wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 10:31 PM GMT

PDB ID	:	1TWA
Title	:	RNA polymerase II complexed with ATP
Authors	:	Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on	:	2004-06-30
Resolution	:	3.20 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:

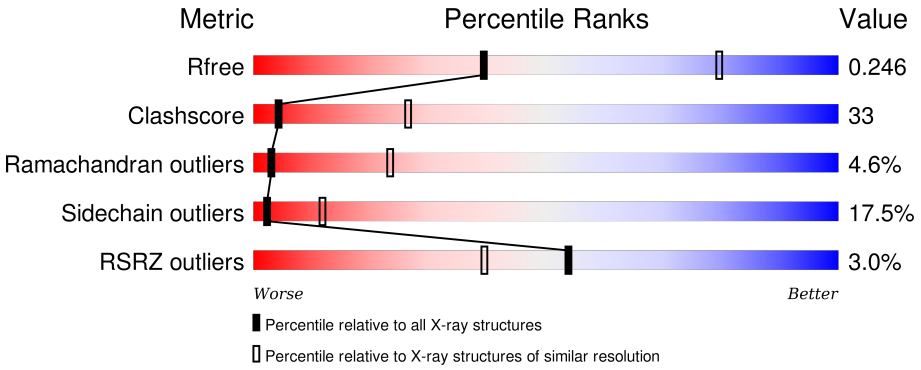
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	A	1733	2% 16% 35% 20% 8% 22%
2	B	1224	4% 18% 40% 23% 8% 11%
3	C	318	% 13% 38% 25% 8% 16%
4	E	215	2% 18% 41% 30% 11%
5	F	155	% 11% 21% 16% 5% 46%

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Mol	Chain	Length	Quality of chain
6	H	146	5% 10% 29% 27% 25% 9%
7	I	122	2% 11% 46% 34% 9%
8	J	70	11% 46% 26% 9% 9%
9	K	120	18% 38% 29% 10% 5%
10	L	70	6% 16% 26% 23% 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	C	3002	-	-	X	-
12	ZN	J	3001	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 27757 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	1352	10635	6711	1842	2024	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
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

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

- 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
8	J	64	Total	C	N	O	S	0	0	0
			525	334	92	93	6			

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

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

- 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
10	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

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

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

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

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

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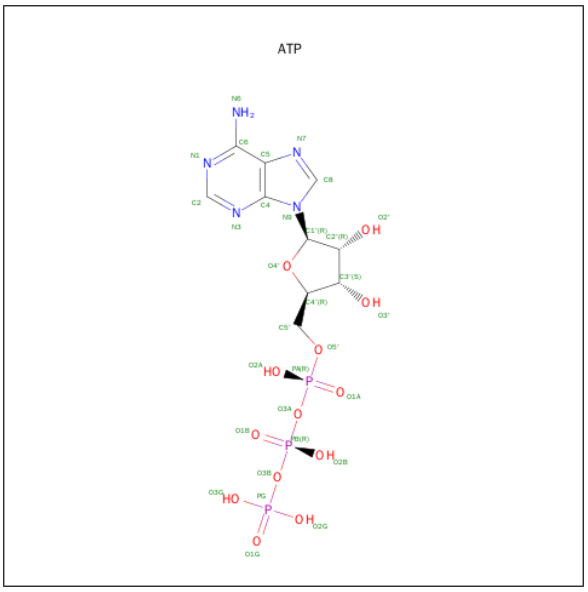
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	I	2	Total Zn 2 2	0	0
12	C	1	Total Zn 1 1	0	0
12	A	2	Total Zn 2 2	0	0
12	L	1	Total Zn 1 1	0	0

- Molecule 13 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



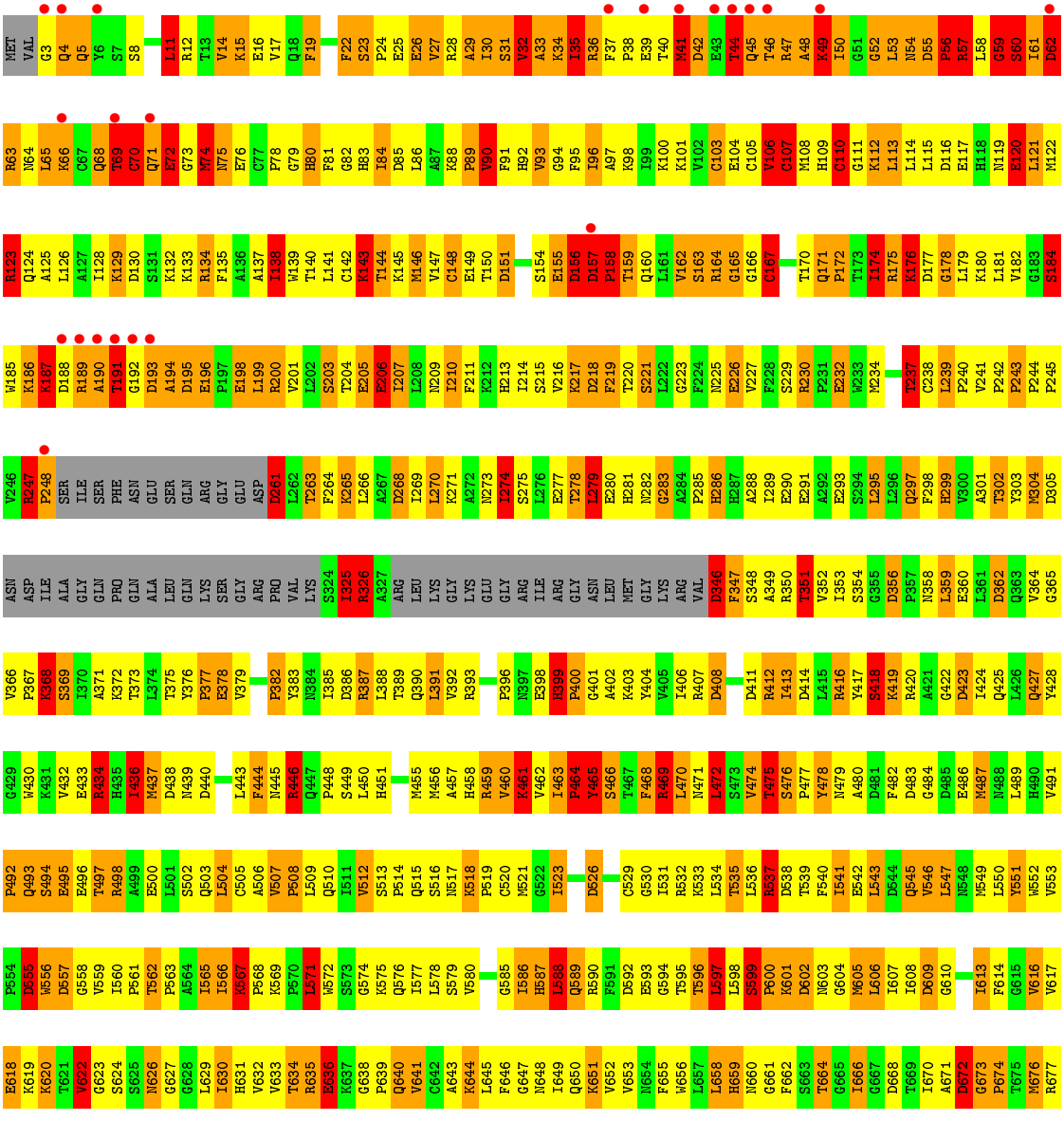
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C N O P 31 10 5 13 3	0	0

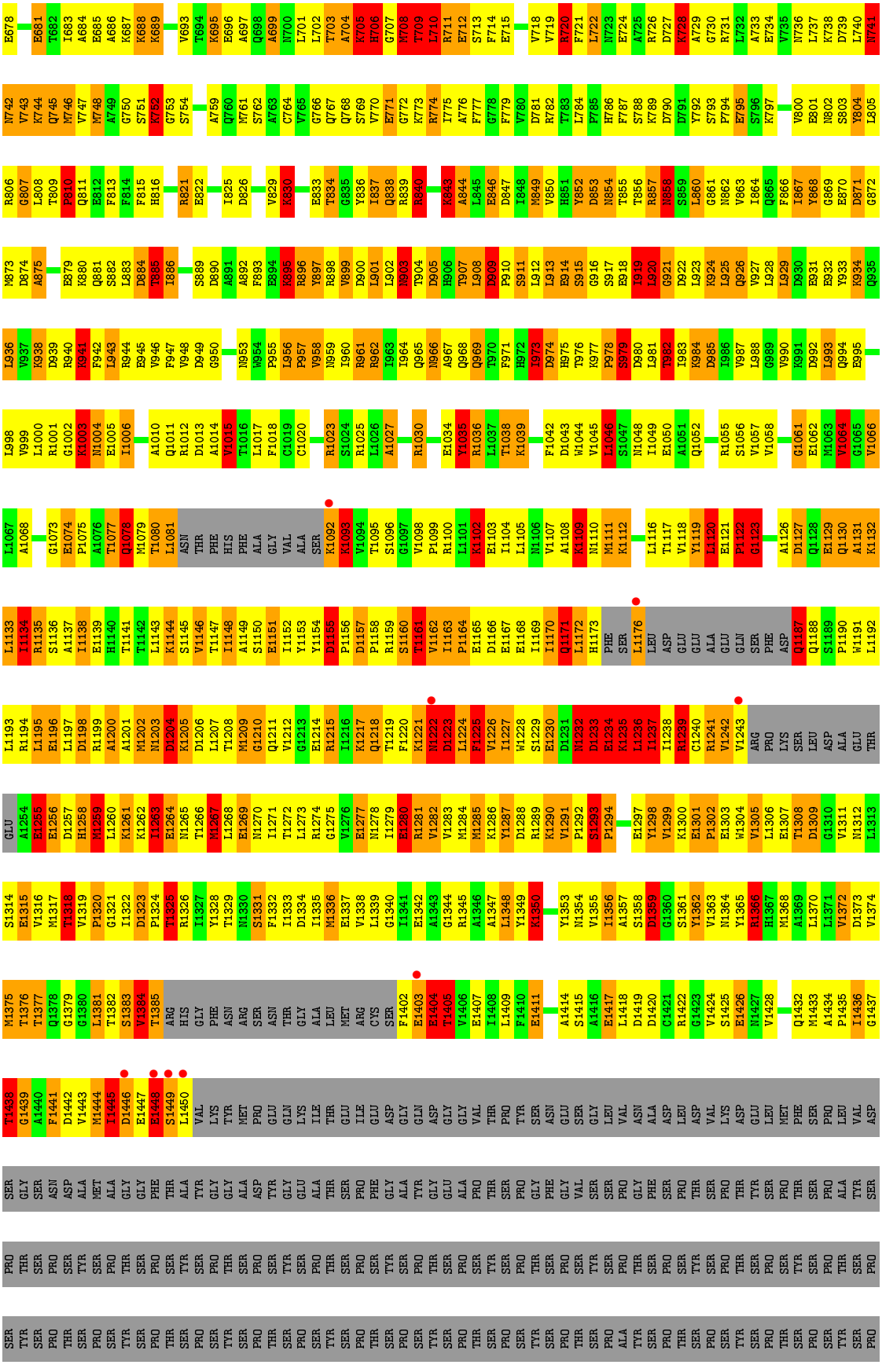
3 Residue-property plots (i)

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: DNA-directed RNA polymerase II largest subunit

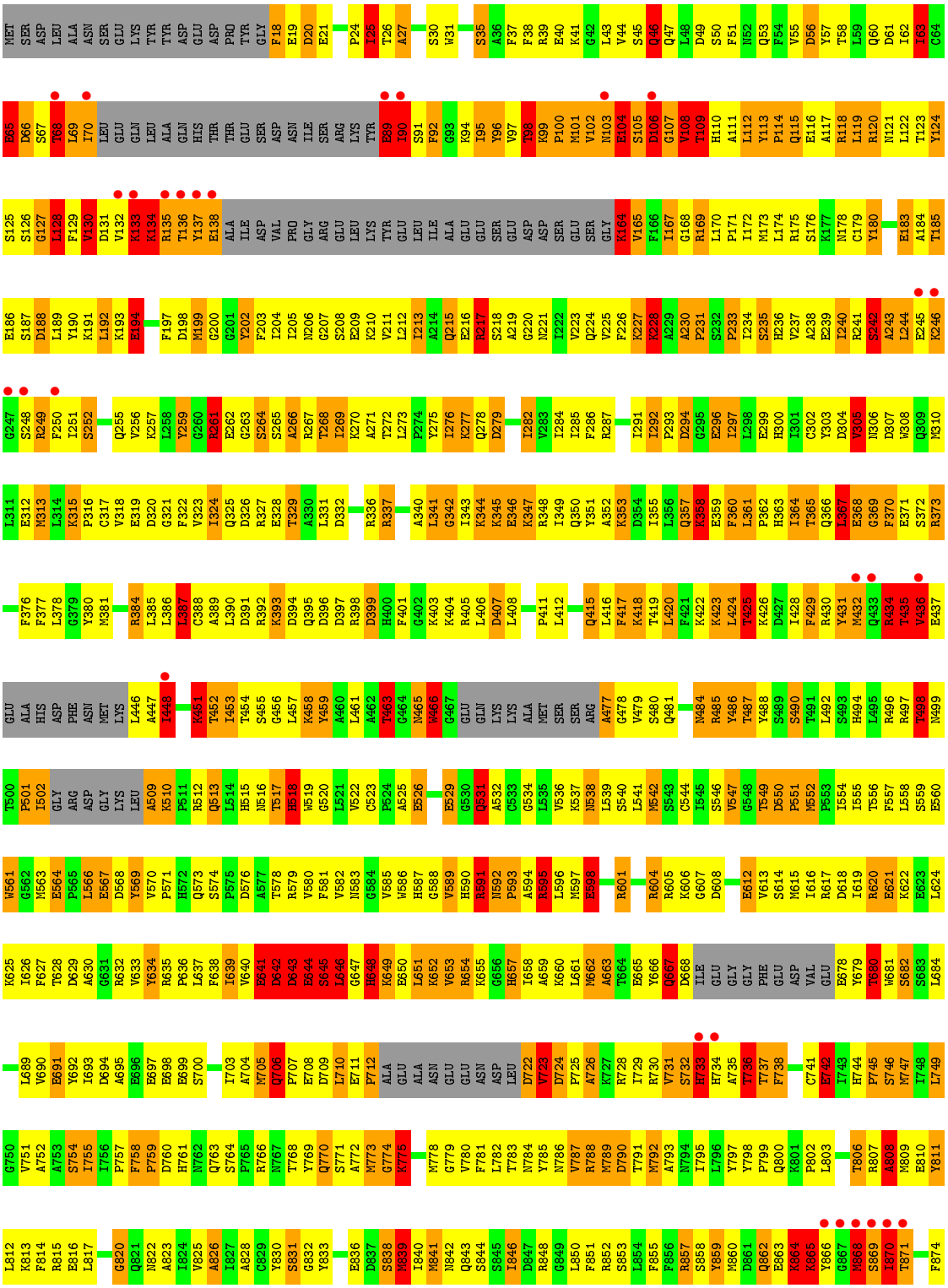
Chain A:

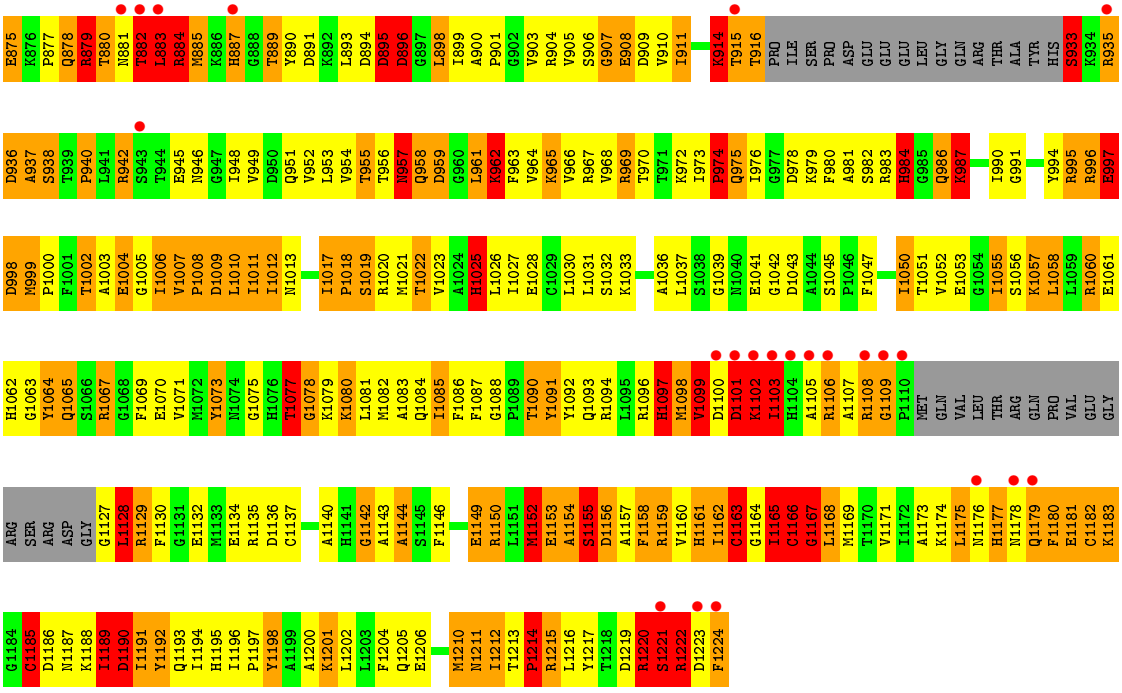




- Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide

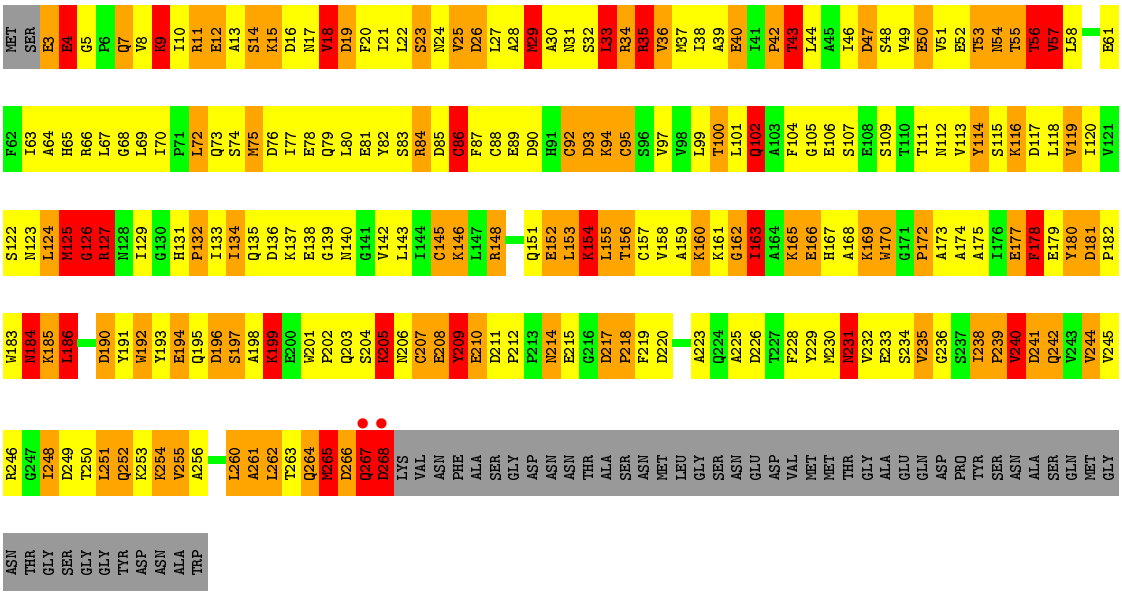
Chain B:





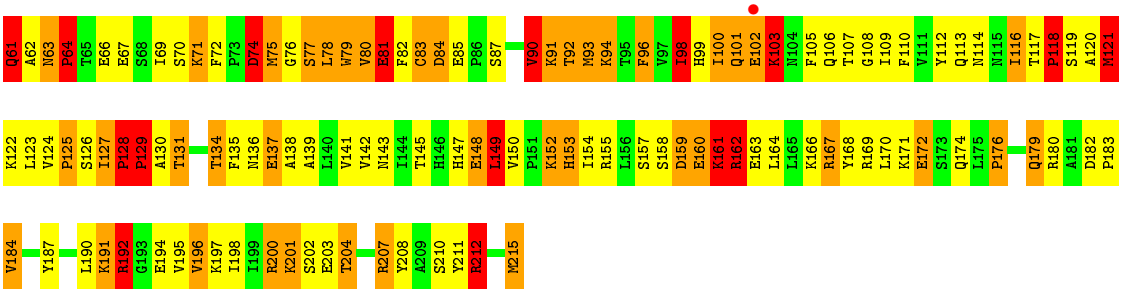
• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide

Chain C:

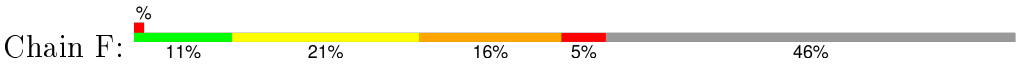


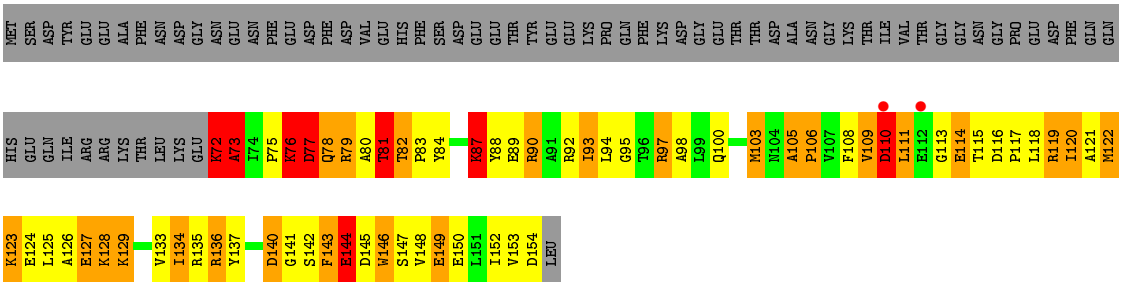
• Molecule 4: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

Chain E:

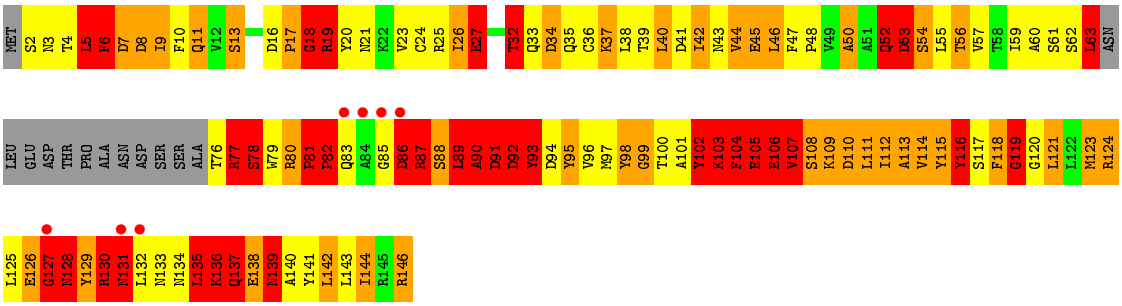


• Molecule 5: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

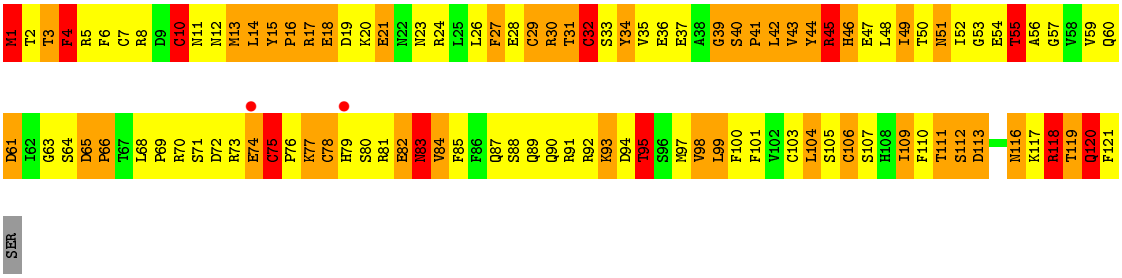




• Molecule 6: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

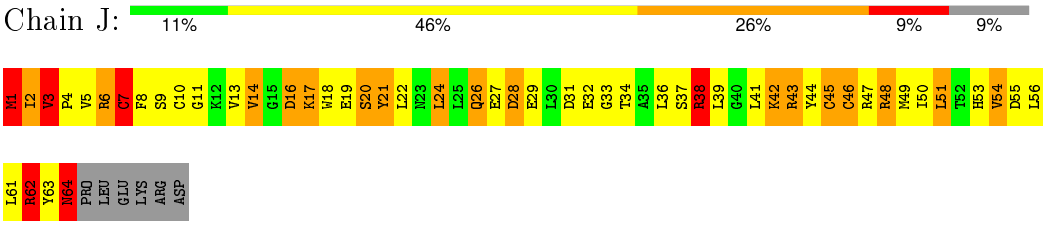


• Molecule 7: DNA-directed RNA polymerase II 14.2 kDa polypeptide



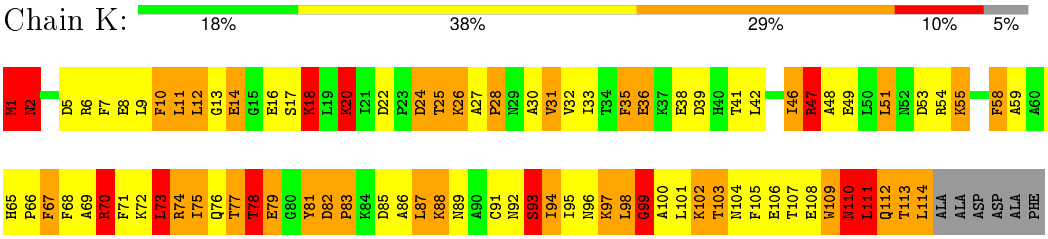
• Molecule 8: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide

Chain J:



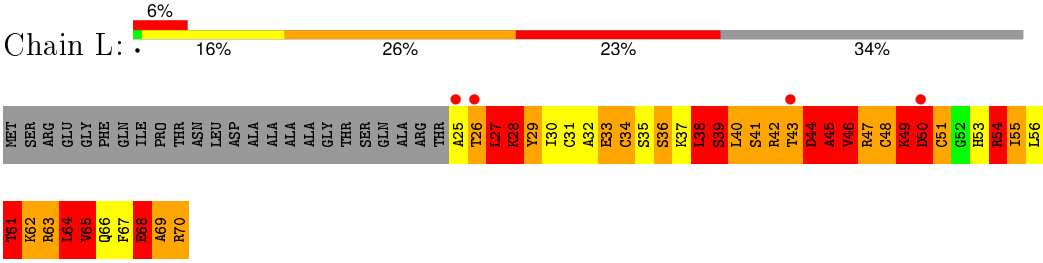
• Molecule 9: DNA-directed RNA polymerase II 13.6 kDa polypeptide

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 – 3.20 39.69 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.20) 97.5 (39.69-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.246 0.205 , 0.246	Depositor DCC
R_{free} test set	2472 reflections (2.97%)	DCC
Wilson B-factor (Å^2)	55.9	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 42.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 93452 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	27757	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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: ZN, MN, ATP

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	3.53	1385/10822 (12.8%)	2.62	715/14641 (4.9%)
2	B	3.54	1164/8860 (13.1%)	2.56	552/11945 (4.6%)
3	C	3.57	288/2133 (13.5%)	2.62	126/2891 (4.4%)
4	E	3.50	210/1796 (11.7%)	2.40	107/2416 (4.4%)
5	F	3.12	78/682 (11.4%)	2.30	35/922 (3.8%)
6	H	3.37	138/1086 (12.7%)	2.46	68/1470 (4.6%)
7	I	3.73	145/1009 (14.4%)	2.69	86/1357 (6.3%)
8	J	3.41	75/533 (14.1%)	3.10	53/715 (7.4%)
9	K	3.36	117/937 (12.5%)	2.65	61/1265 (4.8%)
10	L	3.99	58/366 (15.8%)	2.90	43/485 (8.9%)
All	All	3.52	3658/28224 (13.0%)	2.59	1846/38107 (4.8%)

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	41
2	B	0	40
3	C	0	13
4	E	1	6
5	F	0	2
6	H	0	12
7	I	0	6
8	J	0	1
9	K	0	1
10	L	0	2
All	All	1	124

The worst 5 of 3658 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	552	MET	CG-SD	26.10	2.49	1.81
1	A	728	LYS	CD-CE	24.04	2.11	1.51
2	B	598	GLU	CG-CD	23.97	1.88	1.51
1	A	771	GLU	CD-OE2	23.53	1.51	1.25
3	C	165	LYS	CE-NZ	23.14	2.06	1.49

The worst 5 of 1846 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	774	ARG	NE-CZ-NH1	34.28	137.44	120.30
1	A	469	ARG	NE-CZ-NH2	-32.36	104.12	120.30
1	A	1366	ARG	NE-CZ-NH1	31.49	136.04	120.30
3	C	35	ARG	NE-CZ-NH2	-28.02	106.29	120.30
3	C	34	ARG	NE-CZ-NH2	-27.97	106.32	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	204	THR	CB

5 of 124 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	PRO	Peptide
1	A	165	GLY	Peptide
1	A	44	THR	Peptide
1	A	60	SER	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	10635	0	10688	687	0
2	B	8690	0	8715	513	0
3	C	2095	0	2053	155	0
4	E	1760	0	1788	130	0
5	F	670	0	689	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	1068	0	1040	164	0
7	I	990	0	949	71	0
8	J	525	0	537	42	0
9	K	919	0	929	73	0
10	L	364	0	388	65	0
11	A	2	0	0	0	0
12	A	2	0	0	1	0
12	B	1	0	0	1	0
12	C	1	0	0	2	0
12	I	2	0	0	0	0
12	J	1	0	0	2	0
12	L	1	0	0	1	0
13	A	31	0	12	0	0
All	All	27757	0	27788	1819	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 33.

The worst 5 of 1819 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:1057:LYS:CE	2:B:1057:LYS:CD	1.75	1.65
1:A:368:LYS:CE	1:A:368:LYS:CD	1.75	1.65
4:E:37:LEU:CD1	4:E:37:LEU:CG	1.75	1.64
1:A:919:ILE:CD1	1:A:919:ILE:CG1	1.75	1.64
1:A:1112:LYS:CE	1:A:1112:LYS:CD	1.74	1.64

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	1335/1733 (77%)	1187 (89%)	91 (7%)	57 (4%)	3 25
2	B	1071/1224 (88%)	924 (86%)	104 (10%)	43 (4%)	4 27
3	C	264/318 (83%)	231 (88%)	23 (9%)	10 (4%)	4 28
4	E	213/215 (99%)	183 (86%)	16 (8%)	14 (7%)	1 12
5	F	81/155 (52%)	73 (90%)	6 (7%)	2 (2%)	7 41
6	H	129/146 (88%)	89 (69%)	19 (15%)	21 (16%)	0 1
7	I	119/122 (98%)	110 (92%)	8 (7%)	1 (1%)	24 69
8	J	62/70 (89%)	58 (94%)	4 (6%)	0	100 100
9	K	112/120 (93%)	98 (88%)	12 (11%)	2 (2%)	11 51
10	L	44/70 (63%)	24 (54%)	13 (30%)	7 (16%)	0 1
All	All	3430/4173 (82%)	2977 (87%)	296 (9%)	157 (5%)	3 23

5 of 157 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	45	GLN
1	A	47	ARG
1	A	59	GLY
1	A	60	SER

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	1184/1520 (78%)	998 (84%)	186 (16%)	3 15
2	B	947/1061 (89%)	806 (85%)	141 (15%)	4 17
3	C	234/274 (85%)	194 (83%)	40 (17%)	2 12
4	E	197/197 (100%)	152 (77%)	45 (23%)	1 5
5	F	73/137 (53%)	64 (88%)	9 (12%)	6 27
6	H	117/128 (91%)	73 (62%)	44 (38%)	0 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	I	115/116 (99%)	91 (79%)	24 (21%)	1 7
8	J	59/65 (91%)	49 (83%)	10 (17%)	2 13
9	K	99/102 (97%)	80 (81%)	19 (19%)	2 10
10	L	40/57 (70%)	21 (52%)	19 (48%)	0 0
All	All	3065/3657 (84%)	2528 (82%)	537 (18%)	2 12

5 of 537 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	549	THR
2	B	1056	SER
8	J	48	ARG
2	B	606	LYS
2	B	870	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	433	GLN
2	B	590	HIS
7	I	46	HIS
2	B	513	GLN
2	B	518	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 carbohydrates 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	ATP	A	3011	11	24,33,33	1.10	2 (8%)	31,52,52	2.46	4 (12%)

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	ATP	A	3011	11	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	3011	ATP	C2-N1	2.61	1.38	1.33
13	A	3011	ATP	C2-N3	3.71	1.38	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	3011	ATP	N3-C2-N1	-11.47	120.11	128.89
13	A	3011	ATP	PA-O3A-PB	-4.11	121.17	132.73
13	A	3011	ATP	PB-O3B-PG	-3.48	120.99	132.67
13	A	3011	ATP	C2'-C1'-N9	-2.38	110.65	114.29

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

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

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	A	1352/1733 (78%)	-0.35	32 (2%) 62 47	9, 38, 105, 151	0
2	B	1091/1224 (89%)	-0.24	52 (4%) 34 21	10, 36, 111, 138	0
3	C	266/318 (83%)	-0.44	2 (0%) 87 80	21, 42, 72, 123	0
4	E	215/215 (100%)	-0.23	5 (2%) 64 49	13, 51, 102, 134	0
5	F	83/155 (53%)	-0.35	2 (2%) 62 47	18, 36, 64, 73	0
6	H	133/146 (91%)	0.24	7 (5%) 30 17	41, 79, 121, 132	0
7	I	121/122 (99%)	-0.20	2 (1%) 73 60	23, 44, 78, 108	0
8	J	64/70 (91%)	-0.53	0 100 100	21, 35, 61, 76	0
9	K	114/120 (95%)	-0.29	0 100 100	21, 50, 72, 81	0
10	L	46/70 (65%)	0.30	4 (8%) 13 7	39, 89, 118, 121	0
All	All	3485/4173 (83%)	-0.28	106 (3%) 54 39	9, 41, 107, 151	0

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1109	GLY	9.8
1	A	69	THR	7.9
2	B	1110	PRO	7.7
1	A	248	PRO	7.3
6	H	85	GLY	7.1

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
13	ATP	A	3011	31/31	0.89	0.23	0.63	69,74,83,83	0
12	ZN	C	3002	1/1	0.98	0.06	-1.21	78,78,78,78	0
12	ZN	I	3004	1/1	0.97	0.05	-1.34	144,144,144,144	0
12	ZN	L	3005	1/1	0.69	0.06	-1.45	139,139,139,139	0
12	ZN	A	3008	1/1	0.97	0.03	-1.62	96,96,96,96	0
12	ZN	A	3006	1/1	0.96	0.04	-2.02	124,124,124,124	0
12	ZN	I	3003	1/1	0.87	0.06	-2.24	144,144,144,144	0
12	ZN	J	3001	1/1	0.99	0.09	-3.00	84,84,84,84	0
11	MN	A	3009	1/1	0.98	0.12	-	24,24,24,24	0
11	MN	A	3010	1/1	0.97	0.12	-	29,29,29,29	0
12	ZN	B	3007	1/1	0.93	0.06	-	108,108,108,108	0

6.5 Other polymers (i)

There are no such residues in this entry.