



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:26 AM GMT

PDB ID : 3I4M  
Title : 8-oxoguanine containing RNA polymerase II elongation complex D  
Authors : Damsma, G.E.; Cramer, P.  
Deposited on : 2009-07-02  
Resolution : 3.70 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

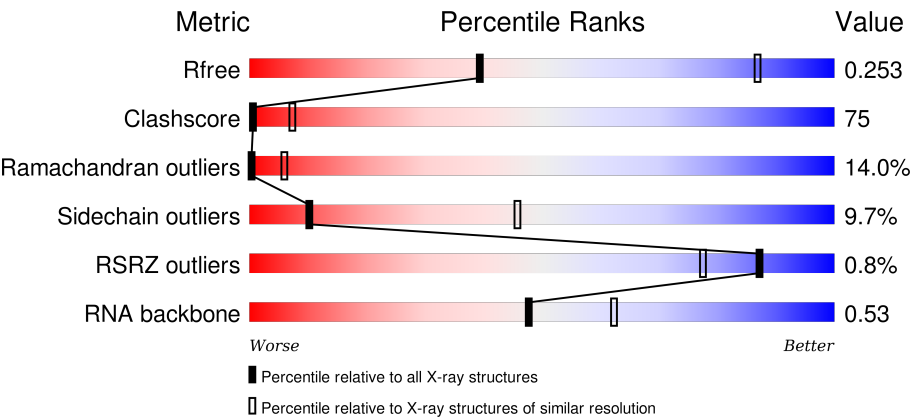
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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))
$R_{free}$	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)
RNA backbone	2183	1067 (4.60-2.80)

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. 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>16%</div><div>53%</div><div>13%</div><div>•</div><div>18%</div></div></div>
2	B	1224	<div><div>%</div><div><div>17%</div><div>58%</div><div>16%</div><div>•</div><div>8%</div></div></div>
3	C	324	<div><div></div><div><div>18%</div><div>50%</div><div>15%</div><div>•</div><div>17%</div></div></div>
4	D	221	<div><div>2%</div><div><div>19%</div><div>51%</div><div>13%</div><div>•</div><div>15%</div></div></div>

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	T	26	
14	N	12	
15	P	16	

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32355 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	1429	Total	C	N	O	S	0	0	0
			11240	7079	1966	2133	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1125	Total	C	N	O	S	0	0	0
			8942	5659	1571	1657	55			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	270	Total	C	N	O	S	0	0	0
			2125	1336	353	422	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	EXPRESSION TAG	UNP P16370
C	-4	HIS	-	EXPRESSION TAG	UNP P16370
C	-3	HIS	-	EXPRESSION TAG	UNP P16370
C	-2	HIS	-	EXPRESSION TAG	UNP P16370
C	-1	HIS	-	EXPRESSION TAG	UNP P16370
C	0	HIS	-	EXPRESSION TAG	UNP P16370

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	187	Total	C	N	O	S	0	0	0
			1504	930	269	301	4			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	88	Total	C	N	O	S	0	0	0
			712	455	120	134	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	137	Total	C	N	O	S	0	0	0
			1101	693	185	218	5			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	116	Total	C	N	O	S	0	0	0
			944	581	172	181	10			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	116	Total	C	N	O	S	0	0	0
			929	596	158	173	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	47	Total	C	N	O	S	0	0	0
			370	228	73	65	4			

- Molecule 13 is a DNA chain called DNA (5'-D(\*AP\*G\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*AP\*(8OG)P\*GP\*CP\*CP\*(BRU)P\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	T	21	Total	Br	C	N	O	P	0	0	0
			426	1	203	75	127	20			

- Molecule 14 is a DNA chain called DNA (5'-D(\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*GP\*AP\*GP\*CP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	11	Total	C	N	O	P	0	0	0
			224	108	42	64	10			

- Molecule 15 is a RNA chain called RNA (5'-R(\*UP\*GP\*CP\*AP\*UP\*C\*UP\*UP\*CP\*CP\*AP\*GP\*GP\*CP\*CP\*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	10	Total	C	N	O	P	0	0	0
			205	93	33	70	9			

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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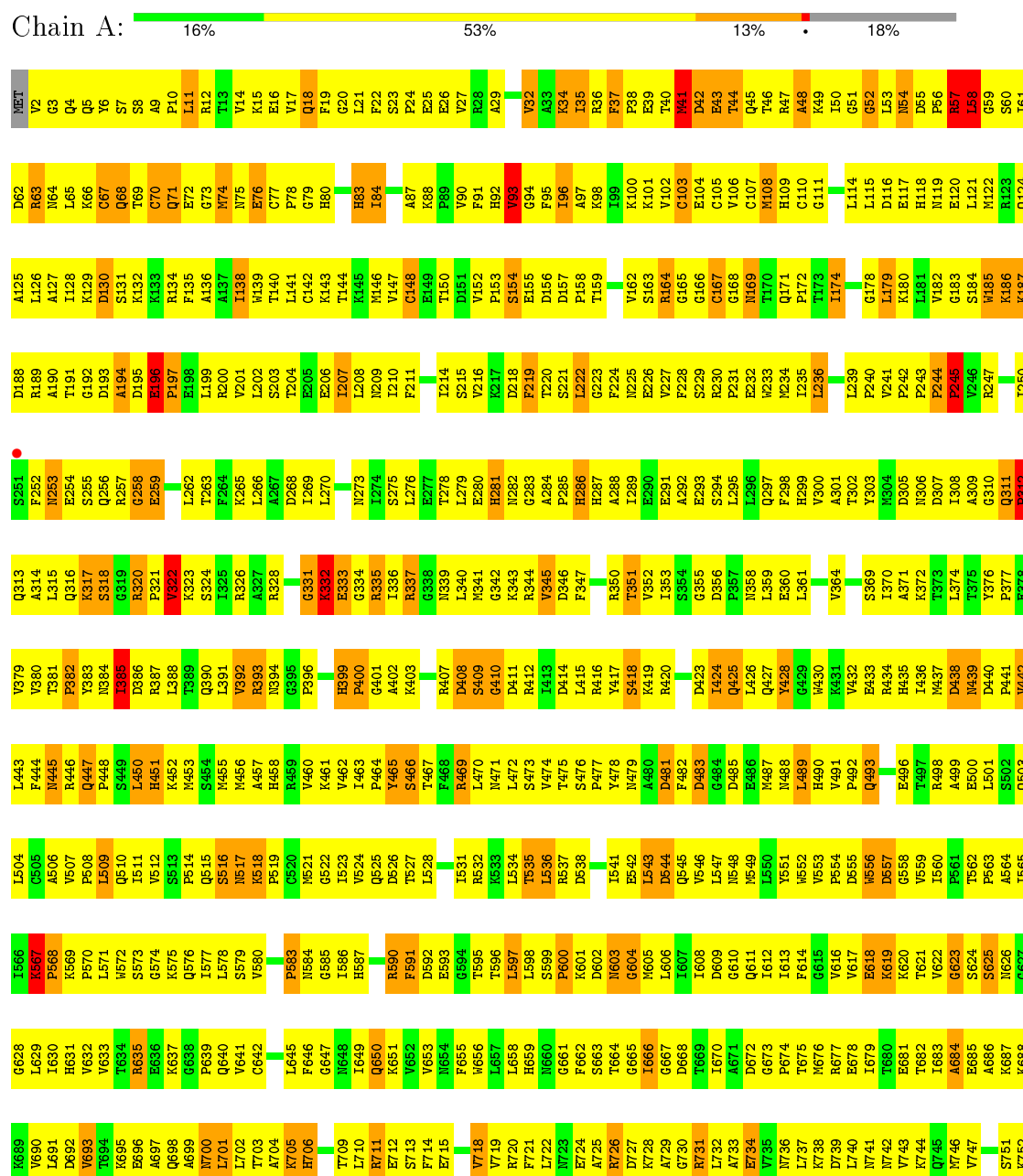
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	2	Total 2	Zn 2	0	0
17	L	1	Total 1	Zn 1	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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





[illegible]

- Molecule 2: DNA-directed RNA polymerase II subunit RPB2

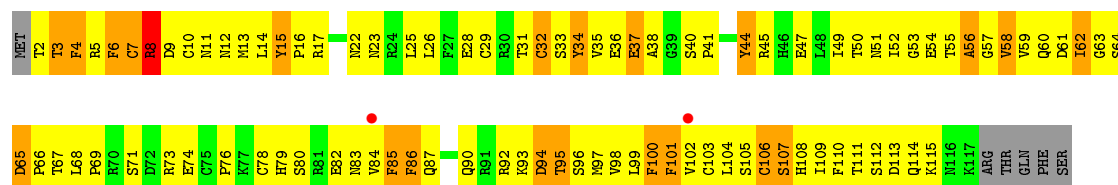
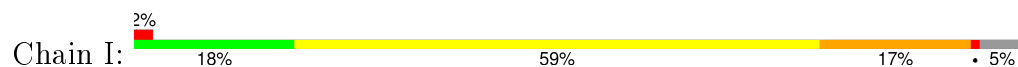




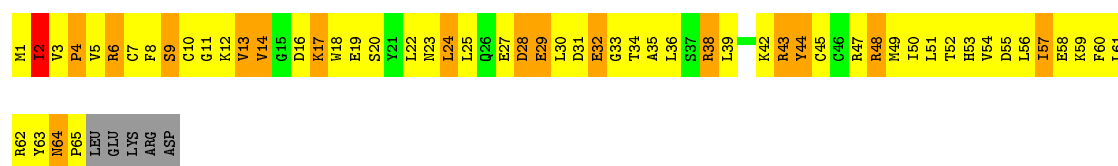
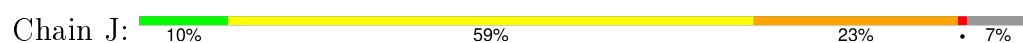
M64	M65	M66	ASP	THR	PRO	ALA	ASN	ASP	SER	PER	ALA	T76	R77	S78	T79	R80	P81	Q82	Q83	R84	G85	D86	S87	S88	L89	A90	D91	D92	Y93	Y94	Y95	P96	M97	Y98	G99	T100	A101	Y102	K103	F104	M105	E106	T107	S108	K109	D110	D111	L111	I112	A113	Y116	S117	F118	G119	G120	L121	L122	M123	P124		
M1	S2	N3	T4	L5	F6	D7	D8	I9	F10	I11	V12	S13	E14	V15	D16	P17	G18	R19	Y20		G24	R25	T26	E27	A28	A29	S30	T31	T32	Q33	D34	Q35	G36	K37	L38	T39	L40	D41	I42	M43	V44	E45	L46	F47	K48	P49	V49		Q52	D53	S54	L55	T56	Y57	T58	I59	A60	S61	S62	R63	P64



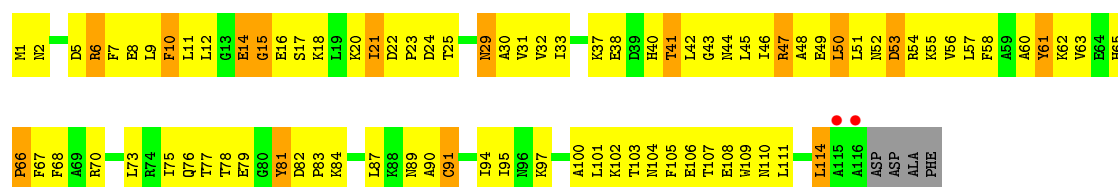
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



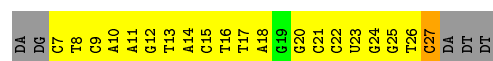
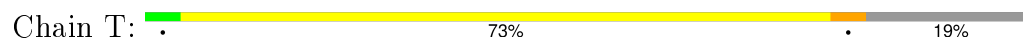
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



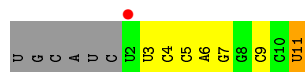
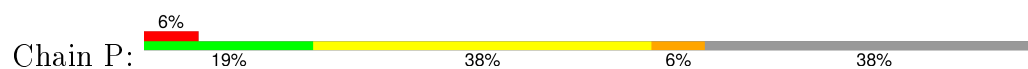
- Molecule 13: DNA (5'-D(\*AP\*G\*CP\*TP\*CP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*AP\*(8OG)P\*GP\*CP\*CP\*(BRU)P\*GP\*GP\*TP\*CP\*AP\*TP\*T)-3')



- Molecule 14: DNA (5'-D(\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*GP\*AP\*GP\*CP\*T)-3')



- Molecule 15: RNA (5'-R(\*UP\*GP\*CP\*AP\*UP\*C\*UP\*UP\*CP\*CP\*AP\*GP\*GP\*CP\*CP\*U)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	220.65Å 392.00Å 281.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.70 49.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-3.70) 100.0 (49.00-3.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 3.67Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.225 , 0.258 0.227 , 0.253	Depositor DCC
$R_{free}$ test set	2439 reflections (1.92%)	DCC
Wilson B-factor (Å <sup>2</sup> )	114.2	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 97.9	EDS
Estimated twinning fraction	0.029 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.034 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 129421 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	32355	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, 8OG, ZN, BRU

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	0.44	0/11441	0.74	3/15473 (0.0%)
2	B	0.41	0/9116	0.70	0/12291
3	C	0.42	0/2163	0.69	0/2930
4	D	0.38	0/1516	0.63	0/2031
5	E	0.39	0/1788	0.64	0/2406
6	F	0.52	0/724	0.82	0/977
7	G	0.44	0/1368	0.72	0/1844
8	H	0.37	0/1119	0.68	0/1514
9	I	0.38	0/962	0.66	0/1295
10	J	0.44	0/541	0.74	0/727
11	K	0.46	0/947	0.68	0/1279
12	L	0.39	0/372	0.68	0/495
13	T	0.56	1/426 (0.2%)	0.87	0/650
14	N	0.41	0/251	0.81	0/386
15	P	0.42	0/227	0.80	0/351
All	All	0.43	1/32961 (0.0%)	0.71	3/44649 (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	1
2	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	27	DC	C1'-N1	5.98	1.57	1.49



All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	567	LYS	C-N-CD	5.82	140.63	128.40
1	A	3	GLY	N-CA-C	-5.75	98.73	113.10
1	A	509	LEU	CA-CB-CG	-5.00	103.79	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1035	TYR	Sidechain
2	B	797	TYR	Sidechain

## 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	11240	0	11311	1819	0
2	B	8942	0	8986	1481	0
3	C	2125	0	2090	340	0
4	D	1504	0	1518	205	0
5	E	1752	0	1776	286	0
6	F	712	0	738	138	0
7	G	1340	0	1357	217	0
8	H	1101	0	1075	206	0
9	I	944	0	901	162	0
10	J	532	0	542	129	0
11	K	929	0	939	135	0
12	L	370	0	394	90	0
13	T	426	0	236	37	0
14	N	224	0	126	11	0
15	P	205	0	109	8	0
16	A	1	0	0	0	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	L	1	0	0	0	0
All	All	32355	0	32098	4821	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 75.

The worst 5 of 4821 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:69:LEU:HD13	2:B:429:PHE:CD1	1.39	1.55
2:B:69:LEU:HD13	2:B:429:PHE:CE1	1.66	1.30
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.24	1.17
2:B:806:THR:HG22	2:B:808:ALA:H	1.08	1.16
2:B:340:ALA:HB3	2:B:343:ILE:HG12	1.29	1.15

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	1421/1733 (82%)	909 (64%)	310 (22%)	202 (14%)	0	6
2	B	1111/1224 (91%)	694 (62%)	257 (23%)	160 (14%)	0	6
3	C	268/324 (83%)	164 (61%)	66 (25%)	38 (14%)	0	6
4	D	183/221 (83%)	108 (59%)	49 (27%)	26 (14%)	0	6
5	E	212/215 (99%)	134 (63%)	49 (23%)	29 (14%)	0	6
6	F	86/155 (56%)	60 (70%)	20 (23%)	6 (7%)	1	22
7	G	169/171 (99%)	127 (75%)	32 (19%)	10 (6%)	2	27
8	H	133/146 (91%)	72 (54%)	37 (28%)	24 (18%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	114/122 (93%)	73 (64%)	26 (23%)	15 (13%)	0	6
10	J	63/70 (90%)	34 (54%)	13 (21%)	16 (25%)	0	1
11	K	114/120 (95%)	79 (69%)	26 (23%)	9 (8%)	1	18
12	L	45/70 (64%)	19 (42%)	11 (24%)	15 (33%)	0	0
All	All	3919/4571 (86%)	2473 (63%)	896 (23%)	550 (14%)	0	6

5 of 550 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	41	MET
1	A	43	GLU
1	A	48	ALA
1	A	58	LEU

### 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	1249/1520 (82%)	1135 (91%)	114 (9%)	12	49
2	B	974/1061 (92%)	879 (90%)	95 (10%)	10	45
3	C	238/280 (85%)	215 (90%)	23 (10%)	10	46
4	D	167/200 (84%)	145 (87%)	22 (13%)	5	31
5	E	196/197 (100%)	179 (91%)	17 (9%)	13	51
6	F	78/137 (57%)	69 (88%)	9 (12%)	7	37
7	G	152/152 (100%)	138 (91%)	14 (9%)	11	49
8	H	121/128 (94%)	112 (93%)	9 (7%)	17	58
9	I	110/116 (95%)	98 (89%)	12 (11%)	8	40
10	J	60/65 (92%)	55 (92%)	5 (8%)	14	53
11	K	99/102 (97%)	87 (88%)	12 (12%)	6	34
12	L	41/57 (72%)	35 (85%)	6 (15%)	4	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3485/4015 (87%)	3147 (90%)	338 (10%)	10	46

5 of 338 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	591	ARG
2	B	1048	THR
9	I	94	ASP
2	B	615	MET
2	B	830	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	357	GLN
2	B	821	GLN
9	I	89	GLN
2	B	383	ASN
2	B	518	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/16 (56%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	11	U

There are no RNA pucker outliers to report.

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

2 non-standard protein/DNA/RNA residues are 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
13	8OG	T	19	13,15	16,25,26	1.31	2 (12%)	21,37,40	2.69	4 (19%)
13	BRU	T	23	13,15	13,21,22	4.58	4 (30%)	16,30,33	4.31	3 (18%)

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
13	8OG	T	19	13,15	-	0/3/21/22	0/3/3/3
13	BRU	T	23	13,15	-	0/3/21/22	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	23	BRU	BR-C5	-15.18	1.49	1.90
13	T	19	8OG	C8-N7	-2.70	1.31	1.34
13	T	23	BRU	C6-N1	2.18	1.38	1.35
13	T	23	BRU	C4-N3	2.41	1.37	1.33
13	T	19	8OG	C6-N1	3.57	1.39	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	19	8OG	C5-C6-N1	-8.75	111.62	123.59
13	T	23	BRU	C5-C4-N3	-8.30	115.14	124.00
13	T	23	BRU	O3'-C3'-C2'	-2.33	103.03	110.74
13	T	19	8OG	N3-C2-N1	-2.28	123.98	127.44
13	T	19	8OG	C2'-C1'-N9	3.43	119.27	115.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T	23	BRU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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 [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	1429/1733 (82%)	-0.29	1 (0%) 95 94	15, 73, 135, 195	0
2	B	1125/1224 (91%)	-0.12	15 (1%) 79 66	11, 88, 154, 194	0
3	C	270/324 (83%)	-0.27	1 (0%) 93 88	34, 73, 131, 174	0
4	D	187/221 (84%)	-0.12	4 (2%) 67 52	58, 98, 152, 197	0
5	E	214/215 (99%)	-0.24	2 (0%) 85 75	42, 112, 155, 161	0
6	F	88/155 (56%)	-0.44	0 100 100	24, 48, 91, 122	0
7	G	171/171 (100%)	-0.21	0 100 100	48, 74, 117, 128	0
8	H	137/146 (93%)	0.17	3 (2%) 65 50	91, 125, 152, 157	0
9	I	116/122 (95%)	-0.09	2 (1%) 73 58	65, 121, 152, 153	0
10	J	65/70 (92%)	-0.39	0 100 100	48, 67, 106, 121	0
11	K	116/120 (96%)	-0.29	2 (1%) 73 58	32, 79, 108, 160	0
12	L	47/70 (67%)	-0.03	1 (2%) 67 52	73, 124, 147, 159	0
13	T	19/26 (73%)	0.46	0 100 100	128, 194, 200, 200	0
14	N	11/12 (91%)	0.93	1 (9%) 11 7	186, 198, 200, 200	0
15	P	10/16 (62%)	0.33	1 (10%) 9 6	177, 193, 199, 200	0
All	All	4005/4625 (86%)	-0.20	33 (0%) 87 77	11, 83, 152, 200	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	471	LYS	6.2
2	B	883	LEU	3.7
2	B	722	ASP	3.4
11	K	116	ALA	3.2
2	B	504	ARG	3.2

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
13	8OG	T	19	23/24	0.89	0.17	-	131,141,154,155	0
13	BRU	T	23	20/21	0.68	0.27	-	153,162,167,170	0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
17	ZN	I	1121	1/1	0.99	0.12	-0.71	70,70,70,70	0
17	ZN	C	1269	1/1	1.00	0.12	-0.72	39,39,39,39	0
17	ZN	A	2457	1/1	1.00	0.14	-1.17	38,38,38,38	0
17	ZN	I	1122	1/1	0.91	0.04	-1.72	134,134,134,134	0
17	ZN	L	1071	1/1	0.97	0.06	-2.00	111,111,111,111	0
17	ZN	J	1066	1/1	0.99	0.23	-2.36	47,47,47,47	0
17	ZN	A	2456	1/1	0.96	0.07	-2.64	96,96,96,96	0
16	MG	A	2458	1/1	0.95	0.09	-3.37	69,69,69,69	0
17	ZN	B	2225	1/1	0.99	0.21	-	43,43,43,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.