44	102.44	118.33
12	T	20	02I	N3-C2-N1	-6.33	120.08	128.67
12	T	20	02I	O4'-C1'-C2'	-4.47	97.89	106.24
12	T	20	02I	C2'-C1'-N9	-2.53	105.65	110.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	T	20	02I	5	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	1395/1733 (80%)	-0.25	13 (0%) 81 66	84, 144, 236, 306	0
2	B	1104/1224 (90%)	-0.30	7 (0%) 85 72	76, 131, 209, 281	0
3	C	266/318 (83%)	-0.41	0 100 100	89, 133, 192, 229	0
4	E	214/215 (99%)	-0.36	1 (0%) 87 75	99, 166, 231, 267	0
5	F	84/155 (54%)	-0.51	0 100 100	102, 142, 185, 209	0
6	H	133/146 (91%)	-0.23	2 (1%) 71 55	119, 168, 238, 262	0
7	I	119/122 (97%)	-0.41	0 100 100	96, 151, 190, 216	0
8	J	65/70 (92%)	-0.43	0 100 100	98, 128, 168, 192	0
9	K	114/120 (95%)	-0.51	0 100 100	94, 137, 177, 200	0
10	L	46/70 (65%)	-0.01	1 (2%) 62 46	119, 180, 250, 264	0
11	R	9/9 (100%)	-0.47	0 100 100	102, 124, 217, 261	0
12	T	10/29 (34%)	-0.23	0 100 100	108, 136, 243, 256	0
All	All	3559/4211 (84%)	-0.31	24 (0%) 84 70	76, 141, 224, 306	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	997	LEU	6.4
1	A	1108	ALA	4.1
1	A	1002	GLY	3.1
1	A	144	THR	3.0
2	B	335	GLY	2.9

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
12	02I	T	20	21/22	0.55	0.13	204,227,305,321	0

### 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
13	ZN	A	1801	1/1	0.89	0.07	244,244,244,244	0
13	ZN	J	101	1/1	0.98	0.04	124,124,124,124	0
13	ZN	B	1301	1/1	0.99	0.03	202,202,202,202	0
13	ZN	I	201	1/1	0.99	0.03	161,161,161,161	0
13	ZN	A	1802	1/1	0.99	0.02	170,170,170,170	0
13	ZN	L	101	1/1	0.99	0.03	175,175,175,175	0
13	ZN	C	401	1/1	1.00	0.02	135,135,135,135	0
13	ZN	I	202	1/1	1.00	0.02	128,128,128,128	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.