wwPDB X-ray Structure Validation Summary Report (i)

Aug 30, 2023 – 02:24 AM EDT

PDB ID	:	3M3Y
Title	:	RNA polymerase II elongation complex C
Authors	:	Wang, D.; Zhu, G.; Huang, X.; Lippard, S.J.
Deposited on	:	2010-03-10
Resolution	:	3.18 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

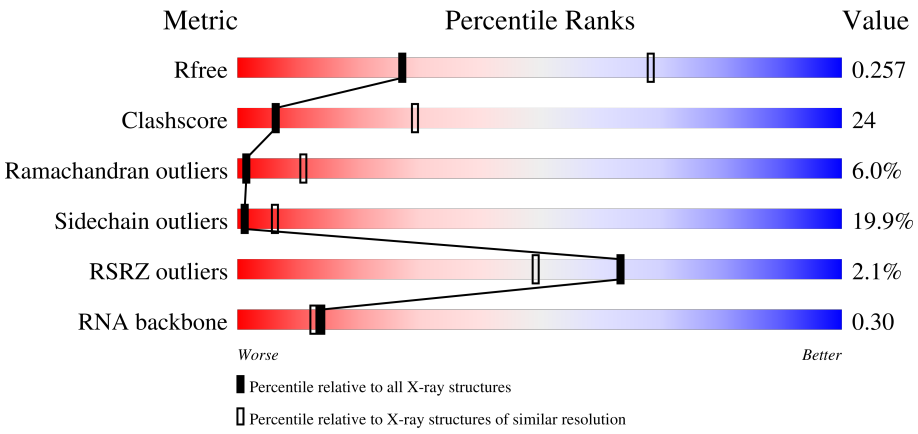
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.18 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)
RNA backbone	3102	1054 (3.50-2.86)

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 >=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 <=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	.% 41% 30% 9% • 20%
2	B	1224	2% 46% 33% 9% • 10%
3	C	318	40% 32% 12% 16%
4	E	215	2% 57% 34% 8%

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Mol	Chain	Length	Quality of chain
5	F	155	29% 20% 5% 46%
6	H	146	3% 45% 32% 13% 9%
7	I	122	56% 29% 13%
8	J	70	37% 37% 16% 7%
9	K	120	% 68% 25% 5%
10	L	70	7% 34% 19% 13% 34%
11	R	11	9% 27% 27% 45%
12	T	28	36% 18% 50% 32%
13	N	14	21% 100%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 29241 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
			Total	C	N	O	S			
1	A	1395	10969	6917	1923	2068	61	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1106	8792	5568	1538	1631	55	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 11 is a RNA chain called RNA (5'-R(*AP*UP*GP*GP*AP*GP*AP*GP*GP*AP *C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
11	R	11	240	108	50	72	10	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
12	T	28	550	265	92	166	27	0	0	0

- Molecule 13 is a DNA chain called DNA (5'-D(*GP*TP*GP*GP*TP*TP*AP*TP*GP*GP *GP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
13	N	14	293	140	55	85	13	0	0	0

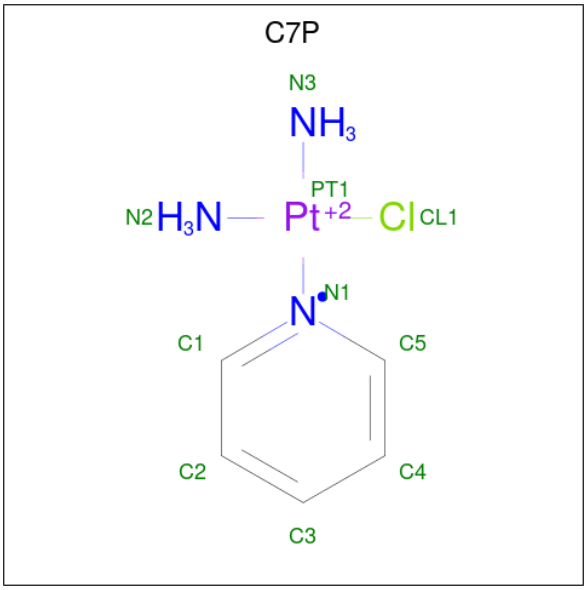
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

- Molecule 16 is cis-diammine(pyridine)chloroplatinum(II) (three-letter code: C7P) (formula: $C_5H_{11}ClN_3Pt$).



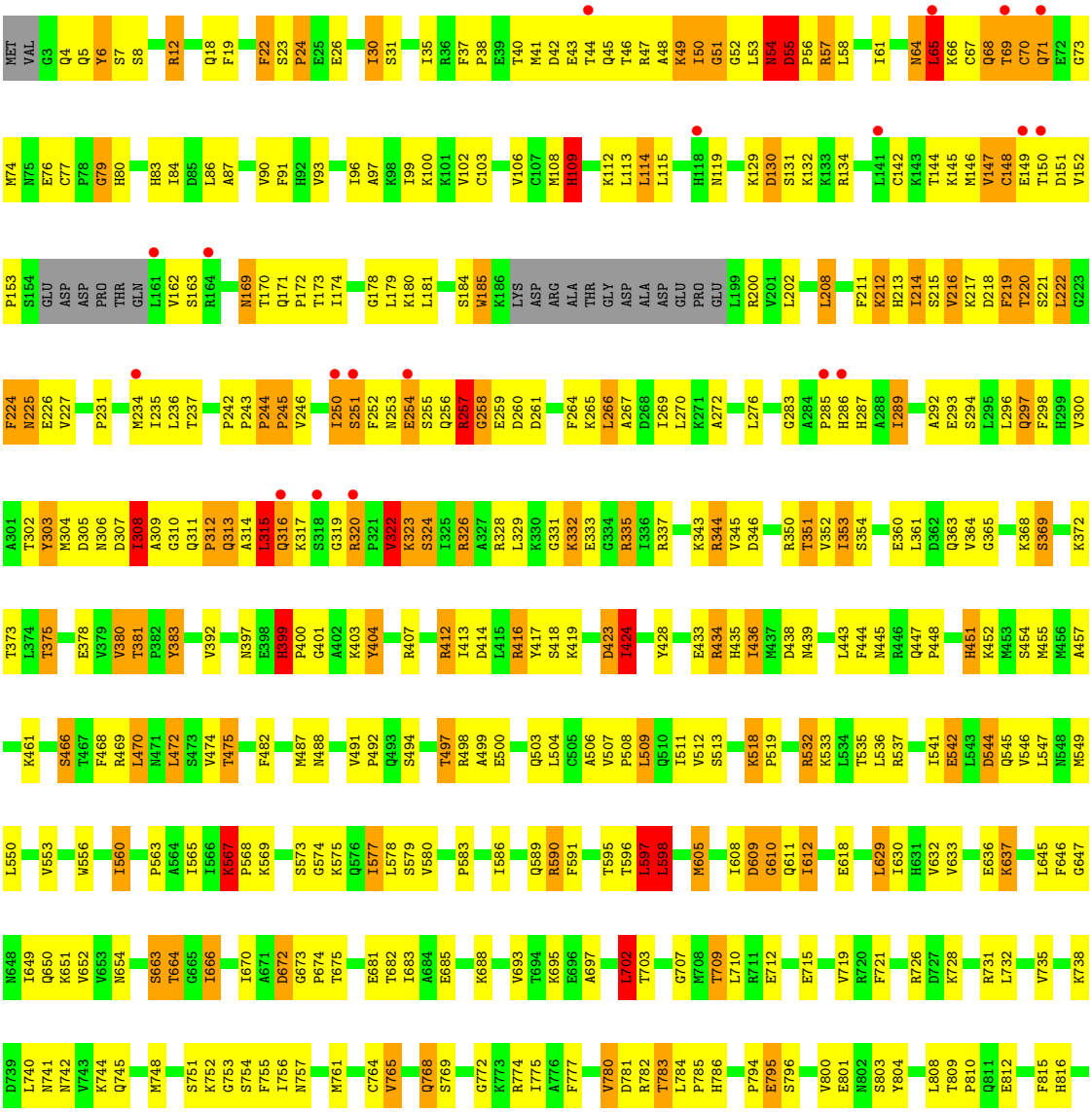
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	T	1	Total C N Pt 9 5 3 1	0	0

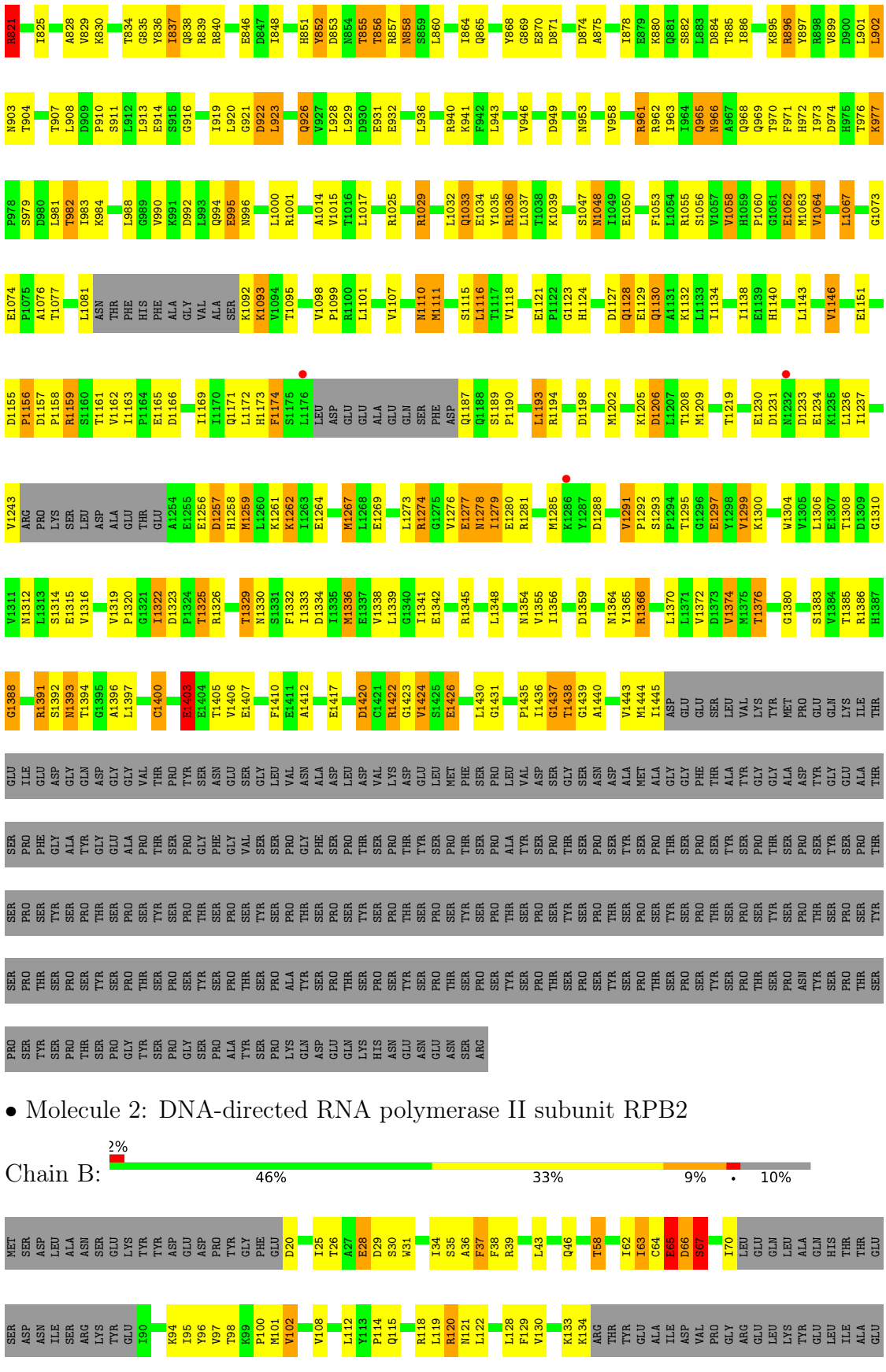
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

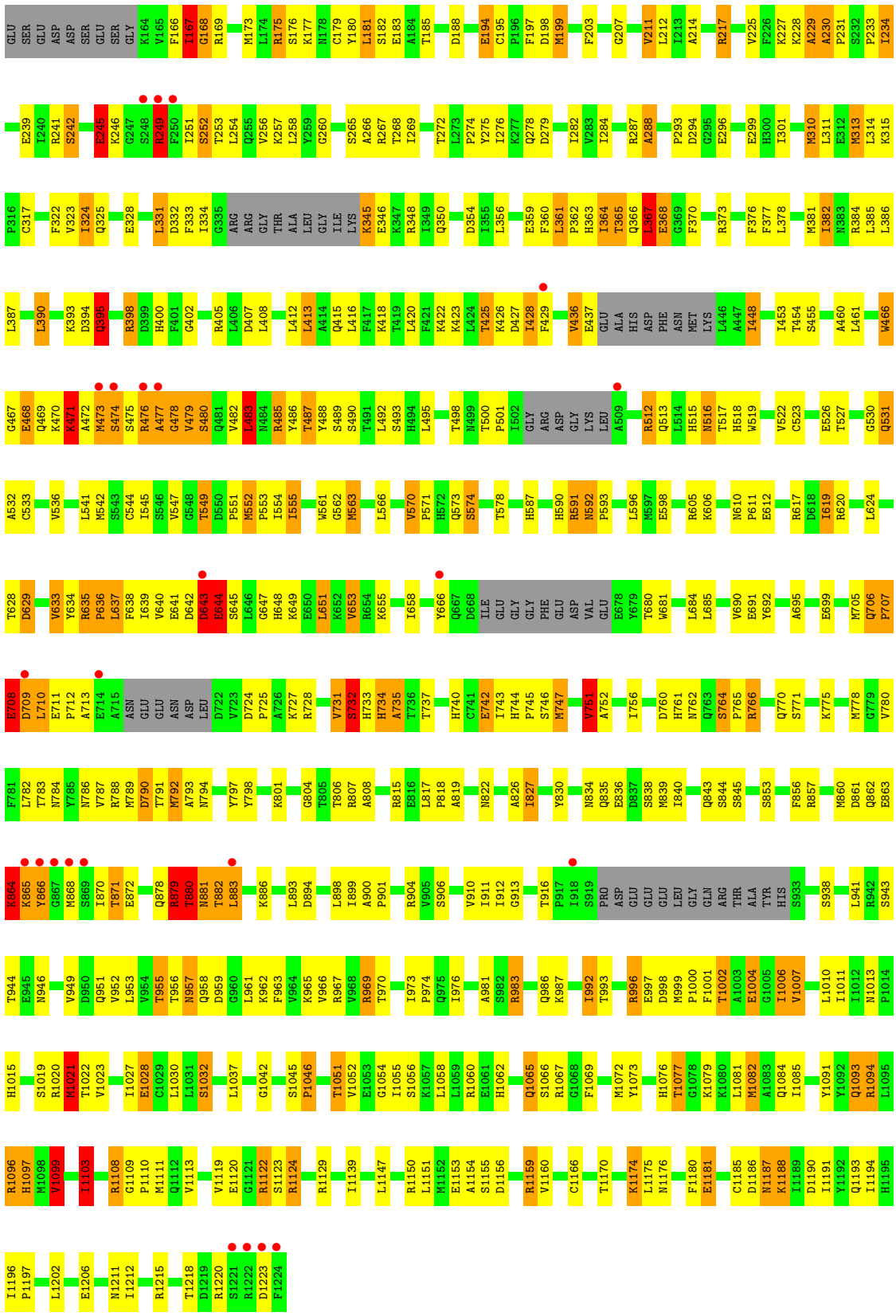
Chain A:





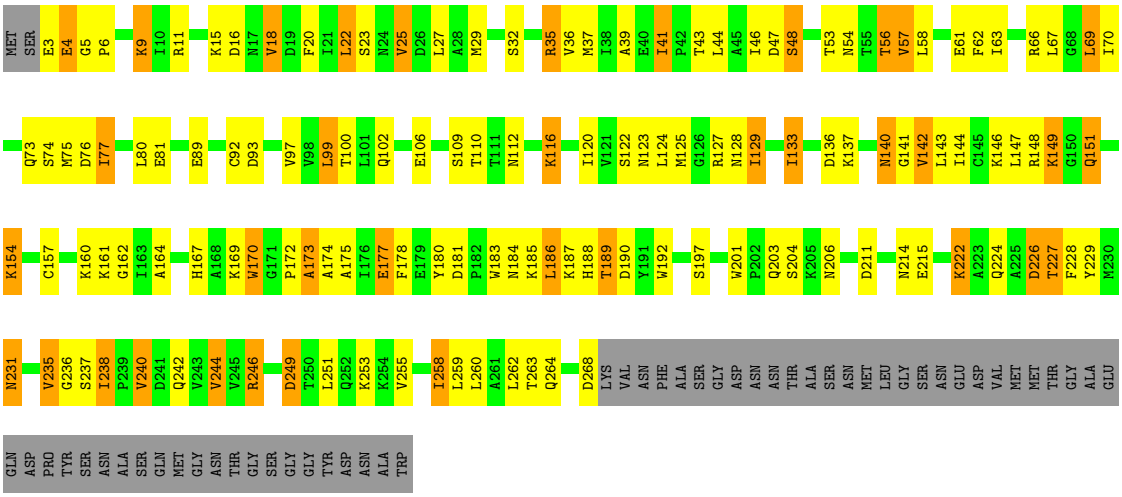
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:



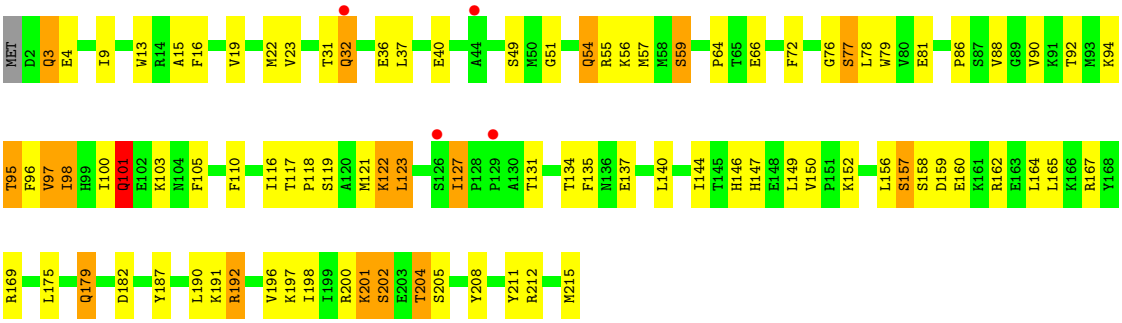
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 40% 32% 12% 16%



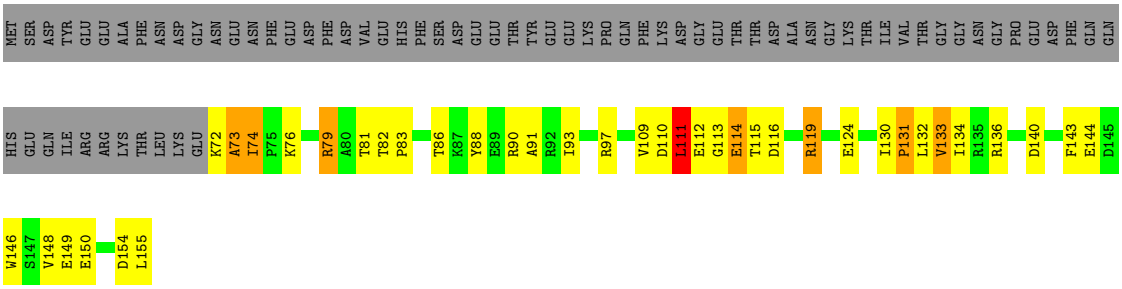
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 2% 57% 34% 8%



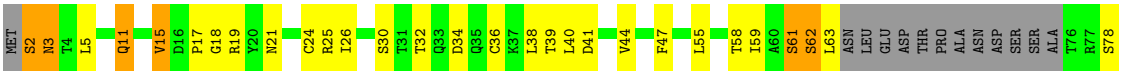
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

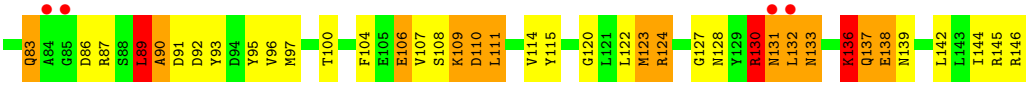
Chain F: 29% 20% 5% • 46%



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

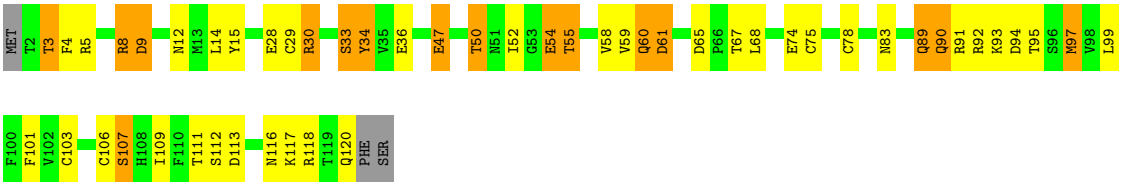
Chain H: 3% 45% 32% 13% • 9%





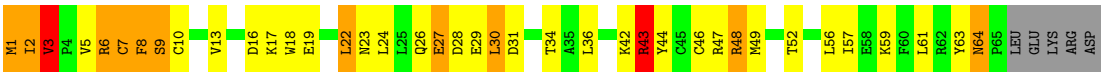
• Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I:



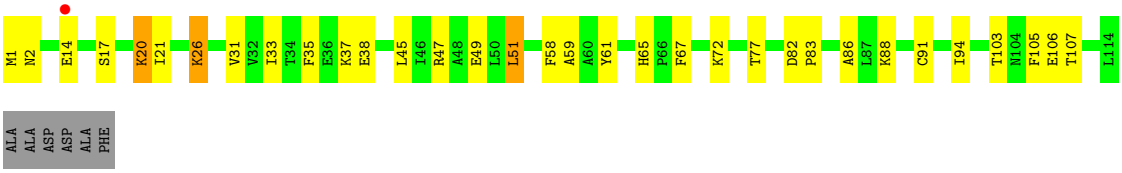
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



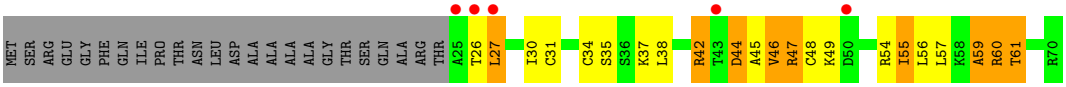
• Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K:



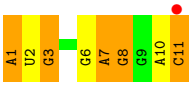
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



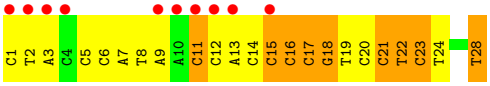
• Molecule 11: RNA (5'-R(*AP*UP*GP*GP*AP*GP*AP*GP*GP*AP*C)-3')

Chain R:



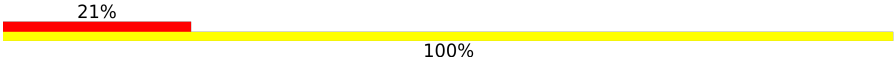
• Molecule 12: DNA (28-MER)

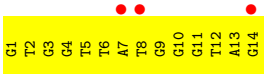
Chain T:



• Molecule 13: DNA (5'-D(*GP*TP*GP*GP*TP*TP*AP*TP*GP*GP*GP*TP*AP*G)-3')

Chain N:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	169.48Å 223.12Å 193.81Å 90.00° 101.47° 90.00°	Depositor
Resolution (Å)	40.00 – 3.18 36.31 – 3.18	Depositor EDS
% Data completeness (in resolution range)	98.6 (40.00-3.18) 98.6 (36.31-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.207 , 0.255 0.222 , 0.257	Depositor DCC
R_{free} test set	5827 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	77.3	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 57.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	29241	wwPDB-VP
Average B, all atoms (Å^2)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, C7P, 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	0.73	1/11163 (0.0%)	0.87	8/15091 (0.1%)
2	B	0.84	2/8963 (0.0%)	0.94	11/12086 (0.1%)
3	C	0.84	1/2133 (0.0%)	0.93	0/2891
4	E	0.60	0/1788	0.75	1/2406 (0.0%)
5	F	0.71	0/691	0.79	0/933
6	H	0.69	0/1086	0.91	1/1470 (0.1%)
7	I	0.81	1/989 (0.1%)	0.94	1/1331 (0.1%)
8	J	0.85	0/541	1.01	2/727 (0.3%)
9	K	0.74	0/937	0.82	0/1265
10	L	0.88	0/365	1.10	0/485
11	R	1.25	0/270	2.01	15/421 (3.6%)
12	T	1.34	5/612 (0.8%)	2.03	35/937 (3.7%)
13	N	0.50	0/329	0.94	0/509
All	All	0.79	10/29867 (0.0%)	0.96	74/40552 (0.2%)

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	3
2	B	0	5
4	E	0	1
6	H	0	3
8	J	0	1
10	L	0	1
All	All	0	14

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	18	DG	C8-N7	9.27	1.36	1.30
12	T	21	DC	C3'-O3'	-6.85	1.35	1.44
12	T	18	DG	C6-N1	-6.38	1.35	1.39
12	T	18	DG	N9-C4	-5.70	1.33	1.38
1	A	795	GLU	CG-CD	5.61	1.60	1.51

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	T	18	DG	N3-C4-C5	-16.47	120.37	128.60
12	T	18	DG	C2-N3-C4	14.35	119.07	111.90
12	T	18	DG	C5-C6-N1	12.95	117.97	111.50
12	T	18	DG	N3-C4-N9	11.38	132.83	126.00
12	T	18	DG	O4'-C1'-N9	10.61	115.43	108.00

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1391	ARG	Peptide
1	A	252	PHE	Peptide
1	A	71	GLN	Peptide
2	B	245	GLU	Peptide
2	B	265	SER	Peptide

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	10969	0	11071	589	0
2	B	8792	0	8824	445	0
3	C	2095	0	2051	114	0
4	E	1752	0	1776	63	0
5	F	679	0	701	26	0
6	H	1068	0	1040	69	0
7	I	971	0	927	36	0
8	J	532	0	543	40	0
9	K	919	0	929	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	L	363	0	387	13	0
11	R	240	0	122	2	0
12	T	550	0	316	66	0
13	N	293	0	161	75	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	1	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
16	T	9	0	5	0	0
All	All	29241	0	28853	1398	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 1398 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)
12:T:2:DT:H2"	12:T:3:DA:C5'	1.47	1.44
12:T:2:DT:C2'	12:T:3:DA:H5'	1.42	1.43
1:A:567:LYS:CG	1:A:568:PRO:HD2	1.60	1.30
13:N:1:DG:H2"	13:N:2:DT:C7	1.71	1.19
12:T:8:DT:H2"	12:T:9:DA:C8	1.79	1.18

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%)	1094 (79%)	201 (14%)	88 (6%)	1	9
2	B	1088/1224 (89%)	900 (83%)	126 (12%)	62 (6%)	1	12
3	C	264/318 (83%)	226 (86%)	30 (11%)	8 (3%)	4	25
4	E	212/215 (99%)	173 (82%)	28 (13%)	11 (5%)	2	13
5	F	82/155 (53%)	63 (77%)	13 (16%)	6 (7%)	1	6
6	H	129/146 (88%)	94 (73%)	23 (18%)	12 (9%)	0	3
7	I	117/122 (96%)	97 (83%)	13 (11%)	7 (6%)	1	11
8	J	63/70 (90%)	52 (82%)	6 (10%)	5 (8%)	1	5
9	K	112/120 (93%)	105 (94%)	7 (6%)	0	100	100
10	L	44/70 (63%)	25 (57%)	10 (23%)	9 (20%)	0	0
All	All	3494/4173 (84%)	2829 (81%)	457 (13%)	208 (6%)	1	11

5 of 208 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	55	ASP
1	A	57	ARG
1	A	65	LEU
1	A	73	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1218/1520 (80%)	974 (80%)	244 (20%)	1	6
2	B	960/1061 (90%)	772 (80%)	188 (20%)	1	7
3	C	234/274 (85%)	180 (77%)	54 (23%)	1	3
4	E	196/197 (100%)	160 (82%)	36 (18%)	1	8
5	F	74/137 (54%)	62 (84%)	12 (16%)	2	10
6	H	117/128 (91%)	95 (81%)	22 (19%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	I	113/116 (97%)	87 (77%)	26 (23%)	1 3
8	J	60/65 (92%)	42 (70%)	18 (30%)	0 1
9	K	99/102 (97%)	87 (88%)	12 (12%)	5 20
10	L	40/57 (70%)	33 (82%)	7 (18%)	2 9
All	All	3111/3657 (85%)	2492 (80%)	619 (20%)	1 6

5 of 619 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	154	LYS
7	I	91	ARG
3	C	235	VAL
3	C	151	GLN
4	E	204	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	794	ASN
3	C	112	ASN
2	B	843	GLN
2	B	1084	GLN
3	C	188	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	10/11 (90%)	2 (20%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	3	G
11	R	11	C

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
16	C7P	T	29	12	3,9,10	0.42	0	2,11,14	0.68	0

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
16	C7P	T	29	12	-	-	0/0/1/1

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 (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, 95th 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^2)	Q<0.9
1	A	1395/1733 (80%)	-0.25	22 (1%) 72 59	47, 104, 216, 308	0
2	B	1106/1224 (90%)	-0.34	24 (2%) 62 48	43, 86, 154, 209	0
3	C	266/318 (83%)	-0.43	0 100 100	62, 91, 135, 158	0
4	E	214/215 (99%)	-0.04	4 (1%) 66 53	81, 159, 225, 242	0
5	F	84/155 (54%)	-0.26	0 100 100	77, 110, 142, 150	0
6	H	133/146 (91%)	0.06	4 (3%) 50 34	101, 153, 199, 211	0
7	I	119/122 (97%)	-0.11	0 100 100	74, 118, 158, 172	0
8	J	65/70 (92%)	-0.65	0 100 100	56, 73, 100, 116	0
9	K	114/120 (95%)	-0.40	1 (0%) 84 75	59, 103, 131, 141	0
10	L	46/70 (65%)	0.40	5 (10%) 5 3	72, 144, 173, 182	0
11	R	11/11 (100%)	0.88	1 (9%) 9 5	141, 156, 210, 217	0
12	T	28/28 (100%)	1.91	10 (35%) 0 0	146, 286, 394, 400	0
13	N	14/14 (100%)	1.67	3 (21%) 0 0	309, 352, 380, 391	0
All	All	3595/4226 (85%)	-0.24	74 (2%) 63 49	43, 103, 203, 400	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	LEU	9.0
1	A	44	THR	7.7
2	B	866	TYR	7.7
2	B	1223	ASP	5.7
1	A	318	SER	5.6

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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, 95th 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^2)	Q<0.9
15	MG	A	2001	1/1	0.84	0.08	67,67,67,67	0
14	ZN	A	1734	1/1	0.89	0.09	113,113,113,113	0
16	C7P	T	29	9/10	0.92	0.33	205,229,260,269	1
14	ZN	B	1307	1/1	0.95	0.04	92,92,92,92	0
14	ZN	J	101	1/1	0.96	0.06	61,61,61,61	0
14	ZN	L	105	1/1	0.96	0.05	101,101,101,101	1
14	ZN	A	1735	1/1	0.98	0.04	83,83,83,83	0
14	ZN	I	204	1/1	0.98	0.07	59,59,59,59	0
14	ZN	I	203	1/1	0.99	0.03	74,74,74,74	0
14	ZN	C	319	1/1	0.99	0.04	63,63,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.