



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 06:33 AM GMT

PDB ID : 3H0G  
Title : RNA Polymerase II from Schizosaccharomyces pombe  
Authors : Spahr, H.; Calero, G.; Bushnell, D.A.; Kornberg, R.D.  
Deposited on : 2009-04-09  
Resolution : 3.65 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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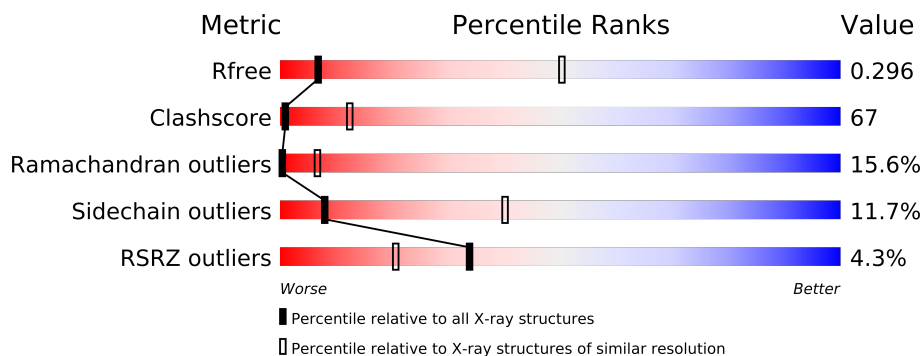
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.65 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.







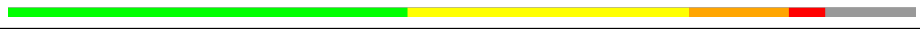
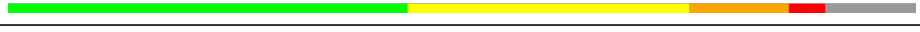



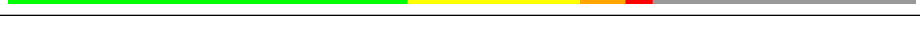
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1021 (3.94-3.38)
Clashscore	79885	1025 (3.90-3.42)
Ramachandran outliers	78287	1195 (3.92-3.40)
Sidechain outliers	78261	1193 (3.92-3.40)
RSRZ outliers	66119	1021 (3.94-3.38)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1752	
1	M	1752	
2	B	1210	
2	N	1210	
3	C	297	
3	O	297	
4	D	135	
4	P	135	
5	E	210	
5	Q	210	
6	F	142	
6	R	142	
7	G	172	
7	S	172	

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Mol	Chain	Length	Quality of chain
8	H	125	
8	T	125	
9	I	113	
9	U	113	
10	J	71	
10	V	71	
11	K	123	
11	W	123	
12	L	63	
12	X	63	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
14	MG	A	2458	-	X

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 62870 atoms, of which 0 are hydrogen and 0 are deuterium.

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	1496	Total	C	N	O	S	0	0	0
			11802	7415	2071	2246	70			
1	M	1476	Total	C	N	O	S	0	0	0
			11666	7334	2047	2216	69			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1150	Total	C	N	O	S	0	0	0
			9180	5772	1630	1716	62			
2	N	1150	Total	C	N	O	S	0	0	0
			9180	5772	1630	1716	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	263	Total	C	N	O	S	0	0	0
			2088	1315	355	406	12			
3	O	263	Total	C	N	O	S	0	0	0
			2088	1315	355	406	12			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit rpb4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	130	Total	C	N	O	S	0	0	0
			1036	649	176	205	6			
4	P	130	Total	C	N	O	S	0	0	0
			1036	649	176	205	6			

- 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	207	Total	C	N	O	S	0	0	0
			1663	1050	301	306	6			
5	Q	207	Total	C	N	O	S	0	0	0
			1663	1050	301	306	6			

- 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	83	Total	C	N	O	S	0	0	0
			656	416	112	125	3			
6	R	83	Total	C	N	O	S	0	0	0
			656	416	112	125	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit rpb7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	170	Total	C	N	O	S	0	0	0
			1330	860	217	247	6			
7	S	170	Total	C	N	O	S	0	0	0
			1330	860	217	247	6			

- 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	124	Total	C	N	O	S	0	0	0
			996	631	167	195	3			
8	T	124	Total	C	N	O	S	0	0	0
			996	631	167	195	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	111	Total	C	N	O	S	0	0	0
			902	551	164	176	11			
9	U	111	Total	C	N	O	S	0	0	0
			902	551	164	176	11			

- 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	64	Total	C	N	O	S	0	0	0
			518	330	87	94	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	V	64	Total	C	N	O	S	0	0	0
			518	330	87	94	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			955	608	159	182	6			
11	W	119	Total	C	N	O	S	0	0	0
			955	608	159	182	6			

- 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	45	Total	C	N	O	S	0	0	0
			368	225	74	61	8			
12	X	45	Total	C	N	O	S	0	0	0
			368	225	74	61	8			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		
13	B	1	Total	Zn	0	0
			1	1		
13	I	2	Total	Zn	0	0
			2	2		
13	C	1	Total	Zn	0	0
			1	1		
13	V	1	Total	Zn	0	0
			1	1		
13	A	2	Total	Zn	0	0
			2	2		
13	N	1	Total	Zn	0	0
			1	1		
13	U	2	Total	Zn	0	0
			2	2		
13	X	1	Total	Zn	0	0
			1	1		
13	O	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	L	1	Total 1	Zn 1	0	0
13	M	2	Total 2	Zn 2	0	0

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

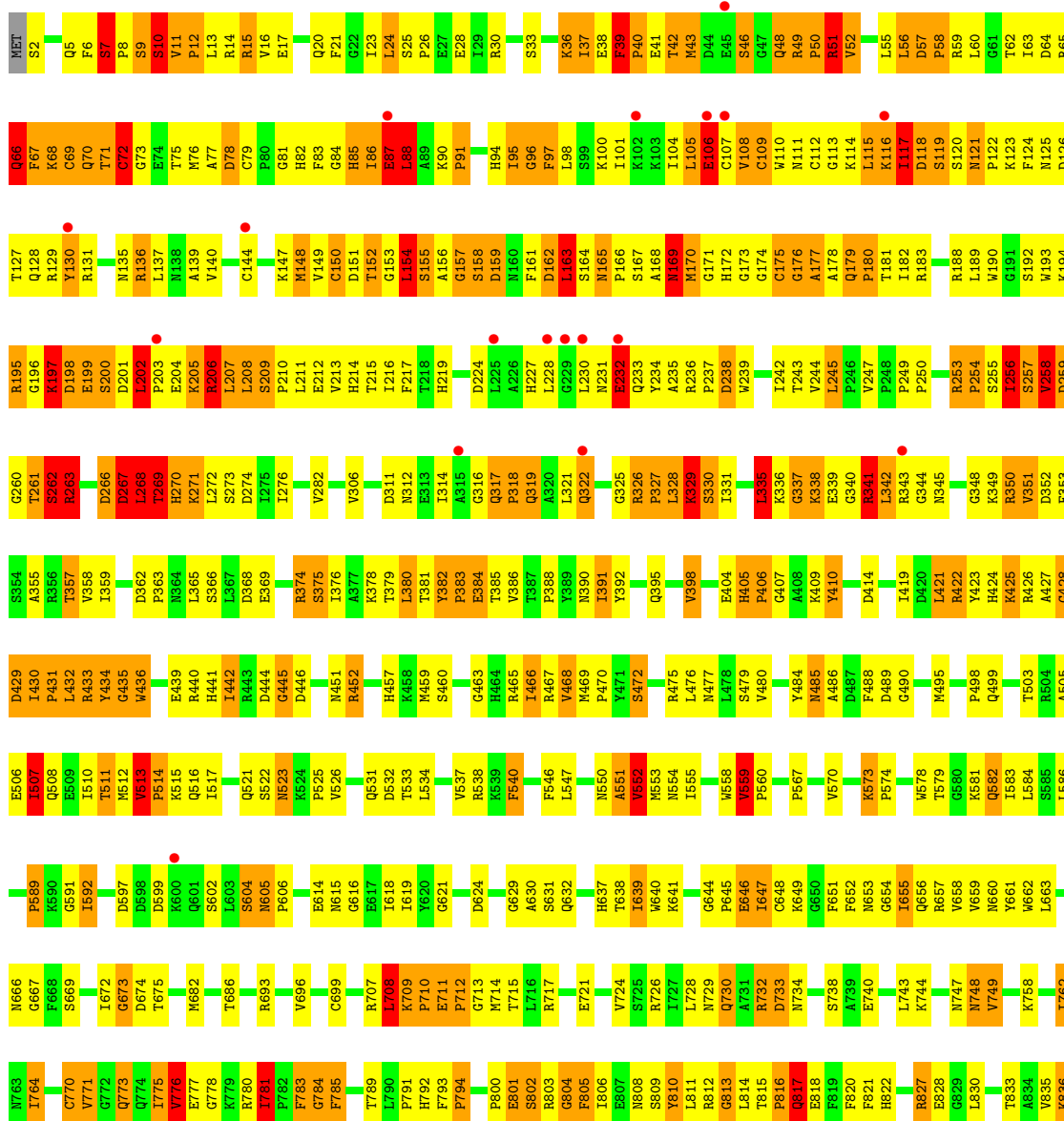
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total 1	Mg 1	0	0
14	M	1	Total 1	Mg 1	0	0

### 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 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 subunit rpb1

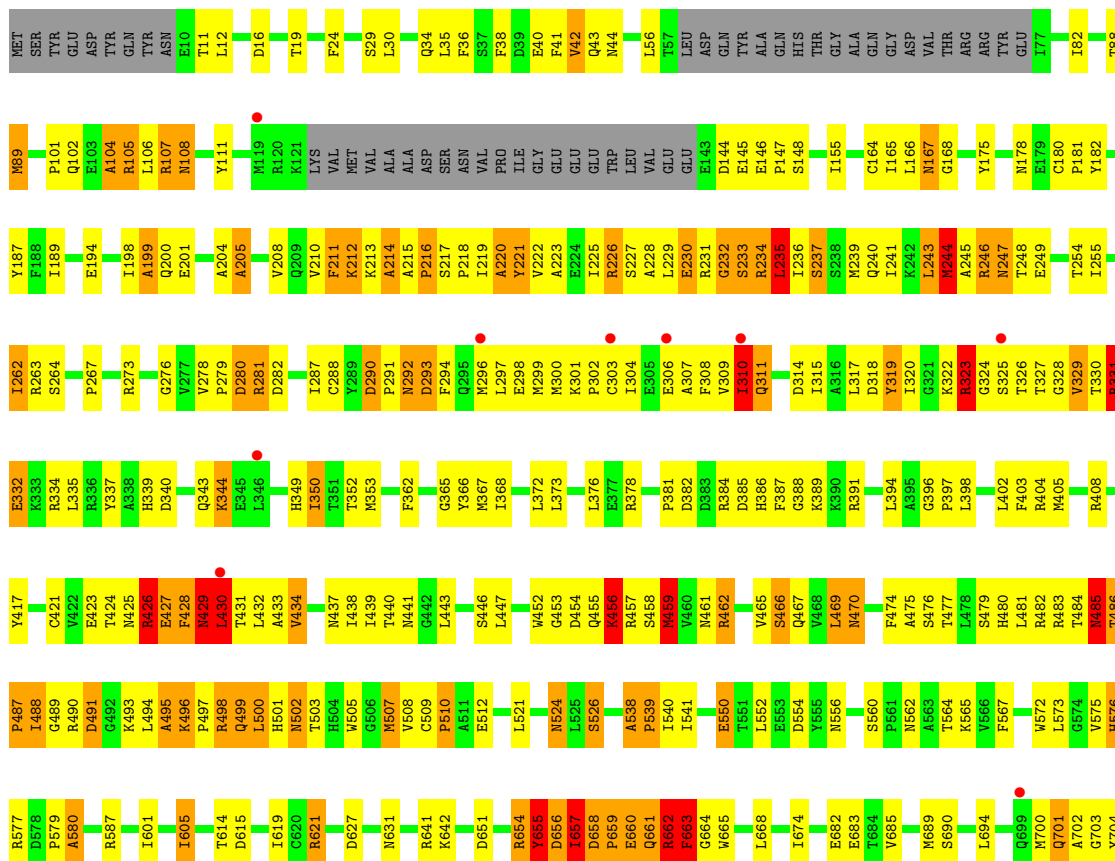
Chain A: 

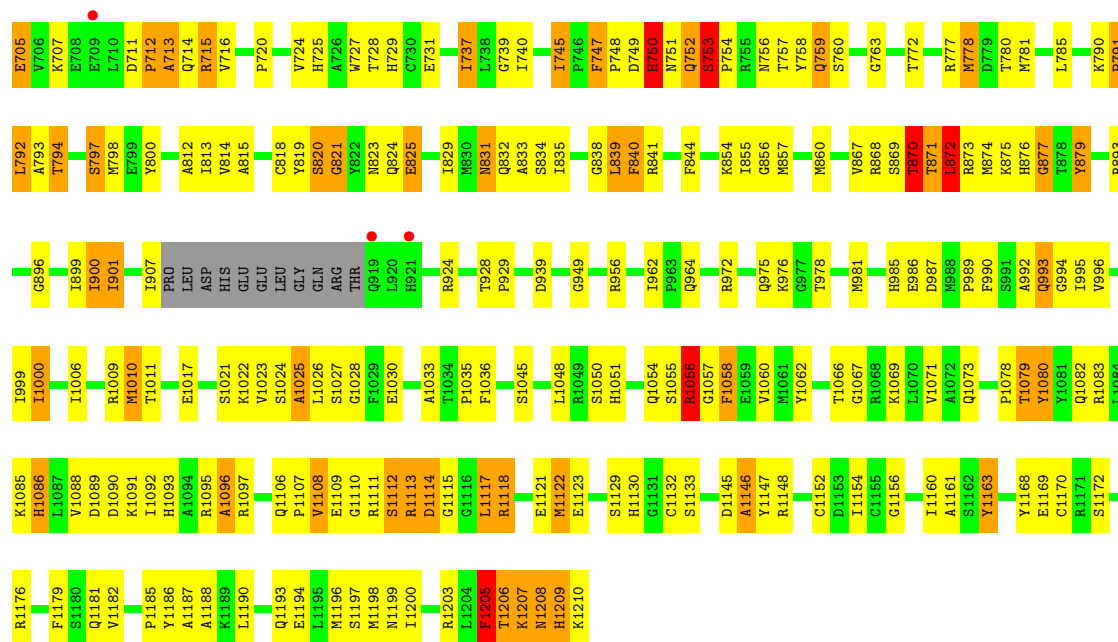


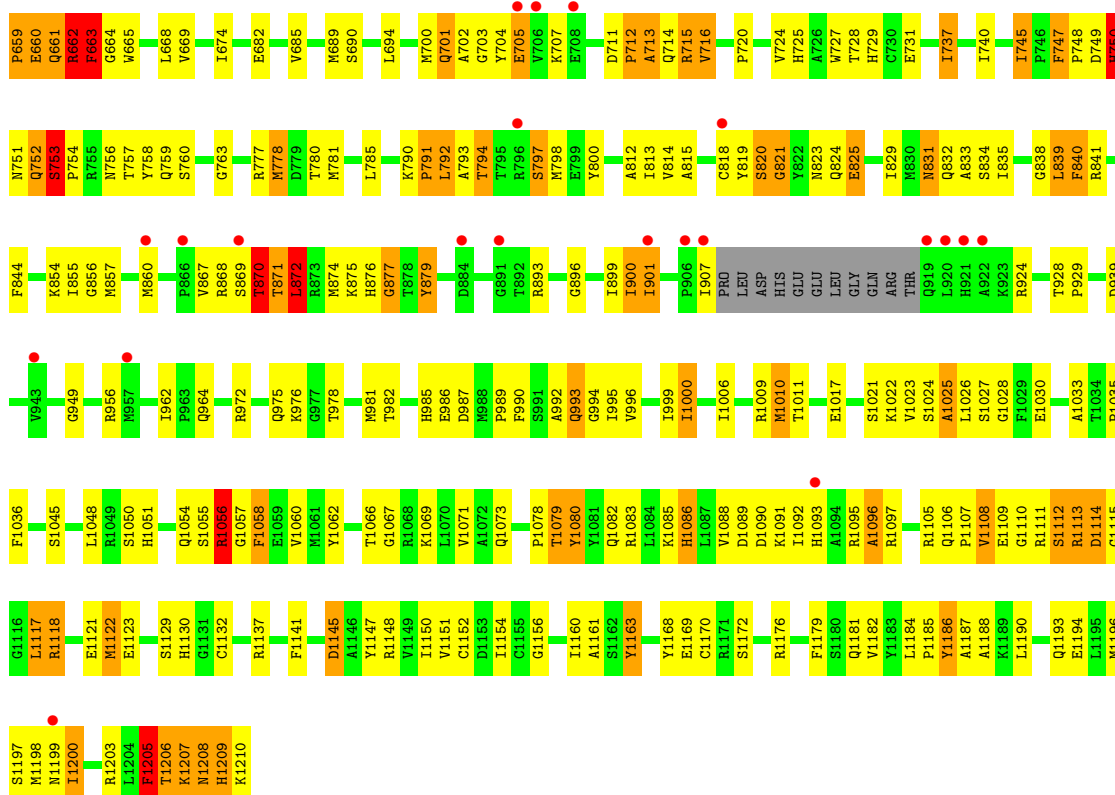




K1252	P1180	A1111	L1040	H917	R827	K744	I655	K573	F488	D414	R341	P254	R188	D126
A1253	D1181	K1112	N1041	E918	E828	N747	Q656	F574	D489	T419	L342	S255	L189	T127
D1254	E1183	N1113	V1042	N919	G829	N748	R657	W578	M495	G420	G343	S256	W190	Q128
D1255	E1184	N1114	S920	N920	L830	V749	R658	T579	M496	L421	G344	S257	G191	R129
D1256	E1185	K1115	A1044	I921	V749	V749	V659	T579	V497	R422	N345	D258	S192	Y130
M1259	E1186	T1116	E922	E922	T833	K758	N660	G580	V497	R422	G348	G260	W193	R131
I1260	N1187	S1117	N923	N923	A834	K758	Y661	K581	P498	Y423	G349	T261	K194	N135
E1261	L1188	M1048	D924	D924	V835	I762	W662	Q582	Q499	H424	R350	S262	R195	R136
E1262	L1189	G1049	S925	S925	R836	I762	L663	L583	T503	R425	V351	R263	G196	L137
D1263	K1189	E1051	N926	N926	T837	N763	N666	L584	R504	R426	G352	R264	D197	N138
D1264	K1190	N927	S927	S927	A838	I764	N666	S585	R504	A427	F353	E265	E199	A139
V1265	Q1191	V928	V928	V928	E839	I764	G667	L586	A505	G428	S354	D266	S200	V140
L1266	S1192	D928	D928	D928	T840	C770	F668	F589	I507	D429	A355	D267	S201	W141
M1273	P1193	P1125	S1062	S1062	G841	V771	S669	I592	Q508	I430	R356	L268	L202	N142
L1274	W1194	W1126	G1064	G1064	T842	G772	I672	I592	Q508	P431	R356	L269	L203	V143
E1275	L1195	C946	C946	C946	T843	G773	G673	G509	E509	L432	V352	E270	E204	K144
L1276	L1196	E1065	E1065	E1065	Q844	Q774	G674	D597	T511	R433	V358	H270	K205	K145
S1276	A1129	M1066	M1066	M1066	R845	I775	D674	D597	T511	Y434	V359	K271	K206	T146
I1277	N1130	V1067	V1067	V1067	R846	N776	T675	D599	V513	C435	D362	L272	R206	T146
S1278	M1131	M1131	L1070	L1070	K849	E777	M652	D599	V513	W436	D362	S273	L207	K147
R1278	A1203	A1071	A1071	A1071	G778	G778	I672	S602	K515	E439	L365	D274	L208	M148
L1279	K1204	K952	K952	K952	K779	K779	I672	S602	K515	R440	S366	I275	S209	V149
G1281	M1205	G953	G953	G953	R780	R780	G673	L603	Q516	R440	S366	I276	P210	C150
V1282	D1207	D954	D954	D954	I781	I781	G674	S604	I517	H441	L367	K277	L211	D151
P1283	K1208	W957	W957	W957	F782	F782	T675	N605	I517	I442	D368	V282	E212	T152
M1284	K1209	P957	P957	P957	F783	F783	V696	P606	Q521	R443	E369	V282	V213	G153
L1286	M1212	P957	P957	P957	G785	G785	V696	P606	S222	D444	E369	V282	E212	T152
T1286	S1213	V961	V961	V961	F785	F785	E614	E614	S522	R444	E369	V282	E212	T152
V1288	M1214	G962	G962	G962	T789	T789	C699	C699	N523	G445	R374	E286	T215	S155
L1289	V1215	V963	V963	V963	I790	I790	L703	L703	K524	D446	R374	E286	T215	S155
M1290	A1216	R964	R964	R964	F791	F791	K709	K709	N615	D446	R374	E286	T215	S155
M1291	G1217	R965	R965	R965	H792	H792	P710	P710	K524	D446	R374	E286	T215	S155
K1294	F1223	N969	N969	N969	F793	F793	E711	E711	K524	D446	R374	E286	T215	S155
I1295	R1225	N969	N969	N969	F794	F794	P712	P712	K524	D446	R374	E286	T215	S155
T1303	D1226	N969	N969	N969	F794	F794	P712	P712	K524	D446	R374	E286	T215	S155
A1307	F1228	N969	N969	N969	F794	F794	P712	P712	K524	D446	R374	E286	T215	S155
D1308	T1229	N969	N969	N969	F794	F794	P712	P712	K524	D446	R374	E286	T215	S155
E1309	I1230	N969	N969	N969	F794	F794	P712	P712	K524	D446	R374	E286	T215	S155
V1310	D1234	N969	N969	N969	F794	F794	P712	P712	K524	D446	R374	E286	T215	S155
L1311	R1234	N969	N969	N969	F794	F794	P712	P712	K524	D446	R374	E286	T215	S155
L1312	K1238	N969	N969	N969	F794	F794	P712	P712	K524	D446	R374	E286	T215	S155
E1313	L1239	N969	N969	N969	F794	F794	P712	P712	K524	D446	R374	E286	T215	S155
T1314	I1240	N969	N969	N969	F794	F794	P712	P712	K524	D446	R374	E286	T215	S155
A1317	H1241	N969	N969	N969	F794	F794	P712	P712	K524	D446	R374	E286	T215	S155
N1316	R1242	N969	N969	N969	F794	F794	P712	P712	K524	D446	R374	E286	T215	S155
L1319	C1243	N969	N969	N969	F794	F794	P712	P712	K524	D446	R374	E286	T215	S155
T1320	R1244	N969	N969	N969	F794	F794	P712	P712	K524	D446	R374	E286	T215	S155
E1321	I1245	N969	N969	N969	F794	F794	P712	P712	K524	D446	R374	E286	T215	S155
A1322	L1246	N969	N969	N969	F794	F794	P712	P712	K524	D446	R374	E286	T215	S155
M1323	R1247	N969	N969	N969	F794	F794	P712	P712	K524	D446	R374	E286	T215	S155
G1327	D1248	N969	N969	N969	F794	F794	P712	P712	K524	D446	R374	E286	T215	S155
V1328	C1250	N969	N969	N969	F794	F794	P712	P712	K524	D446	R374	E286	T215	S155
D1329	R1251	N969	N969	N969	F794	F794	P712	P712	K524	D446	R374	E286	T215	S155

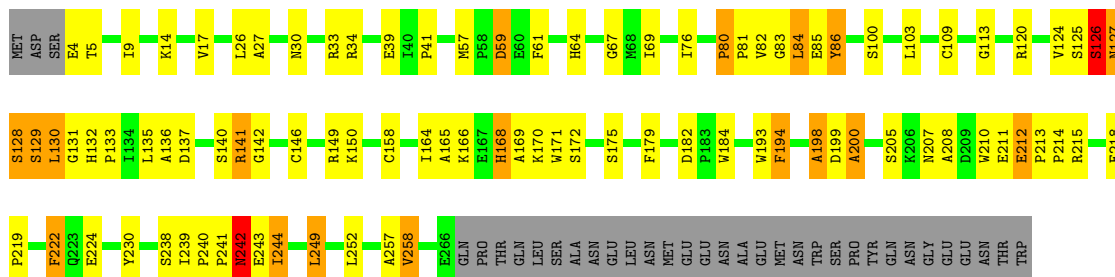






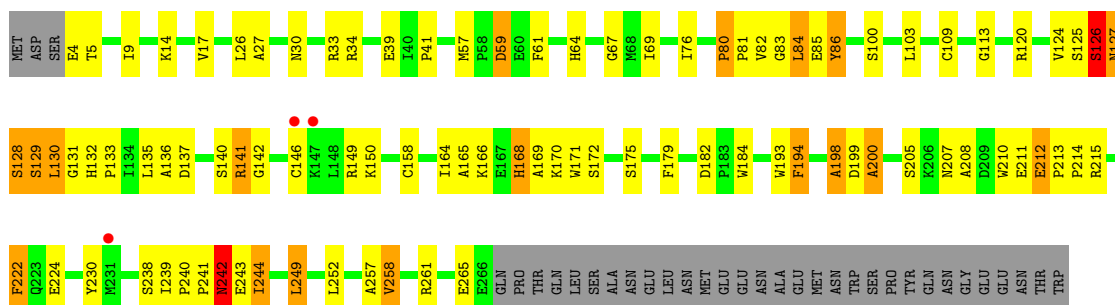
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



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

Chain O:



- Molecule 4: DNA-directed RNA polymerase II subunit rpb4

A66	R67	F68	K69	T70	A71	E72	G73	T74	Y75		L80	L81	R84	F85	H86	K87	F88	E89	R90	A91	G92	L93	G94	T95	L96	C97	G98	E99	D100	A101	E102	E103	A104		L111	A112		T115	D116	D117	Q118	N119	L120		L124		T129	L130	R131	K132	F133	Q134	D135
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- Molecule 4: DNA-directed RNA polymerase II subunit rpb4

F65	A66	R67	F68	K69	T70	A71	E72	A73	T74	Y75	E78	R79	L80	L81	R84	F85	H86	K87	F88	E89	R90	A91	T95	L96	C97	C98	E99	D100	A101	E102	F103	A104	L111	A112	L115	D116	L117	Q118	N119	L120	L124	T129	L130	R131	K132	F133	D134	Q135
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- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

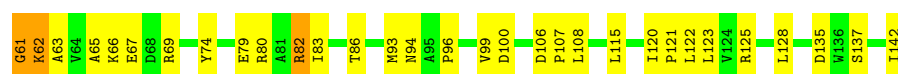
A210

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

S197	E198	T199	S200	G201	R202		C209	A210
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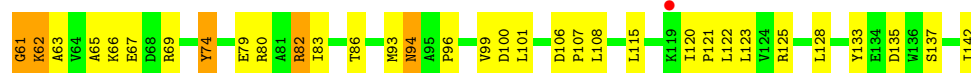
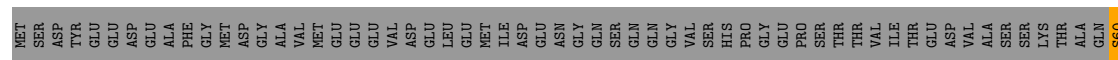
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

[illegible]



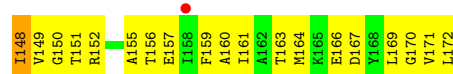
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain R:



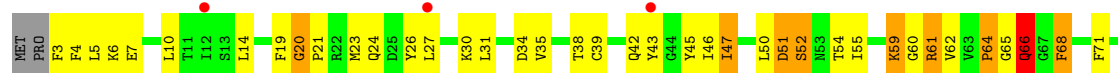
- Molecule 7: DNA-directed RNA polymerase II subunit rpb7

Chain G:



- Molecule 7: DNA-directed RNA polymerase II subunit rpb7

Chain S:



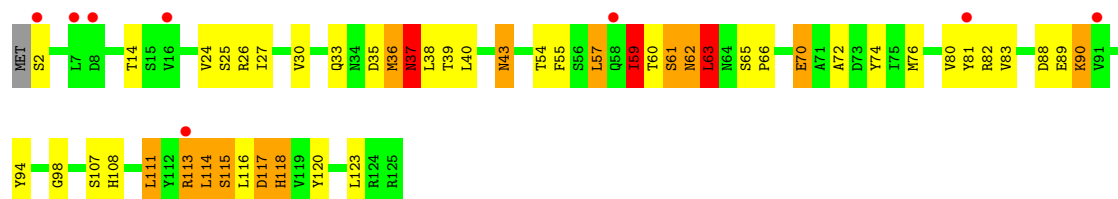
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



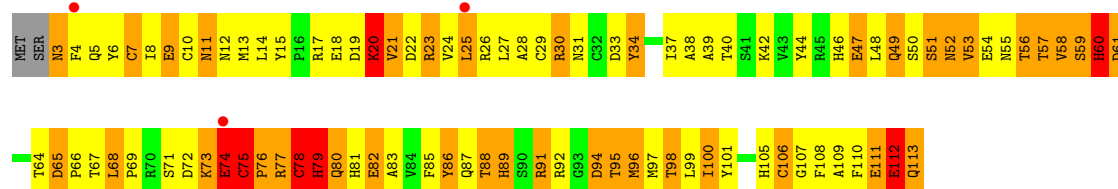
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain T:



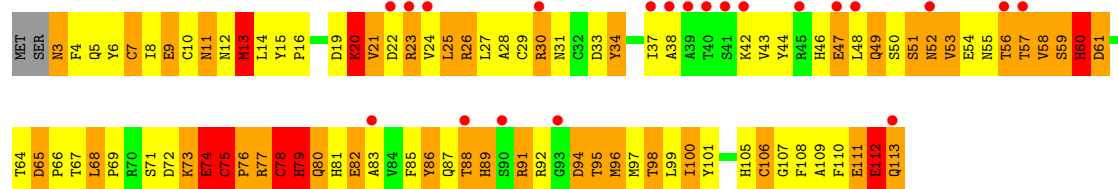
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



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

Chain U:



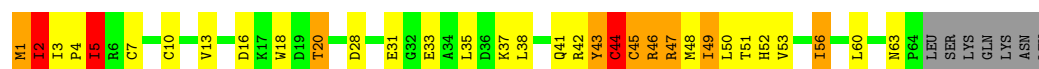
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



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

Chain V:



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

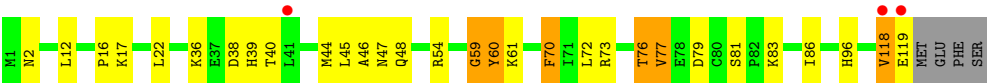
Chain K:



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

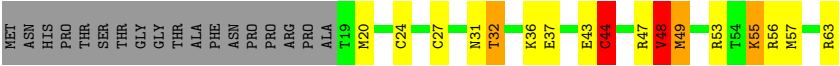
Chain W:





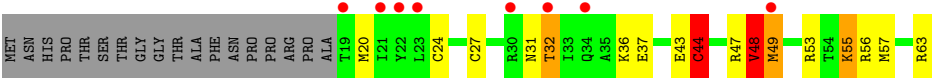
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



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

Chain X:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.03Å 202.68Å 391.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 3.65 48.69 – 3.65	Depositor EDS
% Data completeness (in resolution range)	92.8 (48.70-3.65) 96.2 (48.69-3.65)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.297 , 0.321 0.292 , 0.296	Depositor DCC
$R_{free}$ test set	6923 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	125.6	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 115.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	1 of 138803 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	62870	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	203.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.41	0/12026	0.57	1/16260 (0.0%)
1	M	0.42	0/11887	0.56	1/16069 (0.0%)
2	B	0.44	0/9360	0.60	5/12643 (0.0%)
2	N	0.43	0/9360	0.59	5/12643 (0.0%)
3	C	0.44	0/2135	0.60	0/2904
3	O	0.44	0/2135	0.59	0/2904
4	D	0.24	0/1049	0.38	0/1412
4	P	0.24	0/1049	0.38	0/1412
5	E	0.38	0/1695	0.60	0/2287
5	Q	0.39	0/1695	0.60	0/2287
6	F	0.50	0/666	0.67	0/901
6	R	0.50	0/666	0.67	0/901
7	G	0.26	0/1361	0.57	3/1847 (0.2%)
7	S	0.26	0/1361	0.57	3/1847 (0.2%)
8	H	0.42	0/1010	0.65	0/1363
8	T	0.42	0/1010	0.65	0/1363
9	I	0.22	0/921	0.37	0/1246
9	U	0.24	0/921	0.37	0/1246
10	J	0.57	0/526	0.77	0/709
10	V	0.57	0/526	0.76	0/709
11	K	0.47	0/972	0.61	0/1317
11	W	0.47	0/972	0.61	0/1317
12	L	0.36	0/371	0.57	0/491
12	X	0.37	0/371	0.57	0/491
All	All	0.41	0/64045	0.58	18/86569 (0.0%)

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	992	ALA	N-CA-C	-5.71	95.59	111.00
2	N	992	ALA	N-CA-C	-5.69	95.65	111.00
7	G	167	ASP	CB-CG-OD2	5.38	123.14	118.30
7	S	167	ASP	CB-CG-OD2	5.35	123.12	118.30
2	N	711	ASP	CB-CG-OD2	5.30	123.07	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11802	0	378	1195	0
1	M	11666	0	241	1154	0
2	B	9180	0	30	486	0
2	N	9180	0	30	493	0
3	C	2088	0	0	65	0
3	O	2088	0	0	66	0
4	D	1036	0	0	145	0
4	P	1036	0	0	128	0
5	E	1663	0	0	54	0
5	Q	1663	0	0	56	0
6	F	656	0	0	22	0
6	R	656	0	0	27	0
7	G	1330	0	0	145	0
7	S	1330	0	0	148	0
8	H	996	0	0	35	0
8	T	996	0	0	36	0
9	I	902	0	0	121	0
9	U	902	0	0	120	0
10	J	518	0	0	23	0
10	V	518	0	0	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	955	0	2	15	0
11	W	955	0	2	16	0
12	L	368	0	0	7	0
12	X	368	0	0	7	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
13	M	2	0	0	0	0
13	N	1	0	0	0	0
13	O	1	0	0	0	0
13	U	2	0	0	0	0
13	V	1	0	0	0	0
13	X	1	0	0	0	0
14	A	1	0	0	0	0
14	M	1	0	0	0	0
All	All	62870	0	683	4253	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 67.

The worst 5 of 4253 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:1498:GLY:CA	1:M:1500:PRO:HD3	1.46	1.43
1:A:1489:SER:HB3	1:A:1490:PRO:CD	1.61	1.29
1:M:1498:GLY:HA3	1:M:1500:PRO:CD	1.61	1.28
4:D:24:MET:SD	4:D:88:PHE:CD1	2.30	1.24
4:P:24:MET:SD	4:P:88:PHE:CD1	2.30	1.24

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	1494/1752 (85%)	939 (63%)	280 (19%)	275 (18%)	0	4
1	M	1472/1752 (84%)	932 (63%)	281 (19%)	259 (18%)	0	5
2	B	1142/1210 (94%)	735 (64%)	245 (22%)	162 (14%)	0	9
2	N	1142/1210 (94%)	738 (65%)	243 (21%)	161 (14%)	0	9
3	C	261/297 (88%)	178 (68%)	56 (22%)	27 (10%)	1	16
3	O	261/297 (88%)	178 (68%)	56 (22%)	27 (10%)	1	16
4	D	128/135 (95%)	86 (67%)	20 (16%)	22 (17%)	0	5
4	P	128/135 (95%)	86 (67%)	20 (16%)	22 (17%)	0	5
5	E	205/210 (98%)	137 (67%)	43 (21%)	25 (12%)	1	12
5	Q	205/210 (98%)	137 (67%)	43 (21%)	25 (12%)	1	12
6	F	81/142 (57%)	58 (72%)	15 (18%)	8 (10%)	1	18
6	R	81/142 (57%)	57 (70%)	16 (20%)	8 (10%)	1	18
7	G	168/172 (98%)	128 (76%)	24 (14%)	16 (10%)	1	20
7	S	168/172 (98%)	128 (76%)	24 (14%)	16 (10%)	1	20
8	H	122/125 (98%)	73 (60%)	27 (22%)	22 (18%)	0	4
8	T	122/125 (98%)	73 (60%)	27 (22%)	22 (18%)	0	4
9	I	109/113 (96%)	46 (42%)	27 (25%)	36 (33%)	0	0
9	U	109/113 (96%)	45 (41%)	25 (23%)	39 (36%)	0	0
10	J	62/71 (87%)	41 (66%)	15 (24%)	6 (10%)	1	19
10	V	62/71 (87%)	41 (66%)	15 (24%)	6 (10%)	1	19
11	K	117/123 (95%)	80 (68%)	24 (20%)	13 (11%)	1	14
11	W	117/123 (95%)	80 (68%)	24 (20%)	13 (11%)	1	14
12	L	43/63 (68%)	23 (54%)	12 (28%)	8 (19%)	0	4
12	X	43/63 (68%)	23 (54%)	12 (28%)	8 (19%)	0	4
All	All	7842/8826 (89%)	5042 (64%)	1574 (20%)	1226 (16%)	0	7

5 of 1226 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	12	PRO
1	A	37	ILE
1	A	42	THR
1	A	50	PRO

### 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	1301/1536 (85%)	1113 (86%)	188 (14%)	5	28
1	M	1286/1536 (84%)	1097 (85%)	189 (15%)	4	28
2	B	1012/1064 (95%)	914 (90%)	98 (10%)	12	51
2	N	1012/1064 (95%)	914 (90%)	98 (10%)	12	51
3	C	236/267 (88%)	220 (93%)	16 (7%)	22	71
3	O	236/267 (88%)	220 (93%)	16 (7%)	22	71
4	D	111/115 (96%)	94 (85%)	17 (15%)	4	26
4	P	111/115 (96%)	94 (85%)	17 (15%)	4	26
5	E	182/184 (99%)	169 (93%)	13 (7%)	21	69
5	Q	182/184 (99%)	169 (93%)	13 (7%)	21	69
6	F	71/121 (59%)	64 (90%)	7 (10%)	11	50
6	R	71/121 (59%)	64 (90%)	7 (10%)	11	50
7	G	146/148 (99%)	139 (95%)	7 (5%)	35	81
7	S	146/148 (99%)	139 (95%)	7 (5%)	35	81
8	H	113/114 (99%)	99 (88%)	14 (12%)	7	37
8	T	113/114 (99%)	99 (88%)	14 (12%)	7	37
9	I	103/105 (98%)	80 (78%)	23 (22%)	1	9
9	U	103/105 (98%)	80 (78%)	23 (22%)	1	9
10	J	59/66 (89%)	46 (78%)	13 (22%)	1	9
10	V	59/66 (89%)	46 (78%)	13 (22%)	1	9
11	K	109/113 (96%)	104 (95%)	5 (5%)	37	82
11	W	109/113 (96%)	103 (94%)	6 (6%)	30	78
12	L	39/53 (74%)	34 (87%)	5 (13%)	6	35
12	X	39/53 (74%)	34 (87%)	5 (13%)	6	35
All	All	6949/7772 (89%)	6135 (88%)	814 (12%)	8	40

5 of 814 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	47	GLU
1	M	262	SER
7	S	114	HIS
9	I	94	ASP
1	M	48	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 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 ⓘ

Of 18 ligands modelled in this entry, 18 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.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1496/1752 (85%)	0.27	42 (2%) 50 30	51, 150, 385, 628	0
1	M	1476/1752 (84%)	0.51	124 (8%) 11 8	83, 199, 449, 672	0
2	B	1150/1210 (95%)	0.22	12 (1%) 79 56	69, 143, 314, 580	0
2	N	1150/1210 (95%)	0.57	64 (5%) 24 14	85, 222, 419, 618	0
3	C	263/297 (88%)	0.03	0 100 100	80, 126, 252, 477	0
3	O	263/297 (88%)	0.27	3 (1%) 77 53	125, 190, 350, 511	0
4	D	130/135 (96%)	0.43	3 (2%) 57 35	128, 240, 360, 596	0
4	P	130/135 (96%)	0.55	6 (4%) 31 19	152, 287, 414, 545	0
5	E	207/210 (98%)	0.05	3 (1%) 72 47	70, 164, 293, 516	0
5	Q	207/210 (98%)	0.15	3 (1%) 72 47	119, 181, 373, 501	0
6	F	83/142 (58%)	-0.22	0 100 100	70, 97, 170, 232	0
6	R	83/142 (58%)	-0.07	1 (1%) 75 51	111, 126, 200, 335	0
7	G	170/172 (98%)	0.42	5 (2%) 49 30	92, 199, 323, 514	0
7	S	170/172 (98%)	1.01	28 (16%) 2 3	122, 240, 388, 494	0
8	H	124/125 (99%)	0.16	3 (2%) 56 34	82, 138, 298, 408	0
8	T	124/125 (99%)	0.45	8 (6%) 18 12	115, 197, 344, 429	0
9	I	111/113 (98%)	0.42	3 (2%) 52 31	98, 239, 367, 549	0
9	U	111/113 (98%)	1.25	21 (18%) 2 2	151, 330, 482, 585	0
10	J	64/71 (90%)	0.05	0 100 100	85, 108, 220, 304	0
10	V	64/71 (90%)	0.15	0 100 100	137, 203, 326, 373	0
11	K	119/123 (96%)	-0.06	0 100 100	60, 126, 221, 319	0
11	W	119/123 (96%)	0.39	3 (2%) 54 33	76, 168, 295, 470	0
12	L	45/63 (71%)	-0.03	0 100 100	93, 177, 299, 481	0
12	X	45/63 (71%)	0.82	8 (17%) 2 3	153, 277, 425, 580	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	7904/8826 (89%)	0.36	340 (4%) 34 20	51, 181, 397, 672	0

The worst 5 of 340 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	W	119	GLU	14.3
9	U	39	ALA	10.7
1	A	107	CYS	9.2
1	M	1239	LEU	8.6
1	A	1195	LEU	8.4

## 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
14	MG	A	2458	1/1	1.66	37.54	109,109,109,109	0
13	ZN	A	2457	1/1	0.20	-0.22	122,122,122,122	0
13	ZN	N	2225	1/1	0.22	-0.66	180,180,180,180	0
13	ZN	I	1122	1/1	0.12	-0.79	126,126,126,126	0
13	ZN	B	2225	1/1	0.18	-0.90	149,149,149,149	0
13	ZN	X	1071	1/1	0.07	-1.04	195,195,195,195	0
13	ZN	M	2456	1/1	0.17	-1.09	432,432,432,432	0
13	ZN	C	1269	1/1	0.08	-1.16	122,122,122,122	0
13	ZN	L	1071	1/1	0.10	-1.18	123,123,123,123	0
13	ZN	M	2457	1/1	0.15	-1.36	172,172,172,172	0
13	ZN	J	1066	1/1	0.23	-1.49	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
13	ZN	A	2456	1/1	0.07	-1.70	245,245,245,245	0
13	ZN	V	1066	1/1	0.20	-1.90	155,155,155,155	0
13	ZN	O	1269	1/1	0.11	-1.92	189,189,189,189	0
14	MG	M	2458	1/1	0.26	-2.10	197,197,197,197	0
13	ZN	I	1121	1/1	0.07	-2.34	160,160,160,160	0
13	ZN	U	1121	1/1	0.06	-2.43	284,284,284,284	0
13	ZN	U	1122	1/1	0.05	-4.42	240,240,240,240	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.