



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 08:00 am BST

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

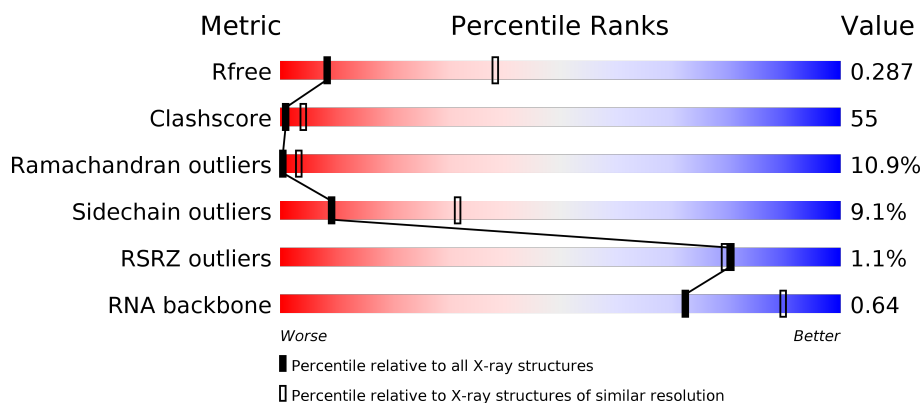
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	
4	D	221	

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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
1	A	1418	Total	C	N	O	S	0	0	0
			11158	7032	1949	2115	62			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 13 is a protein called AMATOXIN.

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

- 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
14	N	13	Total	C	N	O	P	0	0	0
			262	127	47	76	12			

- 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
15	P	10	Total	C	N	O	P	0	0	0
			214	97	44	64	9			

- 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
16	T	25	Total	Br	C	N	O	P	0	0
			509	1	243	92	149	24		

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

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

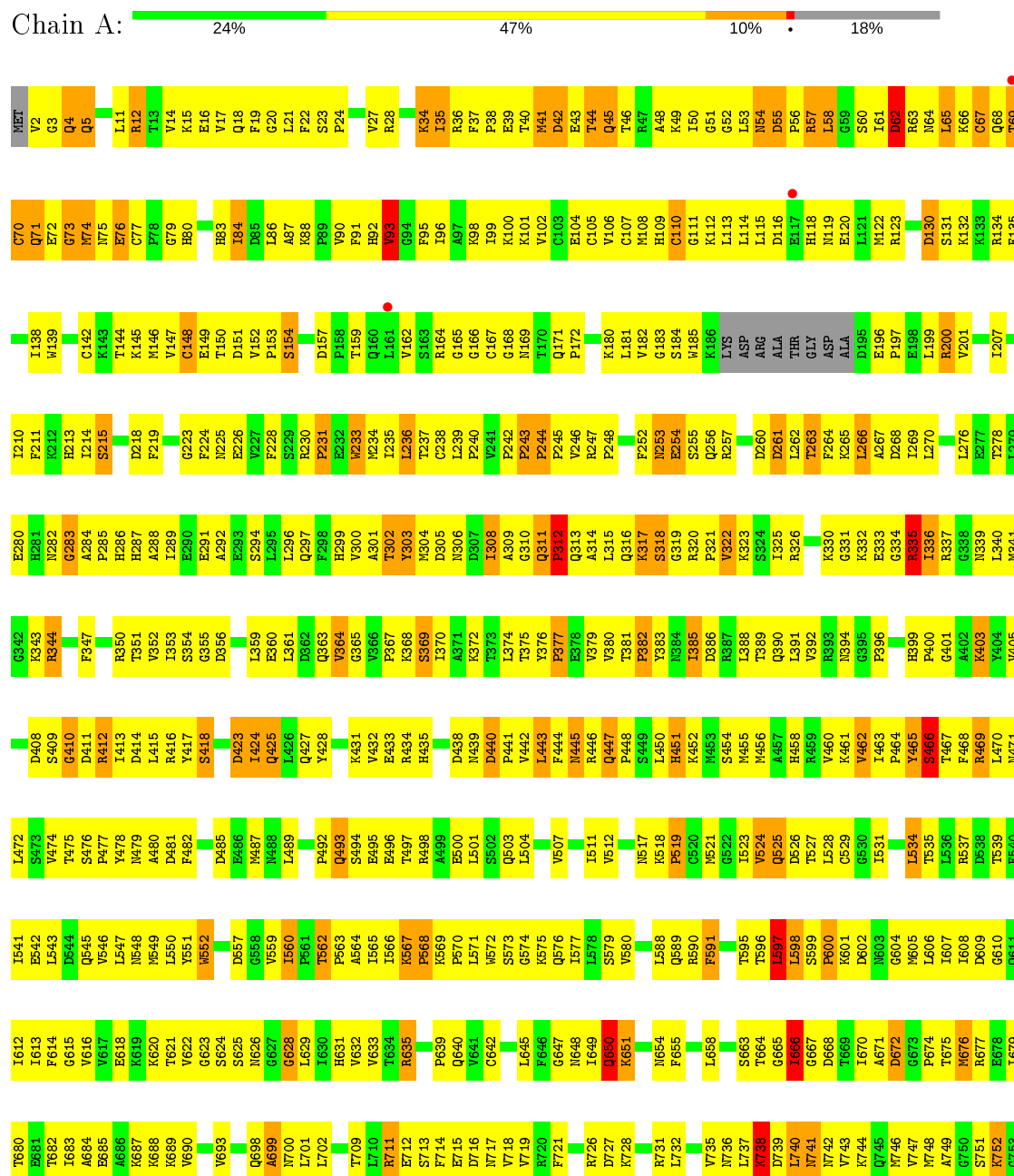
- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

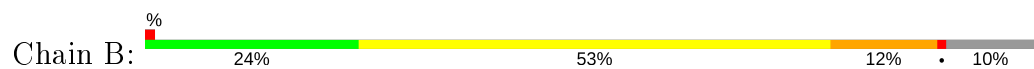
3 Residue-property plots

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

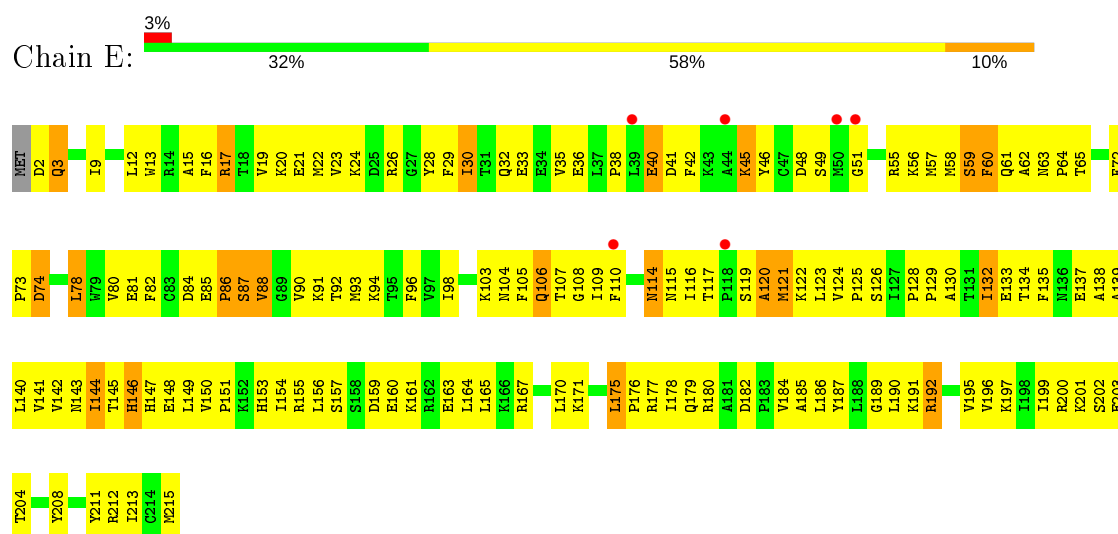
• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1



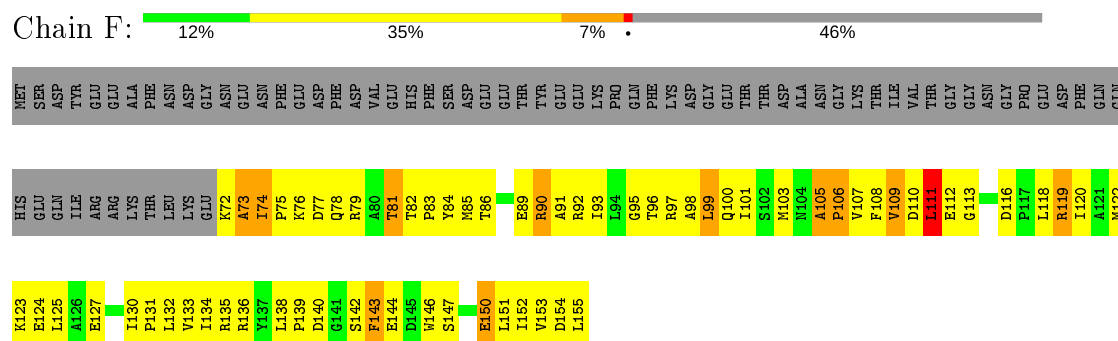
- Molecule 2: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2



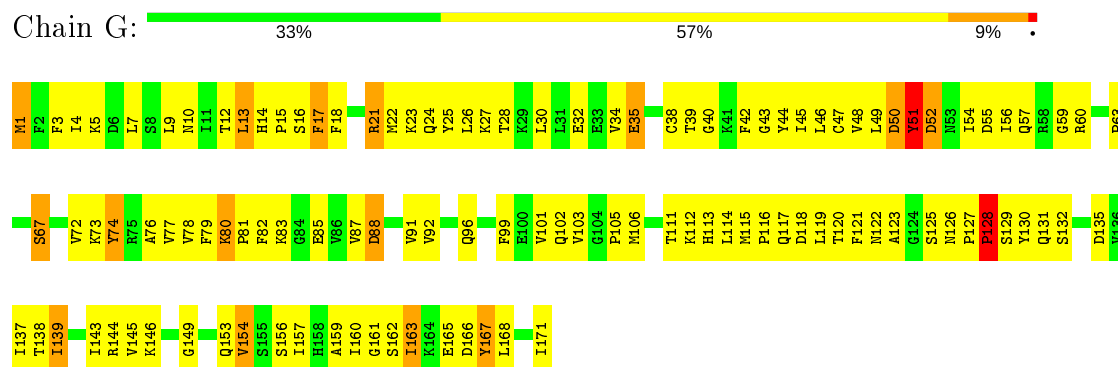
9007	G907	Q843	M778	A713	V653	H590	L521	Y459	K393	L324	L254	T185	S125	162	NET
E908	S844	S845	F781	E714	R654	R591	V522	A460	D393	Q325	K257	E186	S126	163	SER
D909	S845	S845	F781	A715	R654	R592	V522	A461	D394	Q326	K257	E186	S127	164	ASP
V910	I846	I846	L782	ASN	R655	R593	A525	A462	D395	R327	K258	D188	L128	654	LEU
I911	D847	D847	I783	GLU	H657	A594	E526	T463	D396	E328	Y259	L189	F129	D66	ALA
I912	R848	R848	I784	GLU	H658	A595	Q520	G464	H400	T329	G260	Y190	V130	S67	ASN
Q913	G849	G849	Y785	ASN	A659	L596	Q531	I465	H401	A330	R261	K191	D131	T68	SER
K914	L850	L850	N786	ASP	R660	M597	Q531	I466	F401	A332	E262	K192	V132	L69	GLU
T915	F851	F851	N787	LEU	L661	M597	Q531	I467	G402	D332	E263	K193	V133	L70	LYS
T916	R852	R852	N788	LEU	M662	L600	L535	E468	R405	F333	S264	E194	K134	170	LEU
P917	S853	S853	N789	LEU	A663	R601	L536	E469	R405	F334	S265	E195	ARG	GLU	TYR
S918	L854	L854	D790	W723	T664	T602	K537	K470	L408	I334	A266	P196	THR	GLN	TYR
S919	F855	F855	T791	W724	E685	L603	K538	K471	L409	ARG	A267	P197	GLU	GLN	ASP
PRU	F856	F856	M792	W725	T686	R604	L539	A472	A409	G335	T268	D198	ASP	ALA	ASP
ASP	R857	R857	L796	K727	Q687	R605	M542	M473	G410	ARG	L273	I204	THR	ALA	GLU
GLU	S858	S858	L796	R728	Q687	R606	M543	S474	G411	GLY	L274	I205	ALA	GLN	PRO
GLU	Y859	Y859	Y797	I729	D687	G607	S543	S475	L412	THR	P274	I206	ILE	HIS	THR
GLU	Y860	Y860	Y798	R730	ILE	D608	S544	S476	L413	LEU	P275	I207	VAL	THR	THR
LEU	Y861	Y861	Y799	S732	GLY	I609	I545	A477	L414	GLY	I276	N206	PRO	GLU	GLU
GLY	E863	E863	Q800	H733	GLY	M810	S546	G478	F417	LYS	K277	G207	GLY	SER	D20
K864	K864	K864	R801	H734	PHE	P611	G548	V479	K418	ARG	Q278	S208	ARG	ASP	E21
K865	K865	K865	P802	A735	GLU	B612	G549	S480	K419	ASN	Q279	E209	ASN	S22	ASN
Y866	Y866	Y866	L803	T736	ASP	V613	T549	Q481	T419	GLU	D279	K210	ILE	A23	A23
G867	G867	G867	G804	T737	VAL	S614	D550	V482	L420	LYS	K347	V211	LYS	SER	P24
M868	M868	M868	T805	T738	GLU	M615	P551	L483	F421	GLY	I282	L212	TYR	ARG	T25
S869	S869	S869	T806	T738	E678	I616	M552	M484	K422	Y351	I285	L213	GLU	LYS	E28
I870	I870	I870	R807	C741	T679	R617	P553	R485	K423	Y352	F286	Q215	LEU	TYR	D29
K871	K871	K871	A808	E742	T680	D618	P554	Y486	L424	I355	E216	E216	ILE	GLU	S30
E872	E872	E872	M809	I743	W681	I619	I555	T487	L425	Y353	E217	S218	ALA	I90	S30
R873	R873	R873	E810	H744	S682	R620	T556	Y488	L426	E359	L289	S219	GLU	S91	W31
F874	F874	F874	Y811	P745	S683	B621	F557	S489	D427	E359	G290	A219	GLU	A32	A32
E875	E875	E875	L812	S746	L684	K622	L558	S490	F428	F360	G291	G220	SER	F92	V33
K876	K876	K876	K813	S746	L685	K623	S559	S491	F429	L361	I291	G221	GLU	I95	I34
P877	P877	P877	F814	I748	S686	L624	S560	T491	R430	P362	I292	I222	ASP	S35	S35
Q878	Q878	Q878	R815	T748	E687	M625	W561	L492	Y431	H363	D294	V223	ASP	V97	A36
R879	R879	R879	E816	A752	G562	I626	G562	L495	Q433	T365	G295	Q224	SER	T98	F37
T880	T880	T880	L817	A752	G563	P627	M563	R496	R434	Q366	E296	V225	GLU	K39	F38
N881	N881	N881	P813	I755	E564	T628	P564	T497	T435	L367	I297	F226	SER	R39	R39
T882	T882	T882	Q821	I756	L566	D629	P565	T498	V436	L367	L298	K227	GLY	E40	E40
R883	R883	R883	Q822	I757	E567	V633	E567	M499	E437	F370	E299	K228	GLY	K41	K41
R884	R884	R884	N822	P757	E567	V634	E567	I502	GLU	E371	H300	A229	V165	M103	Q42
S886	S886	S886	A823	P758	E567	R635	H572	GLY	ALA	S372	E302	A230	F166	E104	L43
R887	R887	R887	I824	P759	E567	R636	Q573	ARG	HIS	R373	G302	P231	I167	S105	V44
G888	G888	G888	V825	H761	E696	R637	S574	ASP	ASP	K374	Y303	S232	G168	D106	S45
T889	T889	T889	A826	H762	E697	L637	S574	ASP	PHE	A375	D304	F233	R169	G107	Q46
Y890	Y890	Y890	A828	Q763	E698	F638	P575	GLY	ASN	F376	V305	I234	P171	V108	Q47
D891	D891	D891	C829	S764	E699	V640	D576	LYS	MET	F377	N306	H236	I172	L112	L48
T892	T892	T892	S831	P765	S700	V641	A577	LEU	LYS	L378	D307	H237	M173	Y113	D49
K893	K893	K893	Y830	R766	I701	B641	T578	A509	L446	G379	K308	V237	M174	P114	S50
L894	L894	L894	S832	N767	I702	D642	R579	K510	A447	V380	Q309	A238	L174	F151	F51
D895	D895	D895	Q833	T768	I703	D643	V580	P511	I448	M381	N310	E239	R175	Q115	N52
L896	L896	L896	A704	Y769	A704	D644	F581	R512	N449	L382	L311	I240	R176	Q116	N53
L897	L897	L897	M705	Q770	M705	S645	V582	Q513	N450	E312	E312	I241	K177	A117	Q53
Q898	Q898	Q898	Q835	S771	L646	L646	N583	L514	K451	R383	E312	I242	N178	R118	F54
I899	I899	I899	P707	T708	G647	H648	H515	H515	T452	L385	L314	L244	C179	R119	V55
L900	L900	L900	S838	N773	H648	H648	V585	H516	T453	L386	L315	I245	C180	Y57	D56
G902	G902	G902	N839	G774	K649	K649	V586	T517	T454	L387	P316	R249	L181	N121	T58
V903	V903	V903	L710	G775	H587	H587	H587	T518	T455	L388	P317	R250	S182	L122	L59
R967	R967	R967	N841	Q776	G588	G588	H588	H519	L457	C389	F322	F250	E183	Q60	Q60
V968	V968	V968	N842	A777	V589	V589	V589	G520	K458	L390	V323	T253	A184	Y124	D61



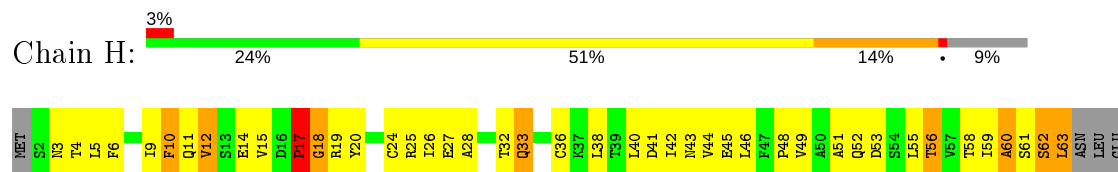
• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC2

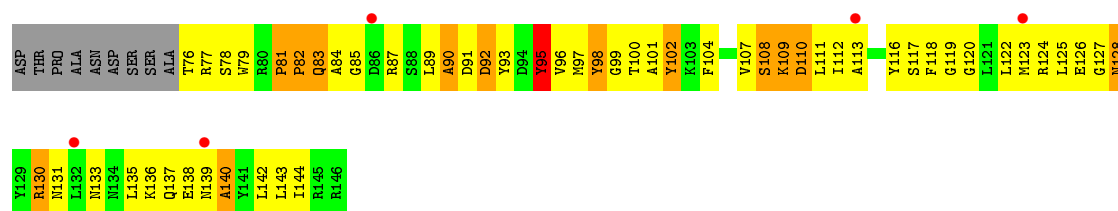


• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

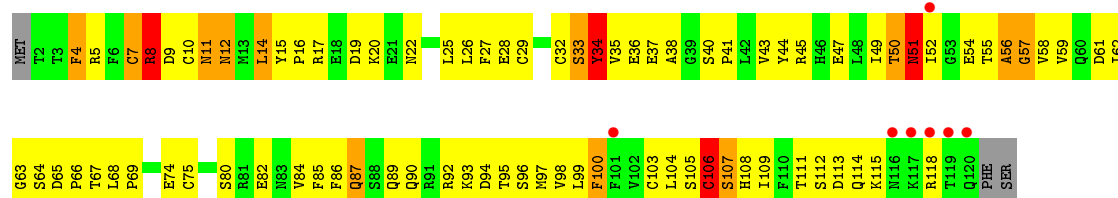


• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC3

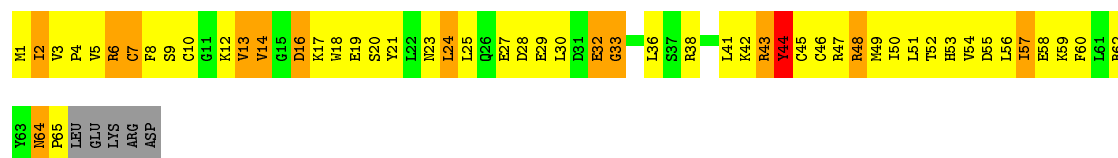
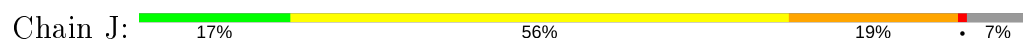




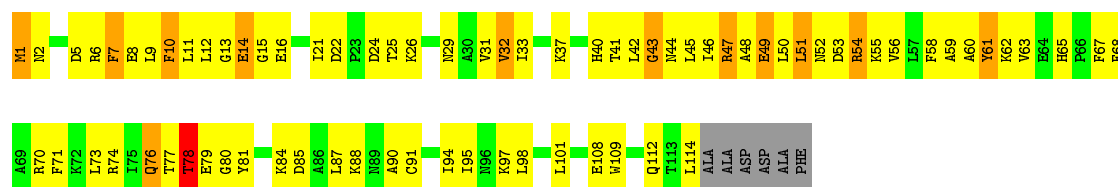
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



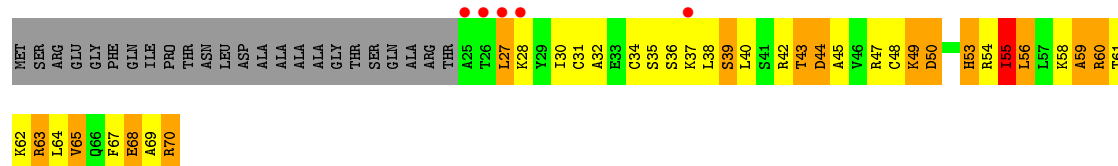
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC5



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

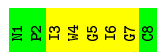


• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC4

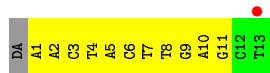


• Molecule 13: AMATOXIN

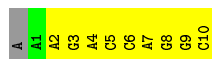
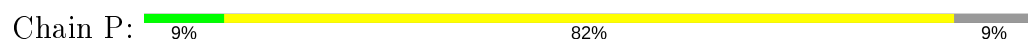




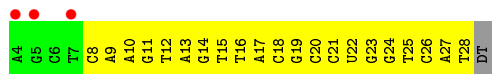
- Molecule 14: 5'-D(*AP*AP*AP*CP*TP*AP*CP*TP*TP*GP *AP*GP*CP*T)-3'



- 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

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)	Xtriage
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	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
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	Xtriage
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

Xtriage'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: MG, BRU, ZN, HYP, TRX, CSX, ILX

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

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 ⓘ

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
2	B	603	LEU
2	B	1021	MET
10	J	7	CYS
2	B	635	ARG
2	B	811	TYR

Some 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	449	ASN
2	B	822	ASN
9	I	12	ASN
2	B	465	ASN
2	B	572	HIS

5.3.3 RNA ⓘ

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 ⓘ

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	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	CSX	M	8	13	3,6,7	1.01	0	1,6,8	1.64	0
16	BRU	T	22	15,16	15,21,22	1.70	3 (20%)	17,30,33	4.08	4 (23%)
13	HYP	M	2	13	6,8,9	0.89	0	5,10,12	1.70	2 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	T	22	BRU	C4-C5	5.05	1.44	1.38
16	T	22	BRU	C4-N3	3.27	1.38	1.33
13	M	4	TRX	CZ3-CH2	3.06	1.44	1.38
13	M	3	ILX	CB-CA	-3.03	1.51	1.54
16	T	22	BRU	C6-C5	-2.04	1.34	1.39

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	22	BRU	C4-N3-C2	14.47	127.36	115.14
13	M	4	TRX	CB-CG-CD1	-7.20	119.07	127.97
16	T	22	BRU	C5-C4-N3	-6.94	115.34	123.64
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

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	49, 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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	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	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
17	ZN	A	2457	1/1	0.99	0.14	53,53,53,53	0
17	ZN	I	1121	1/1	0.99	0.16	96,96,96,96	0
17	ZN	J	1066	1/1	0.99	0.21	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.