



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 03:48 am BST

PDB ID : 3HOV
Title : Complete RNA polymerase II elongation complex II
Authors : Sydow, J.F.; Brueckner, F.; Cheung, A.C.M.; Damsma, G.E.; Dengl, S.;
Lehmann, E.; Vassilyev, D.; Cramer, P.
Deposited on : 2009-06-03
Resolution : 3.50 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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	:	2.11
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

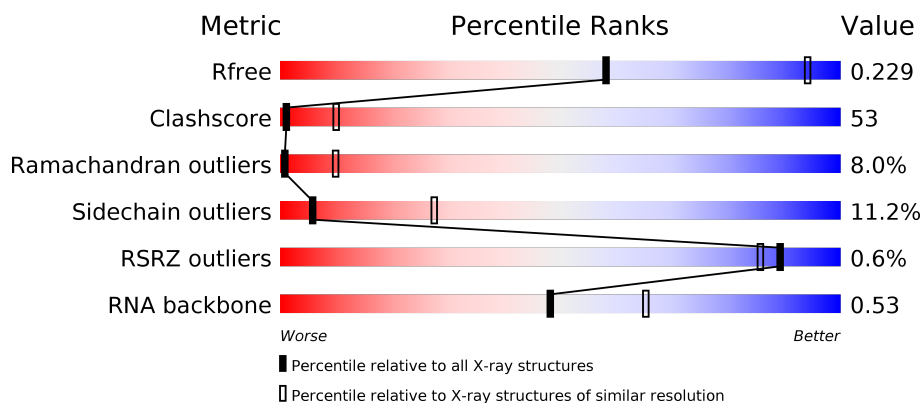
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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.



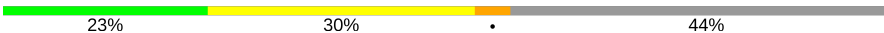
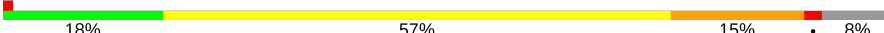

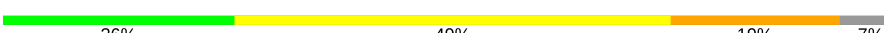
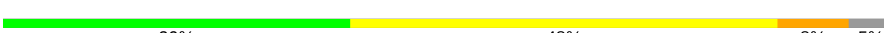
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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 $\leq 5\%$. 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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 15%, yellow 44%, green 27%, grey 18%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 27% 44% 9% • 18% </div> </div>
2	B	1224	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 15%, yellow 52%, green 25%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 25% 52% 12% 10% </div> </div>
3	C	318	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 46%, green 26%, grey 16%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 26% 46% 11% 16% </div> </div>
4	D	221	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, orange 15%, yellow 44%, green 25%, grey 19%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 25% 44% 10% • 19% </div> </div>

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	T	26	
14	N	13	
15	P	17	

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 31777 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1416	Total	C	N	O	S	0	0	0
			11143	7021	1949	2111	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1104	Total	C	N	O	S	0	0	0
			8779	5560	1537	1627	55			

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

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

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	134	Total	C	N	O	S	0	0	0
			1076	677	182	213	4			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 13 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*AP*A*GP*TP*AP*GP*TP*TP*AP*TP*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	T	17	Total	Br	C	N	O	P	0	0	0
			347	1	166	61	103	16			

- Molecule 14 is a DNA chain called 5'-D(*T*AP*CP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	5	Total	C	N	O	P	0	0	0
			97	48	18	27	4			

- Molecule 15 is a RNA chain called 5'-R(*UP*GP*CP*AP*UP*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	10	Total	C	N	O	P	0	0	0
			215	96	42	67	10			

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

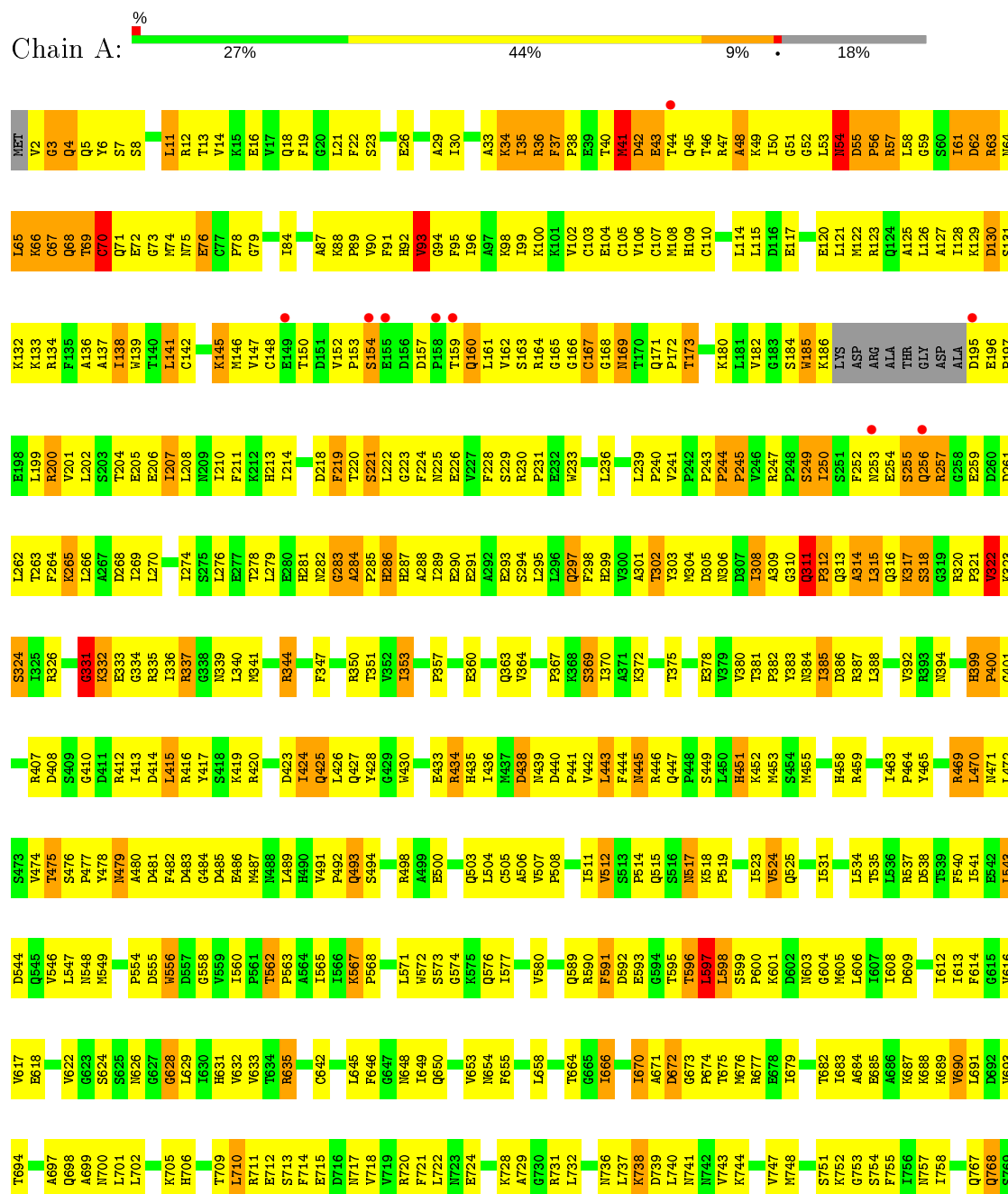
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

3 Residue-property plots

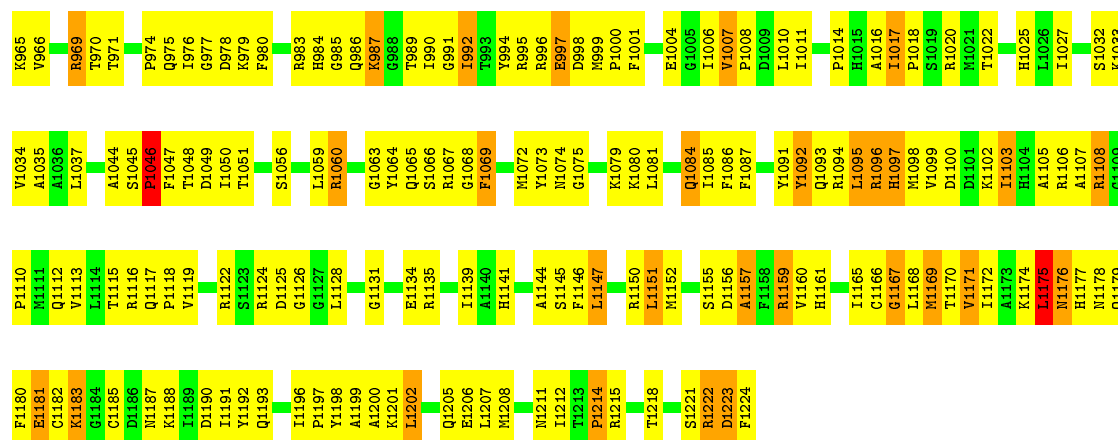
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

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



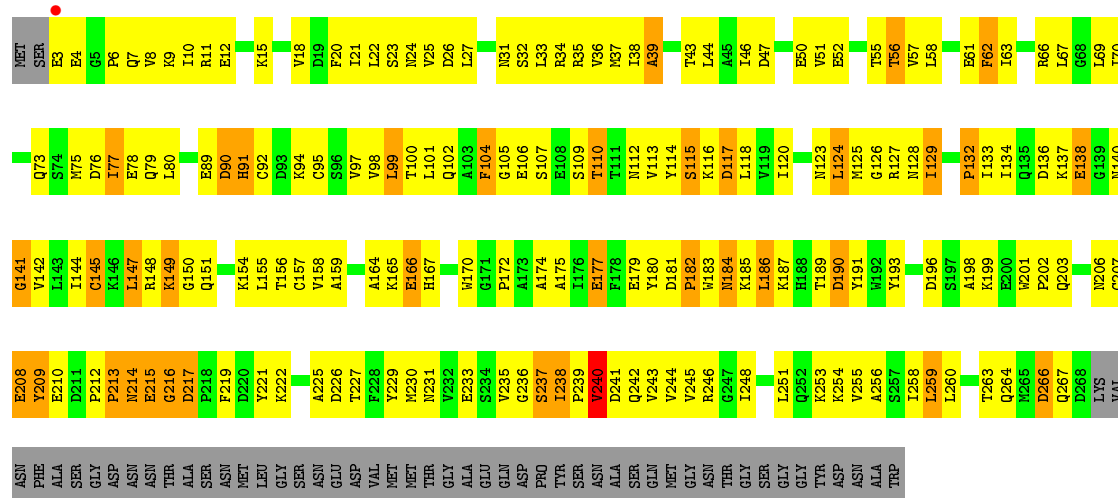


L898	S771	D642	V580	B512	A447	F377	P316	Q255	T185	T123	D61	NET
I899	A772	D643	F581	Q513	I448	L378	C317	Q256	E186	Y124	I62	SER
A900	G773	E644	M583	H514	M449	G379	V318	E187	S187	S125	I63	ASP
	G774	S645	M583	H515	A450	Y380	F319	K258	D188	S126	C64	LEU
S906	K775	L646	M586	M516	K451	M381	D320	K259	B65	G127	B66	ALA
G907	D708	G647	M586	T517	K452	I382		G260	L189	L128	F129	ASN
	L710	H648		H518	K453	N383	V823	K261	S67	F129	S67	SER
V910	E711	K649	V589	H519	K454	N384	I324	E262	T68	V130	T68	GLU
I911	F712	E650	H590	G520	S455	L385	D326	S265	L69	L192	L69	LYS
I912	A713	L651	M592	L521	G456	L386	D327	S266	E194	E194		
G913	E714	K652	N592		L457	L387	R327	S267		K133	I70	TYR
K914	A715	V653	P593	E526	K458		E328	A266	M199	ARG	LEU	THR
T915	ASN	R654	A594	T527	K459		T329	R267	GLN	THR	GLN	ASP
G949	GLU	K655	R595	P528	A460	A330	A330	R267	LEU	TYR	LEU	ASP
L850	GLU	G656	L596	E529	L461	R382	L331	T268		GLU	ALA	PRO
F851	ASN	G656	L597	E530		K393	D332			ALA	ALA	TYR
	M597	E531	G530	K393	G464	D384	D332	I126	I126	I126	HIS	GLY
S919	ASP	L658	E531	Q531	M465	Q395	I334	T272	ASP	VAL	THR	PHE
PRO	LEU	K660	L600	A532	G467	F401	G335	T273	ASP	PRO	GLU	GLU
ASP	D722	L661	R601	L535	E468	F401	ARG	I275	GLY	GLY	GLU	D20
GLU	V723	M662	T602	V536	Q469	F401	GLY	I276	GLY	ARG	SER	E21
GLU		A663	L603	K537	K470	G402	THR	Q278	ASP	ASP	ASP	S22
GLU	R728	T664	R604	M538	L470		ALA	Q278	ASN	GLU	ASN	A23
LEU	R729	E665	R605	L539	LYS		LEU	D279	I126	LEU	I126	P24
GLY	R730	G666	K606		A472		LEU	I280	SER	LYS	SER	I25
GLN	V731	V666	G607	M542	M473	R405	GLY	P281	ARG	TYR	ARG	T26
ARG	S732	Q667	G607		S474	L406	I126		LYS	GLU	LYS	A27
THR	H733	D668	D608	T545	S475	D407	LYS	V283	N221	LEU	TYR	E28
ALA	H734	ILE	I609	S546	R476	L408	K345	I284	I222	ILE	GLU	D29
TYR	A735	GLU	N610	V547	A477		E346	I285	V233	ALA	I90	S30
HIS	T736	GLY	P611	M547	G478	P411	K347	I286	Q224	GLU	S91	X31
S933	T737	PHE	P612	G548	V479		R348	R287	V225	GLU	F92	A32
K934	F738	GLU	V613	T549	S480	F417	I349	A288	F226	SER	G93	V33
R935	T739	ASP	S614	D550		K418	Q350	L289	K227	GLU	I94	I34
D936	H740	VAL	M615	P551	L483	K422	A352	G290	K228	ASP	S95	S35
A937	C741	GLU	R617	P552	M484	K423	K353	I291	Y96	ASP	A36	A36
S938	E742	GLU	D618	I554	R485	K423	L434	I292	SER	SER	V97	F37
	I743	PHE	I619	I555	Y486	L434	D354	P293	A230	GLU	T98	F38
L941	H744	GLU	R620	T556	T487	T425	I355	D294	R99	SER	R99	R39
R942	F745		R621	P557		K426	L355	G295	GLY	P100	E40	E40
S943	S746		K622	L558	S490	K426	L355	G295	M101	M101	M101	K41
T944	M747		G623	S559	T491	I428	Q357	E296	Q42	V102	V102	Q42
E945	I748		L624	E560	L492	F429	E358	L298	N103	N103	N103	L43
N946	L749		G625	W561	S493	R430	F360	E299	V44	E104	E104	V44
G947	G750		I626	G562	Y431	Y431	L361	H300	S45	S105	S105	S45
I948	V751		P627	M563	M432	M432	P362	I301	Q46	Q46	Q46	Q46
V949	A752		D629		R497	R497	R363	C302	R241	G107	G107	Q47
			A630	L566	T498	R434	I364	Y303	S242	V108	V108	L48
V952	I756		G631		P501	T435	T365	D304	A243	T109	T109	D49
L953	P757		R632	Y569	I502	V436	Q366	V305	E245	H110	H110	S50
V954	F758		V570	V570	E437	E437	L367	N306	E245	L111	L111	F51
T955	F759		P571	H572	GLU	GLU	E368	D307	K246	L112	L112	B52
G956	D760		G633	H572	ARG	ALA	G369	W308	Q347	Y113	Y113	Q53
N957			Y634	E696	ASP	HIS	F370	Q309	S248	K177	P114	F54
Q958	Q763		R635	Q573	ASP	ASP	F370	N310	R249	N178	Q115	V55
D959	S764		P636	S574	GLY	ASP	E371	M310	R249	C179	Q115	
G960	S765		L637	P575	LYS	PHE	S372	L311	F250	L178	D56	D56
L961	R766		P638	D576	L508	ASN	R373	E312	I251	Y180	R118	Y57
R962	R766		P639	A577	A509	NET	K374	M313	T252	Y180	L119	T58
F963	Y769		L702	T578	M509	LYS	A375	L314	S252	S182	R120	L59
V964	Q770		B641	R579	P511	L446	F376	K315	L254	S182	R120	Q60



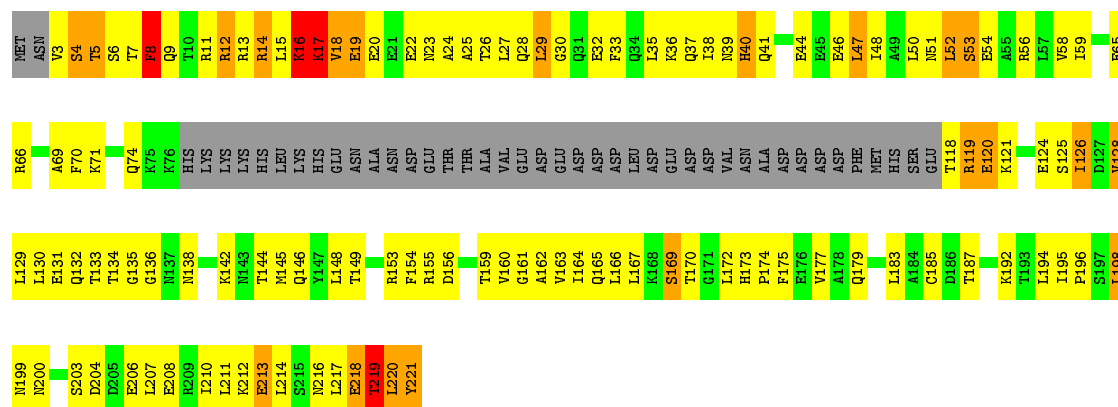
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 26% 46% 11% 16%



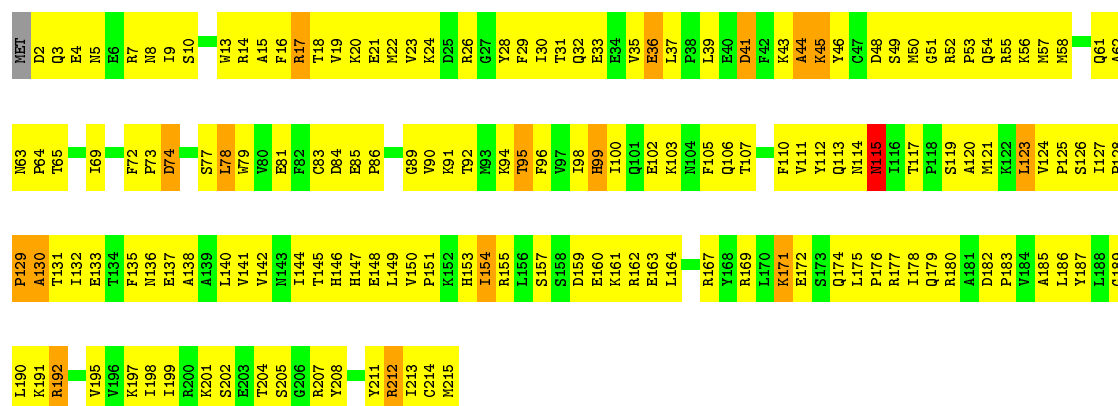
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D: 25% 44% 10% 19%

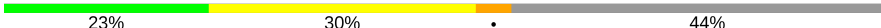


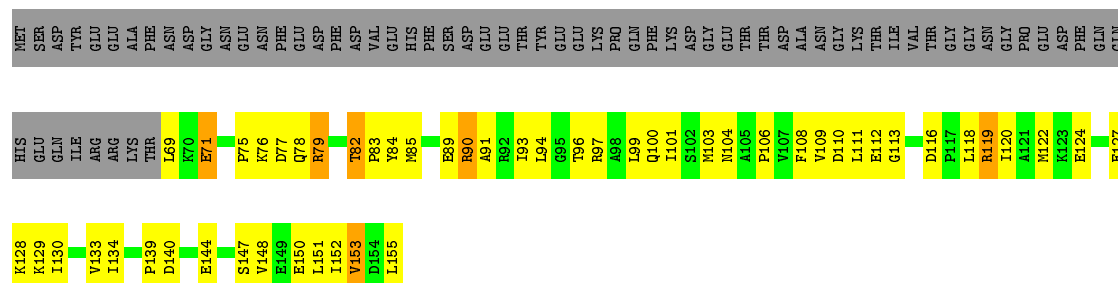
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 



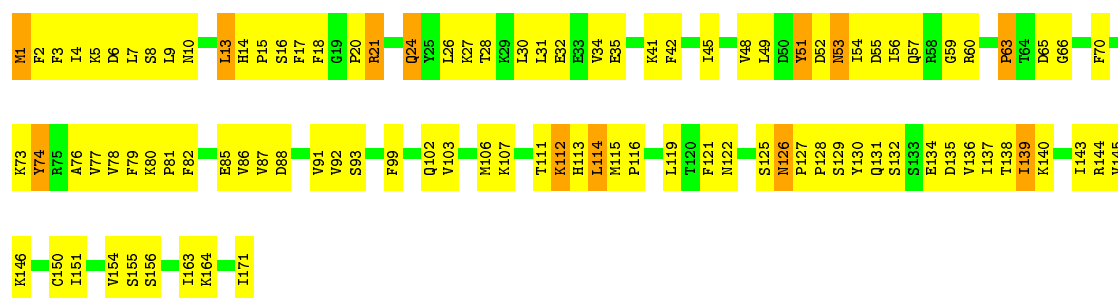
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 



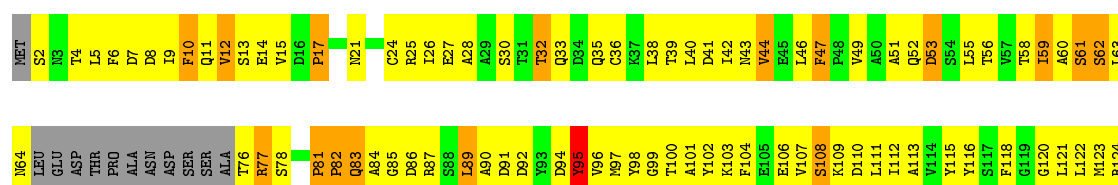
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G: 



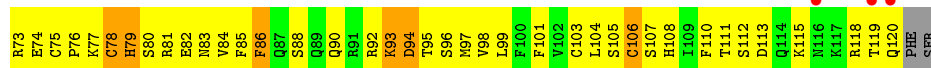
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 

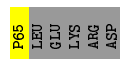




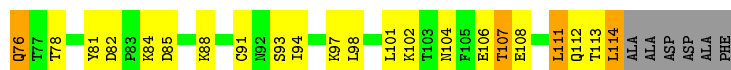
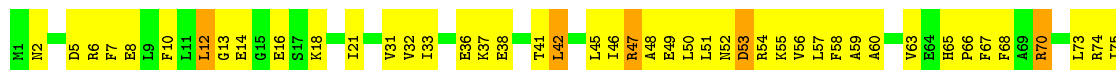
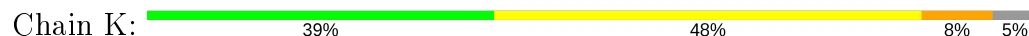
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9



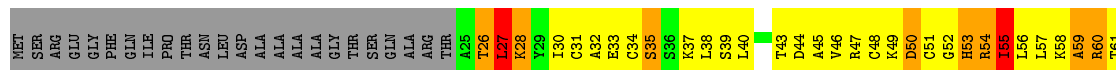
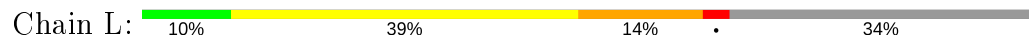
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11



- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 13: 5'-D(*AP*GP*CP*TP*CP*AP*A*GP*TP*AP*GP*TP*TP*AP*TP*GP*CP*C
P*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3'

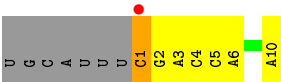




● Molecule 14: 5'-D(*T*AP*CP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3'



● Molecule 15: 5'-R(*UP*GP*CP*AP*UP*UP*UP*CP*GP*AP*CP*CP*AP*GP*GP*CP*A)-3',



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.25Å 393.38Å 283.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50 49.17 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.50) 99.9 (49.17-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.210 , 0.226 0.214 , 0.229	Depositor DCC
R_{free} test set	4056 reflections (2.61%)	wwPDB-VP
Wilson B-factor (Å ²)	85.9	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 99.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.024 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	31777	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, BRU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/11342	0.77	12/15337 (0.1%)
2	B	0.48	0/8948	0.74	1/12062 (0.0%)
3	C	0.47	0/2133	0.75	1/2891 (0.0%)
4	D	0.45	0/1444	0.72	1/1935 (0.1%)
5	E	0.45	0/1788	0.68	1/2406 (0.0%)
6	F	0.56	0/717	0.80	1/967 (0.1%)
7	G	0.48	0/1368	0.76	1/1844 (0.1%)
8	H	0.43	0/1094	0.72	0/1481
9	I	0.44	0/989	0.71	0/1331
10	J	0.50	0/541	0.83	0/727
11	K	0.48	0/937	0.67	0/1265
12	L	0.57	0/365	0.84	0/485
13	T	0.54	0/365	0.85	0/560
14	N	0.57	0/108	0.78	0/164
15	P	0.45	0/240	0.82	1/372 (0.3%)
All	All	0.48	0/32379	0.75	19/43827 (0.0%)

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
2	B	0	1
8	H	0	1
13	T	0	3
All	All	0	5

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	PRO	N-CA-C	-6.45	95.34	112.10
3	C	39	ALA	N-CA-C	6.38	128.24	111.00
1	A	55	ASP	N-CA-CB	6.13	121.63	110.60
1	A	3	GLY	N-CA-C	-6.04	97.99	113.10
15	P	1	C	N1-C1'-C2'	5.90	121.67	114.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1192	TYR	Sidechain
8	H	102	TYR	Sidechain
13	T	18	DA	Sidechain
13	T	19	DT	Sidechain
13	T	21	DC	Sidechain

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	A	11143	0	11217	1194	0
2	B	8779	0	8808	1069	0
3	C	2095	0	2051	259	0
4	D	1434	0	1460	156	0
5	E	1752	0	1776	193	0
6	F	705	0	731	75	0
7	G	1340	0	1357	133	0
8	H	1076	0	1046	159	0
9	I	971	0	929	118	0
10	J	532	0	542	77	0
11	K	919	0	929	82	0
12	L	363	0	388	85	0
13	T	347	0	192	20	0
14	N	97	0	58	6	0
15	P	215	0	111	7	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
All	All	31777	0	31595	3348	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 53.

The worst 5 of 3348 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:559:SER:HA	2:B:563:MET:HB3	1.20	1.18
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.08	1.17
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.28	1.14
2:B:261:ARG:HH11	2:B:261:ARG:HB3	1.12	1.13
1:A:53:LEU:HD23	1:A:54:ASN:N	1.65	1.12

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	1406/1733 (81%)	1062 (76%)	240 (17%)	104 (7%)	1	11
2	B	1082/1224 (88%)	795 (74%)	188 (17%)	99 (9%)	1	8
3	C	264/318 (83%)	200 (76%)	45 (17%)	19 (7%)	1	11
4	D	174/221 (79%)	131 (75%)	29 (17%)	14 (8%)	1	10
5	E	212/215 (99%)	159 (75%)	40 (19%)	13 (6%)	1	15
6	F	85/155 (55%)	72 (85%)	12 (14%)	1 (1%)	13	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	169/171 (99%)	143 (85%)	20 (12%)	6 (4%)	3	26
8	H	130/146 (89%)	86 (66%)	23 (18%)	21 (16%)	0	2
9	I	117/122 (96%)	76 (65%)	31 (26%)	10 (8%)	1	9
10	J	63/70 (90%)	44 (70%)	10 (16%)	9 (14%)	0	3
11	K	112/120 (93%)	90 (80%)	19 (17%)	3 (3%)	5	33
12	L	44/70 (63%)	18 (41%)	16 (36%)	10 (23%)	0	1
All	All	3858/4565 (84%)	2876 (74%)	673 (17%)	309 (8%)	1	10

5 of 309 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	43	GLU
1	A	54	ASN
1	A	57	ARG
1	A	58	LEU

5.3.2 Protein sidechains ⓘ

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	1239/1520 (82%)	1099 (89%)	140 (11%)	6	27
2	B	958/1061 (90%)	845 (88%)	113 (12%)	5	25
3	C	234/274 (85%)	205 (88%)	29 (12%)	4	23
4	D	160/200 (80%)	134 (84%)	26 (16%)	2	13
5	E	196/197 (100%)	180 (92%)	16 (8%)	11	40
6	F	77/137 (56%)	70 (91%)	7 (9%)	9	36
7	G	152/152 (100%)	138 (91%)	14 (9%)	9	36
8	H	118/128 (92%)	105 (89%)	13 (11%)	6	29
9	I	113/116 (97%)	106 (94%)	7 (6%)	18	51
10	J	60/65 (92%)	53 (88%)	7 (12%)	5	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	99/102 (97%)	91 (92%)	8 (8%)	11	41
12	L	40/57 (70%)	35 (88%)	5 (12%)	4	23
All	All	3446/4009 (86%)	3061 (89%)	385 (11%)	6	27

5 of 385 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	452	THR
2	B	889	THR
8	H	138	GLU
2	B	475	SER
2	B	645	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	484	ASN
2	B	835	GLN
8	H	128	ASN
2	B	513	GLN
2	B	573	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/17 (52%)	0	0

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 ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	BRU	T	23	13,15	15,21,22	4.02	4 (26%)	17,30,33	3.98	4 (23%)

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	BRU	T	23	13,15	-	1/4/21/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	23	BRU	BR-C5	-14.02	1.50	1.90
13	T	23	BRU	C4-C5	5.17	1.45	1.38
13	T	23	BRU	C4-N3	3.57	1.39	1.33
13	T	23	BRU	C6-C5	-2.23	1.34	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	23	BRU	C4-N3-C2	14.05	127.01	115.14
13	T	23	BRU	C5-C4-N3	-6.94	115.33	123.64
13	T	23	BRU	C5-C6-N1	2.97	123.81	119.97
13	T	23	BRU	BR-C5-C6	2.56	123.13	117.31

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	T	23	BRU	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T	23	BRU	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 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	1416/1733 (81%)	-0.27	10 (0%) 87 83	28, 72, 115, 145	0
2	B	1104/1224 (90%)	-0.22	8 (0%) 87 83	28, 85, 126, 140	0
3	C	266/318 (83%)	-0.24	1 (0%) 92 90	41, 71, 107, 125	0
4	D	178/221 (80%)	-0.11	0 100 100	52, 84, 120, 134	0
5	E	214/215 (99%)	-0.05	0 100 100	52, 103, 130, 138	0
6	F	87/155 (56%)	-0.56	0 100 100	32, 51, 81, 91	0
7	G	171/171 (100%)	-0.24	0 100 100	48, 71, 104, 117	0
8	H	134/146 (91%)	0.23	1 (0%) 87 83	79, 109, 127, 139	0
9	I	119/122 (97%)	0.03	3 (2%) 57 51	66, 106, 126, 144	0
10	J	65/70 (92%)	-0.39	0 100 100	49, 68, 95, 107	0
11	K	114/120 (95%)	-0.24	0 100 100	36, 76, 95, 112	0
12	L	46/70 (65%)	0.01	0 100 100	48, 111, 129, 130	0
13	T	16/26 (61%)	0.46	0 100 100	99, 137, 166, 166	0
14	N	5/13 (38%)	1.41	1 (20%) 1 1	143, 147, 156, 171	0
15	P	10/17 (58%)	0.64	1 (10%) 7 8	122, 129, 147, 153	0
All	All	3945/4621 (85%)	-0.20	25 (0%) 89 86	28, 80, 124, 171	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1455	PRO	4.0
2	B	918	ILE	3.3
9	I	120	GLN	3.0
15	P	1	C	2.9
14	N	1	DA	2.9

6.2 Non-standard residues in protein, DNA, RNA chains [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	BRU	T	23	20/21	0.74	0.26	127,131,137,139	0

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. 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
17	MG	A	2458	1/1	0.73	0.32	123,123,123,123	0
16	ZN	L	1071	1/1	0.91	0.08	111,111,111,111	0
16	ZN	I	1122	1/1	0.95	0.05	122,122,122,122	0
16	ZN	A	2456	1/1	0.97	0.05	86,86,86,86	0
16	ZN	J	1066	1/1	0.99	0.21	61,61,61,61	0
16	ZN	C	1269	1/1	0.99	0.10	49,49,49,49	0
16	ZN	I	1121	1/1	0.99	0.10	90,90,90,90	0
16	ZN	B	2225	1/1	0.99	0.17	54,54,54,54	0
16	ZN	A	2457	1/1	0.99	0.14	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.