



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 4, 2023 – 05:00 pm GMT

PDB ID : 2VUM
Title : Alpha-amanitin inhibited complete RNA polymerase II elongation complex
Authors : Brueckner, F.; Cramer, P.
Deposited on : 2008-05-27
Resolution : 3.40 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

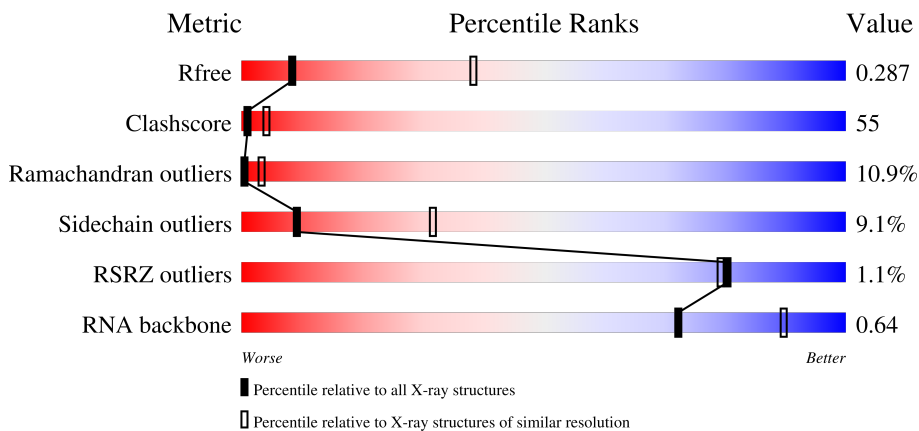
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 24% 47% 10% 18%
2	B	1224	 24% 53% 12% 10%
3	C	318	 28% 43% 12% 16%
4	D	221	 29% 42% 9% 20%

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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	M	8	
14	N	14	
15	P	11	
16	T	26	

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 32083 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
			Total	C	N	O	S			
1	A	1418	11158	7032	1949	2115	62	0	0	0

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

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

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

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

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	177	1356	840	241	273	2	0	0	0

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC1.

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

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2.

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

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

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

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3.

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

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

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

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5.

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

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

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

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4.

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

- Molecule 13 is a protein called AMATOXIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	N	O				S
13	M	8	64	39	10	14	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
14	N	13	262	127	47	76	12	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
15	P	10	214	97	44	64	9	0	0	0

- Molecule 16 is a DNA chain called 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*GP*TP*TP*AP*CP*GP*CP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	Br	C	N	O	P			
16	T	25	509	1	243	92	149	24	0	0	0

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

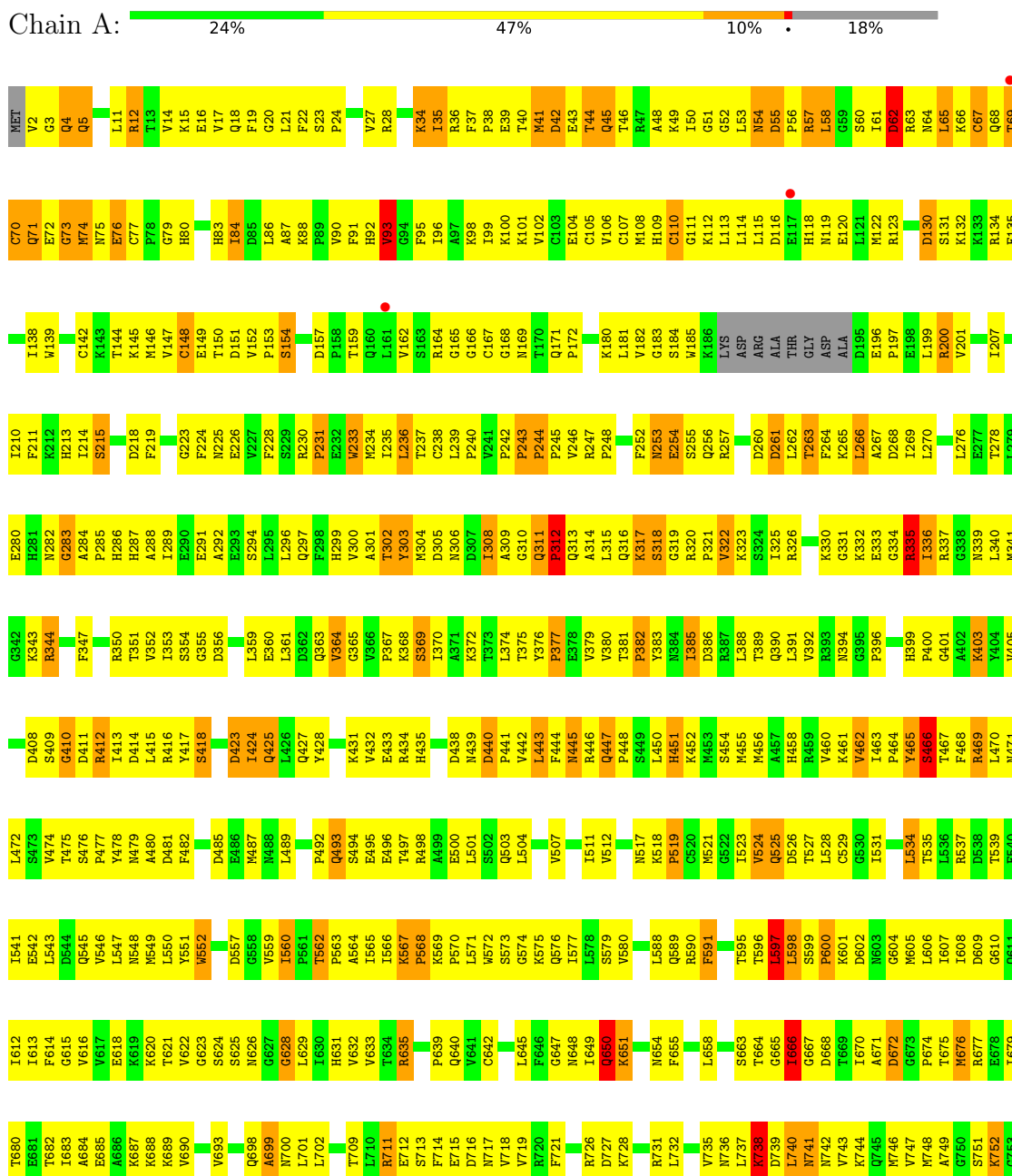
- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

3 Residue-property plots

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

• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1

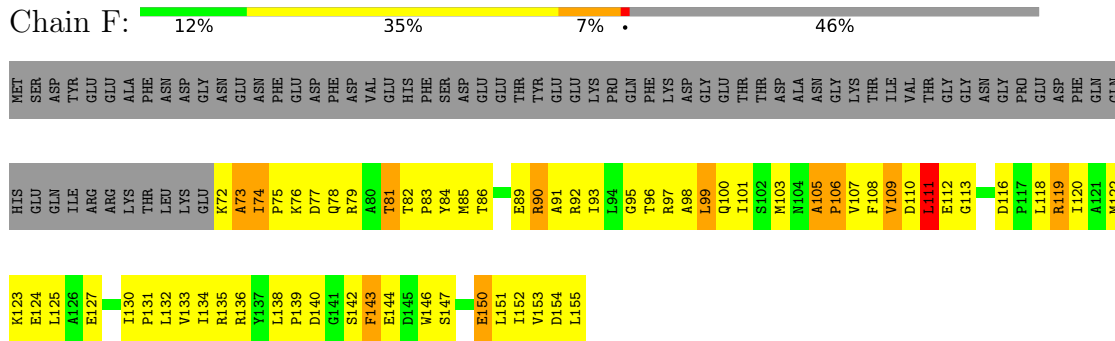




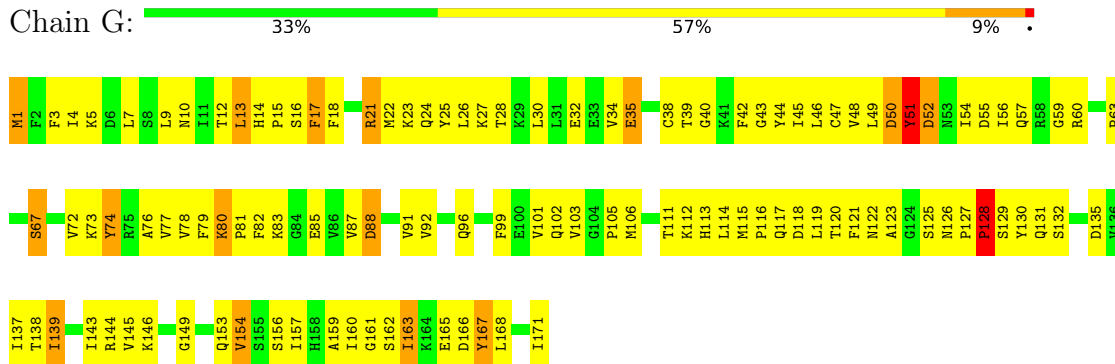
NET	E28	E29	S30	S31	S32	S33	S34	S35	S36	S37	S38	S39	S40	S41	S42	S43	S44	S45	S46	S47	S48	S49	S50	S51	S52	S53	S54	S55	S56	S57	S58	S59	S60	S61	S62	S63	S64	S65	S66	S67	S68	S69	S70	S71	S72	S73	S74	S75	S76	S77	S78	S79	S80	S81	S82	S83	S84	S85	S86	S87	S88	S89	S90	S91	S92	S93	S94	S95	S96	S97	S98	S99	S100																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
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LEU	T25	T26	T27	T28	T29	T30	T31	T32	T33	T34	T35	T36	T37	T38	T39	T40	T41	T42	T43	T44	T45	T46	T47	T48	T49	T50	T51	T52	T53	T54	T55	T56	T57	T58	T59	T60	T61	T62	T63	T64	T65	T66	T67	T68	T69	T70	T71	T72	T73	T74	T75	T76	T77	T78	T79	T80	T81	T82	T83	T84	T85	T86	T87	T88	T89	T90	T91	T92	T93	T94	T95	T96	T97	T98	T99	T100																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
ALA	D20	D21	D22	D23	D24	D25	D26	D27	D28	D29	D30	D31	D32	D33	D34	D35	D36	D37	D38	D39	D40	D41	D42	D43	D44	D45	D46	D47	D48	D49	D50	D51	D52	D53	D54	D55	D56	D57	D58	D59	D60	D61	D62	D63	D64	D65	D66	D67	D68	D69	D70	D71	D72	D73	D74	D75	D76	D77	D78	D79	D80	D81	D82	D83	D84	D85	D86	D87	D88	D89	D90	D91	D92	D93	D94	D95	D96	D97	D98	D99	D100																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
ASN	L62	L63	L64	L65	L66	L67	L68	L69	L70	L71	L72	L73	L74	L75	L76	L77	L78	L79	L80	L81	L82	L83	L84	L85	L86	L87	L88	L89	L90	L91	L92	L93	L94	L95	L96	L97	L98	L99	L100	L101	L102	L103	L104	L105	L106	L107	L108	L109	L110	L111	L112	L113	L114	L115	L116	L117	L118	L119	L120	L121	L122	L123	L124	L125	L126	L127	L128	L129	L130	L131	L132	L133	L134	L135	L136	L137	L138	L139	L140	L141	L142	L143	L144	L145	L146	L147	L148	L149	L150	L151	L152	L153	L154	L155	L156	L157	L158	L159	L160	L161	L162	L163	L164	L165	L166	L167	L168	L169	L170	L171	L172	L173	L174	L175	L176	L177	L178	L179	L180	L181	L182	L183	L184	L185	L186	L187	L188	L189	L190	L191	L192	L193	L194	L195	L196	L197	L198	L199	L200																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
SER	T185	T186	T187	T188	T189	T190	T191	T192	T193	T194	T195	T196	T197	T198	T199	T200	T201	T202	T203	T204	T205	T206	T207	T208	T209	T210	T211	T212	T213	T214	T215	T216	T217	T218	T219	T220	T221	T222	T223	T224	T225	T226	T227	T228	T229	T230	T231	T232	T233	T234	T235	T236	T237	T238	T239	T240	T241	T242	T243	T244	T245	T246	T247	T248	T249	T250	T251	T252	T253	T254	T255	T256	T257	T258	T259	T260	T261	T262	T263	T264	T265	T266	T267	T268	T269	T270	T271	T272	T273	T274	T275	T276	T277	T278	T279	T280	T281	T282	T283	T284	T285	T286	T287	T288	T289	T290	T291	T292	T293	T294	T295	T296	T297	T298	T299	T300																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
GLU	L254	L255	L256	L257	L258	L259	L260	L261	L262	L263	L264	L265	L266	L267	L268	L269	L270	L271	L272	L273	L274	L275	L276	L277	L278	L279	L280	L281	L282	L283	L284	L285	L286	L287	L288	L289	L290	L291	L292	L293	L294	L295	L296	L297	L298	L299	L300	L301	L302	L303	L304	L305	L306	L307	L308	L309	L310	L311	L312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	S101
LEU	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	S101																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													



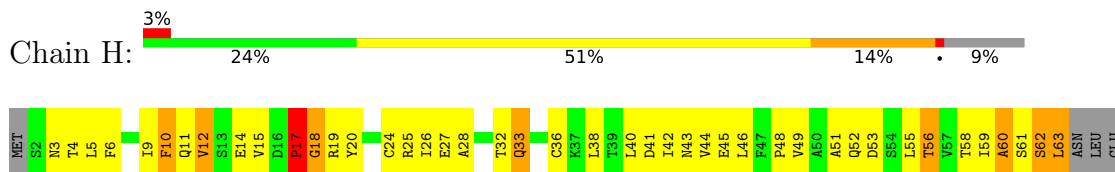
- Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2

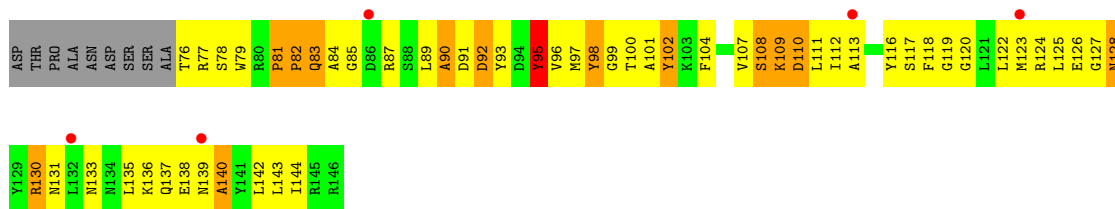


- Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

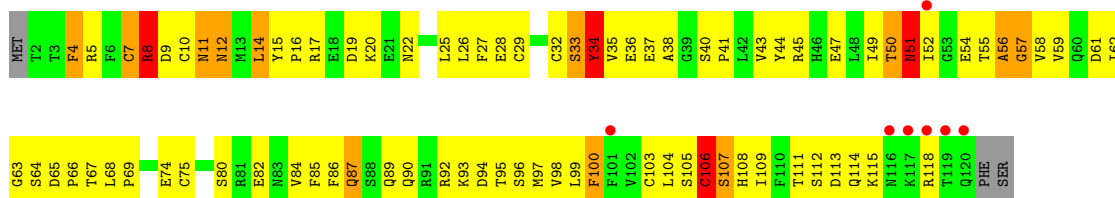


- Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3

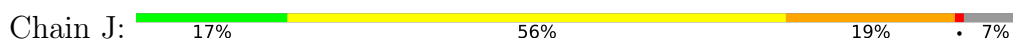




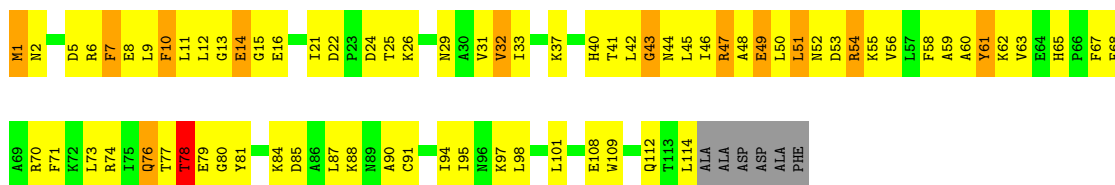
● Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



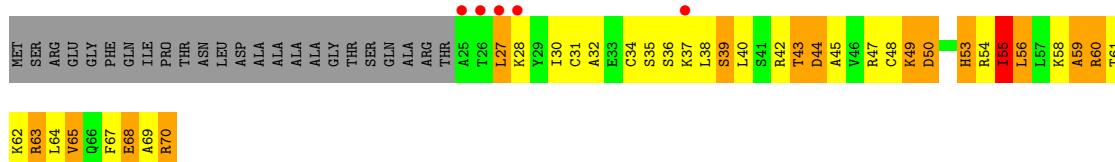
● Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5



● Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



● Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4

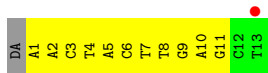
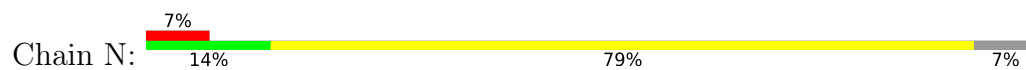


● Molecule 13: AMATOXIN

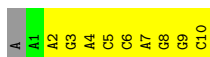
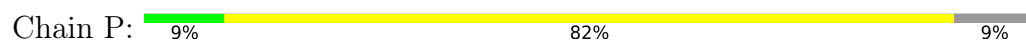




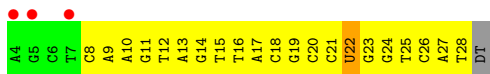
- Molecule 14: 5'-D(*AP*AP*AP*CP*TP*AP*CP*TP*TP*GP *AP*GP*CP*T)-3'



- Molecule 15: 5'-R(*AP*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3'



- Molecule 16: 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP *GP*TP*TP*AP*CP*GP*CP*CP*BRUP*GP*GP*TP*CP*AP*TP*T)-3'



4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	220.62Å 394.23Å 283.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.40 49.75 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.40) 99.9 (49.75-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.19Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.255 , 0.288 0.251 , 0.287	Depositor DCC
R_{free} test set	7809 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	72.7	Xtrriage
Anisotropy	0.244	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	0.077 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.085 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	32083	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TRX, ILX, ZN, MG, CSX, HYP, 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	0.44	0/11359	0.73	1/15364 (0.0%)
2	B	0.43	0/8963	0.73	0/12086
3	C	0.44	0/2133	0.71	1/2891 (0.0%)
4	D	0.40	0/1365	0.65	0/1837
5	E	0.40	0/1788	0.63	0/2406
6	F	0.49	0/691	0.75	0/933
7	G	0.45	0/1368	0.71	0/1844
8	H	0.41	0/1086	0.66	0/1470
9	I	0.39	0/989	0.67	0/1331
10	J	0.46	0/541	0.76	0/727
11	K	0.48	0/937	0.71	0/1265
12	L	0.44	0/365	0.77	0/485
13	M	1.80	1/22 (4.5%)	1.60	0/26
14	N	0.59	0/293	0.84	0/450
15	P	0.45	0/240	0.77	0/373
16	T	0.55	0/547	0.95	0/840
All	All	0.44	1/32687 (0.0%)	0.72	2/44328 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	7	GLY	N-CA	5.81	1.54	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	39	ALA	N-CA-C	5.43	125.66	111.00
1	A	266	LEU	N-CA-C	-5.29	96.70	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11158	0	11222	1335	0
2	B	8792	0	8823	1107	0
3	C	2095	0	2051	245	0
4	D	1356	0	1319	127	0
5	E	1752	0	1776	162	0
6	F	679	0	701	86	0
7	G	1340	0	1357	170	0
8	H	1068	0	1040	160	0
9	I	971	0	931	108	0
10	J	532	0	543	128	0
11	K	919	0	929	103	0
12	L	363	0	388	54	0
13	M	64	0	50	4	0
14	N	262	0	149	20	0
15	P	214	0	111	7	0
16	T	509	0	281	41	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	32083	0	31671	3527	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 55.

The worst 5 of 3527 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)
1:A:1329:THR:HG22	1:A:1331:SER:H	1.05	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.14	1.10
6:F:109:VAL:HG12	6:F:110:ASP:H	1.15	1.09
1:A:40:THR:HB	1:A:41:MET:HE2	1.15	1.09
3:C:43:THR:HG22	3:C:44:LEU:H	1.08	1.08

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	1408/1733 (81%)	984 (70%)	283 (20%)	141 (10%)	0	4
2	B	1088/1224 (89%)	740 (68%)	220 (20%)	128 (12%)	0	3
3	C	264/318 (83%)	187 (71%)	52 (20%)	25 (10%)	0	4
4	D	173/221 (78%)	116 (67%)	37 (21%)	20 (12%)	0	3
5	E	212/215 (99%)	150 (71%)	41 (19%)	21 (10%)	0	4
6	F	82/155 (53%)	58 (71%)	14 (17%)	10 (12%)	0	2
7	G	169/171 (99%)	126 (75%)	30 (18%)	13 (8%)	1	6
8	H	129/146 (88%)	95 (74%)	17 (13%)	17 (13%)	0	1
9	I	117/122 (96%)	74 (63%)	28 (24%)	15 (13%)	0	2
10	J	63/70 (90%)	38 (60%)	14 (22%)	11 (18%)	0	0
11	K	112/120 (93%)	86 (77%)	17 (15%)	9 (8%)	1	6
12	L	44/70 (63%)	19 (43%)	13 (30%)	12 (27%)	0	0
13	M	3/8 (38%)	3 (100%)	0	0	100	100
All	All	3864/4573 (84%)	2676 (69%)	766 (20%)	422 (11%)	0	3

5 of 422 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	54	ASN
1	A	57	ARG
1	A	67	CYS
1	A	71	GLN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1241/1520 (82%)	1134 (91%)	107 (9%)	10	35
2	B	960/1061 (90%)	870 (91%)	90 (9%)	8	30
3	C	234/274 (85%)	207 (88%)	27 (12%)	5	20
4	D	140/200 (70%)	125 (89%)	15 (11%)	6	24
5	E	196/197 (100%)	185 (94%)	11 (6%)	21	51
6	F	74/137 (54%)	65 (88%)	9 (12%)	5	18
7	G	152/152 (100%)	142 (93%)	10 (7%)	16	46
8	H	117/128 (91%)	107 (92%)	10 (8%)	10	35
9	I	113/116 (97%)	103 (91%)	10 (9%)	10	33
10	J	60/65 (92%)	53 (88%)	7 (12%)	5	20
11	K	99/102 (97%)	88 (89%)	11 (11%)	6	22
12	L	40/57 (70%)	34 (85%)	6 (15%)	3	12
13	M	2/2 (100%)	2 (100%)	0	100	100
All	All	3428/4011 (86%)	3115 (91%)	313 (9%)	9	32

5 of 313 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	148	LEU
9	I	87	GLN
4	D	221	TYR
7	G	13	LEU
11	K	47	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	975	GLN
4	D	137	ASN
2	B	1065	GLN
3	C	73	GLN
4	D	173	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/11 (81%)	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 [i](#)

5 non-standard protein/DNA/RNA residues are 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	CSX	M	8	13	3,6,7	1.01	0	1,6,8	1.64	0
13	TRX	M	4	13	14,16,17	1.18	1 (7%)	15,22,24	2.63	4 (26%)
13	ILX	M	3	13	8,9,10	1.35	1 (12%)	9,11,13	2.14	2 (22%)
13	HYP	M	2	13	6,8,9	0.89	0	5,10,12	1.70	2 (40%)
16	BRU	T	22	16,15	18,21,22	0.38	0	26,30,33	0.95	2 (7%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CSX	M	8	13	-	0/1/5/7	-
13	TRX	M	4	13	-	0/4/6/8	0/2/2/2
13	ILX	M	3	13	-	0/11/12/14	-
13	HYP	M	2	13	-	0/0/11/13	0/1/1/1
16	BRU	T	22	16,15	-	0/7/21/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	4	TRX	CZ3-CH2	3.06	1.44	1.38
13	M	3	ILX	CB-CA	-3.03	1.51	1.54

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	4	TRX	CB-CG-CD1	-7.20	119.07	127.97
13	M	3	ILX	CB-CA-C	-5.50	105.52	112.94
13	M	4	TRX	CB-CG-CD2	4.90	133.87	126.25
13	M	4	TRX	CZ2-CE2-CD2	3.01	125.04	121.16
16	T	22	BRU	C6-C5-C4	-2.88	117.74	120.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	4	TRX	1	0
13	M	3	ILX	1	0
16	T	22	BRU	4	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1418/1733 (81%)	-0.26	6 (0%) 92 92	37, 86, 139, 189	0
2	B	1106/1224 (90%)	-0.15	9 (0%) 86 85	37, 96, 148, 181	0
3	C	266/318 (83%)	-0.33	0 100 100	48, 83, 117, 141	0
4	D	177/221 (80%)	-0.24	0 100 100	66, 107, 145, 149	0
5	E	214/215 (99%)	-0.01	6 (2%) 53 51	66, 127, 171, 180	0
6	F	84/155 (54%)	-0.45	0 100 100	42, 70, 99, 108	0
7	G	171/171 (100%)	-0.21	0 100 100	70, 90, 126, 136	0
8	H	133/146 (91%)	0.25	5 (3%) 40 39	91, 125, 152, 168	0
9	I	119/122 (97%)	0.03	7 (5%) 22 23	84, 125, 158, 175	0
10	J	65/70 (92%)	-0.35	0 100 100	44, 76, 113, 128	0
11	K	114/120 (95%)	-0.34	0 100 100	56, 83, 109, 133	0
12	L	46/70 (65%)	0.50	5 (10%) 5 6	76, 152, 166, 169	0
13	M	4/8 (50%)	-0.51	0 100 100	88, 90, 91, 97	0
14	N	13/14 (92%)	0.64	1 (7%) 13 15	151, 178, 218, 221	0
15	P	10/11 (90%)	-0.35	0 100 100	89, 111, 162, 172	0
16	T	24/26 (92%)	0.19	3 (12%) 3 4	80, 159, 224, 233	0
All	All	3964/4624 (85%)	-0.19	42 (1%) 80 79	37, 93, 152, 233	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	27	LEU	6.8
1	A	1176	LEU	6.7
2	B	471	LYS	5.9
16	T	4	DA	5.3
2	B	883	LEU	4.9

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
16	BRU	T	22	20/21	0.82	0.18	69,75,79,82	0
13	TRX	M	4	15/16	0.95	0.26	88,91,93,93	0
13	CSX	M	8	7/8	0.97	0.15	92,94,95,97	0
13	HYP	M	2	8/9	0.97	0.12	84,85,86,87	0
13	ILX	M	3	10/11	0.98	0.17	85,86,88,91	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	ZN	I	1122	1/1	0.94	0.09	144,144,144,144	0
17	ZN	L	1071	1/1	0.95	0.09	107,107,107,107	0
17	ZN	A	2456	1/1	0.97	0.08	78,78,78,78	0
17	ZN	C	1269	1/1	0.99	0.13	67,67,67,67	0
17	ZN	I	1121	1/1	0.99	0.16	96,96,96,96	0
17	ZN	A	2457	1/1	0.99	0.14	53,53,53,53	0
17	ZN	J	1066	1/1	0.99	0.21	72,72,72,72	0
17	ZN	B	2225	1/1	0.99	0.18	65,65,65,65	0
18	MG	A	2458	1/1	0.99	0.16	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.