wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 06:58 AM GMT

PDB ID	:	2YU9
Title	:	RNA polymerase II elongation complex in 150 mm MG+2 with UTP
Authors	:	Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.
Deposited on	:	2007-04-06
Resolution	:	3.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

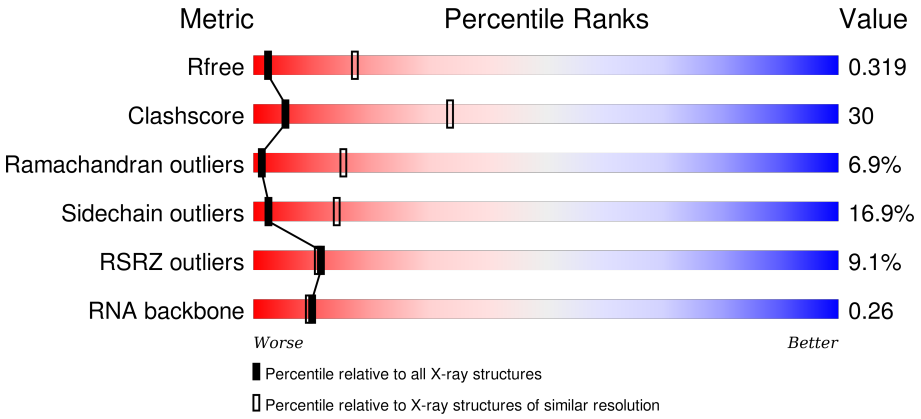
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)
RNA backbone	2183	1041 (4.00-2.80)

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 >=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 <=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	R	10	70% 30%
2	T	28	43% 29% 43% 29%
3	N	14	64% 43% 43% 14%
4	A	1733	7% 41% 30% 9% • 19%

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Mol	Chain	Length	Quality of chain
5	B	1224	7% 40% 39% 10% 8%
6	C	318	5% 45% 32% 7% 16%
7	E	215	11% 65% 27% 8%
8	F	155	3% 32% 19% 5% 45%
9	H	146	10% 59% 27% 5% 9%
10	I	122	12% 60% 30% 8%
11	J	70	% 19% 46% 24% 7%
12	K	120	4% 49% 37% 9% 5%
13	L	70	17% 40% 19% 7% 34%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	UTP	A	2003[A]	-	-	X	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29530 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 RNA chain called 5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	R	10	216	98	45	64	9	0	0	0

- Molecule 2 is a DNA chain called 28-MER DNA template strand.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	1411	11094	6994	1945	2094	61	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	1121	8914	5643	1563	1653	55	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	85	Total	C	N	O	S	0	0	0
			688	439	116	130	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit 9.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypep-

tide.

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

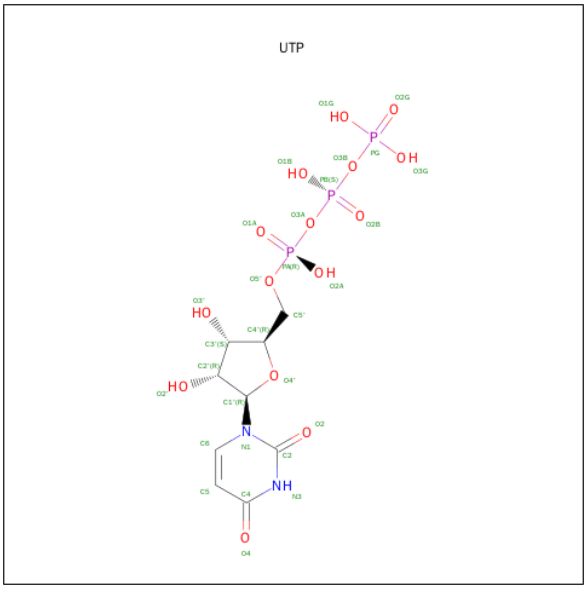
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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	2	Total	Mg	0	0
			2	2		

- Molecule 16 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$).



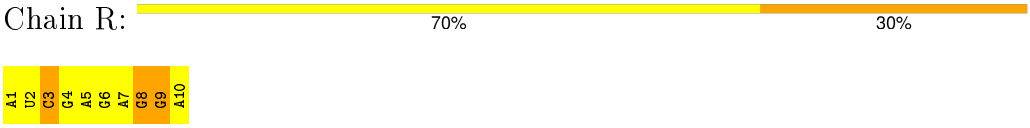
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	A	1	Total	C	N	O	P	0	1
			58	18	4	30	6		

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 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.

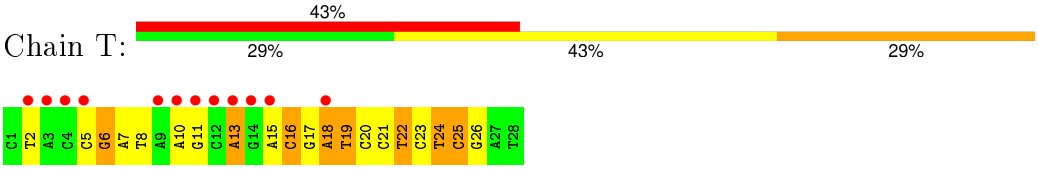
- Molecule 1: 5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*A)-3'

Chain R:



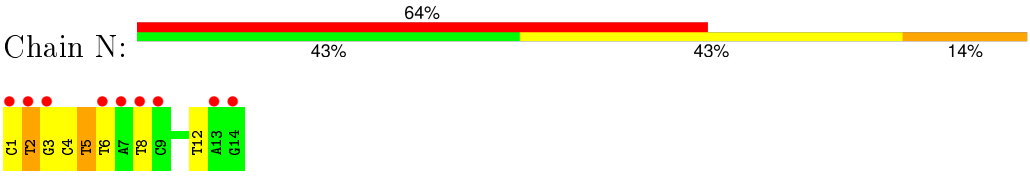
- Molecule 2: 28-MER DNA template strand

Chain T:



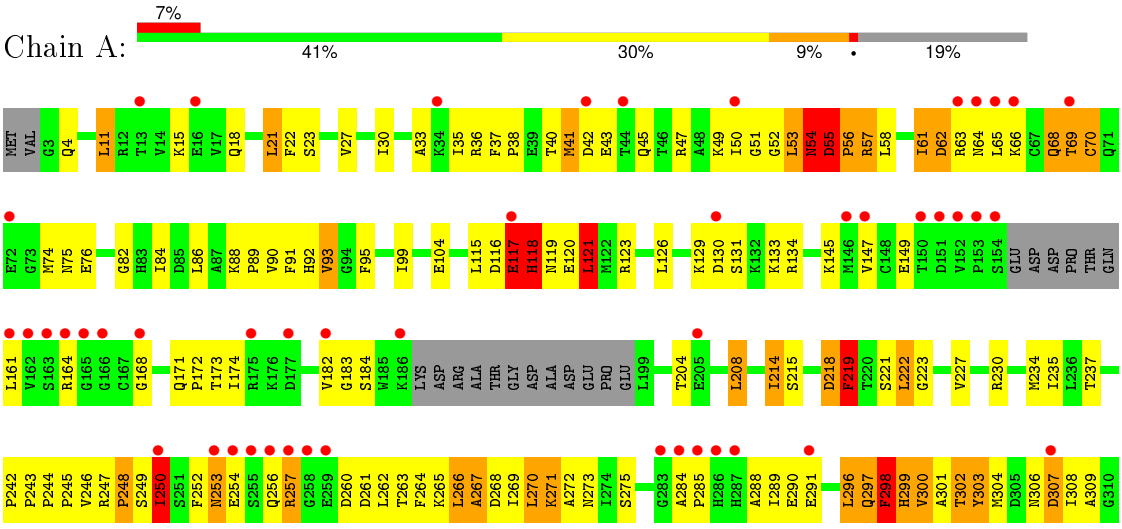
- Molecule 3: 5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3'

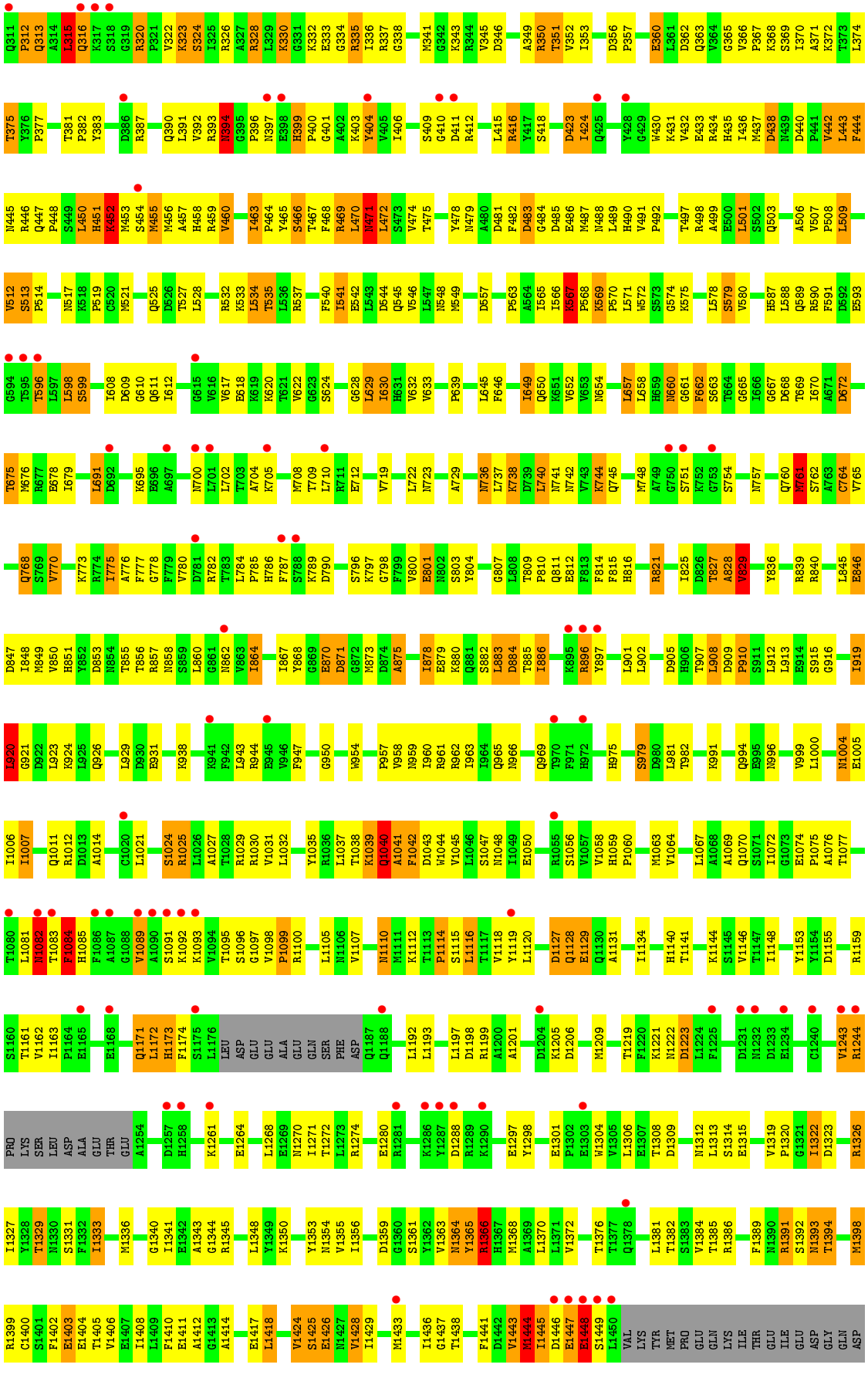
Chain N:

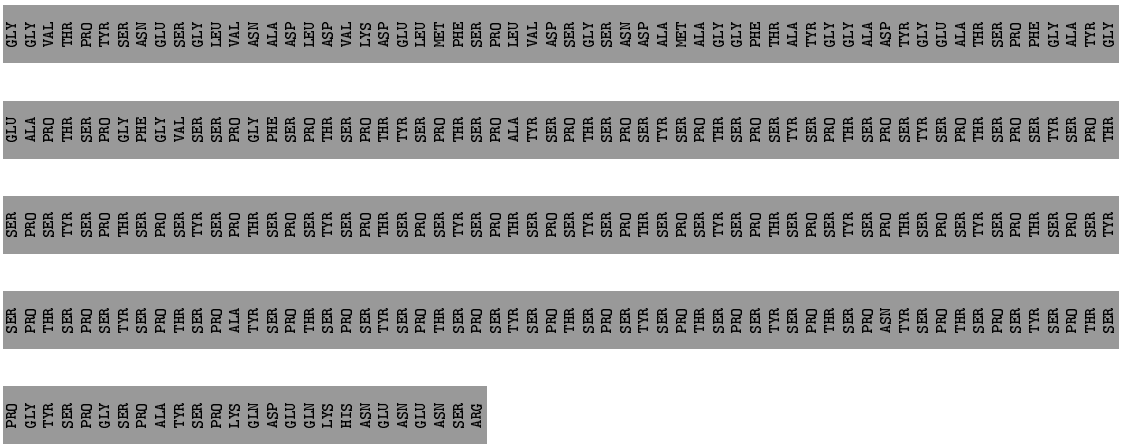


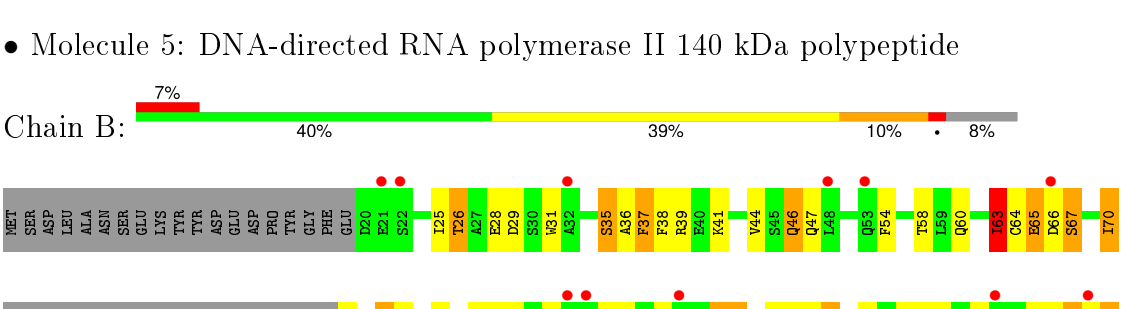
- Molecule 4: DNA-directed RNA polymerase II largest subunit

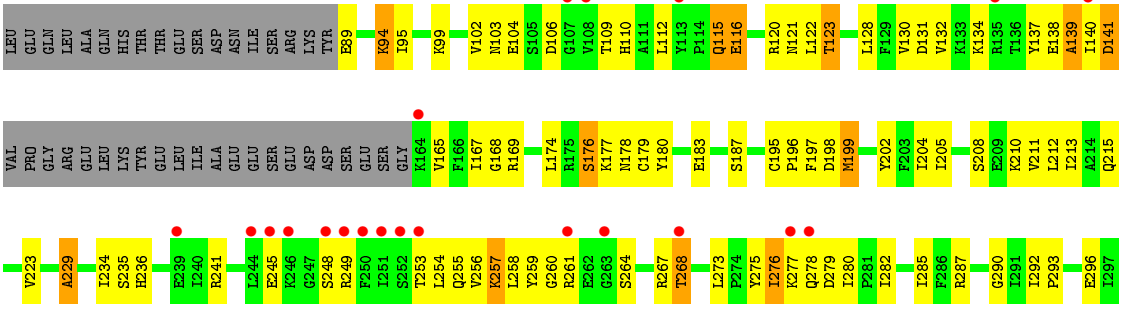
Chain A:

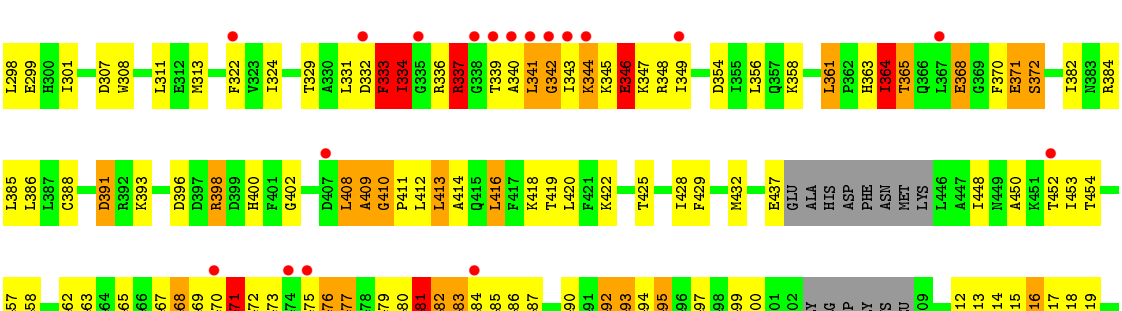


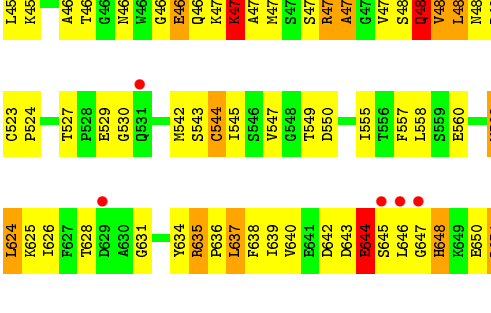






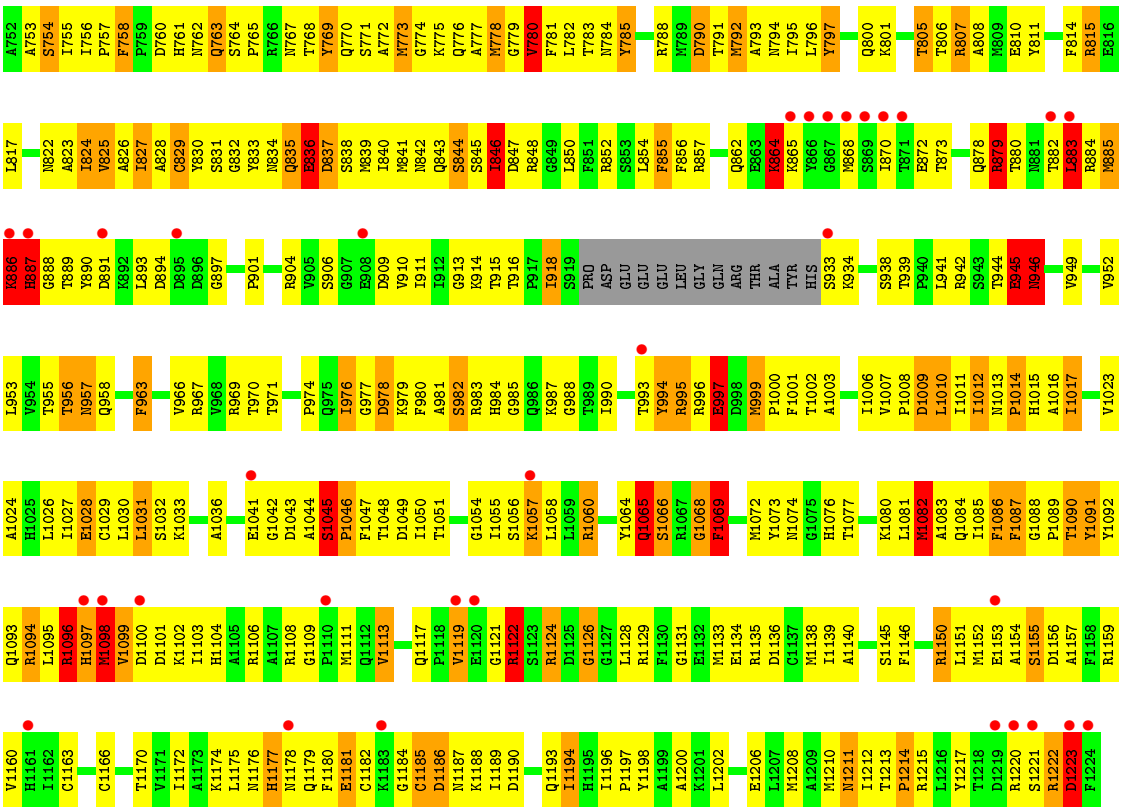






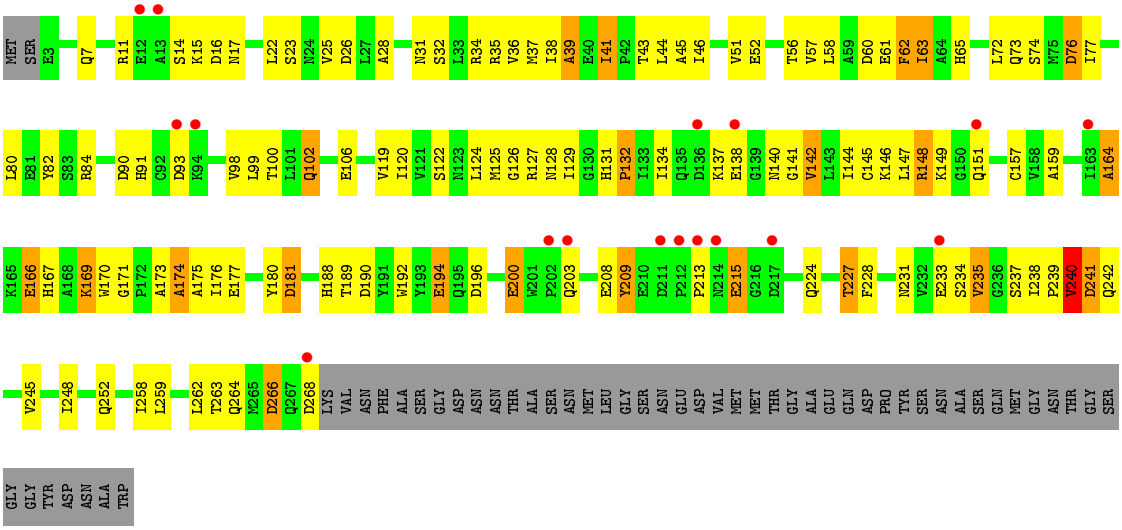
• Molecule 5: DNA-directed RNA polymerase II 140 kDa polypeptide

Chain B:



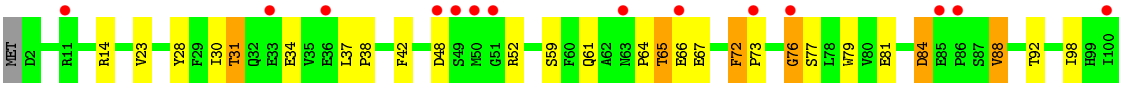
• Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide

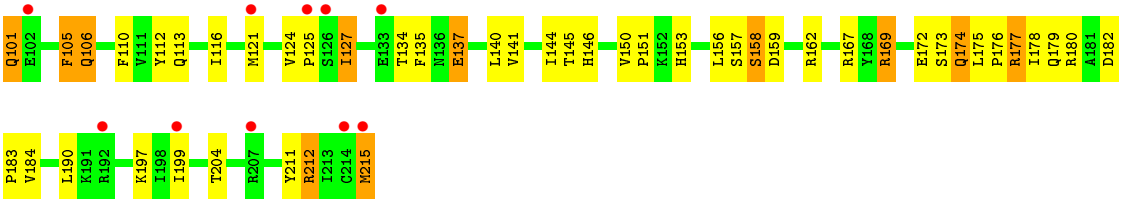
Chain C:



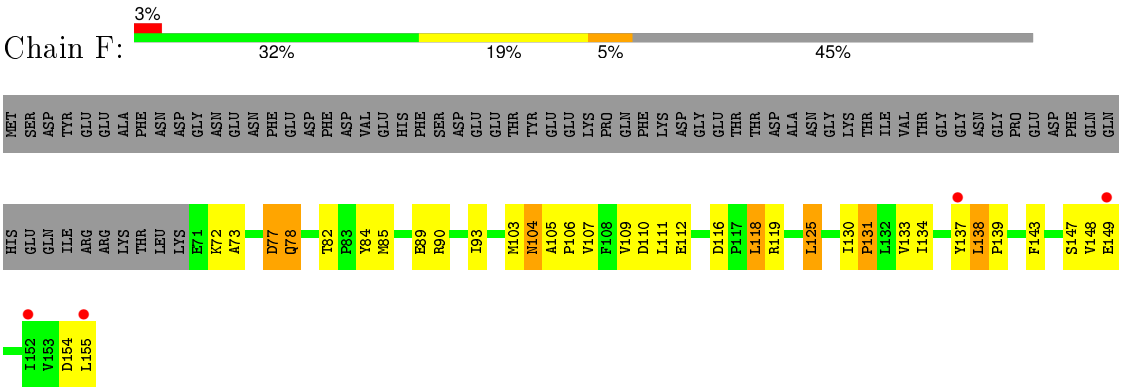
• Molecule 7: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

Chain E:

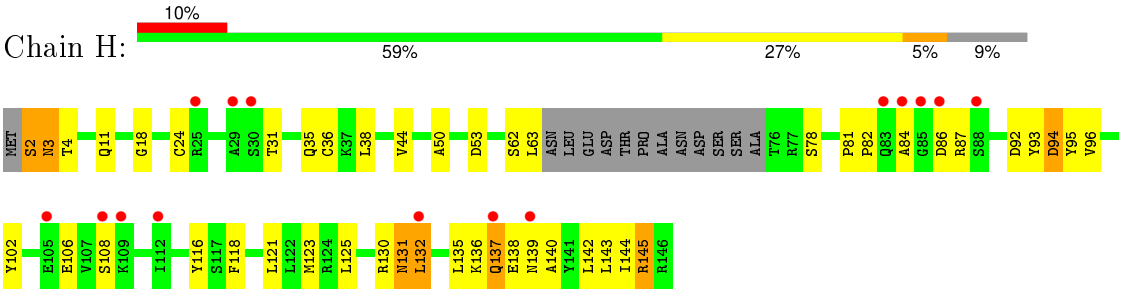




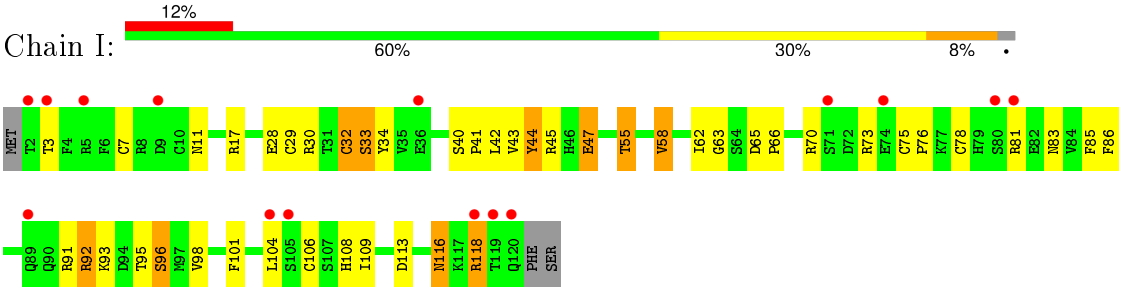
• Molecule 8: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



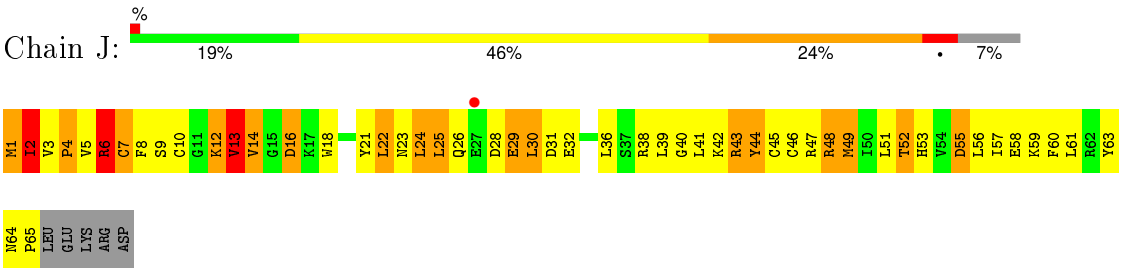
• Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



• Molecule 10: DNA-directed RNA polymerase II subunit 9

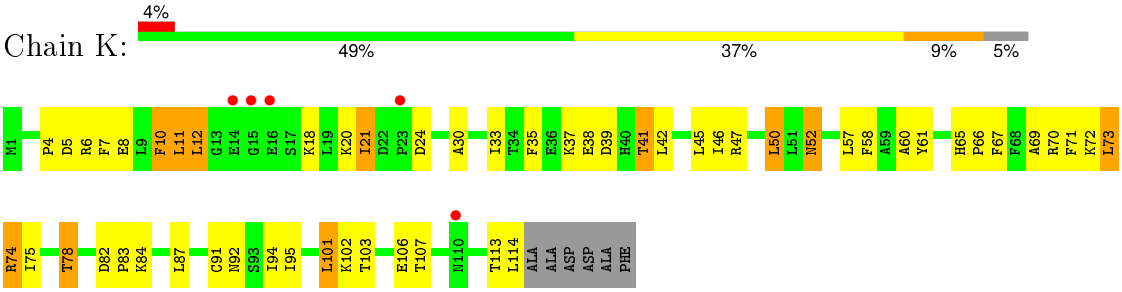


• Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10



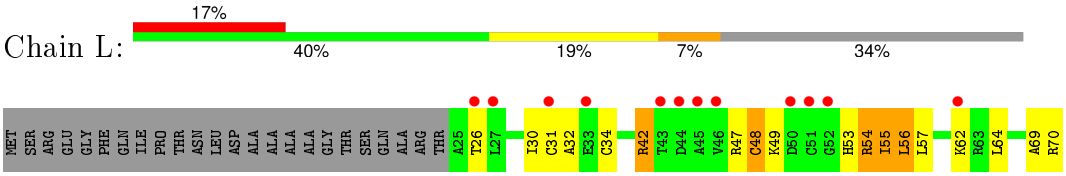
• Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K:



• Molecule 13: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	170.61Å 222.73Å 196.16Å 90.00° 101.87° 90.00°	Depositor
Resolution (Å)	19.98 – 3.40 19.97 – 3.40	Depositor EDS
% Data completeness (in resolution range)	90.0 (19.98-3.40) 90.0 (19.97-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 3.44Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.283 , 0.344 0.271 , 0.319	Depositor DCC
R_{free} test set	2609 reflections (3.06%)	DCC
Wilson B-factor (Å^2)	101.5	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 121.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 87950 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	29530	wwPDB-VP
Average B, all atoms (Å^2)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: UTP, MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	R	0.58	0/243	1.05	1/378 (0.3%)
2	T	0.91	1/634 (0.2%)	1.72	18/975 (1.8%)
3	N	1.12	1/317 (0.3%)	1.59	6/488 (1.2%)
4	A	0.49	0/11292	0.66	0/15267
5	B	0.54	0/9087	0.68	0/12253
6	C	0.56	0/2133	0.68	0/2891
7	E	0.46	0/1788	0.61	0/2406
8	F	0.46	0/700	0.65	0/945
9	H	0.44	0/1086	0.66	0/1470
10	I	0.46	0/989	0.65	0/1331
11	J	0.50	0/541	0.65	0/727
12	K	0.53	0/937	0.64	0/1265
13	L	0.59	0/365	0.83	0/485
All	All	0.53	2/30112 (0.0%)	0.73	25/40881 (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
4	A	0	18
5	B	0	20
6	C	0	1
9	H	0	1
11	J	0	4
All	All	0	44

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	12	DT	C5-C7	10.67	1.56	1.50
2	T	18	DA	O3'-P	7.41	1.70	1.61

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	25	DC	O4'-C1'-N1	13.75	117.62	108.00
3	N	1	DC	O4'-C1'-N1	10.87	115.61	108.00
2	T	16	DC	O4'-C1'-N1	10.29	115.21	108.00
2	T	25	DC	C1'-O4'-C4'	-10.21	99.89	110.10
2	T	25	DC	O4'-C4'-C3'	-9.01	100.60	106.00

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	117	GLU	Peptide
4	A	218	ASP	Peptide
4	A	222	LEU	Peptide
4	A	53	LEU	Peptide
4	A	54	ASN	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	R	216	0	109	58	0
2	T	566	0	316	43	0
3	N	284	0	161	3	0
4	A	11094	0	11178	663	0
5	B	8914	0	8953	727	0
6	C	2095	0	2051	120	0
7	E	1752	0	1776	52	0
8	F	688	0	707	23	0
9	H	1068	0	1040	38	0
10	I	971	0	927	30	0
11	J	532	0	542	121	0
12	K	919	0	929	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	L	363	0	386	10	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	2	0	0	0	0
16	A	58	0	22	12	0
All	All	29530	0	29097	1745	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 30.

The worst 5 of 1745 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)
16:A:2003[A]:UTP:H5'2	16:A:2003[A]:UTP:C6	1.44	1.52
9:H:2:SER:CB	9:H:3:ASN:HB2	1.35	1.50
4:A:1444:MET:CG	4:A:1445:ILE:HG13	1.49	1.42
9:H:2:SER:HB2	9:H:3:ASN:CB	1.52	1.40
4:A:1040:GLN:N	4:A:1041:ALA:HB3	1.43	1.31

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
4	A	1401/1733 (81%)	1052 (75%)	250 (18%)	99 (7%)	1 15
5	B	1105/1224 (90%)	836 (76%)	177 (16%)	92 (8%)	1 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	C	264/318 (83%)	197 (75%)	54 (20%)	13 (5%)	3 25
7	E	212/215 (99%)	184 (87%)	22 (10%)	6 (3%)	6 41
8	F	83/155 (54%)	70 (84%)	7 (8%)	6 (7%)	1 14
9	H	129/146 (88%)	99 (77%)	22 (17%)	8 (6%)	2 18
10	I	117/122 (96%)	88 (75%)	22 (19%)	7 (6%)	2 19
11	J	63/70 (90%)	49 (78%)	7 (11%)	7 (11%)	0 6
12	K	112/120 (93%)	96 (86%)	14 (12%)	2 (2%)	11 50
13	L	44/70 (63%)	26 (59%)	14 (32%)	4 (9%)	1 9
All	All	3530/4173 (85%)	2697 (76%)	589 (17%)	244 (7%)	1 15

5 of 244 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	55	ASP
4	A	68	GLN
4	A	93	VAL
4	A	117	GLU
4	A	118	HIS

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
4	A	1231/1520 (81%)	1016 (82%)	215 (18%)	2 13
5	B	972/1061 (92%)	799 (82%)	173 (18%)	2 12
6	C	234/274 (85%)	204 (87%)	30 (13%)	5 26
7	E	196/197 (100%)	173 (88%)	23 (12%)	7 30
8	F	75/137 (55%)	68 (91%)	7 (9%)	11 42
9	H	117/128 (91%)	102 (87%)	15 (13%)	5 26
10	I	113/116 (97%)	93 (82%)	20 (18%)	2 12
11	J	60/65 (92%)	40 (67%)	20 (33%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	K	99/102 (97%)	80 (81%)	19 (19%)	2 9
13	L	40/57 (70%)	32 (80%)	8 (20%)	1 8
All	All	3137/3657 (86%)	2607 (83%)	530 (17%)	2 14

5 of 530 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	245	GLU
5	B	662	MET
11	J	16	ASP
5	B	344	LYS
5	B	487	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	178	ASN
5	B	657	HIS
11	J	53	HIS
5	B	278	GLN
5	B	499	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	8/10 (80%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	8	G
1	R	9	G

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 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	UTP	A	2003[A]	-	20,30,30	1.66	4 (20%)	30,47,47	1.97	4 (13%)
16	UTP	A	2003[B]	-	20,30,30	1.66	4 (20%)	30,47,47	1.97	4 (13%)

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	UTP	A	2003[A]	-	-	0/18/38/38	0/2/2/2
16	UTP	A	2003[B]	-	-	0/18/38/38	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	2003[A]	UTP	O4'-C1'	2.17	1.43	1.41
16	A	2003[B]	UTP	O4'-C1'	2.22	1.44	1.41
16	A	2003[A]	UTP	PG-O2G	3.11	1.61	1.51
16	A	2003[B]	UTP	PG-O2G	3.14	1.61	1.51
16	A	2003[B]	UTP	C6-N1	3.31	1.40	1.35

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	2003[B]	UTP	C4'-O4'-C1'	-5.15	104.06	109.72
16	A	2003[A]	UTP	C4'-O4'-C1'	-5.09	104.12	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	A	2003[A]	UTP	PB-O3A-PA	-4.52	120.03	132.73
16	A	2003[B]	UTP	PB-O3A-PA	-4.52	120.03	132.73
16	A	2003[A]	UTP	PB-O3B-PG	-3.79	119.95	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	2003[A]	UTP	9	0
16	A	2003[B]	UTP	3	0

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^{th} 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	R	10/10 (100%)	0.64	0 100 100	118, 142, 150, 153	0
2	T	28/28 (100%)	1.81	12 (42%) 0 0	138, 167, 200, 200	0
3	N	14/14 (100%)	2.90	9 (64%) 0 0	155, 184, 200, 200	0
4	A	1411/1733 (81%)	0.44	126 (8%) 12 11	101, 149, 166, 193	0
5	B	1121/1224 (91%)	0.40	90 (8%) 15 14	84, 141, 159, 176	0
6	C	266/318 (83%)	0.33	17 (6%) 23 21	109, 139, 155, 178	0
7	E	214/215 (99%)	0.60	24 (11%) 7 7	147, 163, 172, 177	0
8	F	85/155 (54%)	0.37	4 (4%) 35 32	144, 160, 173, 178	0
9	H	133/146 (91%)	0.54	15 (11%) 7 7	141, 154, 173, 182	0
10	I	119/122 (97%)	0.81	15 (12%) 5 5	134, 153, 169, 171	0
11	J	65/70 (92%)	0.10	1 (1%) 76 71	99, 120, 137, 144	0
12	K	114/120 (95%)	0.30	5 (4%) 38 34	130, 147, 166, 171	0
13	L	46/70 (65%)	1.29	12 (26%) 1 1	148, 174, 178, 179	0
All	All	3626/4225 (85%)	0.46	330 (9%) 11 11	84, 147, 169, 200	0

The worst 5 of 330 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	250	PHE	11.2
5	B	1221	SER	10.5
5	B	339	THR	9.3
4	A	1090	ALA	8.2
7	E	48	ASP	7.6

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. 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^{th} 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^2)	Q<0.9
16	UTP	A	2003[A]	29/29	0.82	0.39	2.04	132,133,138,138	29
16	UTP	A	2003[B]	29/29	0.82	0.39	1.90	137,137,137,137	29
14	ZN	B	1307	1/1	0.96	0.20	-0.36	142,142,142,142	0
14	ZN	L	105	1/1	0.97	0.28	-0.63	175,175,175,175	0
14	ZN	A	1734	1/1	0.87	0.25	-0.75	157,157,157,157	0
14	ZN	C	319	1/1	0.95	0.09	-0.87	149,149,149,149	0
14	ZN	I	203	1/1	0.91	0.10	-1.25	141,141,141,141	0
15	MG	A	2001	1/1	0.92	0.15	-1.36	124,124,124,124	0
14	ZN	I	204	1/1	0.83	0.12	-1.47	154,154,154,154	0
14	ZN	A	1735	1/1	0.93	0.08	-3.00	149,149,149,149	0
14	ZN	J	101	1/1	0.98	0.07	-3.12	109,109,109,109	0
15	MG	A	2002	1/1	0.96	0.35	-	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.