



wwPDB X-ray Structure Validation Summary Report

Oct 31, 2023 – 09:58 AM EDT

PDB ID : 3I4N
Title : 8-oxoguanine containing RNA polymerase II elongation complex E
Authors : Damsma, G.E.; Cramer, P.
Deposited on : 2009-07-02
Resolution : 3.90 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 : 1.8.5 (274361), 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

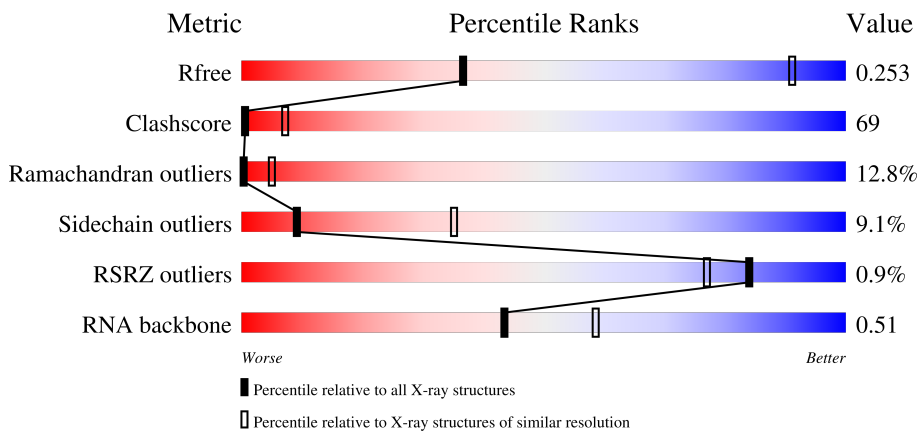
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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.



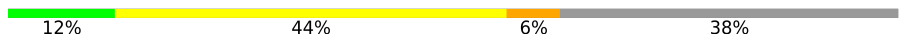
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)
RNA backbone	3102	1040 (4.76-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	 17% 52% 12% 18%
2	B	1224	 21% 56% 13% 8%
3	C	324	 19% 52% 12% 17%
4	D	221	 19% 48% 14% 18%

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Mol	Chain	Length	Quality of chain
5	E	215	 23% 63% 13% .
6	F	155	 10% 39% 6% . 43%
7	G	171	 35% 57% 8%
8	H	146	 5% 16% 58% 18% . 6%
9	I	122	 3% 29% 52% 15% . .
10	J	70	 16% 51% 26% 7%
11	K	120	 2% 26% 62% 8% .
12	L	70	 . 39% 26% . 33%
13	T	26	 69% 8% 23%
14	N	12	 25% 67% 8%
15	P	16	 12% 44% 6% 38%

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 32307 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	1429	11240	7079	1966	2133	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	1125	8942	5659	1571	1657	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	270	2125	1336	353	422	14	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	EXPRESSION TAG	UNP P16370
C	-4	HIS	-	EXPRESSION TAG	UNP P16370
C	-3	HIS	-	EXPRESSION TAG	UNP P16370
C	-2	HIS	-	EXPRESSION TAG	UNP P16370
C	-1	HIS	-	EXPRESSION TAG	UNP P16370
C	0	HIS	-	EXPRESSION TAG	UNP P16370

- 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	182	1465	904	262	296	3	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	88	712	455	120	134	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	137	1101	693	185	218	5	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	117	952	586	173	182	11	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	116	929	596	158	173	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	47	370	228	73	65	4	0	0	0

- Molecule 13 is a DNA chain called DNA (5'-D(*AP*G*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP*(8OG)P*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	Br	C	N	O	P			
13	T	20	407	1	194	72	121	19	0	0	0

- Molecule 14 is a DNA chain called DNA (5'-D(*AP*GP*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	11	224	108	42	64	10	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
15	P	10	207	94	35	69	9	0	0	0

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

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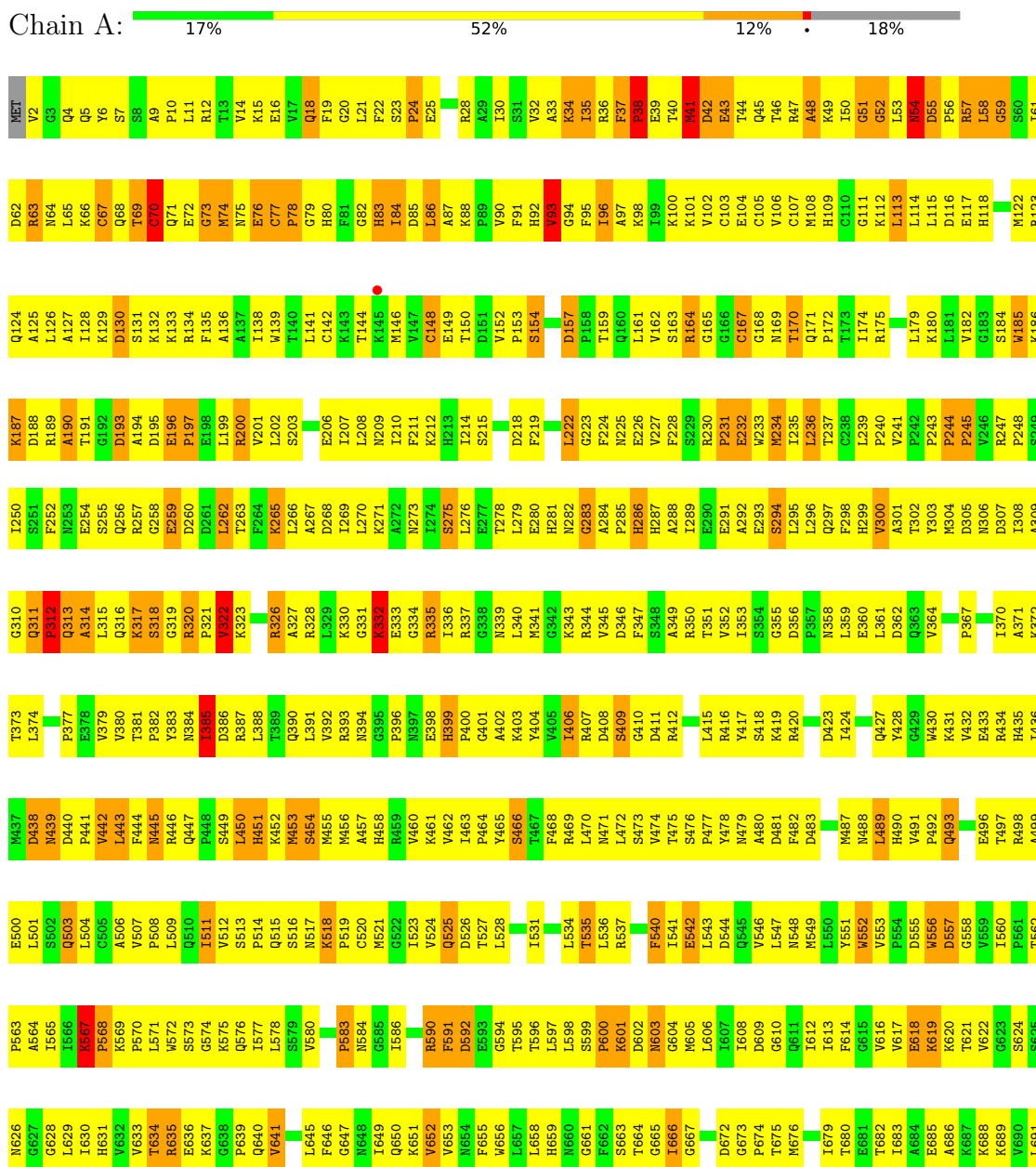
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	J	1	Total 1	Zn 1	0	0
17	L	1	Total 1	Zn 1	0	0

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



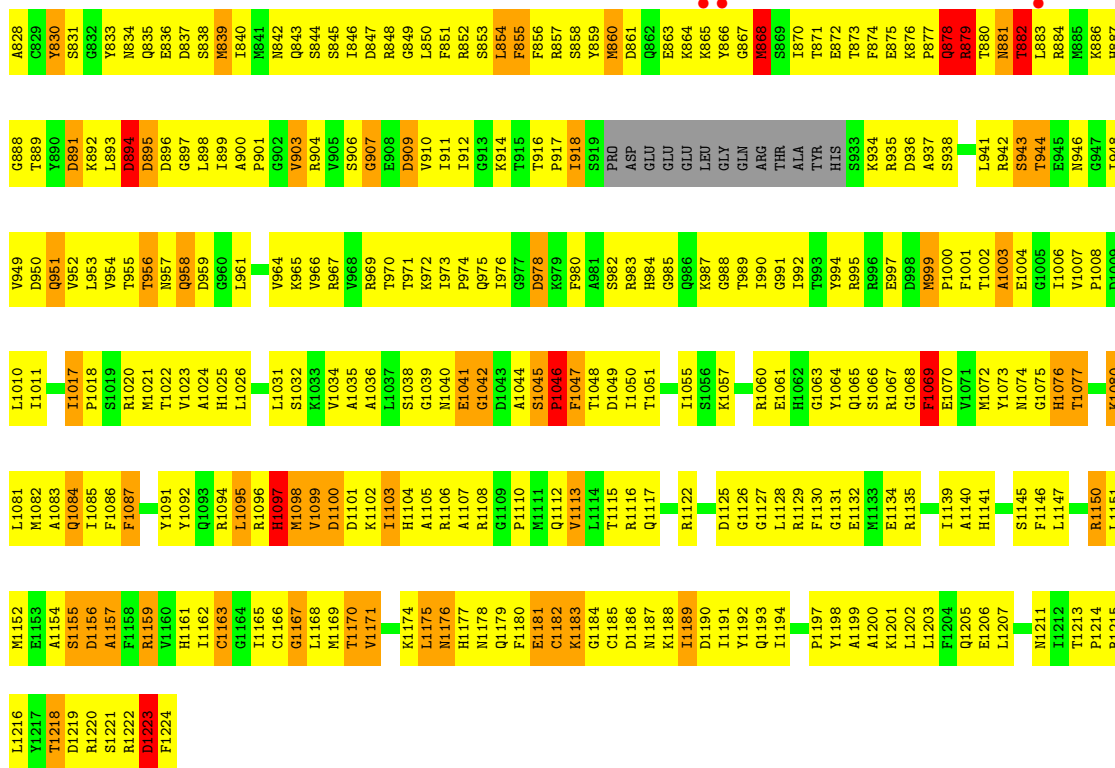
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PRO	ASP	ASP	GLY	ASP	P1324	H1258	L1197	I1072	D1012	E945	E879	M818	K695
PRO	ASP	ASP	GLY	ASP	T1325	L1260	D1198	G1073	D1013	V946	K880	G819	E696
PRO	ASP	ASP	GLY	ASP	R1326	K1261	A1201	P1074	V1015	V948	L883	G820	A697
PRO	ASP	ASP	GLY	ASP	I1327	K1262	M1202	P1075	T1016	D949	D884	R821	K698
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PRO	ASP	ASP	GLY	ASP	M1330	M1265	M1210	Q1079	C1019	E952	I886	D826	L701
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PRO	ASP	ASP	GLY	ASP	D1334	E1269	L1144	THR	R1023	G766	G766	K830	K705
PRO	ASP	ASP	GLY	ASP	M1335	R1270	V1146	THR	S1024	V958	F893	T831	H706
PRO	ASP	ASP	GLY	ASP	M1336	L1271	V1147	PHE	R1025	E959	E894	A832	G707
PRO	ASP	ASP	GLY	ASP	M1337	L1272	L1148	HIS	R1026	N960	E894	A832	G707
PRO	ASP	ASP	GLY	ASP	L1339	L1273	L1149	PHE	L1026	I966	K895	E833	M708
PRO	ASP	ASP	GLY	ASP	G1340	L1274	A1149	ALA	A1027	R961	E771	T834	T709
PRO	ASP	ASP	GLY	ASP	I1341	G1275	S1150	GLY	T1028	R962	G772	G836	L710
PRO	ASP	ASP	GLY	ASP	E1342	E1276	E1151	VAL	R1029	I963	K773	R711	R710
PRO	ASP	ASP	GLY	ASP	E1343	R1276	L1152	ALA	R1030	I964	R774	R774	E712
PRO	ASP	ASP	GLY	ASP	G1344	E1277	Y1153	SER	L1031	Q965	I775	Q838	S713
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PRO	ASP	ASP	GLY	ASP	A1347	E1280	P1156	K1094	E1034	Q968	G778	L841	F716
PRO	ASP	ASP	GLY	ASP	L1348	M1284	D1157	T1095	Y1035	Q969	F779	V842	D716
PRO	ASP	ASP	GLY	ASP	L1349	M1285	P1158	S1096	R1036	T970	V760	K843	M717
PRO	ASP	ASP	GLY	ASP	E1351	M1286	R1159	S1097	L1037	F971	V760	K843	V718
PRO	ASP	ASP	GLY	ASP	F1352	D1288	S1160	V1098	T1038	H972	D781	V719	V719
PRO	ASP	ASP	GLY	ASP	G1353	R1289	T1161	P1099	K1039	H972	R782	R846	R720
PRO	ASP	ASP	GLY	ASP	V1355	K1290	V1162	R1100	Q1040	I973	T763	E846	F721
PRO	ASP	ASP	GLY	ASP	L1356	L1291	L1163	L1101	A1041	I976	V765	L848	L722
PRO	ASP	ASP	GLY	ASP	D1359	P1292	E1165	E1103	D1043	K977	H766	M849	A725
PRO	ASP	ASP	GLY	ASP	G1360	S1293	D1166	E1104	V1044	P978	K977	V850	R726
PRO	ASP	ASP	GLY	ASP	S1361	P1294	E1167	L1105	V1045	S916	S768	H851	D727
PRO	ASP	ASP	GLY	ASP	Y1362	T1295	E1168	M1106	L1046	D980	K728	Y852	K728
PRO	ASP	ASP	GLY	ASP	V1363	G1296	I1169	V1107	S1047	T982	K769	D853	A729
PRO	ASP	ASP	GLY	ASP	M1364	E1297	Q1171	A1108	I1048	L920	G730	M854	G730
PRO	ASP	ASP	GLY	ASP	Y1365	M1298	L1172	M1111	I1050	X984	R731	T855	R731
PRO	ASP	ASP	GLY	ASP	H1366	V1299	H1173	K1112	A1051	D985	E795	T856	L732
PRO	ASP	ASP	GLY	ASP	M1367	K1300	F1174	T1113	E1052	I986	S796	R857	A733
PRO	ASP	ASP	GLY	ASP	A1368	E1301	S1175	P1114	Q1053	L983	K797	M858	E734
PRO	ASP	ASP	GLY	ASP	L1369	E1302	L1176	S1115	F1054	L994	G798	S859	V735
PRO	ASP	ASP	GLY	ASP	L1370	E1303	L1177	S1115	L1054	Q994	V800	G861	L736
PRO	ASP	ASP	GLY	ASP	L1371	M1304	D1178	T1117	R1055	E995	E801	M862	K738
PRO	ASP	ASP	GLY	ASP	V1372	V1305	E1179	L1118	S1056	N996	N802	V863	D739
PRO	ASP	ASP	GLY	ASP	D1373	L1306	GLU	Y1119	V1057	L997	L929	R864	L740
PRO	ASP	ASP	GLY	ASP	V1374	T1308	ALA	L1120	V1058	V999	E931	Q865	M741
PRO	ASP	ASP	GLY	ASP	M1375	D1309	GLU	E1121	H1059	L1000	E932	R866	W742
PRO	ASP	ASP	GLY	ASP	T1376	G1310	GLN	P1122	P1060	L1001	E932	I867	V743
PRO	ASP	ASP	GLY	ASP	T1377	V1311	SER	G1123	Q1061	Y868	Y933	V868	K744
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PRO	ASP	ASP	GLY	ASP	F1389	L1317	P1190	A1254	A1068	Q1008	F813	D874	G750
PRO	ASP	ASP	GLY	ASP	N1390	T1318	W1191	Q1130	A1069	M1009	F815	A876	K752

THR	SER	PRO	ASN	TYR	TRP	PRO	THR	THR	LYS	SER	PRO	THR	THR	GLY	GLY	TYR	SER	PRO	THR
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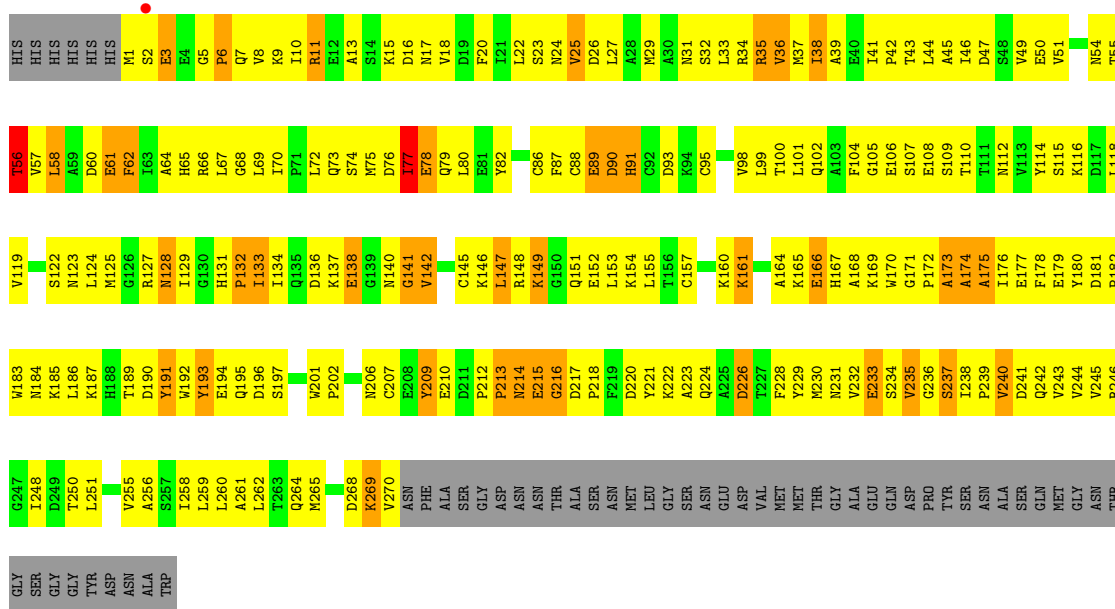
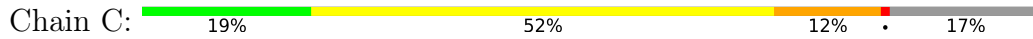
● Molecule 2: DNA-directed RNA polymerase II subunit RPB2



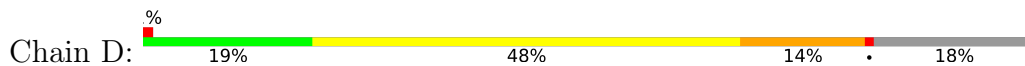
MET	SER	I62	I63	C64	E65	D66	A67	A68	S67	T68	L69	I70	LEU	LEU	GLM	ASP	ASP	ASP	PRO	THR	THR	THR	GLY	GLY	TYR	SER	SER	PRO	D20	E21	S22	A23	P24	I25	T26	D29	S30	W31	S91	F92	A32	V83	I34	S35	A36	F37	F38	R39	E40	K41	G42	L43	V44	S45	T109	H110	A111	L48	D49	S50	P114	Q115	F51	N52	Q53	F54	V55	D56	Y57	T58	L59	Q60	S125	S126	G127	L128	F129	L130	D131	V132	K133	K134	R135	E136	D188	L189	Y190	K191	L192	K193	E194	P196	F197	Y202	F203	I204	I205	N206	G207	K210	V211	L212	I213	A214	Q215	E216	R217	S218	A219	G220	N221	I222	V223	Q224	K227	K228	A229	A230	P231	T234	S235	H236	V237	A238	E239	T240	R241	S242	A243	L244	G247	L118	L119	V55	D56	N121	L122	T58	L184	T185	S252	T253	L254	Q255	K256	Y257	L258	Y259	G260	R261	S265	A266	E267	R268	I269	K270	F333	A271	T272	L273	P274	Y275	I276	K277	Q278	D279	I280	P281	I282	V283	I284	I285	F286	R287	A288	G289	G290	I291	L292	P293	D294	E296	I297	L298	E299	H300	Y303	D304	V305	N306	D307	W308	M310	Q309	F370	E371	L311	E312	M313	L314	K315	P316	C317	V318	E319	D320	V323	L324	G325	D326	R327	E328	T329	A330	L331	D332	F333	I334	G335	Q336	R337	G338	T339	K403	A340	L341	G342	I343	K344	K345	E346	K347	I348	R349	G350	Y351	A352	K353	L354	L355	L356	Q357	K358	E359	F360	L361	P362	H363	L364	T365	Q366	L367	E368	G369	W436	E437	GLU	ALA	S372	R373	K374	A375	F376	ASN	MET	L378	G379	Y380	M381	I382	N383	R384	L385	L386	L387	C388	S389	L390	D391	R392	K393	D394	Q395	R396	F401	G402	K403	K404	R405	L406	P407	L408	A409	C410	P411	L412	L413	A414	L416	F417	K418	F419	L420	F421	K422	K423	L424	T425	F429	R430	R434	T435	R496	R497	T498	R499	T500	P501	H502	G503	R504	P505	A577	L446	A447	L448	A449	A450	K451	F452	L453	T454	S455	A456	L457	K458	F459	A460	L461	G466	N466	G467	E468	Q469	K470	K471	N472	K473	S474	S475	R476	A477	G478	F479	S480	Q481	L482	L483	N484	R485	F486	L487	L488	P489	S490	T491	L492	L495	R496	R497	T498	R499	T500	P501	H502	G503	R504	P505	A577	L508	A509	K510	P511	R512	Q513	L514	H515	N516	G517	S518	V519	H520	R521	L521	A525	E526	T527	P528	E529	T599	L600	Q531	V536	K537	N538	R604	G605	K606	G607	S608	D609	I610	P611	E612	V613	S614	M615	L616	R617	D618	I619	R620	E621	G622	M625	E626	P627	F627	L628	D629	A630	G631	R632	P571	V633	H572	O573	S574	P635	R636	L637	D656	F638	I639	V640	E641	D642	D643	H648	K649	E650	L651	K652	G653	V654	R655	K656	G657	I658	A659	K660	L661	M662	A663	T664	E665	D668	I703	A704	M705	Q706	F707	E708	D709	L710	E711	P712	A715	ASN	GLU	GLU	ASN	ASN	ASP	LEU	D722	V723	D724	K727	R728	I729	R730	S731	S732	H733	H734	G735	A736	T737	F738	T739	H740	C741	E742	I743	H744	P745	S746	M747	I748	L749	G750	V751	A752	F753	S754	I755	I756	F757	F758	E696	E697	V633	H572	O573	S574	P635	R636	L637	D656	F638	T806	R807	A808	M809	E810	Y811	L812	K813	F814	R815	E816	L817	Q821	N822	P823	I824	V825	A826	I827
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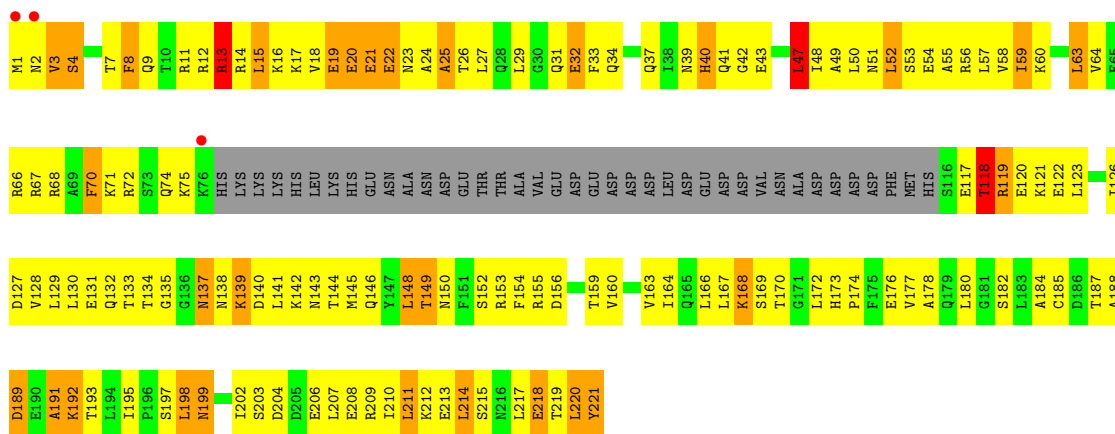


● Molecule 3: DNA-directed RNA polymerase II subunit RPB3



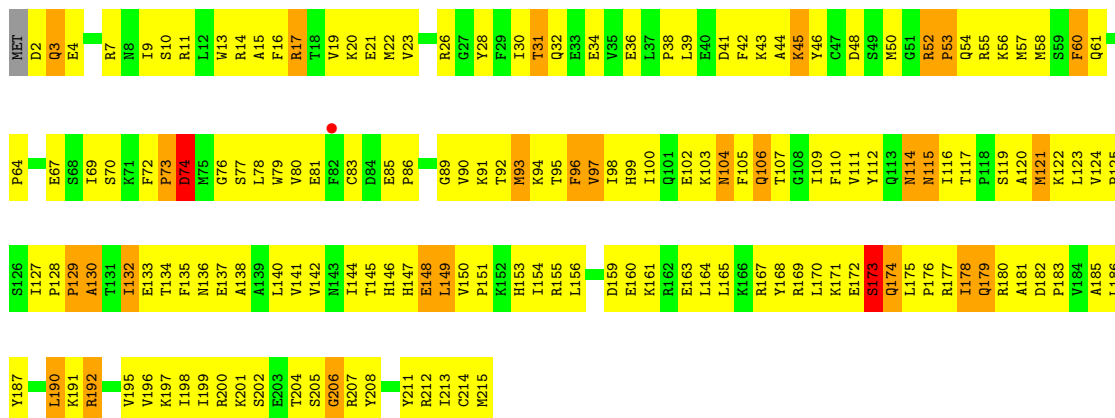
● Molecule 4: DNA-directed RNA polymerase II subunit RPB4





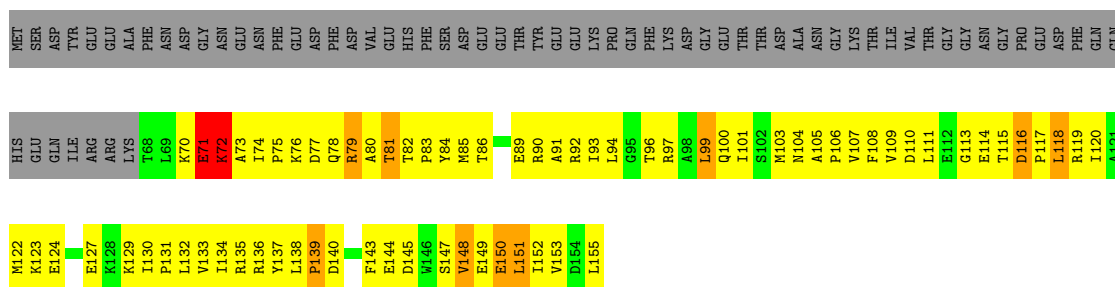
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 23% 63% 13%



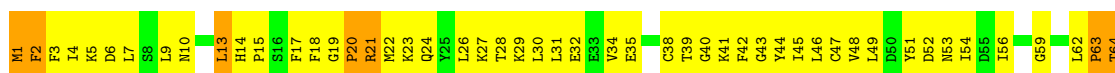
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

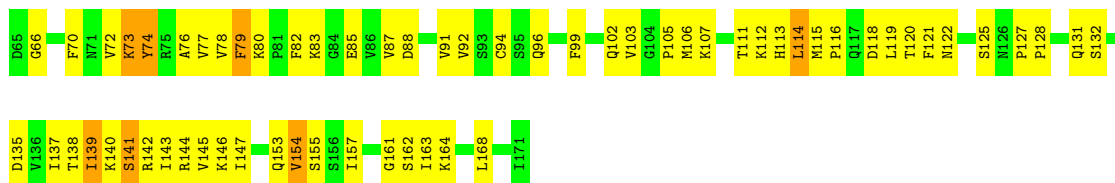
Chain F: 10% 39% 6% 43%



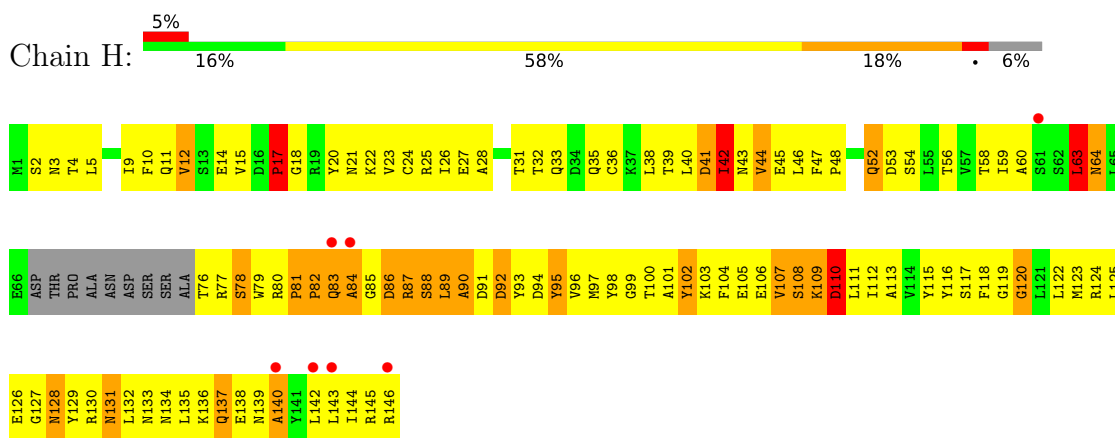
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G: 35% 57% 8%

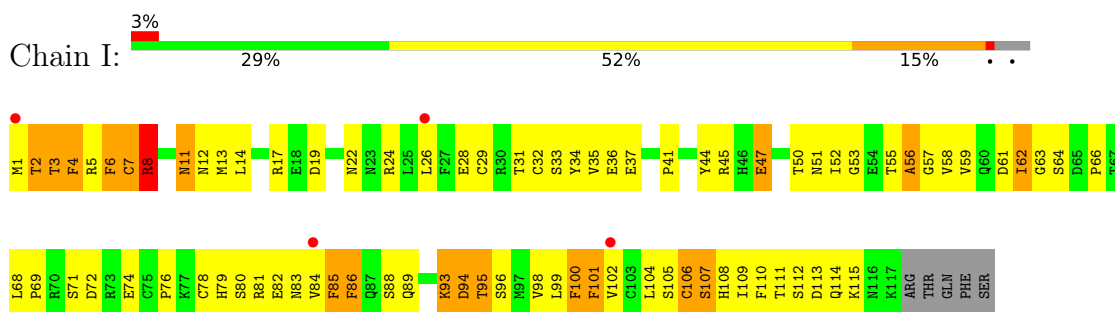




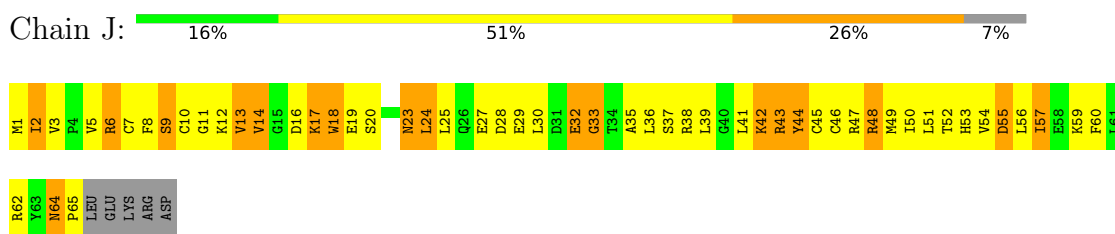
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



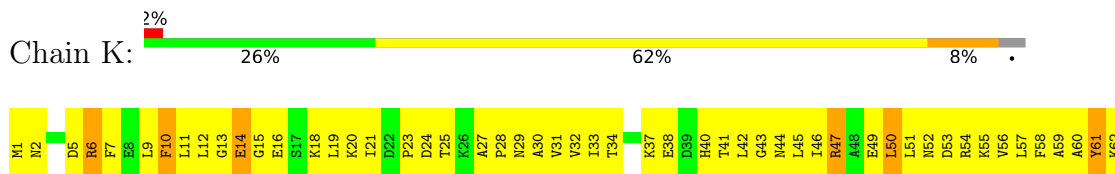
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9



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

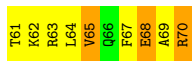


• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

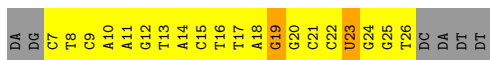




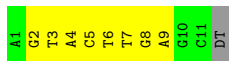
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



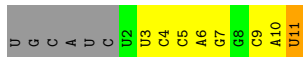
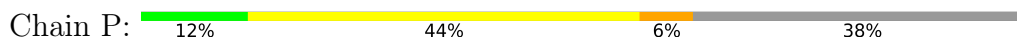
- Molecule 13: DNA (5'-D(*AP*G*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP*(8OG)P*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3')



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



- Molecule 15: RNA (5'-R(*UP*GP*CP*AP*UP*C*UP*UP*CP*CP*AP*GP*GP*CP*AP*U)-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	221.17Å 394.15Å 282.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.90 49.81 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-3.90) 100.0 (49.81-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 3.88Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.228 , 0.266 0.214 , 0.253	Depositor DCC
R_{free} test set	4364 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	128.1	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 95.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.019 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32307	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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, 8OG

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	0.43	0/11441	0.73	1/15473 (0.0%)
2	B	0.41	0/9116	0.69	1/12291 (0.0%)
3	C	0.42	0/2163	0.72	0/2930
4	D	0.39	0/1475	0.64	0/1976
5	E	0.39	0/1788	0.66	0/2406
6	F	0.46	0/724	0.82	0/977
7	G	0.44	0/1368	0.68	0/1844
8	H	0.38	0/1119	0.69	0/1514
9	I	0.36	0/970	0.66	0/1305
10	J	0.43	0/541	0.71	0/727
11	K	0.44	0/947	0.68	0/1279
12	L	0.45	0/372	0.75	0/495
13	T	0.61	0/405	0.84	0/618
14	N	0.67	0/251	0.93	0/386
15	P	0.54	0/230	0.82	0/356
All	All	0.42	0/32910	0.71	2/44577 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	882	THR	N-CA-C	5.61	126.14	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	567	LYS	C-N-CD	5.18	139.27	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	797	TYR	Sidechain

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	11240	0	11313	1726	0
2	B	8942	0	8987	1312	0
3	C	2125	0	2090	327	0
4	D	1465	0	1489	212	0
5	E	1752	0	1776	229	0
6	F	712	0	738	127	0
7	G	1340	0	1357	167	0
8	H	1101	0	1075	211	0
9	I	952	0	913	140	0
10	J	532	0	542	113	0
11	K	929	0	939	132	0
12	L	370	0	394	89	0
13	T	407	0	225	43	0
14	N	224	0	126	11	0
15	P	207	0	109	9	0
16	A	1	0	0	0	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
All	All	32307	0	32073	4433	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 69.

The worst 5 of 4433 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.19	1.14
1:A:320:ARG:HB2	1:A:320:ARG:HH11	1.07	1.14
8:H:33:GLN:HE21	8:H:35:GLN:HB2	1.12	1.13
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.25	1.12
1:A:590:ARG:HH21	1:A:620:LYS:HB3	1.06	1.12

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1421/1733 (82%)	929 (65%)	311 (22%)	181 (13%)	0	5
2	B	1111/1224 (91%)	712 (64%)	251 (23%)	148 (13%)	0	4
3	C	268/324 (83%)	165 (62%)	69 (26%)	34 (13%)	0	5
4	D	178/221 (80%)	125 (70%)	29 (16%)	24 (14%)	0	4
5	E	212/215 (99%)	145 (68%)	42 (20%)	25 (12%)	0	6
6	F	86/155 (56%)	60 (70%)	21 (24%)	5 (6%)	1	21
7	G	169/171 (99%)	133 (79%)	25 (15%)	11 (6%)	1	19
8	H	133/146 (91%)	78 (59%)	26 (20%)	29 (22%)	0	1
9	I	115/122 (94%)	72 (63%)	29 (25%)	14 (12%)	0	6
10	J	63/70 (90%)	35 (56%)	14 (22%)	14 (22%)	0	1
11	K	114/120 (95%)	80 (70%)	31 (27%)	3 (3%)	5	35
12	L	45/70 (64%)	18 (40%)	13 (29%)	14 (31%)	0	0
All	All	3915/4571 (86%)	2552 (65%)	861 (22%)	502 (13%)	0	5

5 of 502 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	41	MET
1	A	43	GLU
1	A	48	ALA
1	A	54	ASN

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	1249/1520 (82%)	1126 (90%)	123 (10%)	8 31
2	B	974/1061 (92%)	888 (91%)	86 (9%)	10 37
3	C	238/280 (85%)	219 (92%)	19 (8%)	12 41
4	D	164/200 (82%)	145 (88%)	19 (12%)	5 26
5	E	196/197 (100%)	182 (93%)	14 (7%)	14 44
6	F	78/137 (57%)	70 (90%)	8 (10%)	7 30
7	G	152/152 (100%)	144 (95%)	8 (5%)	22 52
8	H	121/128 (94%)	111 (92%)	10 (8%)	11 39
9	I	111/116 (96%)	102 (92%)	9 (8%)	11 40
10	J	60/65 (92%)	55 (92%)	5 (8%)	11 39
11	K	99/102 (97%)	89 (90%)	10 (10%)	7 30
12	L	41/57 (72%)	34 (83%)	7 (17%)	2 14
All	All	3483/4015 (87%)	3165 (91%)	318 (9%)	9 35

5 of 318 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	21	GLU
8	H	110	ASP
4	D	127	ASP
5	E	190	LEU

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Mol	Chain	Res	Type
10	J	48	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	686	ASN
9	I	114	GLN
2	B	1117	GLN
9	I	108	HIS
11	K	110	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/16 (56%)	2 (22%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	10	A
15	P	11	U

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 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	8OG	T	19	15,13	22,25,26	1.04	1 (4%)	30,37,40	1.47	3 (10%)
13	BRU	T	23	15,13	18,21,22	3.92	1 (5%)	26,30,33	0.98	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	8OG	T	19	15,13	-	2/7/21/22	0/3/3/3
13	BRU	T	23	15,13	-	1/7/21/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	23	BRU	BR-C5	-16.55	1.49	1.88
13	T	19	8OG	C8-N7	-3.92	1.30	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	19	8OG	N7-C8-N9	5.56	113.18	106.58
13	T	19	8OG	C5-N7-C8	-3.67	104.19	109.47
13	T	23	BRU	C6-C5-C4	-2.58	118.05	120.67
13	T	19	8OG	C4-C5-N7	2.46	110.81	106.08
13	T	23	BRU	O3'-C3'-C2'	-2.17	103.15	110.90

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	T	19	8OG	O4'-C4'-C5'-O5'
13	T	19	8OG	C3'-C4'-C5'-O5'
13	T	23	BRU	C2'-C1'-N1-C2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T	19	8OG	3	0
13	T	23	BRU	2	0

5.5 Carbohydrates

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1429/1733 (82%)	-0.21	3 (0%) 95 93	73, 132, 187, 200	0
2	B	1125/1224 (91%)	-0.05	15 (1%) 77 68	79, 146, 196, 200	0
3	C	270/324 (83%)	-0.21	1 (0%) 92 87	92, 133, 183, 200	0
4	D	182/221 (82%)	-0.18	3 (1%) 72 62	122, 160, 195, 200	0
5	E	214/215 (99%)	-0.21	1 (0%) 91 85	111, 170, 198, 200	0
6	F	88/155 (56%)	-0.26	0 100 100	77, 110, 145, 175	0
7	G	171/171 (100%)	-0.16	0 100 100	113, 140, 176, 182	0
8	H	137/146 (93%)	0.28	7 (5%) 28 23	147, 178, 198, 200	0
9	I	117/122 (95%)	-0.01	4 (3%) 45 35	126, 178, 197, 200	0
10	J	65/70 (92%)	-0.30	0 100 100	112, 129, 171, 180	0
11	K	116/120 (96%)	-0.23	2 (1%) 70 60	96, 135, 160, 199	0
12	L	47/70 (67%)	-0.14	0 100 100	128, 169, 190, 200	0
13	T	18/26 (69%)	0.30	0 100 100	182, 200, 200, 200	0
14	N	11/12 (91%)	0.80	0 100 100	196, 200, 200, 200	0
15	P	10/16 (62%)	-0.14	0 100 100	199, 200, 200, 200	0
All	All	4000/4625 (86%)	-0.14	36 (0%) 84 77	73, 142, 196, 200	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	471	LYS	7.2
2	B	504	ARG	4.0
9	I	1	MET	3.9
4	D	76	LYS	3.5
8	H	140	ALA	3.4

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(\AA^2)	Q<0.9
13	BRU	T	23	20/21	0.71	0.23	198,199,200,200	0
13	8OG	T	19	23/24	0.91	0.17	186,193,198,199	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(\AA^2)	Q<0.9
16	MG	A	2458	1/1	0.93	0.09	200,200,200,200	0
17	ZN	I	1122	1/1	0.95	0.05	198,198,198,198	0
17	ZN	A	2456	1/1	0.97	0.06	150,150,150,150	0
17	ZN	B	2225	1/1	0.99	0.22	106,106,106,106	0
17	ZN	A	2457	1/1	0.99	0.15	107,107,107,107	0
17	ZN	J	1066	1/1	0.99	0.27	135,135,135,135	0
17	ZN	L	1071	1/1	0.99	0.08	158,158,158,158	0
17	ZN	I	1121	1/1	1.00	0.12	140,140,140,140	0
17	ZN	C	1269	1/1	1.00	0.14	101,101,101,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.