



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:57 PM GMT

PDB ID : 1R9T  
Title : RNA POLYMERASE II STRAND SEPARATED ELONGATION COM-  
PLEX, MISMATCHED NUCLEOTIDE  
Authors : Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.  
Deposited on : 2003-10-30  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (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

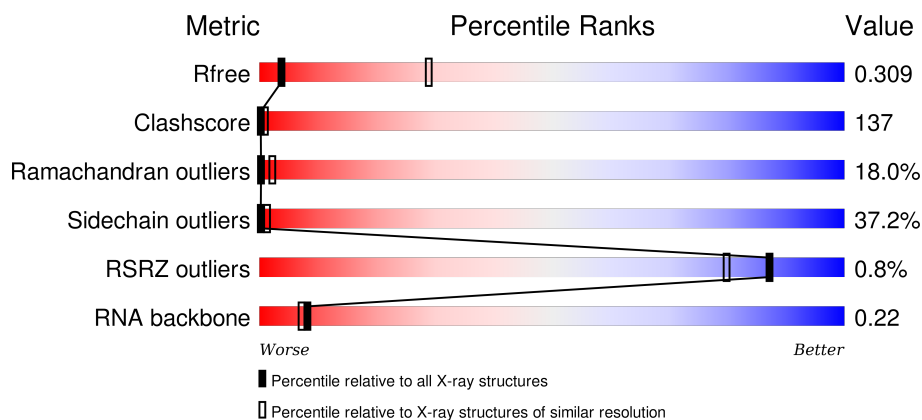
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)

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. 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	R	10	
2	T	28	
3	N	14	
4	A	1733	

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Mol	Chain	Length	Quality of chain
5	B	1224	
6	C	318	
7	E	215	
8	F	155	
9	H	146	
10	I	122	
11	J	70	
12	K	120	
13	L	70	

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
15	MG	A	2002	-	-	-	X
16	ATP	B	1308	-	-	-	X

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29248 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 RNA chain called RNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	10	Total	C	N	O	P	0	0	0
			217	98	45	65	9			

- Molecule 2 is a DNA chain called DNA template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	28	Total	C	N	O	P	0	0	0
			566	271	104	164	27			

- Molecule 3 is a DNA chain called DNA nontemplate strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	14	Total	C	N	O	P	0	0	0
			284	137	49	85	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1395	Total	C	N	O	S	0	0	0
			10969	6917	1923	2068	61			

- Molecule 5 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1106	Total	C	N	O	S	0	0	0
			8792	5568	1538	1631	55			

- Molecule 6 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

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

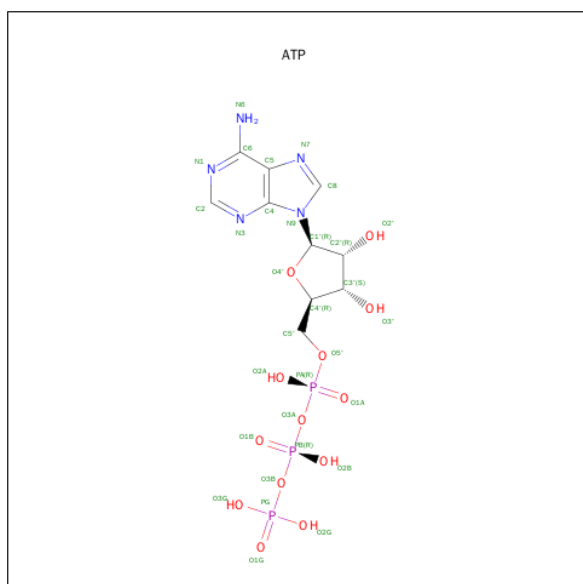
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	2	Total	Mg	0	0
			2	2		

- Molecule 16 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

### 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 ( $\text{RSRZ} > 2$ ). 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.

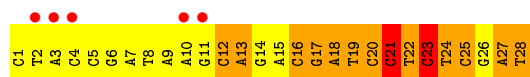
- Molecule 1: RNA strand

Chain R: 



- Molecule 2: DNA template strand

Chain T: 



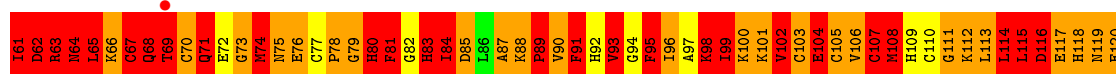
- Molecule 3: DNA nontemplate strand

Chain N: 



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

Chain A: 



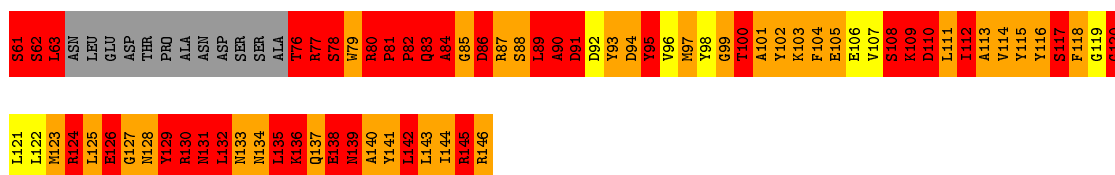


TL142	ASN	L1022	R862	L902	V842	R782	L722	R682	D602	F482	G422	D362	T302	P242
LI143	THR	R1023	R963	R903	K843	T783	N723	S663	M603	D483	D423	Q363	Y303	P243
K1144	PRE	S1024	R964	T904	A844	R784	R724	T664	G604	G484	D424	V364	M304	P244
HI145	HIS	R1025	Q965	T905	L845	P785	A725	G665	M005	D485	G425	G365	N304	P245
VI146	PRE	L1026	R966	H906	D846	H786	R726	T666	L406	E486	L426	V366	N306	R246
TL147	ALA	A1027	A967	T907	D847	F787	D727	G667	L607	M487	Q427	P367	D307	R247
LI148	GLY	T1028	Q968	L908	L848	S788	K728	D688	L608	H488	Y428	K368	L308	P248
AI149	VAL	R1029	D969	D909	M849	K789	A729	T669	D609	L489	G429	S369	A309	S249
SI150	ALA	R1030	T970	P910	V850	D790	G730	L670	G610	H490	W430	I370	I250	P250
E1151	SER	V1031	F971	S911	R851	D791	R731	A671	Q611	A491	K431	A371	Q311	S251
Y1152	K1092	L1032	H972	L912	Y852	D792	L732	D672	L612	P492	K432	K372	P312	F252
Y1153	K1093	Q1033	I973	L913	D853	F793	A733	G673	L613	Q493	E433	T373	Q313	N253
Y1154	W1094	E1034	D974	E914	N854	F794	E734	D674	F614	S494	K434	T374	A314	E254
DI155	T1095	Y1035	H975	S915	T855	E795	V735	T675	G615	E495	H485	T375	L315	S255
P1156	S1096	R1036	T976	G916	T856	S796	M736	T676	V616	E496	L436	Y376	Q316	Q256
DI157	G1097	L1037	K977	S917	R857	K797	L737	T677	E618	T497	K437	P377	K317	R257
RI158	V1098	T1038	P978	E918	N858	G798	K738	E678	G618	R498	D438	E378	S318	G258
RI159	P1099	K1039	S979	I919	S859	F799	D739	T679	E619	A499	I439	V379	G319	E259
SI160	R1100	Q1040	D980	L920	L860	H800	L740	T680	K620	E500	D440	V380	R320	D260
TL161	L1101	A1041	L981	G921	Q861	E801	N741	E681	T621	L501	P441	T381	P321	D261
VI162	K1102	F1042	T982	D922	N862	H802	M742	T682	V622	S502	W442	T382	V322	L262
I1163	E1103	D1043	L983	L923	V863	S803	V743	L683	G623	Q503	L443	T383	K323	T263
P1164	T1104	W1044	K984	K924	L864	H804	K744	A684	S624	L504	F444	N384	S324	F264
E1165	L1105	V1045	D985	L925	Q865	L805	Q745	E685	S625	C505	I445	I385	I325	K265
DI166	M1106	L1046	I986	Q926	P866	R806	M746	A686	N626	E506	K446	D386	R326	L266
E1167	V1107	S1047	V987	V927	L867	G807	V747	K687	G627	V507	Q447	E387	A327	A267
E1168	A1108	N1048	L988	L928	G868	L808	M748	E688	G628	P508	F448	L388	R328	D268
LI169	K1109	T1049	G989	L929	K869	T809	A749	E689	L629	L509	S449	T389	L329	L269
I1170	E1050	E1050	V990	D930	E370	P810	G750	V690	I630	Q150	H450	Q390	K330	L270
Q1171	M1111	A1051	K991	E931	D871	Q811	S751	L691	H631	I511	H451	L391	G331	K271
L1172	L1112	P1052	D992	E932	G872	E812	K752	D692	V632	V512	K452	V392	K332	A272
HI173	T1113	F1053	L993	Y933	K873	F813	G753	V693	V633	S513	K453	R393	E333	N273
F1174	P1114	L1054	Q994	K934	D874	F814	S754	T694	T634	P514	G454	N394	G334	I274
SI175	S1115	R1055	E995	Q935	A875	F815	V755	E695	R635	Q515	M455	P395	R335	S275
L1176	L1116	S1056	L996	L936	K876	H816	L756	E696	E636	S516	K456	L276	L336	L276
LEU	T1117	V1057	V937	V937	H877	A817	N757	A697	K637	N517	A457	N397	R337	E277
ASP	V1118	V1058	L998	K938	L878	R818	L758	Q698	G638	K518	H458	E398	G338	T278
GLU	Y1119	H1059	V999	D939	E879	G819	A759	A699	P639	P519	R459	E399	N339	L279
GLU	L1120	P1060	R940	R940	K880	G820	Q760	N700	Q640	C520	V460	P400	L340	E280
ALA	E1121	G1061	R941	R941	Q881	R821	M761	L701	V641	M521	K461	G401	K341	N281
GLU	P1122	E1062	G1002	F942	S882	E822	S762	L702	C642	G522	V462	A402	G342	N282
GLN	G1123	M1063	L943	L943	L883	G823	A763	T703	A643	I523	L463	K403	K343	G283
SER	H1124	V1064	R944	R944	D884	L824	C764	A704	K644	V524	P464	Y404	R344	A284
PHE	A1125	G1065	E945	E945	T885	L825	V765	T705	L645	Q525	Y465	V405	V345	P285
ASP	A1126	V1066	I1006	V946	L886	D826	G766	H706	F646	D526	S466	I406	D346	H286
Q1187	D1127	L1067	I1007	F947	G887	T827	Q767	G707	G647	T527	T467	R407	F347	H287
Q1188	Q1128	A1068	Q1008	V948	G888	A828	Q768	N708	N648	L528	F468	D408	S348	A288
S1189	E1129	A1069	D949	D949	S889	H829	S769	T709	I649	C529	R469	S409	A349	L289
P1190	Q1130	Q1070	A1010	G950	D890	K830	V770	L710	Q650	G530	L470	G410	R350	E290
H1191	A1131	S1071	E951	E951	A891	T831	E771	R711	K651	I531	N471	D411	T351	E291
L1192	K1132	I1072	R1012	A952	A892	A832	G772	E712	V652	L592	L472	K412	V352	A292
L1193	L1133	G1073	D1013	N953	F893	E833	K773	S713	V653	R593	S473	I413	I353	E293
R1194	L1134	E1074	A1014	N954	E894	T834	R774	F714	M654	L534	V474	D414	S354	S294
L1195	R1135	P1075	K995	P955	K895	G835	I775	E715	F655	T595	T475	L415	G355	L295
E1196	A1136	A1076	L956	L956	R896	H836	A776	D716	V656	L336	S476	R416	D356	L296
L1197	L1137	T1077	P957	P957	V897	T837	F777	N717	L657	R337	P477	Y417	P357	Q297
DI198	T1138	Q1078	F1018	V658	R898	Q838	G778	V718	L658	D338	V478	S418	N358	F298
R1199	E1139	N1079	C1019	N959	V899	R839	F779	W719	M659	T539	N479	R419	L359	H299
H1200	H1140	T1080	D900	P960	D900	R840	V780	W720	M660	F540	A480	R420	E360	V300
A1201	T1141	L1081	R961	R961	L901	L841	D781	F721	G661	I541	D481	A421	L361	A301

L361	T301	R241	L181	M121	D61	MET
P362	C302	S242	S182	L122	I62	SER
H363	C303	A243	E183	T123	I63	LEU
L364	B304	L244	A184	S124	C64	ALA
T365	V305	E245	T185	S125	E65	ASN
Q366	N306	K246	E186	S126	D66	GLU
L367	B307	G247	S187	G127	S67	GLU
E368	N308	S248	D188	L128	T68	LYS
G369	Q309	R249	L189	F129	I69	TYR
F370	N310	F250	V190	N130	I70	LEU
E371	L311	I251	K191	D131	LEU	ASP
S372	E312	S252	L192	V132	GLU	GLU
R373	R313	T253	K193	K133	GLN	GLU
K374	L314	L254	E194	K134	LEU	ASP
L375	R315	Q255	C195	ARG	ALA	PRO
F376	P316	V256	P196	THR	GLN	GLY
F377	G317	K257	F197	TYR	HIS	GLY
L378	V318	L258	D198	GLU	THR	PHE
G379	E319	V259	M199	ALA	THR	GLU
Y380	D320	G260	G200	I1E	GLU	D20
M381	G321	R261	G201	ASP	SER	E21
L382	F322	E262	Y202	VAL	ASP	S22
N383	V323	G263	F203	PRO	ASN	A23
R384	L324	S264	I204	GLY	I1E	F24
L385	Q325	S265	I205	ARG	SER	I25
L386	D326	A266	M206	GLU	ARG	T26
L387	R327	R267	G207	LEU	LYS	A27
C388	E328	T268	S208	LVS	TYR	E28
A389	E329	I269	E209	TYR	GLU	D29
L390	A330	K270	K210	GLU	I90	S30
D391	L331	A271	V211	LEU	S91	N31
R392	R332	T272	L212	I1E	F92	A32
K393	F333	L273	I213	ALA	G93	V33
D394	L334	P274	A214	GLU	K94	I34
Q395	G335	Y275	Q215	GLU	I95	S35
D396	ARG	L276	E216	SER	I96	A36
D397	ARG	K277	R217	GLU	V97	F37
R398	GLY	Q278	S218	ASP	T98	F38
D399	THR	D279	A219	ASP	K99	R39
H400	ALA	L280	G220	SER	P100	E40
F401	LEU	P281	N221	GLU	M101	K41
G402	GLY	L282	I222	SER	V102	G42
K403	I1E	V283	V223	GLY	M103	L43
K404	LVS	L284	Q224	K164	E104	V44
R405	R345	L285	V225	V165	S105	S45
L406	E346	F286	F226	F166	D106	D46
D407	K347	R287	K227	I167	G107	D47
L408	R348	A288	K228	G168	V108	L48
A409	I349	L289	A229	R169	T109	D49
G410	Q350	G290	A230	L170	H110	S50
P411	P351	I291	P231	P171	A111	F51
L412	A352	L292	S232	I172	L112	N52
L413	K353	Q293	S233	M173	Y113	O53
A414	D354	D294	L234	L174	P114	F54
Q415	I355	G295	S235	R175	Q115	V55
L416	L356	E296	D236	E176	E116	D56
F417	Q357	I297	V237	K177	A117	T57
K418	K358	L298	A238	N178	R118	F58
T419	E359	E299	E239	C179	L119	I59
D420	E360	D300	T240	Y180	P120	E60

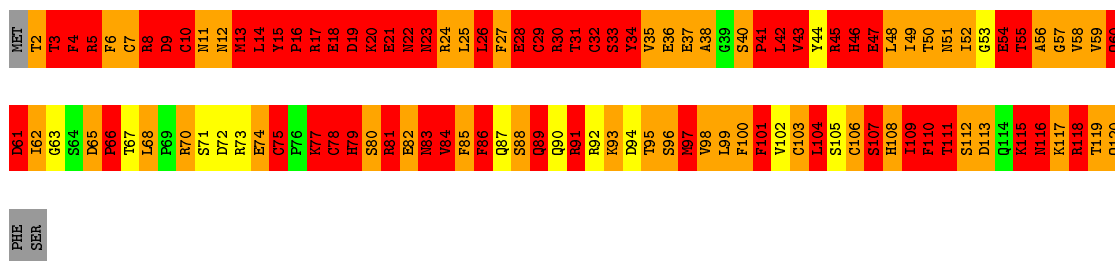
MET	SER	E3	E4	G5	P6	Q7	V8	R9	I10	R11	E12	A13	S14	K15	D16	N17	V18	D19	F20	I21	L22	S23	M24	V25	L27	A28	R29	A30	N31	S32	L33	R34	R35	V36	M37	I38	A39	E40	D47	D48	S49	V49	E50	V51	E52	B53	T54	L55	V56	L57	V58	A59	S60
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E61	F62	I63	A64	H65	R66	L67	G68	L69	I70	P71	L72	L73	L74	M75	L76	L77	E78	G79	L80	E81	L82	L83	L84	L85	L86	L87	L88	L89	L90	L91	L92	L93	L94	L95	L96	L97	L98	L99	T100	L101	Q102	L103	A104	F105	G106	E107	S108	S109	L110	T111	N112	V113	A114	S115	L116	D117	L118	V119	I120																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
V121	S122	M123	L124	M125	G126	R127	N128	L129	G130	H131	P132	L133	L134	Q135	D136	K137	E138	G139	M140	G141	V142	L143	I144	M145	L146	L147	L148	K149	G150	D151	E152	D153	K154	L155	C156	G157	V158	A159	K160	G161	Q162	I163	A164	K165	E166	H167	A168	K169	H170	G171	P172	A173	A174	A175	L176	E177	F178	V179	Y180																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
D181	P182	V183	M184	L185	K186	K187	H188	T189	D190	H191	N192	L193	E194	Q195	D196	S197	L198	K199	E200	G201	P202	Q203	S204	M205	N206	C207	E208	L209	E210	D211	P212	P213	N214	V215	S216	D217	D220	Y221	A222	A223	Q224	A225	D226	T227	F228	M229	V230	N231	V232	E233	T234	V235	G236	S237	T238	P239	V240	D241																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
Q242	V243	V244	V245	G246	L248	L249	D250	L251	Q252	K253	K254	V255	A256	L257	L258	L259	L260	A261	L262	T263	Q264	M265	D266	Q267	D268	L269	V270	P271	P272	P273	P274	P275	P276	P277	P278	P279	P280	P281	P282	P283	P284	P285	P286	P287	P288	P289	P290	P291	P292	P293	P294	P295	P296	P297	P298	P299	P300	P301	P302	P303	P304	P305	P306	P307	P308	P309	P310	P311	P312	P313	P314	P315	P316	P317	P318	P319	P320	P321	P322	P323	P324	P325	P326	P327	P328	P329	P330	P331	P332	P333	P334	P335	P336	P337	P338	P339	P340	P341	P342	P343	P344	P345	P346	P347	P348	P349	P350	P351	P352	P353	P354	P355	P356	P357	P358	P359	P360	P361	P362	P363	P364	P365	P366	P367	P368	P369	P370	P371	P372	P373	P374	P375	P376	P377	P378	P379	P380	P381	P382	P383	P384	P385	P386	P387	P388	P389	P390	P391	P392	P393	P394	P395	P396	P397	P398	P399	P400	P401	P402	P403	P404	P405	P406	P407	P408	P409	P410	P411	P412	P413	P414	P415	P416	P417	P418	P419	P420	P421	P422	P423	P424	P425	P426	P427	P428	P429	P430	P431	P432	P433	P434	P435	P436	P437	P438	P439	P440	P441	P442	P443	P444	P445	P446	P447	P448	P449	P450	P451	P452	P453	P454	P455	P456	P457	P458	P459	P460	P461	P462	P463	P464	P465	P466	P467	P468	P469	P470	P471	P472	P473	P474	P475	P476	P477	P478	P479	P480	P481	P482	P483	P484	P485	P486	P487	P488	P489	P490	P491	P492	P493	P494	P495	P496	P497	P498	P499	P500	P501	P502	P503	P504	P505	P506	P507	P508	P509	P510	P511	P512	P513	P514	P515	P516	P517	P518	P519	P520	P521	P522	P523	P524	P525	P526	P527	P528	P529	P530	P531	P532	P533	P534	P535	P536	P537	P538	P539	P540	P541	P542	P543	P544	P545	P546	P547	P548	P549	P550	P551	P552	P553	P554	P555	P556	P557	P558	P559	P560	P561	P562	P563	P564	P565	P566	P567	P568	P569	P570	P571	P572	P573	P574	P575	P576	P577	P578	P579	P580	P581	P582	P583	P584	P585	P586	P587	P588	P589	P590	P591	P592	P593	P594	P595	P596	P597	P598	P599	P600	P601	P602	P603	P604	P605	P606	P607	P608	P609	P610	P611	P612	P613	P614	P615	P616	P617	P618	P619	P620	P621	P622	P623	P624	P625	P626	P627	P628	P629	P630	P631	P632	P633	P634	P635	P636	P637	P638	P639	P640	P641	P642	P643	P644	P645	P646	P647	P648	P649	P650	P651	P652	P653	P654	P655	P656	P657	P658	P659	P660	P661	P662	P663	P664	P665	P666	P667	P668	P669	P670	P671	P672	P673	P674	P675	P676	P677	P678	P679	P680	P681	P682	P683	P684	P685	P686	P687	P688	P689	P690	P691	P692	P693	P694	P695	P696	P697	P698	P699	P700	P701	P702	P703	P704	P705	P706	P707	P708	P709	P710	P711	P712	P713	P714	P715	P716	P717	P718	P719	P720	P721	P722	P723	P724	P725	P726	P727	P728	P729	P730	P731	P732	P733	P734	P735	P736	P737	P738	P739	P740	P741	P742	P743	P744	P745	P746	P747	P748	P749	P750	P751	P752	P753	P754	P755	P756	P757	P758	P759	P760	P761	P762	P763	P764	P765	P766	P767	P768	P769	P770	P771	P772	P773	P774	P775	P776	P777	P778	P779	P780	P781	P782	P783	P784	P785	P786	P787	P788	P789	P790	P791	P792	P793	P794	P795	P796	P797	P798	P799	P800	P801	P802	P803	P804	P805	P806	P807	P808	P809	P810	P811	P812	P813	P814	P815	P816	P817	P818	P819	P820	P821	P822	P823	P824	P825	P826	P827	P828	P829	P830	P831	P832	P833	P834	P835	P836	P837	P838	P839	P840	P841	P842	P843	P844	P845	P846	P847	P848	P849	P850	P851	P852	P853	P854	P855	P856	P857	P858	P859	P860	P861	P862	P863	P864	P865	P866	P867	P868	P869	P870	P871	P872	P873	P874	P875	P876	P877	P878	P879	P880	P881	P882	P883	P884	P885	P886	P887	P888	P889	P890	P891	P892	P893	P894	P895	P896	P897	P898	P899	P900	P901	P902	P903	P904	P905	P906	P907	P908	P909	P910	P911	P912	P913	P914	P915	P916	P917	P918	P919	P920	P921	P922	P923	P924	P925	P926	P927	P928	P929	P930	P931	P932	P933	P934	P935	P936	P937	P938	P939	P940	P941	P942	P943	P944	P945	P946	P947	P948	P949	P950	P951	P952	P953	P954	P955	P956	P957	P958	P959	P960	P961	P962	P963	P964	P965	P966	P967	P968	P969	P970	P971	P972	P973	P974	P975	P976	P977	P978	P979	P980	P981	P982	P983	P984	P985	P986	P987	P988	P989	P990	P991	P992	P993	P994	P995	P996	P997	P998	P999	P1000	P1001	P1002	P1003	P1004	P1005	P1006	P1007	P1008	P1009	P1010	P1011	P1012	P1013	P1014	P1015	P1016	P1017	P1018	P1019	P1020	P1021	P1022	P1023	P1024	P1025	P1026	P1027	P1028	P1029	P1030	P1031	P1032	P1033	P1034	P1035	P1036	P1037	P1038	P1039	P1040	P1041	P1042	P1043	P1044	P1045	P1046	P1047	P1048	P1049	P1050	P1051	P1052	P1053	P1054	P1055	P1056	P1057	P1058	P1059	P1060	P1061	P1062	P1063	P1064	P1065	P1066	P1067	P1068	P1069	P1070	P1071	P1072	P1073	P1074	P1075	P1076	P1077	P1078	P1079	P1080	P1081	P1082	P1083	P1084	P1085	P1086	P1087	P1088	P1089	P1090	P1091	P1092	P1093	P1094	P1095	P1096	P1097	P1098	P1099	P1100	P1101	P1102	P1103	P1104	P1105	P1106	P1107	P1108	P1109	P1110	P1111	P1112	P1113	P1114	P1115	P1116	P1117	P1118	P1119	P1120	P1121	P1122	P1123	P1124	P1125	P1126	P1127	P1128	P1129	P1130	P1131	P1132	P1133	P1134	P1135	P1136	P1137	P1138	P1139	P1140	P1141	P1142	P1143	P1144	P1145	P1146	P1147	P1148	P1149	P1150	P1151	P1152	P1153	P1154	P1155	P1156	P1157	P1158	P1159	P1160	P1161	P1162	P1163	P1164	P1165	P1166	P1167	P1168	P1169	P1170	P1171	P1172	P1173	P1174	P1175	P1176	P1177	P1178	P1179	P1180	P1181	P1182	P1183	P1184	P1185	P1186	P1187	P1188	P1189	P1190	P1191	P1192	P1193	P1194	P1195	P1196	P1197	P1198	P1199	P1200	P1201	P1202	P1203	P1204	P1205	P1206	P1207	P1208	P1209	P1210	P1211	P1212	P1213	P1214	P1215	P1216	P1217	P1218	P1219	P1220	P1221	P1222	P1223	P1224	P1225	P1226	P1227	P1228	P1229	P1230	P1231	P1232	P1233	P1234	P1235	P1236	P1237	P1238	P1239	P1240	P1241	P1242	P1243	P1244	P1245	P1246	P1247	P1248	P1249	P1250	P1251	P1252	P1253	P1254	P1255	P1256	P1257	P1258	P1259	P1260	P1261	P1262	P1263	P1264	P1265	P1266	P1267	P1268	P1269	P1270	P1271	P1272	P1273	P1274	P1275	P1276	P1277	P1278	P1279	P1280	P1281	P1282	P1283	P1284	P1285	P1286	P1287	P1288	P1289	P1290	P1291	P1292	P1293	P1294	P1295	P1296	P1297	P1298	P1299	P1300	P1301	P1302	P1303	P1304	P1305	P1306	P1307	P1308	P1309	P1310	P1311	P1312	P1313	P1314	P1315	P1316	P1317	P1318	P1319	P1320	P1321	P1322	P1323	P1324	P1325	P1326	P1327	P1328	P1329	P1330	P1331	P1332	P1333	P1334	P1335	P1336	P1337	P1338	P1339	P1340	P1341	P1342	P1343	P1344	P1345	P1346	P1347	P1348	P1349	P1350	P1351	P1352	P1353	P1354	P1355	P1356	P1357	P1358	P1359	P1360	P1361	P1362	P1363	P1364	P1365	P1366	P1367	P1368	P1369	P1370	P1371	P1372	P1373	P1374	P1375	P1376	P1377	P1378	P1379	P1380	P1381	P1382	P1383	P1384	P1385	P1386	P1387	P1388	P1389	P1390	P1391	P1392	P1393	P1394	P1395	P1396	P1397	P1398	P1399	P1400	P1401	P1402	P1403	P1404	P1405	P1406	P1407	P1408	P1409	P1410	P1411	P1412	P1413	P1414	P1415	P1416	P1417	P1418	P1419	P1420	P1421	P1422	P1423	P1424	P1425	P1426	P1427	P1428	P1429	P1430	P1431	P1432	P1433	P1434	P1435	P1436	P1437	P1438	P1439	P1440	P1441	P1442	P1443	P1444	P1445	P1446	P1447	P1448	P1449	P1450	P1451	P1452	P1453	P1454	P1455	P1456	P1457	P1458	P1459	P1460	P1461	P1462	P1463	P1464	P1465	P1466	P1467	P1468	P1469	P1470	P1471	P1472	P1473	P1474	P1475	P1476	P1477	P1478	P1479	P1480	P1481	P1482	P1483	P1484	P1485	P1486	P1487	P1488	P1489	P1490	P1491	P1492	P1493	P1494	P1495	P1496	P1497	P1498	P1499	P1500	P1501	P1502	P1503	P1504	P1505	P1506	P1507	P1508	P1509	P1510	P1511	P1512	P1513	P1514	P1515	P1516	P1517	P1518	P1519	P1520	P1521	P1522	P1523	P1524	P1525	P1526	P1527	P1528	P1529	P



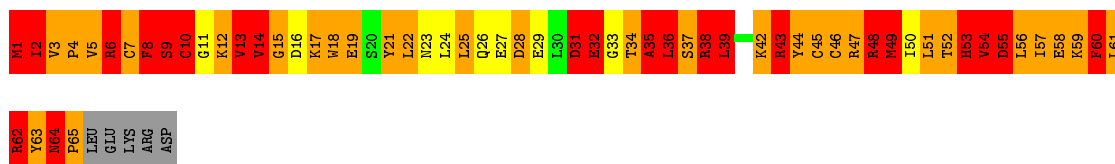
- Molecule 10: DNA-directed RNA polymerase II 14.2 kDa polypeptide

Chain I: 11% 37% 46%



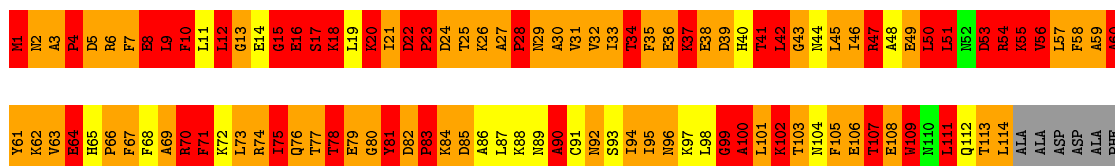
- Molecule 11: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide

Chain J: 6% 13% 41% 33% 7%



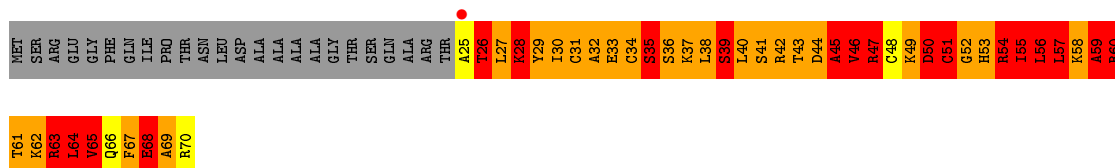
- Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K: 16% 44% 33% 5%



- Molecule 13: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide

Chain L: 6% 33% 27% 34%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.85Å 222.96Å 193.60Å 90.00° 101.17° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 39.98 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.50) 93.7 (39.98-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 3.48Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.230 , 0.317 0.226 , 0.309	Depositor DCC
$R_{free}$ test set	8299 reflections (10.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	80.5	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 81.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 88258 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	29248	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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, MG, 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	R	3.34	30/244 (12.3%)	3.47	35/380 (9.2%)
2	T	2.72	42/633 (6.6%)	2.95	63/971 (6.5%)
3	N	1.33	4/316 (1.3%)	1.10	6/484 (1.2%)
4	A	3.73	1529/11163 (13.7%)	3.57	2038/15091 (13.5%)
5	B	3.68	1206/8963 (13.5%)	3.62	1655/12086 (13.7%)
6	C	3.67	281/2133 (13.2%)	3.42	376/2891 (13.0%)
7	E	3.85	252/1788 (14.1%)	3.52	348/2406 (14.5%)
8	F	3.81	105/691 (15.2%)	3.78	136/933 (14.6%)
9	H	4.17	178/1086 (16.4%)	3.65	243/1470 (16.5%)
10	I	3.97	150/989 (15.2%)	3.89	212/1331 (15.9%)
11	J	3.68	72/541 (13.3%)	3.56	89/727 (12.2%)
12	K	3.73	149/937 (15.9%)	3.38	150/1265 (11.9%)
13	L	4.22	68/365 (18.6%)	3.67	86/485 (17.7%)
All	All	3.71	4066/29849 (13.6%)	3.55	5437/40520 (13.4%)

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	R	0	1
2	T	1	2
4	A	2	121
5	B	4	114
6	C	1	11
7	E	0	17
8	F	0	5
9	H	0	16
10	I	1	18
11	J	0	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
12	K	0	9
13	L	0	5
All	All	9	321

The worst 5 of 4066 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1110	ASN	CB-CG	39.65	2.42	1.51
4	A	820	GLY	C-O	-37.66	0.63	1.23
7	E	117	THR	CA-CB	34.64	2.43	1.53
4	A	437	MET	SD-CE	30.90	3.50	1.77
4	A	322	VAL	CA-CB	-27.33	0.97	1.54

The worst 5 of 5437 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	941	LEU	CB-CG-CD2	37.01	173.92	111.00
4	A	337	ARG	NE-CZ-NH2	-34.93	102.83	120.30
4	A	980	ASP	CB-CG-OD2	33.77	148.69	118.30
5	B	466	TRP	CA-C-N	-31.53	53.14	116.20
4	A	337	ARG	NE-CZ-NH1	31.48	136.04	120.30

5 of 9 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	T	21	DC	C3'
4	A	317	LYS	CA
4	A	324	SER	CA
5	B	636	PRO	CA
5	B	637	LEU	CA

5 of 321 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	3	GLY	Mainchain
4	A	6	TYR	Peptide
1	R	10	A	Sidechain
2	T	21	DC	Sidechain
2	T	23	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	R	217	0	110	34	0
2	T	566	0	314	82	4
3	N	284	0	162	44	0
4	A	10969	0	11061	3443	0
5	B	8792	0	8821	2369	0
6	C	2095	0	2051	490	0
7	E	1752	0	1776	523	0
8	F	679	0	701	194	0
9	H	1068	0	1040	377	0
10	I	971	0	929	310	0
11	J	532	0	543	160	0
12	K	919	0	929	259	0
13	L	363	0	387	98	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	2	0	0	0	0
16	B	31	0	12	7	0
All	All	29248	0	28836	7970	4

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 137.

The worst 5 of 7970 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)
3:N:12:DT:P	7:E:117:THR:HG21	1.32	1.67
4:A:128:ILE:CA	4:A:128:ILE:CB	1.74	1.66
5:B:422:LYS:CB	5:B:422:LYS:CG	1.74	1.65
5:B:866:TYR:CB	5:B:866:TYR:CG	1.80	1.65
4:A:37:PHE:CG	4:A:37:PHE:CB	1.74	1.65

All (4) 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:T:1:DC:C4'	2:T:1:DC:C4'[2_656]	1.63	0.57
2:T:1:DC:C5'	2:T:1:DC:O4'[2_656]	1.69	0.51
2:T:1:DC:O4'	2:T:1:DC:O4'[2_656]	1.78	0.42
2:T:1:DC:C4'	2:T:1:DC:O4'[2_656]	1.80	0.40

## 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	
4	A	1383/1733 (80%)	816 (59%)	306 (22%)	261 (19%)	0	2
5	B	1088/1224 (89%)	708 (65%)	199 (18%)	181 (17%)	0	3
6	C	264/318 (83%)	170 (64%)	58 (22%)	36 (14%)	0	4
7	E	212/215 (99%)	119 (56%)	47 (22%)	46 (22%)	0	1
8	F	82/155 (53%)	45 (55%)	22 (27%)	15 (18%)	0	2
9	H	129/146 (88%)	75 (58%)	28 (22%)	26 (20%)	0	1
10	I	117/122 (96%)	60 (51%)	32 (27%)	25 (21%)	0	1
11	J	63/70 (90%)	41 (65%)	10 (16%)	12 (19%)	0	2
12	K	112/120 (93%)	78 (70%)	18 (16%)	16 (14%)	0	4
13	L	44/70 (63%)	21 (48%)	11 (25%)	12 (27%)	0	0
All	All	3494/4173 (84%)	2133 (61%)	731 (21%)	630 (18%)	0	2

5 of 630 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	34	LYS
4	A	44	THR
4	A	48	ALA
4	A	51	GLY

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Mol	Chain	Res	Type
4	A	55	ASP

### 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	
4	A	1218/1520 (80%)	759 (62%)	459 (38%)	0	1
5	B	960/1061 (90%)	614 (64%)	346 (36%)	0	1
6	C	234/274 (85%)	151 (64%)	83 (36%)	0	1
7	E	196/197 (100%)	116 (59%)	80 (41%)	0	1
8	F	74/137 (54%)	47 (64%)	27 (36%)	0	1
9	H	117/128 (91%)	71 (61%)	46 (39%)	0	1
10	I	113/116 (97%)	70 (62%)	43 (38%)	0	1
11	J	60/65 (92%)	38 (63%)	22 (37%)	0	1
12	K	99/102 (97%)	63 (64%)	36 (36%)	0	1
13	L	40/57 (70%)	24 (60%)	16 (40%)	0	1
All	All	3111/3657 (85%)	1953 (63%)	1158 (37%)	0	1

5 of 1158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	257	LYS
5	B	682	SER
10	I	79	HIS
5	B	319	GLU
5	B	436	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
4	A	1364	ASN
5	B	383	ASN

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Mol	Chain	Res	Type
10	I	60	GLN
4	A	1390	ASN
5	B	115	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	10/10 (100%)	4 (40%)	3 (30%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	U
1	R	5	A
1	R	6	G
1	R	10	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	1	A
1	R	4	G
1	R	5	A

## 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	$\# Z  > 2$
16	ATP	B	1308	-	24,33,33	2.15	6 (25%)	31,52,52	3.35	8 (25%)

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
16	ATP	B	1308	-	-	0/18/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	1308	ATP	O5'-C5'	-5.58	1.22	1.44
16	B	1308	ATP	PA-O5'	-4.12	1.40	1.59
16	B	1308	ATP	C5'-C4'	-2.71	1.42	1.51
16	B	1308	ATP	C2-N1	2.64	1.38	1.33
16	B	1308	ATP	C2-N3	3.73	1.38	1.32

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	1308	ATP	N3-C2-N1	-11.52	120.07	128.89
16	B	1308	ATP	C5'-C4'-C3'	-5.00	95.35	115.21
16	B	1308	ATP	PA-O3A-PB	-4.17	121.03	132.73
16	B	1308	ATP	C1'-N9-C4	-3.94	120.99	126.94
16	B	1308	ATP	PB-O3B-PG	-3.68	120.33	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1308	ATP	7	0

## 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, 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	R	10/10 (100%)	0.40	0 100 100	70, 83, 159, 164	0
2	T	28/28 (100%)	0.93	5 (17%) 2 2	84, 188, 200, 200	0
3	N	14/14 (100%)	1.75	5 (35%) 0 0	185, 198, 200, 200	0
4	A	1395/1733 (80%)	-0.68	11 (0%) 87 80	1, 51, 137, 186	0
5	B	1106/1224 (90%)	-0.70	8 (0%) 89 82	1, 43, 119, 194	0
6	C	266/318 (83%)	-0.80	0 100 100	6, 44, 95, 151	0
7	E	214/215 (99%)	-0.51	0 100 100	13, 79, 141, 165	0
8	F	84/155 (54%)	-0.59	0 100 100	17, 58, 105, 114	0
9	H	133/146 (91%)	-0.57	0 100 100	19, 74, 132, 154	0
10	I	119/122 (97%)	-0.69	0 100 100	4, 56, 105, 146	0
11	J	65/70 (92%)	-0.77	0 100 100	11, 40, 92, 116	0
12	K	114/120 (95%)	-0.71	0 100 100	8, 43, 88, 131	0
13	L	46/70 (65%)	-0.41	1 (2%) 65 55	17, 84, 143, 163	0
All	All	3594/4225 (85%)	-0.65	30 (0%) 87 80	1, 50, 133, 200	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	316	GLN	5.5
4	A	255	SER	4.1
3	N	14	DG	3.8
4	A	44	THR	3.8
4	A	149	GLU	3.6

### 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<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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
15	MG	A	2002	1/1	0.71	0.49	11.34	63,63,63,63	0
16	ATP	B	1308	31/31	0.75	0.35	6.10	64,71,77,78	0
14	ZN	A	1735	1/1	0.98	0.04	-1.42	75,75,75,75	0
14	ZN	I	203	1/1	0.98	0.05	-1.61	98,98,98,98	0
14	ZN	I	204	1/1	0.99	0.05	-1.69	31,31,31,31	0
14	ZN	J	101	1/1	0.97	0.10	-1.79	39,39,39,39	0
14	ZN	C	319	1/1	0.99	0.02	-1.89	31,31,31,31	0
14	ZN	B	1307	1/1	0.99	0.05	-2.32	80,80,80,80	0
14	ZN	A	1734	1/1	0.80	0.05	-2.72	115,115,115,115	0
14	ZN	L	105	1/1	0.98	0.04	-2.77	76,76,76,76	0
15	MG	A	2001	1/1	0.95	0.56	-	55,55,55,55	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.