wwPDB X-ray Structure Validation Summary Report (i)

Aug 15, 2023 – 11:06 PM EDT

PDB ID	:	1TWG
Title	:	RNA polymerase II complexed with CTP
Authors	:	Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on	:	2004-06-30
Resolution	:	3.30 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:

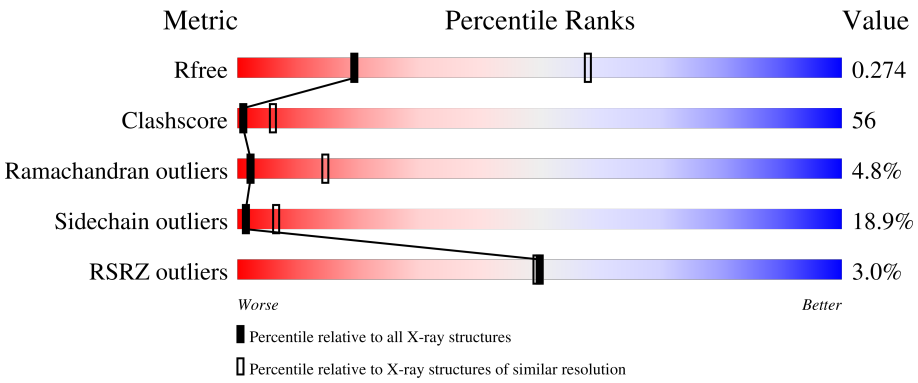
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	2%; 5%, 34%, 28%, 11%, 22%
2	B	1224	4%; 6%, 36%, 33%, 14%, 11%
3	C	318	%; •, 27%, 39%, 13%, 16%
4	E	215	2%; 7%, 29%, 46%, 18%
5	F	155	%; •, 24%, 20%, 6%, 46%

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Mol	Chain	Length	Quality of chain
6	H	146	4% 24% 30% 34% 9%
7	I	122	2% 40% 42% 14%
8	J	70	37% 41% 10% 9%
9	K	120	5% 30% 44% 16% 5%
10	L	70	% 9% 27% 29% 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
12	ZN	J	3001	-	-	X	-
12	ZN	L	3005	-	-	X	-
13	CTP	B	3008	X	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 27731 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 largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1349	10606	6692	1839	2017	58	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1091	8690	5511	1516	1610	53	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	215	1760	1116	310	322	12	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	83	670	428	114	125	3	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

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 14.2 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	I	121	990	610	181	188	11	0	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	J	64	525	334	92	93	6	0	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

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 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	L	46	364	224	72	64	4	0	0	0

- Molecule 11 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
11	A	2	2	2	0	0

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
12	A	2	2	2	0	0
12	B	1	1	1	0	0

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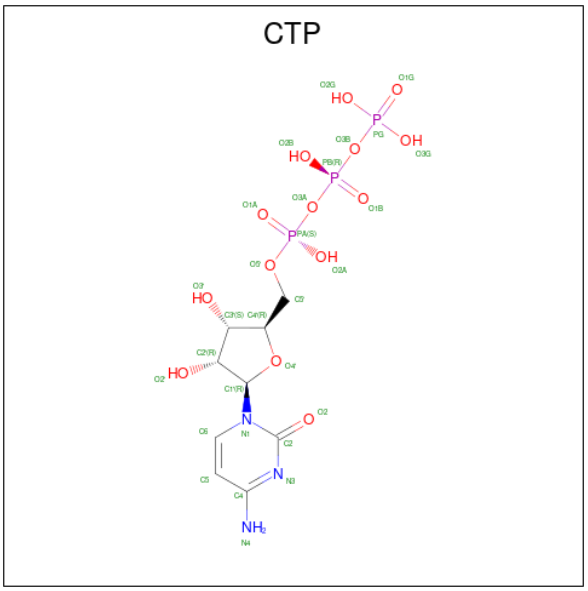
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total Zn 1 1	0	0
12	I	2	Total Zn 2 2	0	0
12	J	1	Total Zn 1 1	0	0
12	L	1	Total Zn 1 1	0	0

- Molecule 13 is CYTIDINE-5'-TRIPHOSPHATE (three-letter code: CTP) (formula: $C_9H_{16}N_3O_{14}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C N O P 29 9 3 14 3	0	0

- Molecule 14 is water.

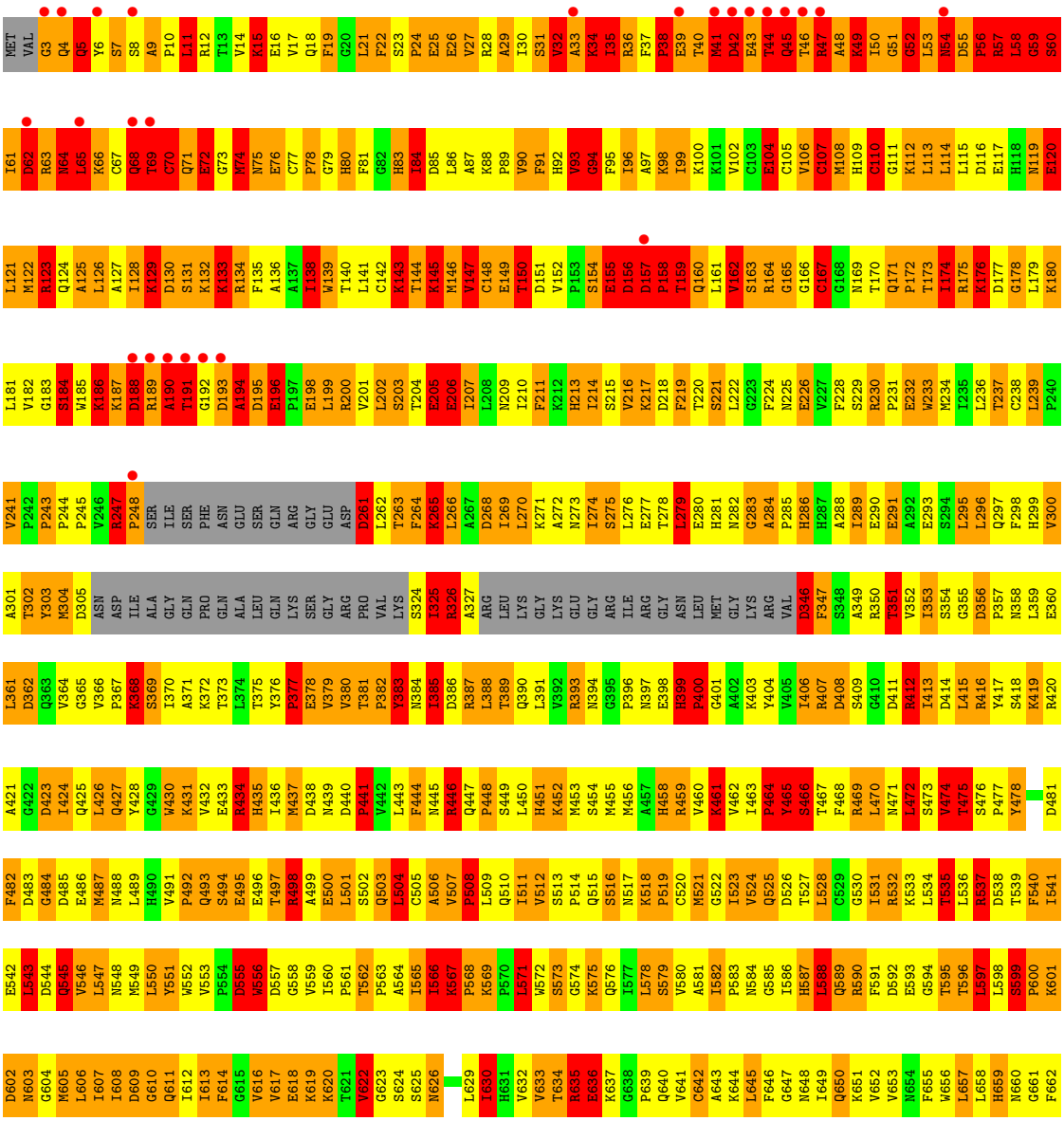
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	2	Total O 2 2	0	0
14	B	3	Total O 3 3	0	0

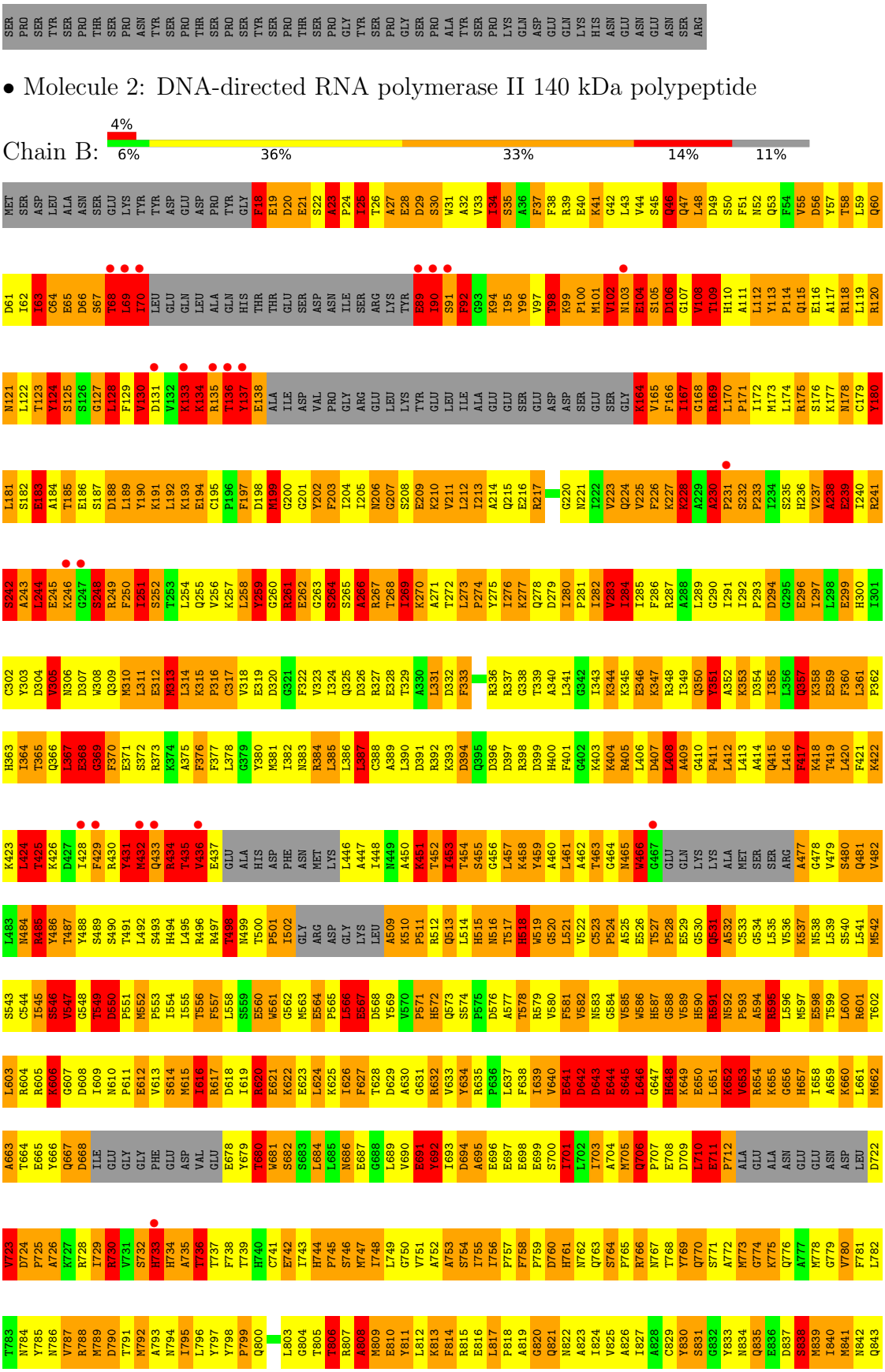
3 Residue-property plots (i)

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 largest subunit

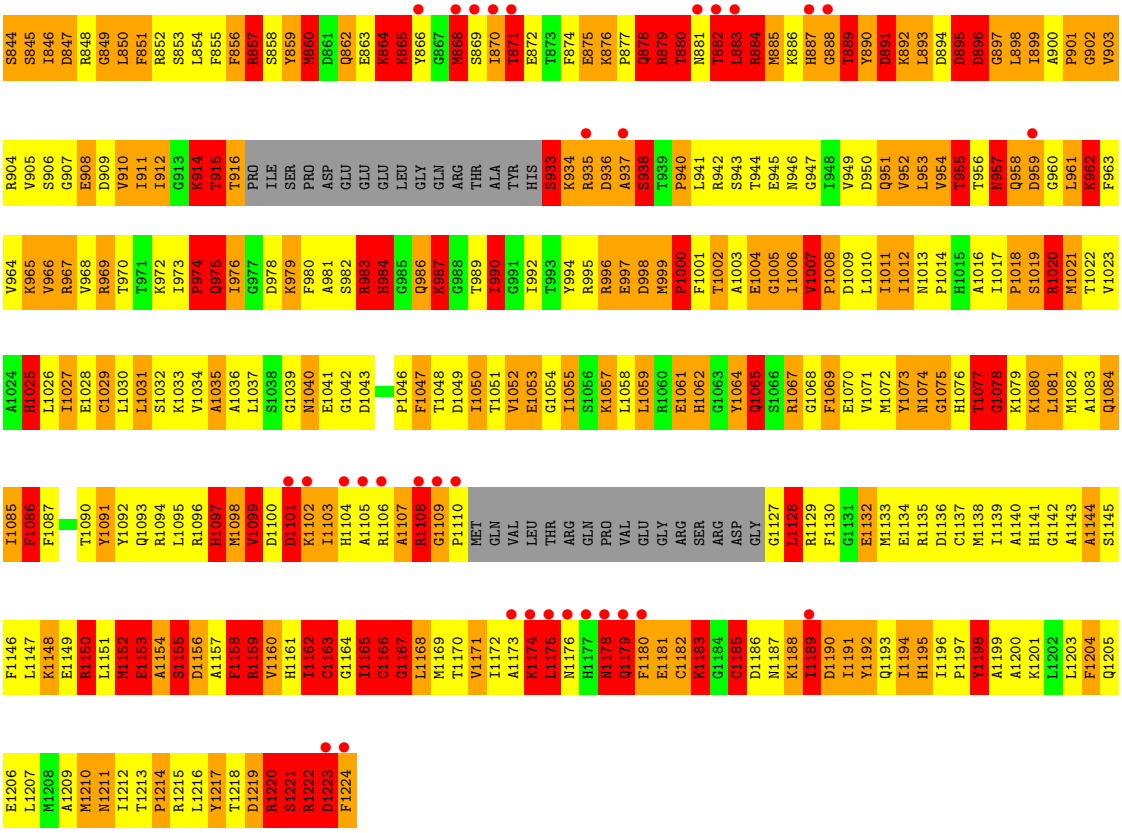
Chain A: 2% 5% 34% 28% 11% 22%





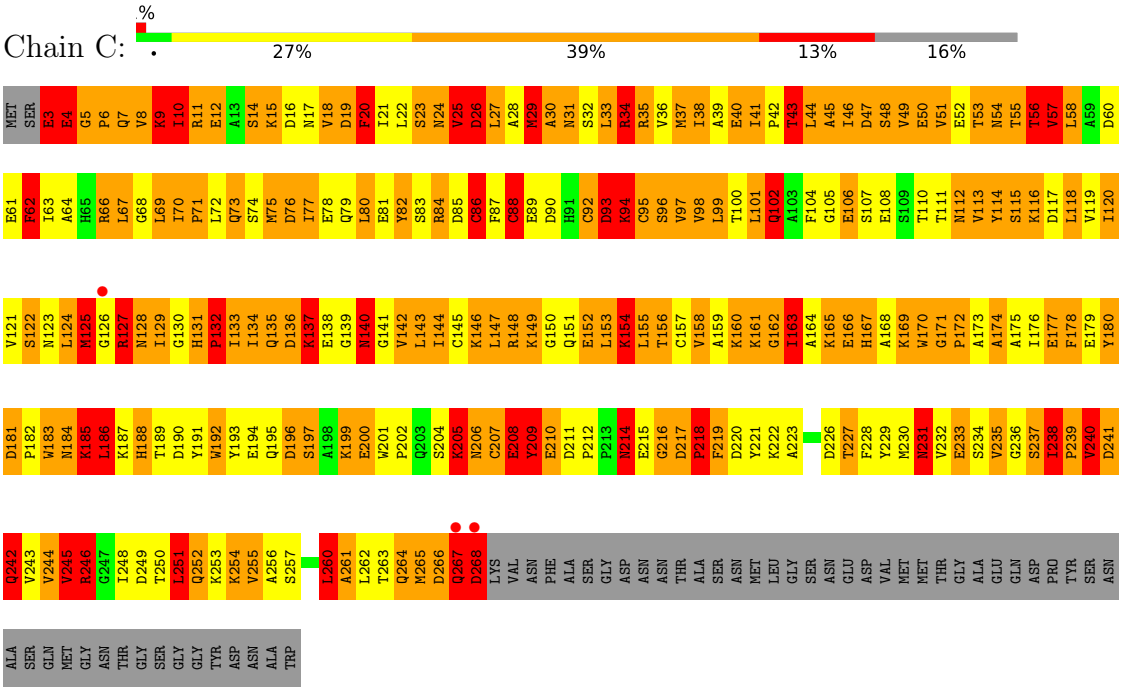
• Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide

Chain B: 4% 6% 36% 33% 14% 11%



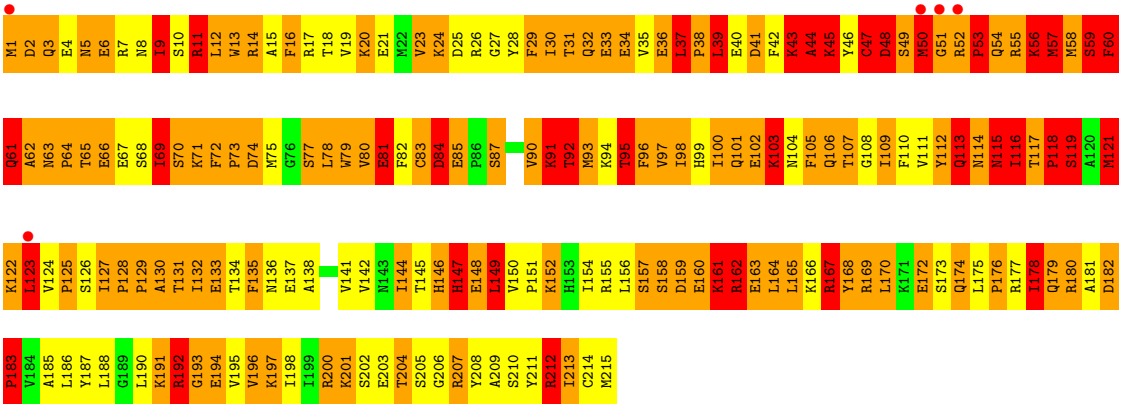
- Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C:



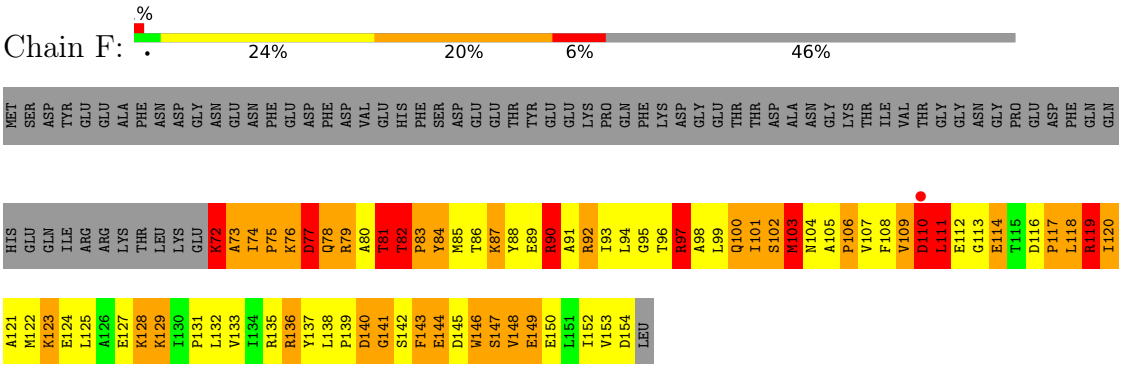
- Molecule 4: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

Chain E:



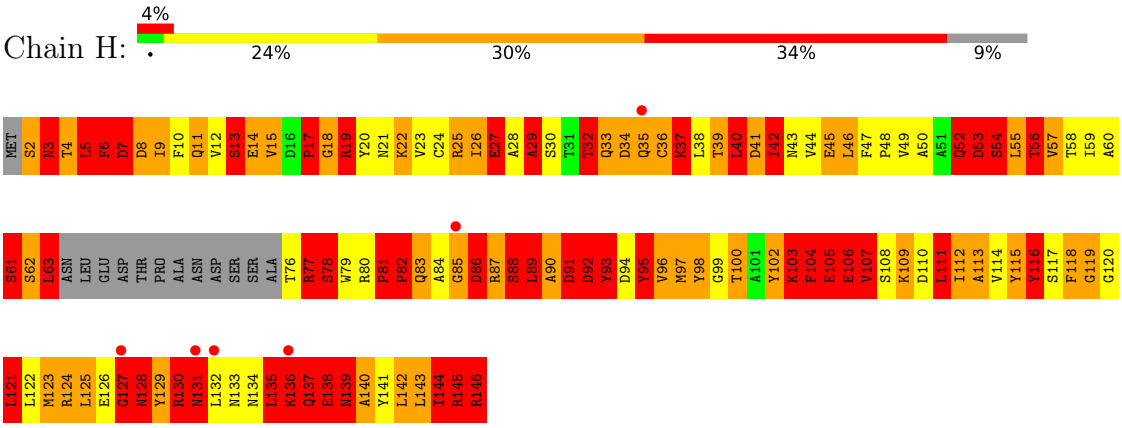
- Molecule 5: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

Chain F:



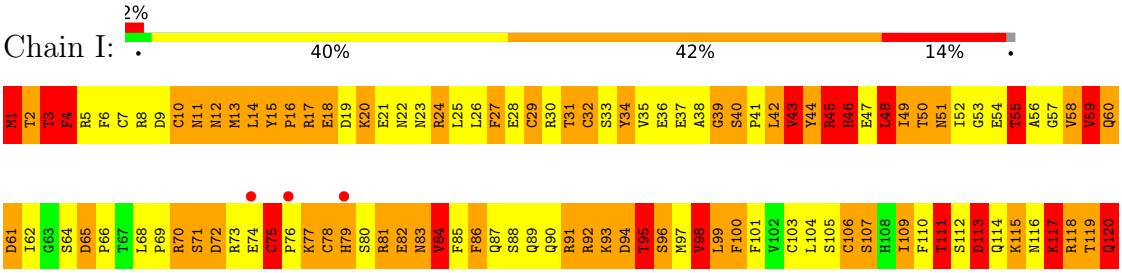
- Molecule 6: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

Chain H:



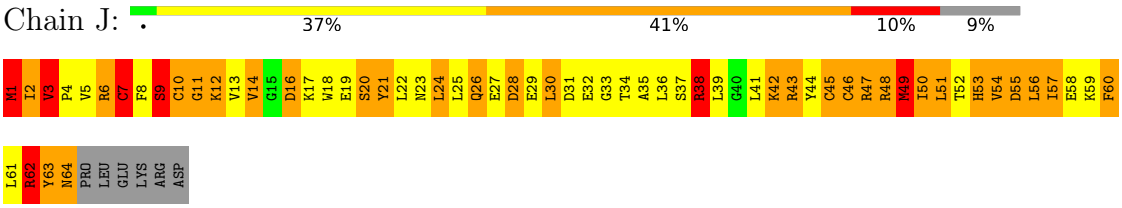
- Molecule 7: DNA-directed RNA polymerase II 14.2 kDa polypeptide

Chain I:



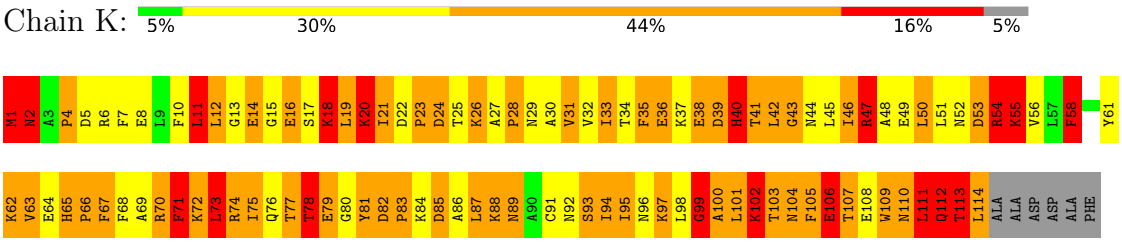
• Molecule 8: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide

Chain J:



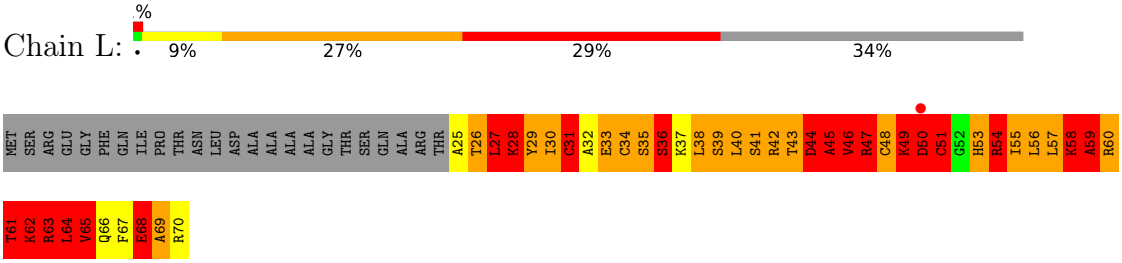
• Molecule 9: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K:



• Molecule 10: 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	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	123.00Å 223.00Å 374.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30 39.42 – 3.29	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.30) 93.0 (39.42-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 3.32Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.263 , 0.281 0.214 , 0.274	Depositor DCC
R_{free} test set	2324 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å^2)	53.7	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	27731	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% 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, CTP, MN

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	4.63	2498/10792 (23.1%)	3.14	1255/14601 (8.6%)
2	B	4.65	2069/8860 (23.4%)	3.12	1000/11945 (8.4%)
3	C	4.80	513/2133 (24.1%)	3.12	254/2891 (8.8%)
4	E	4.70	404/1796 (22.5%)	3.05	209/2416 (8.7%)
5	F	4.16	139/682 (20.4%)	2.87	60/922 (6.5%)
6	H	4.56	229/1086 (21.1%)	3.04	130/1470 (8.8%)
7	I	5.31	288/1009 (28.5%)	3.40	147/1357 (10.8%)
8	J	4.28	125/533 (23.5%)	3.41	78/715 (10.9%)
9	K	4.50	226/937 (24.1%)	3.21	126/1265 (10.0%)
10	L	5.07	98/366 (26.8%)	3.32	59/485 (12.2%)
All	All	4.66	6589/28194 (23.4%)	3.14	3318/38067 (8.7%)

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	69
2	B	0	59
3	C	0	19
4	E	0	9
6	H	0	15
7	I	0	9
8	J	0	2
9	K	0	5
10	L	0	4
All	All	0	191

The worst 5 of 6589 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	564	GLU	CD-OE1	30.56	1.59	1.25
7	I	34	TYR	CD1-CE1	-29.71	0.94	1.39
1	A	1234	GLU	CD-OE1	29.21	1.57	1.25
7	I	34	TYR	CE2-CZ	-28.02	1.02	1.38
1	A	728	LYS	CD-CE	27.41	2.19	1.51

The worst 5 of 3318 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	774	ARG	NE-CZ-NH1	45.06	142.83	120.30
2	B	995	ARG	NE-CZ-NH2	-36.16	102.22	120.30
7	I	91	ARG	NE-CZ-NH1	32.74	136.67	120.30
2	B	995	ARG	NE-CZ-NH1	32.13	136.37	120.30
1	A	469	ARG	NE-CZ-NH1	31.48	136.04	120.30

There are no chirality outliers.

5 of 191 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	44	THR	Peptide
1	A	52	GLY	Peptide
1	A	60	SER	Peptide
1	A	65	LEU	Peptide
1	A	74	MET	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	10606	0	10660	1097	0
2	B	8690	0	8709	1000	2
3	C	2095	0	2053	264	0
4	E	1760	0	1788	203	1
5	F	670	0	690	70	0
6	H	1068	0	1040	223	0
7	I	990	0	948	109	0
8	J	525	0	538	60	0
9	K	919	0	927	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	L	364	0	389	108	0
11	A	2	0	0	0	0
12	A	2	0	0	1	0
12	B	1	0	0	0	0
12	C	1	0	0	1	0
12	I	2	0	0	0	0
12	J	1	0	0	2	0
12	L	1	0	0	2	0
13	B	29	0	11	13	0
14	A	2	0	0	0	0
14	B	3	0	0	7	0
All	All	27731	0	27753	3079	2

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 56.

The worst 5 of 3079 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:226:PHE:CD1	2:B:226:PHE:CE1	1.77	1.67
2:B:370:PHE:CD1	2:B:370:PHE:CE1	1.78	1.67
3:C:165:LYS:CG	3:C:165:LYS:CD	1.74	1.65
2:B:18:PHE:CB	2:B:18:PHE:CG	1.79	1.65
4:E:79:TRP:CB	4:E:79:TRP:CG	1.78	1.65

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:434:ARG:O	2:B:465:ASN:ND2[2_655]	2.11	0.09
2:B:1223:ASP:OD1	4:E:1:MET:CE[8_455]	2.17	0.03

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	1332/1733 (77%)	1160 (87%)	113 (8%)	59 (4%)	2	16
2	B	1071/1224 (88%)	897 (84%)	131 (12%)	43 (4%)	3	18
3	C	264/318 (83%)	218 (83%)	36 (14%)	10 (4%)	3	19
4	E	213/215 (99%)	180 (84%)	20 (9%)	13 (6%)	1	10
5	F	81/155 (52%)	71 (88%)	8 (10%)	2 (2%)	5	27
6	H	129/146 (88%)	85 (66%)	21 (16%)	23 (18%)	0	1
7	I	119/122 (98%)	108 (91%)	8 (7%)	3 (2%)	5	27
8	J	62/70 (89%)	58 (94%)	4 (6%)	0	100	100
9	K	112/120 (93%)	98 (88%)	10 (9%)	4 (4%)	3	20
10	L	44/70 (63%)	26 (59%)	11 (25%)	7 (16%)	0	1
All	All	3427/4173 (82%)	2901 (85%)	362 (11%)	164 (5%)	2	14

5 of 164 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	43	GLU
1	A	45	GLN
1	A	47	ARG
1	A	56	PRO

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	1181/1520 (78%)	984 (83%)	197 (17%)	2	10
2	B	947/1061 (89%)	795 (84%)	152 (16%)	2	10
3	C	234/274 (85%)	192 (82%)	42 (18%)	2	8
4	E	197/197 (100%)	147 (75%)	50 (25%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	73/137 (53%)	61 (84%)	12 (16%)	2	10
6	H	117/128 (91%)	72 (62%)	45 (38%)	0	0
7	I	115/116 (99%)	88 (76%)	27 (24%)	1	3
8	J	59/65 (91%)	48 (81%)	11 (19%)	1	7
9	K	99/102 (97%)	77 (78%)	22 (22%)	1	3
10	L	40/57 (70%)	18 (45%)	22 (55%)	0	0
All	All	3062/3657 (84%)	2482 (81%)	580 (19%)	1	6

5 of 580 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	H	36	CYS
10	L	60	ARG
6	H	83	GLN
6	H	35	GLN
7	I	98	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	73	GLN
9	K	65	HIS
3	C	167	HIS
4	E	147	HIS
1	A	1173	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 11 ligands modelled in this entry, 10 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	$\#\|Z\| > 2$
13	CTP	B	3008	11	26,30,30	2.77	5 (19%)	39,47,47	3.18	12 (30%)

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	CTP	B	3008	11	1/1/7/7	5/22/38/38	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	3008	CTP	C2-N1	9.64	1.60	1.40
13	B	3008	CTP	C1'-N1	7.42	1.69	1.47
13	B	3008	CTP	C6-N1	4.62	1.49	1.38
13	B	3008	CTP	C6-C5	4.21	1.44	1.35
13	B	3008	CTP	C4-N3	2.18	1.39	1.34

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	3008	CTP	O4'-C1'-N1	11.29	134.17	108.36
13	B	3008	CTP	C1'-N1-C2	8.46	137.30	118.42
13	B	3008	CTP	C6-N1-C2	-7.44	107.58	120.49
13	B	3008	CTP	O2-C2-N3	-7.17	110.66	122.33
13	B	3008	CTP	PB-O3A-PA	-3.55	120.63	132.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	B	3008	CTP	C1'

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	B	3008	CTP	C3'-C4'-C5'-O5'
13	B	3008	CTP	O4'-C4'-C5'-O5'
13	B	3008	CTP	PB-O3B-PG-O2G
13	B	3008	CTP	C2'-C1'-N1-C2
13	B	3008	CTP	PB-O3B-PG-O3G

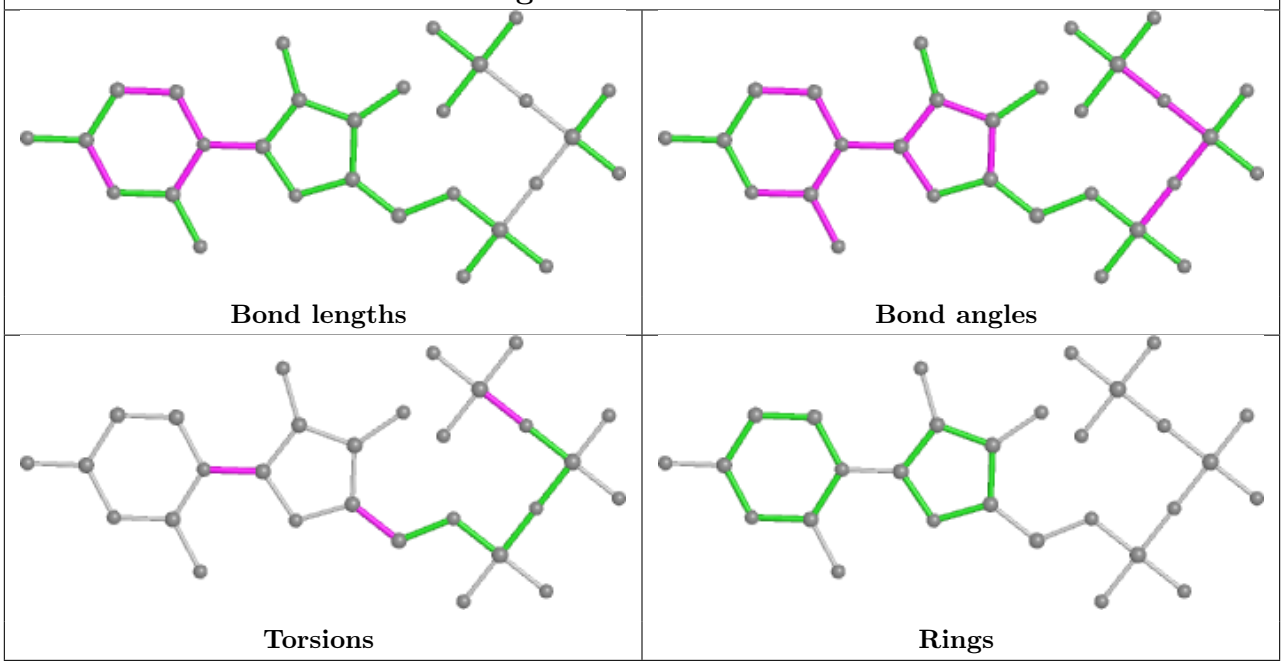
There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	3008	CTP	13	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CTP B 3008



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	13
2	B	13
9	K	3
4	E	2
6	H	1
8	J	1
7	I	1

The worst 5 of 34 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1066:VAL	C	1067:LEU	N	1.20
1	A	1106:ASN	C	1107:VAL	N	1.20
1	A	1191:TRP	C	1192:LEU	N	1.20
1	A	1328:TYR	C	1329:THR	N	1.20
1	B	224:GLN	C	225:VAL	N	1.20

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	1349/1733 (77%)	-0.23	33 (2%)	59	56	1, 24, 101, 195	0
2	B	1091/1224 (89%)	-0.16	54 (4%)	29	27	1, 25, 114, 167	0
3	C	266/318 (83%)	-0.34	3 (1%)	80	81	1, 29, 77, 167	0
4	E	215/215 (100%)	-0.05	5 (2%)	60	59	1, 38, 111, 135	0
5	F	83/155 (53%)	-0.29	1 (1%)	79	78	1, 22, 64, 86	0
6	H	133/146 (91%)	0.17	6 (4%)	33	32	22, 68, 127, 188	0
7	I	121/122 (99%)	-0.03	3 (2%)	57	54	1, 31, 83, 100	0
8	J	64/70 (91%)	-0.37	0	100	100	3, 22, 76, 91	0
9	K	114/120 (95%)	-0.23	0	100	100	3, 36, 73, 99	0
10	L	46/70 (65%)	0.27	1 (2%)	62	60	24, 73, 133, 137	0
All	All	3482/4173 (83%)	-0.18	106 (3%)	50	49	1, 28, 108, 195	0

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	PRO	9.6
2	B	882	THR	9.3
1	A	69	THR	7.0
2	B	1109	GLY	6.9
2	B	1110	PRO	6.1

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)

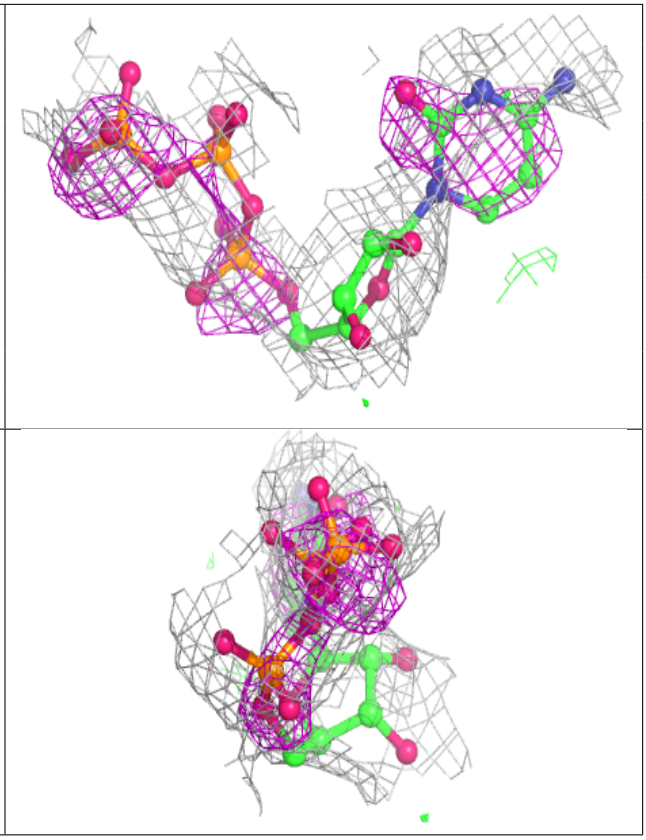
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	CTP	B	3008	29/29	0.82	0.27	26,36,73,77	0
12	ZN	L	3005	1/1	0.89	0.08	84,84,84,84	0
12	ZN	I	3004	1/1	0.89	0.17	49,49,49,49	0
12	ZN	A	3006	1/1	0.92	0.07	48,48,48,48	0
12	ZN	C	3002	1/1	0.94	0.09	35,35,35,35	0
11	MN	A	3010	1/1	0.94	0.07	29,29,29,29	0
12	ZN	B	3007	1/1	0.97	0.08	37,37,37,37	0
11	MN	A	3009	1/1	0.97	0.12	15,15,15,15	0
12	ZN	I	3003	1/1	0.97	0.06	45,45,45,45	0
12	ZN	A	3008	1/1	0.98	0.06	87,87,87,87	0
12	ZN	J	3001	1/1	0.99	0.05	31,31,31,31	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CTP B 3008:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.