



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 03:00 am BST

PDB ID : 3GTL  
Title : Backtracked RNA polymerase II complex with 13mer with G<>U mismatch  
Authors : Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.  
Deposited on : 2009-03-27  
Resolution : 3.38 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

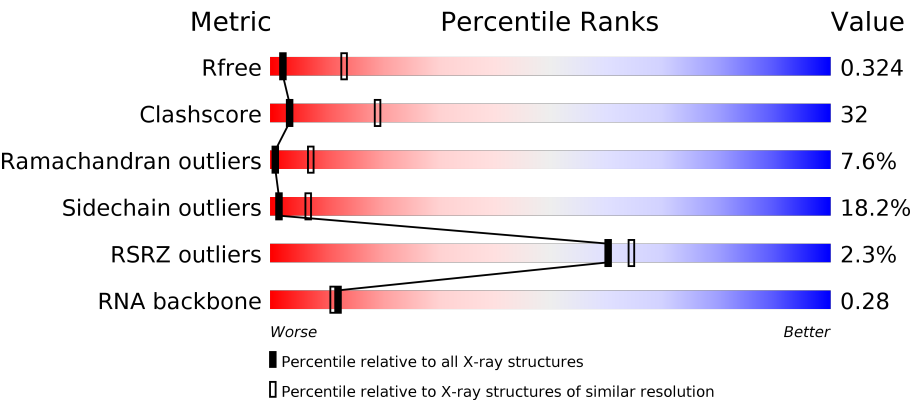
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.38 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>	130704	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)
RNA backbone	3102	1001 (3.80-2.96)

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>2%</div><div><div></div><div>36%</div><div>33%</div><div>10%</div><div>20%</div></div></div>
2	B	1224	<div><div>2%</div><div><div></div><div>38%</div><div>40%</div><div>12%</div><div>10%</div></div></div>
3	C	318	<div><div></div><div><div></div><div>32%</div><div>39%</div><div>12%</div><div>16%</div></div></div>
4	E	215	<div><div>3%</div><div><div></div><div>61%</div><div>33%</div><div>5%</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	13	
12	T	28	
13	N	14	

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 29256 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	1106	Total	C	N	O	S	0	0	0
			8792	5568	1538	1631	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 (5'-R(\*AP\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*GP\*AP\*UP\*UP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	12	Total	C	N	O	P	0	0	0
			257	116	49	81	11			

- Molecule 12 is a DNA chain called DNA (28-MER).

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

- Molecule 13 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
13	N	14	Total	C	N	O	P	0	0	0
			284	137	49	85	13			

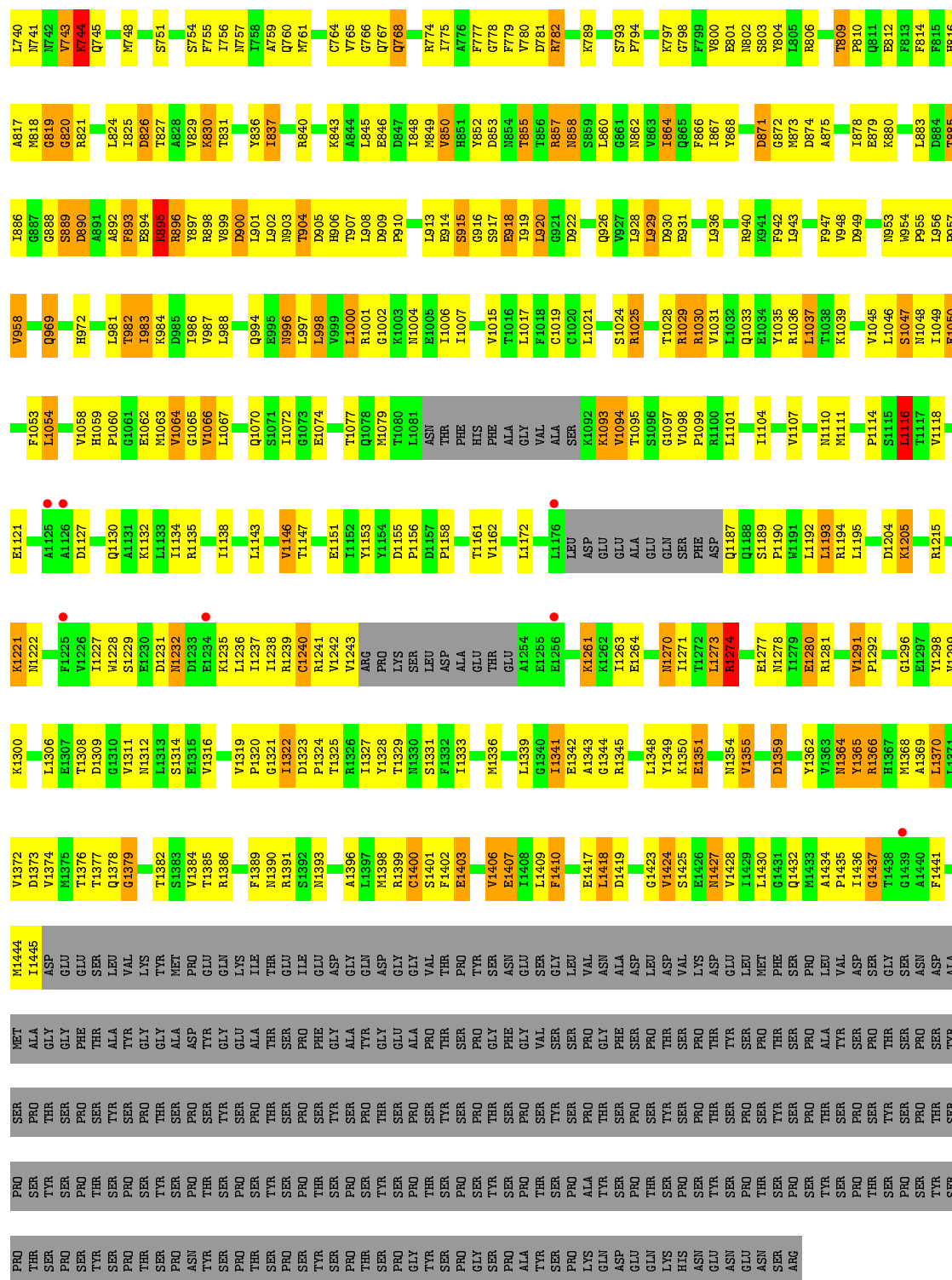
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	J	1	Total	Zn	0	0
			1	1		
14	B	1	Total	Zn	0	0
			1	1		
14	I	2	Total	Zn	0	0
			2	2		
14	C	1	Total	Zn	0	0
			1	1		
14	A	2	Total	Zn	0	0
			2	2		
14	L	1	Total	Zn	0	0
			1	1		

- 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		





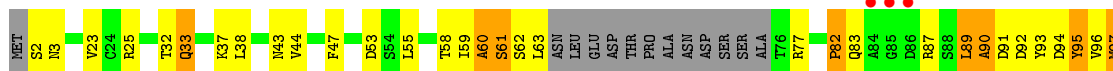




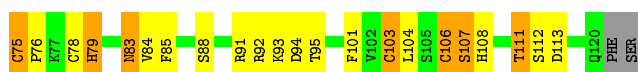




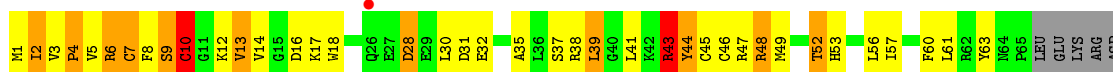
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



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



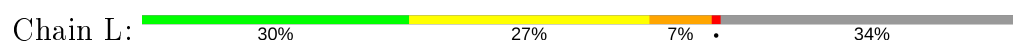
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



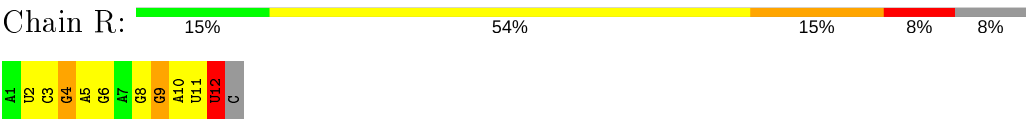
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



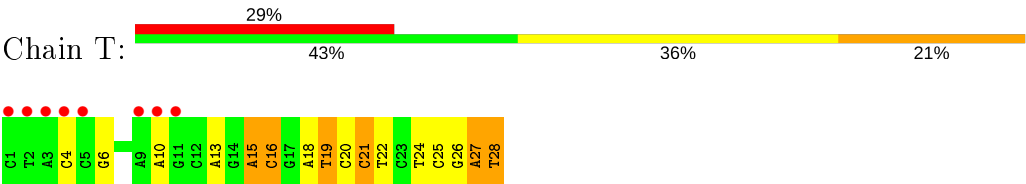
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



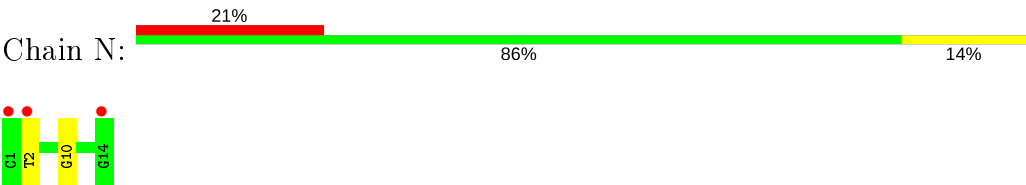
- Molecule 11: RNA (5'-R(\*AP\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*GP\*AP\*UP\*UP\*C)-3')



• Molecule 12: DNA (28-MER)



• Molecule 13: 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, $\alpha$ , $\beta$ , $\gamma$	170.53Å 222.28Å 194.81Å 90.00° 102.19° 90.00°	Depositor
Resolution (Å)	50.00 – 3.38 41.75 – 3.38	Depositor EDS
% Data completeness (in resolution range)	91.1 (50.00-3.38) 91.1 (41.75-3.38)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.270 , 0.322 0.277 , 0.324	Depositor DCC
$R_{free}$ test set	4515 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.7	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 80.4	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	0.89	EDS
Total number of atoms	29256	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: 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	0.57	1/11163 (0.0%)	0.74	5/15091 (0.0%)
2	B	0.62	0/8963	0.79	4/12086 (0.0%)
3	C	0.65	0/2133	0.80	0/2891
4	E	0.46	0/1788	0.60	0/2406
5	F	0.47	0/691	0.71	0/933
6	H	0.45	0/1086	0.71	0/1470
7	I	0.48	0/989	0.66	0/1331
8	J	0.81	1/541 (0.2%)	0.96	1/727 (0.1%)
9	K	0.61	0/937	0.76	1/1265 (0.1%)
10	L	0.59	0/365	0.86	0/485
11	R	1.06	1/288 (0.3%)	1.71	4/448 (0.9%)
12	T	0.91	1/634 (0.2%)	1.69	17/975 (1.7%)
13	N	0.82	0/317	1.43	1/488 (0.2%)
All	All	0.60	4/29895 (0.0%)	0.82	33/40596 (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
8	J	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	R	12	U	C1'-N1	5.54	1.57	1.48
12	T	21	DC	C3'-O3'	-5.29	1.37	1.44
8	J	9	SER	N-CA	5.02	1.56	1.46
1	A	360	GLU	CG-CD	5.01	1.59	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	27	DA	O4'-C4'-C3'	-12.07	98.75	106.00
12	T	16	DC	O4'-C4'-C3'	-9.86	100.08	106.00
2	B	535	LEU	CA-CB-CG	8.83	135.62	115.30
12	T	28	DT	O4'-C1'-N1	7.64	113.34	108.00
2	B	983	ARG	NE-CZ-NH1	7.48	124.04	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	J	4	PRO	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	11071	767	0
2	B	8792	0	8823	775	0
3	C	2095	0	2051	157	0
4	E	1752	0	1776	52	0
5	F	679	0	701	40	0
6	H	1068	0	1040	59	0
7	I	971	0	930	45	0
8	J	532	0	543	71	0
9	K	919	0	929	65	0
10	L	363	0	387	18	0
11	R	257	0	131	15	0
12	T	566	0	316	18	0
13	N	284	0	161	1	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	29256	0	28859	1868	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 32.

The worst 5 of 1868 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:636:PRO:CB	2:B:637:LEU:HA	1.49	1.35
2:B:848:ARG:HD2	8:J:7:CYS:O	1.32	1.26
2:B:827:ILE:HG23	2:B:1012:ILE:CD1	1.68	1.24
2:B:1002:THR:CG2	2:B:1006:ILE:HG12	1.66	1.24
1:A:482:PHE:CD1	2:B:836:GLU:HB3	1.73	1.23

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%)	1021 (74%)	249 (18%)	113 (8%)	1	6
2	B	1088/1224 (89%)	820 (75%)	186 (17%)	82 (8%)	1	7
3	C	264/318 (83%)	192 (73%)	48 (18%)	24 (9%)	1	5
4	E	212/215 (99%)	177 (84%)	28 (13%)	7 (3%)	4	24
5	F	82/155 (53%)	58 (71%)	20 (24%)	4 (5%)	2	15
6	H	129/146 (88%)	101 (78%)	19 (15%)	9 (7%)	1	8
7	I	117/122 (96%)	84 (72%)	22 (19%)	11 (9%)	0	4
8	J	63/70 (90%)	50 (79%)	10 (16%)	3 (5%)	2	16
9	K	112/120 (93%)	88 (79%)	18 (16%)	6 (5%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	L	44/70 (63%)	25 (57%)	12 (27%)	7 (16%)	0	1
All	All	3494/4173 (84%)	2616 (75%)	612 (18%)	266 (8%)	1	7

5 of 266 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	55	ASP
1	A	130	ASP
1	A	226	GLU
1	A	248	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	1218/1520 (80%)	984 (81%)	234 (19%)	1	5
2	B	960/1061 (90%)	779 (81%)	181 (19%)	1	6
3	C	234/274 (85%)	186 (80%)	48 (20%)	1	4
4	E	196/197 (100%)	176 (90%)	20 (10%)	7	28
5	F	74/137 (54%)	65 (88%)	9 (12%)	5	19
6	H	117/128 (91%)	103 (88%)	14 (12%)	5	20
7	I	113/116 (97%)	90 (80%)	23 (20%)	1	4
8	J	60/65 (92%)	47 (78%)	13 (22%)	1	3
9	K	99/102 (97%)	83 (84%)	16 (16%)	2	10
10	L	40/57 (70%)	31 (78%)	9 (22%)	1	3
All	All	3111/3657 (85%)	2544 (82%)	567 (18%)	1	7

5 of 567 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	217	ARG

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Mol	Chain	Res	Type
2	B	614	SER
7	I	83	ASN
2	B	253	THR
2	B	415	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	516	ASN
2	B	822	ASN
7	I	116	ASN
2	B	518	HIS
2	B	744	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	11/13 (84%)	3 (27%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	4	G
11	R	11	U
11	R	12	U

There are no RNA pucker outliers to report.

## 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 9 ligands modelled in this entry, 9 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%)	-0.04	31 (2%) 62 66	13, 87, 161, 194	0
2	B	1106/1224 (90%)	-0.01	24 (2%) 62 66	16, 81, 127, 148	0
3	C	266/318 (83%)	-0.28	1 (0%) 92 95	45, 75, 113, 128	0
4	E	214/215 (99%)	0.00	7 (3%) 46 50	72, 122, 161, 166	0
5	F	84/155 (54%)	-0.12	0 100 100	67, 91, 112, 121	0
6	H	133/146 (91%)	0.09	6 (4%) 33 37	97, 117, 137, 140	0
7	I	119/122 (97%)	-0.08	1 (0%) 86 89	79, 104, 123, 134	0
8	J	65/70 (92%)	-0.27	1 (1%) 73 77	24, 67, 95, 101	0
9	K	114/120 (95%)	-0.20	0 100 100	60, 82, 96, 97	0
10	L	46/70 (65%)	-0.03	0 100 100	86, 138, 153, 154	0
11	R	12/13 (92%)	-0.48	0 100 100	53, 77, 140, 150	0
12	T	28/28 (100%)	1.10	8 (28%) 0 0	52, 198, 323, 324	0
13	N	14/14 (100%)	1.14	3 (21%) 0 1	287, 311, 319, 321	0
All	All	3596/4228 (85%)	-0.04	82 (2%) 60 64	13, 86, 153, 324	0

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	GLU	8.8
13	N	1	DC	6.7
1	A	44	THR	5.5
1	A	1176	LEU	5.4
12	T	2	DT	5.3

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

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
14	ZN	A	1734	1/1	0.93	0.13	150,150,150,150	0
15	MG	A	1736	1/1	0.93	0.12	61,61,61,61	0
14	ZN	I	203	1/1	0.94	0.13	98,98,98,98	0
14	ZN	B	1307	1/1	0.96	0.03	112,112,112,112	0
14	ZN	A	1735	1/1	0.98	0.08	148,148,148,148	0
14	ZN	J	101	1/1	0.99	0.08	66,66,66,66	0
14	ZN	L	105	1/1	0.99	0.08	135,135,135,135	0
14	ZN	I	204	1/1	0.99	0.04	101,101,101,101	0
14	ZN	C	319	1/1	0.99	0.04	59,59,59,59	0

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

There are no such residues in this entry.