wwPDB X-ray Structure Validation Summary Report (i)

May 23, 2020 – 08:15 pm BST

PDB ID	:	1Y1Y
Title	:	RNA Polymerase II-TFIIS-DNA/RNA complex
Authors	:	Cramer, P.; Kettenberger, H.; Armache, K.-J.
Deposited on	:	2004-11-19
Resolution	:	4.00 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 following versions of software and data (see references (1)) were used in the production of this report:

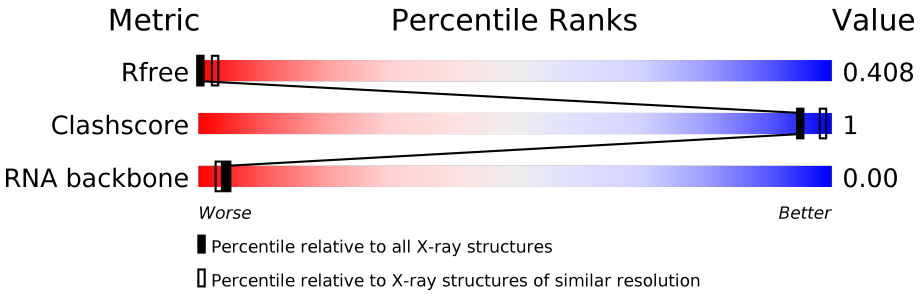
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
RNA backbone	3102	1048 (5.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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%

Mol	Chain	Length	Quality of chain
1	T	7	100%
2	P	4	100%
3	A	1733	82% 18%
4	B	1224	91% 9%
5	C	318	84% 16%
6	D	221	80% 20%
7	E	215	99% .
8	F	155	54% 46%

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Mol	Chain	Length	Quality of chain
9	G	171	99%
10	H	146	91% 9%
11	I	122	98%
12	J	70	93% 7%
13	K	120	95% 5%
14	L	70	66% 34%
15	S	179	95%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 4112 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 DNA chain called 5'-D(P*TP*AP*CP*GP*CP*CP*T)-3'.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	T	7	Total P 7 7	0	0	7

- Molecule 2 is a RNA chain called 5'-R(P*AP*GP*GP*C)-3'.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	P	4	Total P 4 4	0	0	4

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	A	1426	Total C 1426 1426	0	0	1426

- Molecule 4 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	B	1112	Total C 1112 1112	8	0	1112

- Molecule 5 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	C	266	Total C 266 266	0	0	266

- Molecule 6 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	D	177	Total C 177 177	0	0	177

- 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 214 214	0	0	214

- 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	84	Total C 84 84	0	0	84

- Molecule 9 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	G	171	Total C 171 171	0	0	171

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	H	133	Total C 133 133	0	0	133

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit 9.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	I	119	Total C 119 119	0	0	119

- Molecule 12 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	J	65	Total C 65 65	0	0	65

- Molecule 13 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	K	114	Total C 114 114	0	0	114

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	L	46	Total C 46 46	0	0	46

- Molecule 15 is a protein called Transcription elongation factor S-II.

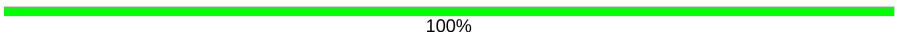
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	S	174	Total C 174 174	0	0	174

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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'-D(P*TP*AP*CP*GP*CP*CP*T)-3'

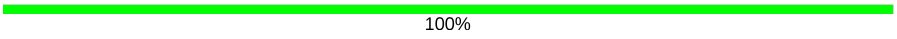
Chain T:



There are no outlier residues recorded for this chain.

- Molecule 2: 5'-R(P*AP*GP*GP*C)-3'

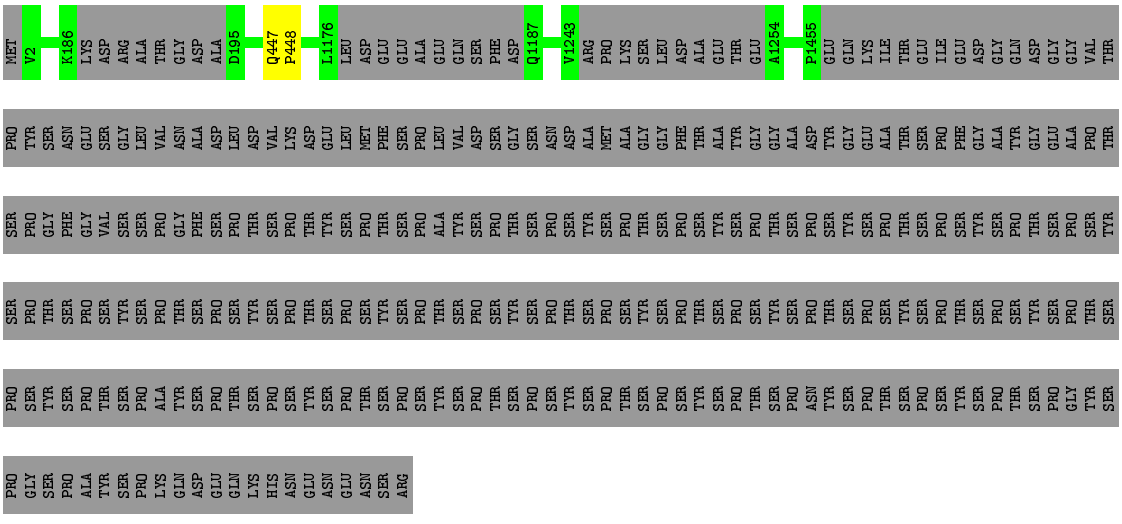
Chain P:



There are no outlier residues recorded for this chain.

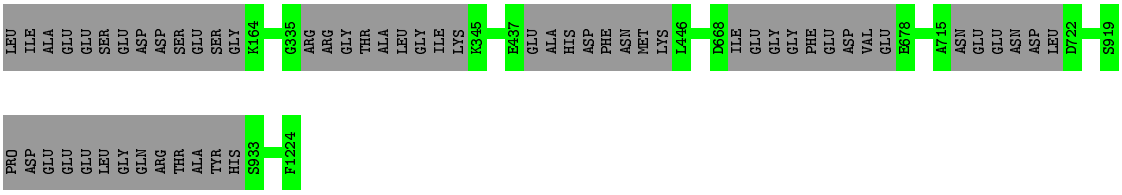
- Molecule 3: DNA-directed RNA polymerase II largest subunit

Chain A:



- Molecule 4: DNA-directed RNA polymerase II 140 kDa polypeptide

Chain B:



• Molecule 5: DNA-directed RNA polymerase II 45 kDa polypeptide

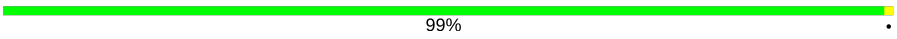
Chain C:

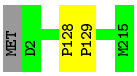
• Molecule 6: DNA-directed RNA polymerase II 32 kDa polypeptide

Chain D:

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

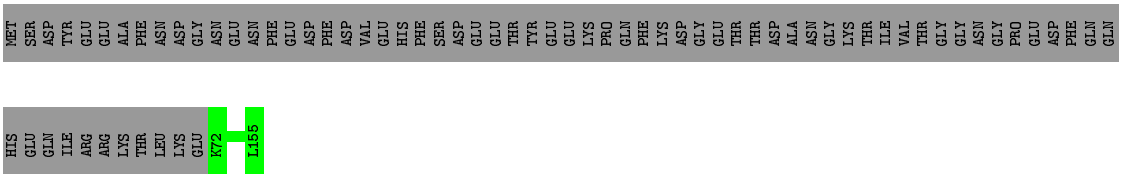
Chain E:





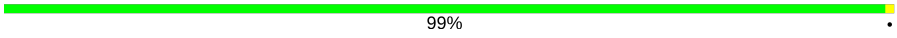
• Molecule 8: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

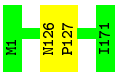
Chain F:



• Molecule 9: DNA-directed RNA polymerase II 19 kDa polypeptide

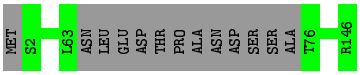
Chain G:





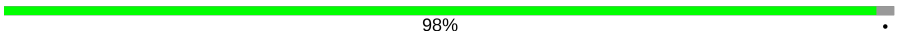
• Molecule 10: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

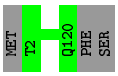
Chain H:



- Molecule 11: DNA-directed RNA polymerase II subunit 9

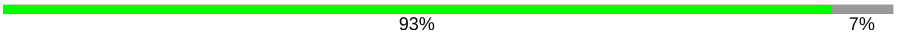
Chain I:





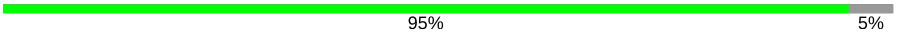
- Molecule 12: DNA-directed RNA polymerases I/II/III subunit 10

Chain J:



- Molecule 13: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K:

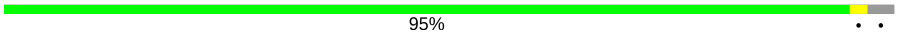


- Molecule 14: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide

Chain L:

- Molecule 15: Transcription elongation factor S-II

Chain S:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	220.20Å 395.70Å 282.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.00 39.19 – 3.98	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-4.00) 98.1 (39.19-3.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.11 (at 4.00Å)	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.281 , (Not available) 0.413 , 0.408	Depositor DCC
R_{free} test set	2038 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å^2)	106.8	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 98.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.004 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.015 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.65	EDS
Total number of atoms	4112	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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

5.1 Standard geometry

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	T	7	0	0	0	0
2	P	4	0	0	0	0
3	A	1426	0	0	1	0
4	B	1112	0	0	0	0
5	C	266	0	0	0	0
6	D	177	0	0	0	0
7	E	214	0	0	1	0
8	F	84	0	0	0	0
9	G	171	0	0	1	0
10	H	133	0	0	0	0
11	I	119	0	0	0	0
12	J	65	0	0	0	0
13	K	114	0	0	0	0
14	L	46	0	0	0	0
15	S	174	0	0	2	0
All	All	4112	0	0	5	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 1.

All (5) 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)
15:S:218:ILE:CA	15:S:219:ALA:CA	2.73	0.66
9:G:126:ASN:CA	9:G:127:PRO:CA	2.78	0.62
3:A:447:GLN:CA	3:A:448:PRO:CA	2.83	0.56
15:S:231:CYS:CA	15:S:232:ASP:CA	2.86	0.53
7:E:128:PRO:CA	7:E:129:PRO:CA	2.90	0.49

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	P	0/4	-	-

There are no RNA backbone outliers to report.

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

There are no ligands in this entry.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.