



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 02:58 am BST

PDB ID : 3GTM  
Title : Co-complex of Backtracked RNA polymerase II with TFIIS  
Authors : Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.  
Deposited on : 2009-03-27  
Resolution : 3.80 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.

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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	:	2.11
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)	:	2.11

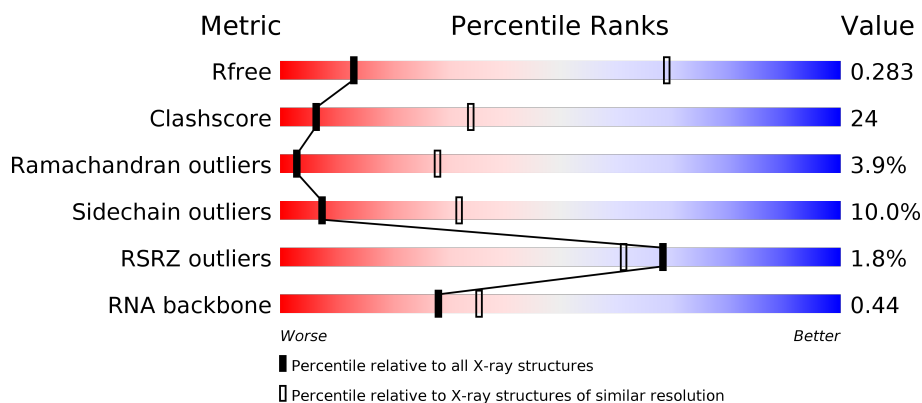
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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 on 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>44%</div> <div>32%</div> <div>6%</div> <div>18%</div> </div>
2	B	1224	<div> <div>46%</div> <div>37%</div> <div>6%</div> <div>10%</div> </div>
3	C	318	<div> <div>51%</div> <div>27%</div> <div>5%</div> <div>16%</div> </div>
4	E	215	<div> <div>63%</div> <div>32%</div> <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	S	173	
12	M	13	
13	N	28	
14	O	14	

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 30560 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	1426	Total	C	N	O	S	0	0	0
			11214	7069	1959	2124	62			

- 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
			8779	5560	1535	1630	54			

- 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
			364	224	72	64	4			

- Molecule 11 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	S	163	Total	C	N	O	S	0	0	0
			1086	655	206	222	3			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	137	MET	-	initiating methionine	UNP P07273
S	138	ARG	-	expression tag	UNP P07273
S	139	GLY	-	expression tag	UNP P07273
S	140	SER	-	expression tag	UNP P07273
S	141	HIS	-	expression tag	UNP P07273
S	142	HIS	-	expression tag	UNP P07273
S	143	HIS	-	expression tag	UNP P07273
S	144	HIS	-	expression tag	UNP P07273
S	291	HIS	GLU	engineered mutation	UNP P07273
S	305	ARG	-	expression tag	UNP P07273
S	306	TRP	-	expression tag	UNP P07273

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Chain	Residue	Modelled	Actual	Comment	Reference
S	307	LYS	-	expression tag	UNP P07273
S	308	PHE	-	expression tag	UNP P07273
S	309	SER	-	expression tag	UNP P07273

- Molecule 12 is a RNA chain called RNA (5'-R(\*AP\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*GP\*AP\*UP\*GP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	12	Total	C	N	O	P	0	0	0
			241	107	47	76	11			

- Molecule 13 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	28	Total	C	N	O	P	0	0	0
			566	271	104	164	27			

- Molecule 14 is a DNA chain called DNA (5'-D(\*CP\*TP\*GP\*CP\*TP\*TP\*AP\*TP\*CP\*GP\*GP\*TP\*AP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	O	14	Total	C	N	O	P	0	0	0
			284	137	49	85	13			

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	J	1	Total	Zn	0	0
			1	1		
16	B	1	Total	Zn	0	0
			1	1		
16	I	2	Total	Zn	0	0
			2	2		
16	C	1	Total	Zn	0	0
			1	1		

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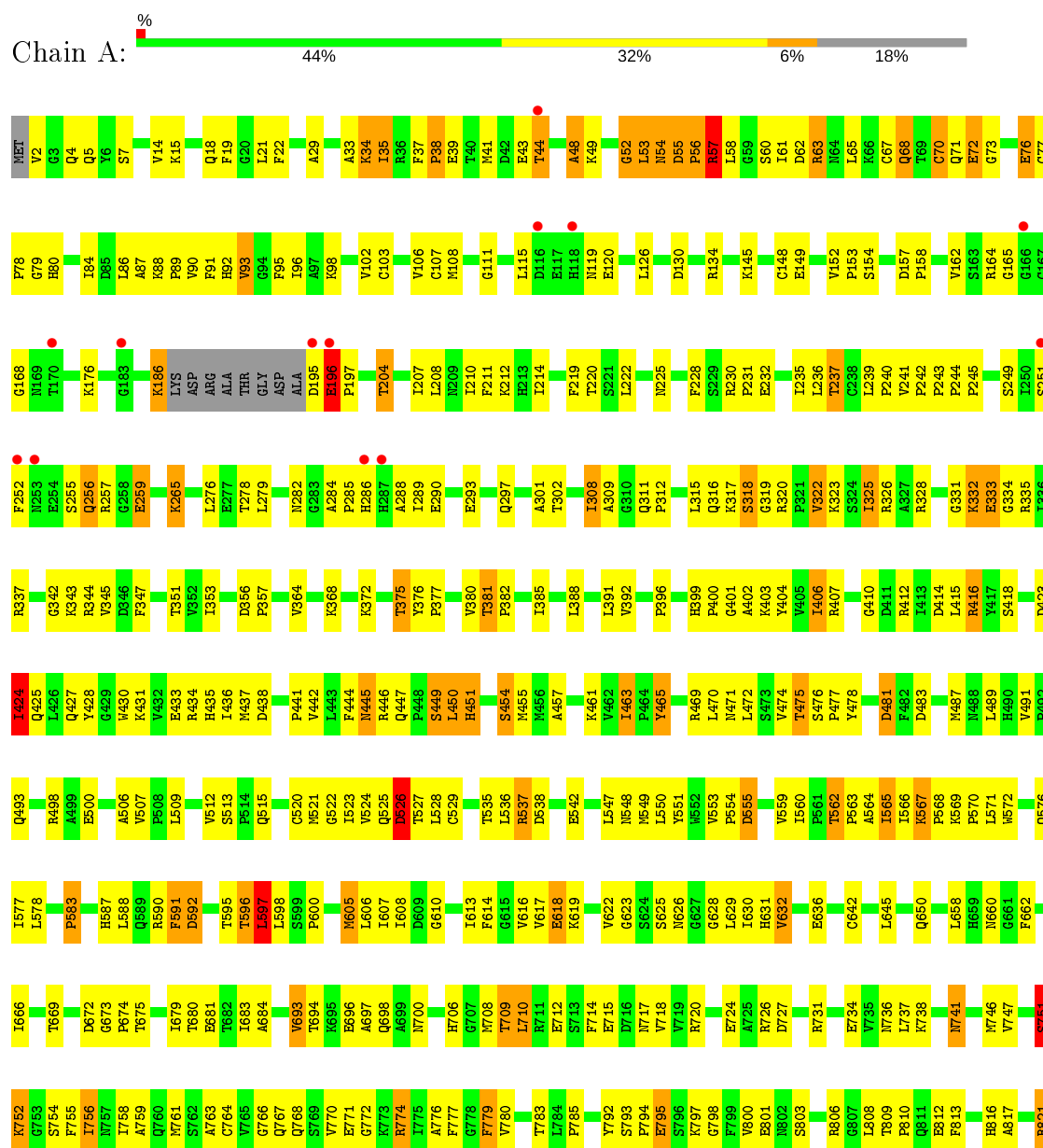
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	2	Total 2	Zn 2	0	0
16	L	1	Total 1	Zn 1	0	0
16	S	1	Total 1	Zn 1	0	0

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

These plots are drawn for all protein, RNA and DNA 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



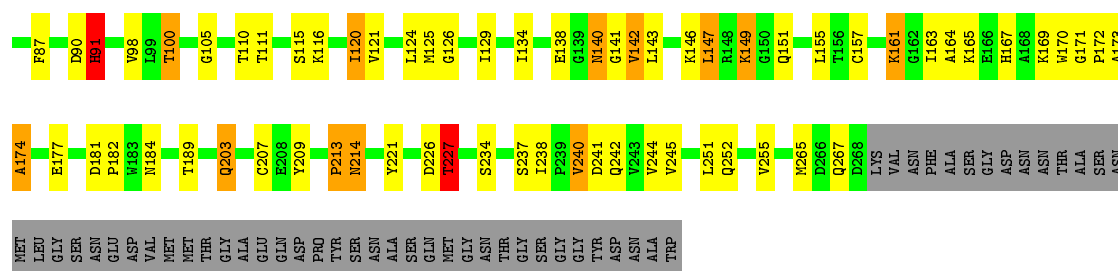




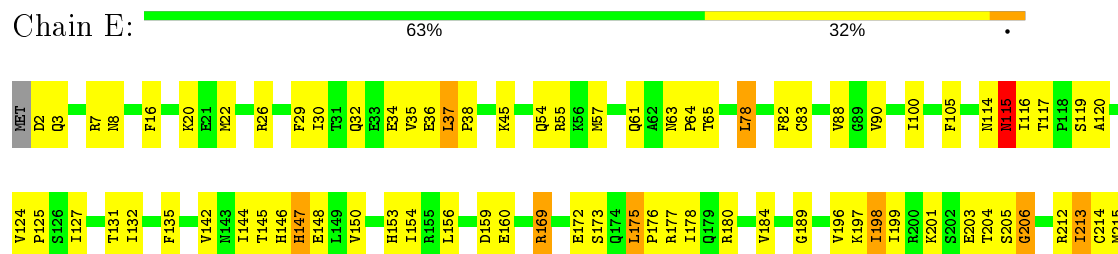
Response	Percentage
Yes	46%
No	37%
Don't know	6%
No answer	10%



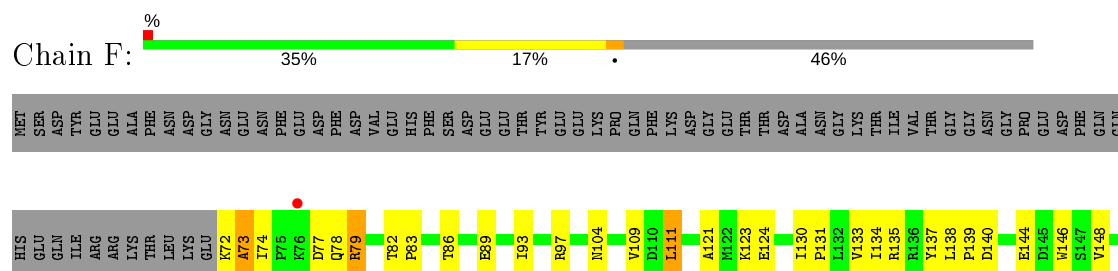




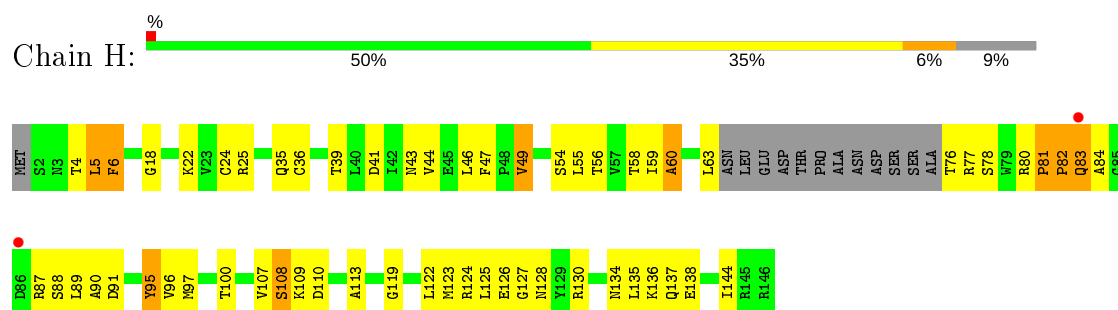
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



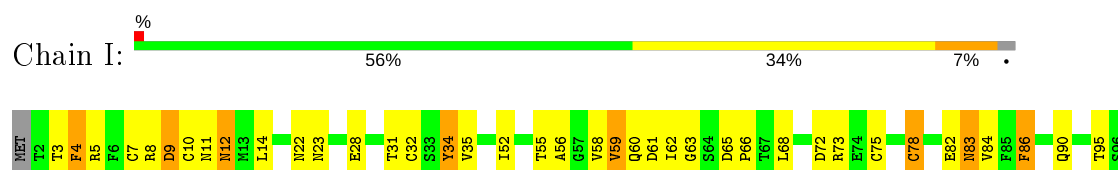
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



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



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

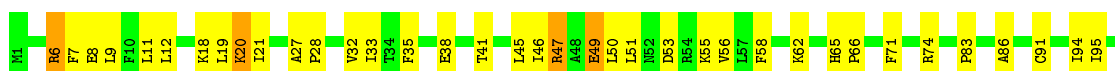




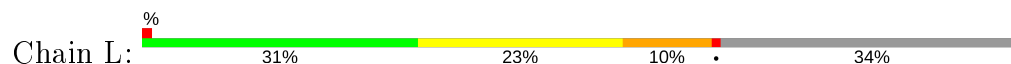
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



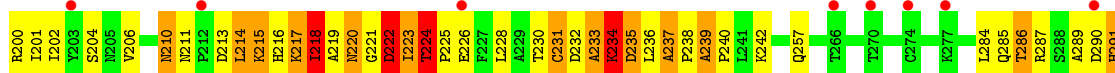
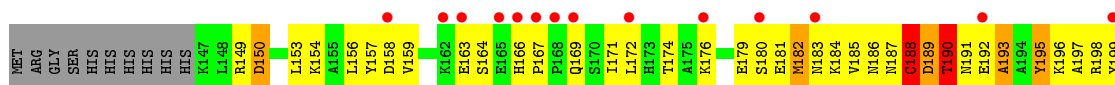
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



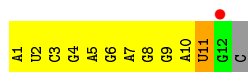
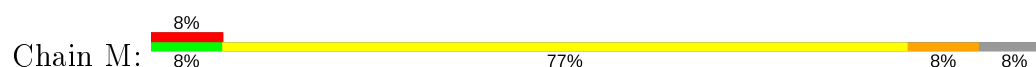
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



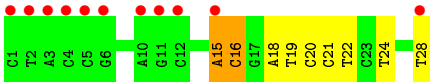
- Molecule 11: Transcription elongation factor S-II



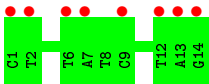
- Molecule 12: RNA (5'-R(\*AP\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*GP\*AP\*UP\*GP\*C)-3')



- Molecule 13: DNA (28-MER)



● Molecule 14: DNA (5'-D(\*CP\*TP\*GP\*CP\*TP\*TP\*AP\*TP\*CP\*GP\*GP\*TP\*AP\*G)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.33Å 218.53Å 193.91Å 90.00° 100.32° 90.00°	Depositor
Resolution (Å)	40.00 – 3.80 39.89 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.80) 94.6 (39.89-3.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 3.76Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.234 , 0.289 0.228 , 0.283	Depositor DCC
$R_{free}$ test set	3320 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.7	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 58.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	30560	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.24	0/11417	0.52	12/15442 (0.1%)
2	B	0.27	0/8949	0.54	10/12066 (0.1%)
3	C	0.25	0/2133	0.49	0/2891
4	E	0.22	0/1788	0.45	1/2406 (0.0%)
5	F	0.24	0/691	0.47	0/933
6	H	0.31	1/1086 (0.1%)	0.54	2/1470 (0.1%)
7	I	0.24	0/989	0.48	0/1331
8	J	0.25	0/541	0.48	0/727
9	K	0.23	0/937	0.42	0/1265
10	L	0.24	0/366	0.65	2/485 (0.4%)
11	S	0.30	0/1100	0.64	1/1466 (0.1%)
12	M	0.42	0/270	0.89	0/421
13	N	0.51	0/634	1.18	5/975 (0.5%)
14	O	0.50	0/317	1.11	0/488
All	All	0.27	1/31218 (0.0%)	0.56	33/42366 (0.1%)

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
11	S	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	127	GLY	N-CA	5.03	1.53	1.46

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	597	LEU	N-CA-CB	-10.25	89.89	110.40
1	A	1189	SER	N-CA-CB	-9.86	95.72	110.50
1	A	596	THR	N-CA-C	-8.47	88.14	111.00
1	A	751	SER	CB-CA-C	-8.05	94.80	110.10
1	A	1188	GLN	N-CA-C	-7.44	90.90	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	S	214	LEU	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	11214	0	11286	566	0
2	B	8779	0	8806	502	0
3	C	2095	0	2051	78	0
4	E	1752	0	1776	59	0
5	F	679	0	701	22	0
6	H	1068	0	1040	63	0
7	I	971	0	927	44	0
8	J	532	0	543	34	0
9	K	919	0	929	32	0
10	L	364	0	387	20	0
11	S	1086	0	947	153	0
12	M	241	0	120	15	0
13	N	566	0	316	9	0
14	O	284	0	161	0	0
15	A	1	0	0	0	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
16	S	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	30560	0	29990	1450	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 24.

The worst 5 of 1450 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)
2:B:507:LYS:C	2:B:508:LEU:HD23	1.55	1.26
1:A:49:LYS:HD2	1:A:55:ASP:CG	1.63	1.18
11:S:183:ASN:HA	11:S:186:ASN:ND2	1.58	1.17
1:A:829:VAL:HG13	2:B:508:LEU:HD12	1.23	1.16
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.22	1.13

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	1418/1733 (82%)	1160 (82%)	210 (15%)	48 (3%)	3	31
2	B	1084/1224 (89%)	882 (81%)	167 (15%)	35 (3%)	4	32
3	C	264/318 (83%)	213 (81%)	37 (14%)	14 (5%)	2	23
4	E	212/215 (99%)	187 (88%)	20 (9%)	5 (2%)	6	37
5	F	82/155 (53%)	70 (85%)	11 (13%)	1 (1%)	13	50
6	H	129/146 (88%)	103 (80%)	17 (13%)	9 (7%)	1	17
7	I	117/122 (96%)	91 (78%)	24 (20%)	2 (2%)	9	43
8	J	63/70 (90%)	50 (79%)	9 (14%)	4 (6%)	1	20
9	K	112/120 (93%)	102 (91%)	9 (8%)	1 (1%)	17	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	L	44/70 (63%)	28 (64%)	11 (25%)	5 (11%)	0	7
11	S	161/173 (93%)	107 (66%)	35 (22%)	19 (12%)	0	6
All	All	3686/4346 (85%)	2993 (81%)	550 (15%)	143 (4%)	3	28

5 of 143 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	55	ASP
1	A	57	ARG
1	A	567	LYS
1	A	709	THR

### 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	1246/1520 (82%)	1123 (90%)	123 (10%)	8	32
2	B	959/1061 (90%)	860 (90%)	99 (10%)	7	31
3	C	234/274 (85%)	213 (91%)	21 (9%)	9	37
4	E	196/197 (100%)	179 (91%)	17 (9%)	10	38
5	F	74/137 (54%)	69 (93%)	5 (7%)	16	47
6	H	117/128 (91%)	109 (93%)	8 (7%)	16	47
7	I	113/116 (97%)	95 (84%)	18 (16%)	2	16
8	J	60/65 (92%)	54 (90%)	6 (10%)	7	32
9	K	99/102 (97%)	93 (94%)	6 (6%)	18	50
10	L	40/57 (70%)	33 (82%)	7 (18%)	2	13
11	S	96/151 (64%)	81 (84%)	15 (16%)	2	17
All	All	3234/3808 (85%)	2909 (90%)	325 (10%)	7	32

5 of 325 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	474	SER
2	B	766	ARG
9	K	47	ARG
2	B	492	LEU
2	B	570	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	236	HIS
2	B	587	HIS
9	K	65	HIS
2	B	357	GLN
2	B	516	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	M	10/13 (76%)	2 (20%)	1 (10%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	M	10	A
12	M	11	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	M	11	U

## 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	1426/1733 (82%)	-0.39	15 (1%) 80 74	26, 75, 156, 230	0
2	B	1104/1224 (90%)	-0.47	6 (0%) 91 87	24, 63, 135, 230	0
3	C	266/318 (83%)	-0.53	0 100 100	30, 61, 101, 141	0
4	E	214/215 (99%)	-0.29	0 100 100	45, 111, 169, 197	0
5	F	84/155 (54%)	-0.26	1 (1%) 79 72	46, 80, 123, 140	0
6	H	133/146 (91%)	-0.27	2 (1%) 73 66	52, 97, 163, 186	0
7	I	119/122 (97%)	-0.21	1 (0%) 86 81	36, 86, 147, 190	0
8	J	65/70 (92%)	-0.54	0 100 100	33, 53, 92, 105	0
9	K	114/120 (95%)	-0.45	0 100 100	38, 69, 104, 150	0
10	L	46/70 (65%)	-0.08	1 (2%) 62 54	34, 99, 161, 185	0
11	S	163/173 (94%)	0.60	22 (13%) 3 3	109, 159, 211, 255	0
12	M	12/13 (92%)	0.19	1 (8%) 11 9	65, 90, 194, 223	0
13	N	28/28 (100%)	1.27	11 (39%) 0 0	66, 232, 305, 320	0
14	O	14/14 (100%)	2.64	8 (57%) 0 0	260, 286, 320, 326	0
All	All	3788/4401 (86%)	-0.34	68 (1%) 68 61	24, 74, 165, 326	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	O	1	DC	5.7
14	O	14	DG	5.4
11	S	176	LYS	5.1
13	N	5	DC	5.0
1	A	253	ASN	4.9

## 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 carbohydrates 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( $\text{\AA}^2$ )	Q<0.9
16	ZN	S	310	1/1	0.83	0.29	228,228,228,228	0
16	ZN	A	1735	1/1	0.96	0.06	128,128,128,128	0
15	MG	A	1734	1/1	0.96	0.15	48,48,48,48	0
16	ZN	L	105	1/1	0.97	0.10	124,124,124,124	0
16	ZN	I	203	1/1	0.98	0.07	73,73,73,73	0
16	ZN	A	1736	1/1	0.98	0.09	73,73,73,73	0
16	ZN	C	319	1/1	0.98	0.08	58,58,58,58	0
16	ZN	J	101	1/1	0.99	0.11	35,35,35,35	0
16	ZN	B	1307	1/1	0.99	0.06	82,82,82,82	0
16	ZN	I	204	1/1	1.00	0.07	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.