



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 25, 2026 – 08:23 AM UTC

PDB ID : 3I4M / pdb_00003i4m
Title : 8-oxoguanine containing RNA polymerase II elongation complex D
Authors : Damsma, G.E.; Cramer, P.
Deposited on : 2009-07-02
Resolution : 3.70 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

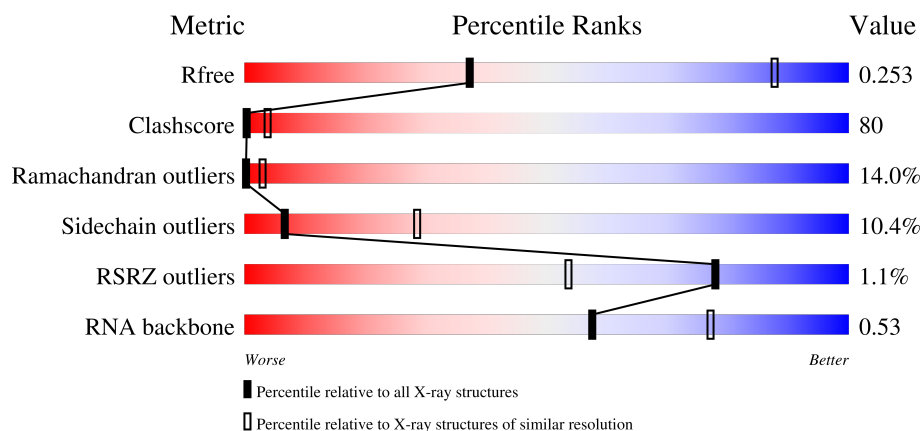
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)
RNA backbone	3983	1007 (4.30-3.08)

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	2% 12% 51% 17% 18%
2	B	1224	2% 15% 56% 18% 8%
3	C	324	15% 51% 16% 17%
4	D	221	2% 15% 52% 15% 15%

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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	T	26	
14	N	12	
15	P	16	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32355 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	1429	Total	C	N	O	S	0	0	0
			11240	7079	1966	2133	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1125	Total	C	N	O	S	0	0	0
			8942	5659	1571	1657	55			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	270	Total	C	N	O	S	0	0	0
			2125	1336	353	422	14			

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
4	D	187	Total	C	N	O	S	0	0	0
			1504	930	269	301	4			

- 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	88	Total	C	N	O	S	0	0	0
			712	455	120	134	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	137	Total	C	N	O	S	0	0	0
			1101	693	185	218	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	116	Total	C	N	O	S	0	0	0
			944	581	172	181	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	116	Total	C	N	O	S	0	0	0
			929	596	158	173	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	47	Total	C	N	O	S	0	0	0
			370	228	73	65	4			

- 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
13	T	21	Total	Br	C	N	O	P	0	0	0
			426	1	203	75	127	20			

- 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
14	N	11	Total	C	N	O	P	0	0	0
			224	108	42	64	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	10	Total	C	N	O	P	0	0	0
			205	93	33	70	9			

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 17 is ZINC ION (CCD ID: 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		

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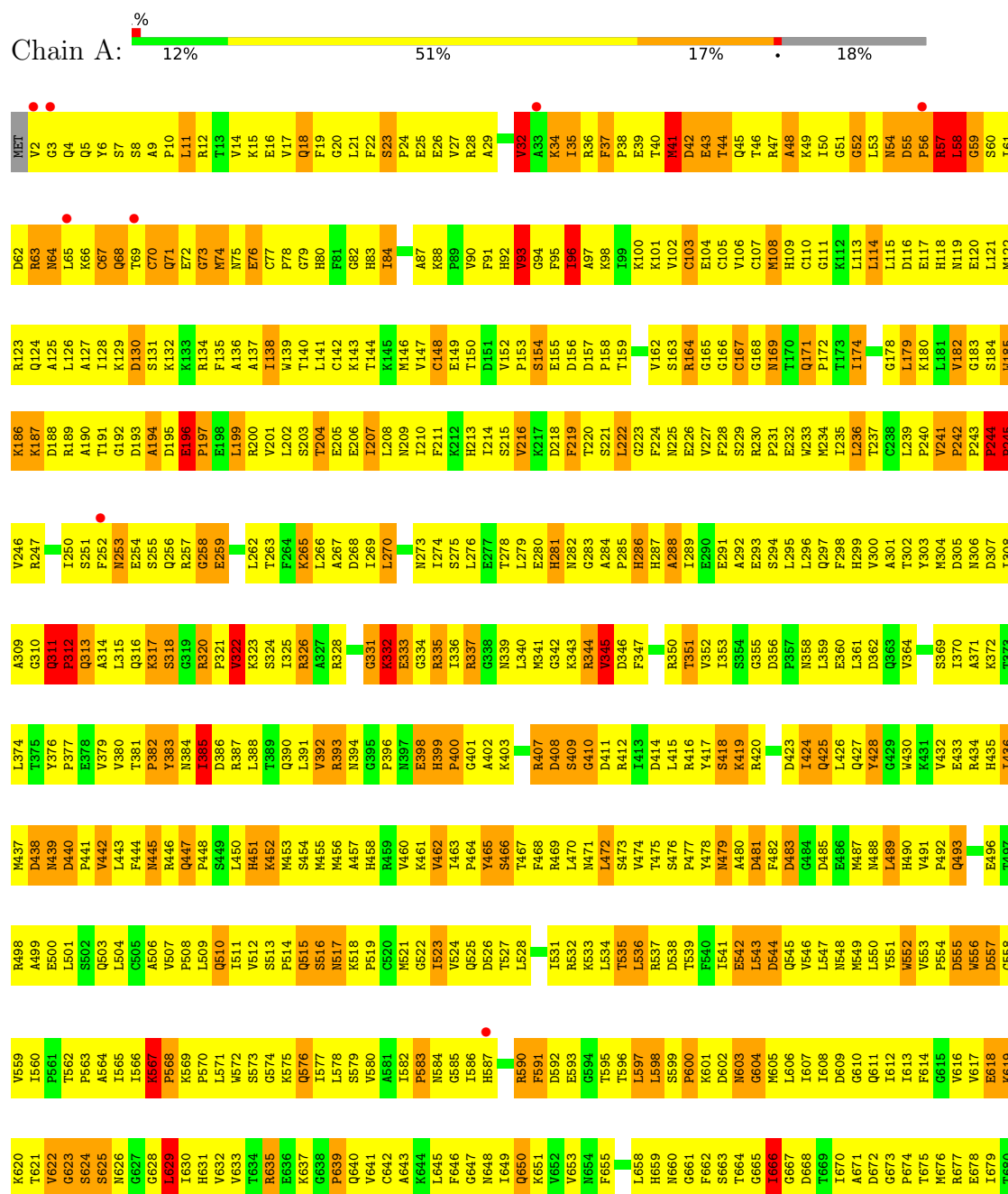
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	J	1	Total 1	Zn 1	0	0
17	L	1	Total 1	Zn 1	0	0

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.

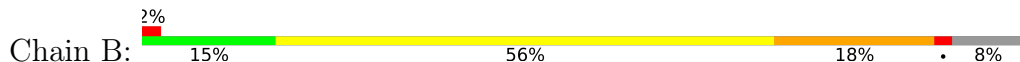
• Molecule 1: DNA-directed RNA polymerase II subunit RPB1



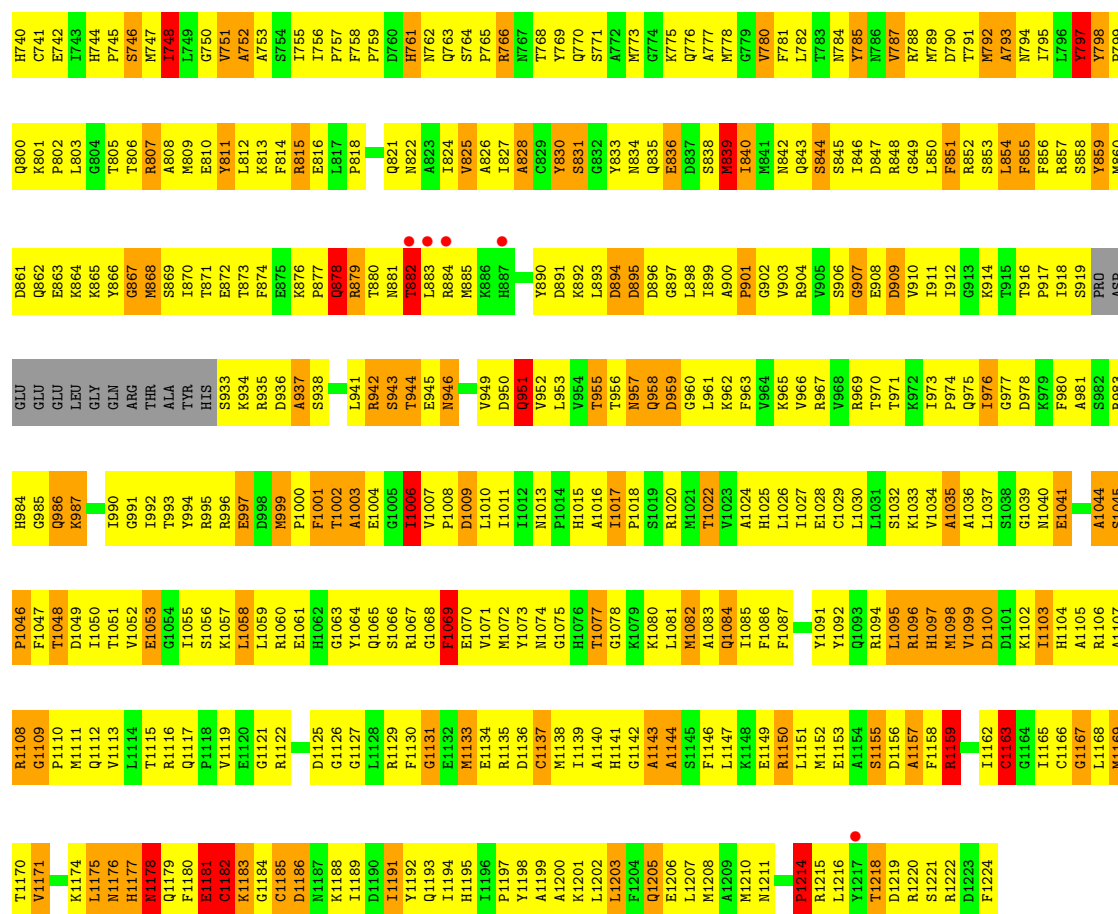


[illegible]

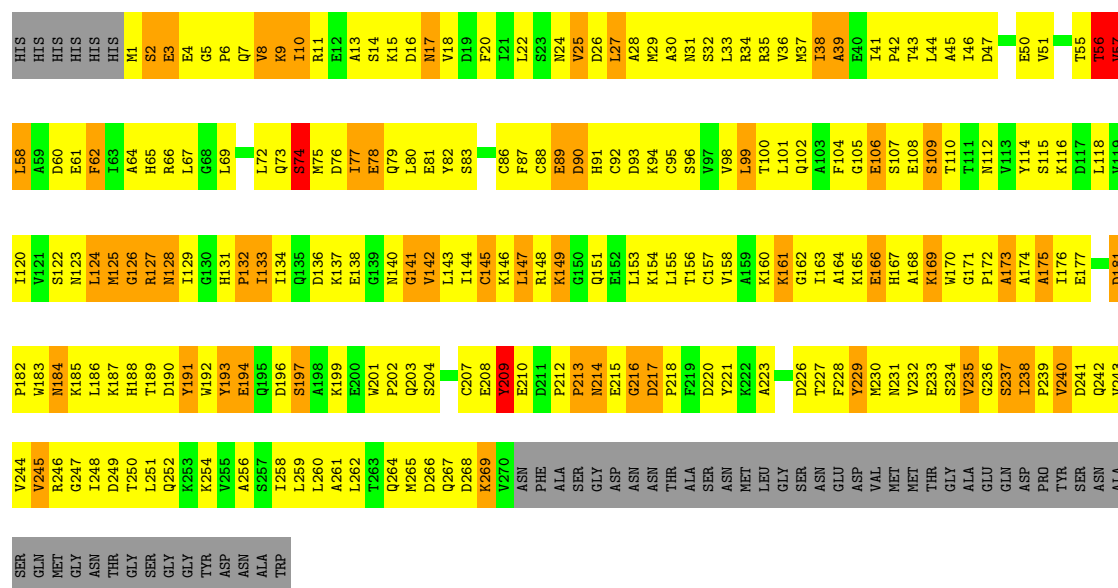
- Molecule 2: DNA-directed RNA polymerase II subunit RPB2

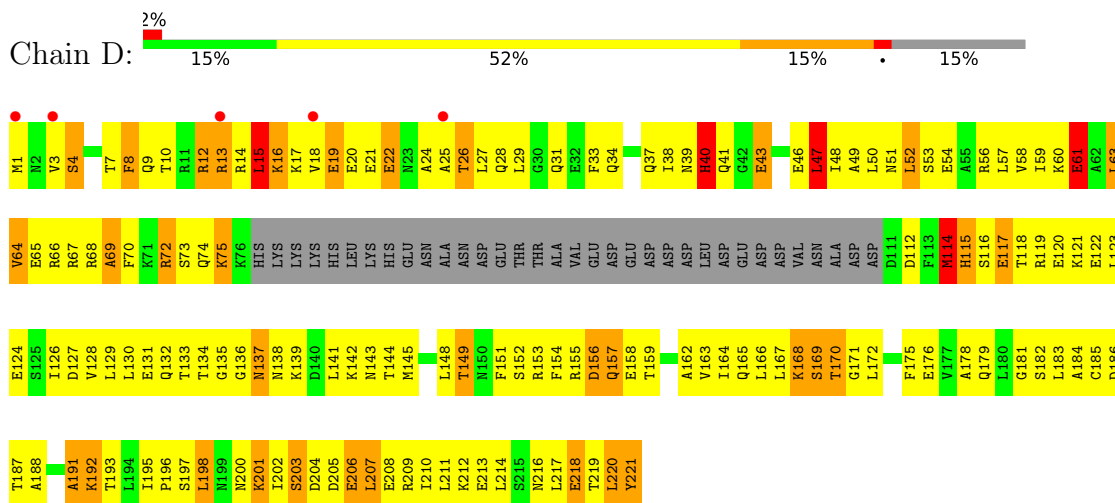


T680	D618	F557	S493	H432	F370	M310	S248	M121	D61
W681	I619	L558	H494	Q433	E371	E312	R249	L122	I62
S682	R620	L495	R434	S372	F250	E185	R249	T185	I63
S683	E560	R496	T435	R373	K374	M313	I251	Y124	C64
K621	E561	R497	V436	K374	A375	K315	S252	S125	E65
L685	G562	T498	E437	F376	F375	K316	T253	D188	ASN
K625	M563		GLJ	F376	F376	P316	L254	G127	S67
I626	E564	P501	ALA	F377	F377	C317	Q255	L128	T68
F688	R627	L502	HIS	L378	L378	V318	V256	F129	LVS
L689	T628	G503	ASP	G379	G379	E319	K257	V130	I70
D629	W690	R504	PHE	Y380	Y380	D320	R258	D131	TVR
A630	D505	R505	ASN	M381	M381	G321	K193	K132	TVR
G631	V570	G506	NET	I382	I382	F322	Y259	K132	ASP
P571	R632	K507	LYS	R383	R382	V323	G260	K133	GLJ
D694	V633	L508	L446	R384	R384	I324	R261	K134	PRO
A695	Y634	A509	A447	L385	L385	Q265	E262	R135	ASP
E696	R635	S574	K510	I448	L386	D326	S264	T136	GLY
E697	P636	P575	R511	N449	L387	R327	S265	Y137	GLY
E698	L637	D576	R512	A450	C388	E328	R266	E138	PHE
E699	R638	E577	Q513	R451	A389	T329	A267	ALA	GLJ
S700	I639	T578	L514	L452	L390	G335	L273	I1E	D20
I701	V640	R579	H515	T453	D391	L331	T268	VAL	E21
L702	E641	V580	N516	T454	R392	D332	I269	PRO	A23
I703	D642	F581	T517	S455	K393	F333	K270	GLY	P24
A704	D643	V582	H518	G456	D394	I334	T272	ARG	I25
M705	E644	N583	G519	L457	Q395	R336	P274	GLU	T26
Q706	S645	G584	G520	R458	D396	L273	T274	LEU	A27
F707	L646	V585	L521	Y459	D397	R337	V275	LYS	TVR
E708	G647	W586	V522	A460	R398	G338	L276	TVR	D29
D709	H648	H587	C523	L461	D399	T339	K277	GLJ	S30
L710	K649	G588		A462	H400	A340	Q278	LEU	S91
E711	R650	V589	E526	T483	F401	L341	D279	I1E	A32
F712	L651	H590	T527	G464	G402	G342	I280	ALA	V33
A713	K652	R591	P528	N465		I343	P281	GLU	K94
E714	V653	N592	E529	V466		R405	G220	GLU	I96
A715	R654	P593	G530	G467		K344	T282	GLU	S96
ASN	K655	A594	Q531	E468	L408	K345	V283	SER	Y96
GLU	G656	R595	A532	Q469	A409	R347	I284	GLU	F37
GLU	H657	L596		G470	G410	F286	T285	ASP	F38
ASN	I658	M597	R591	K471	P411	R287	R287	ASP	R39
ASP	A659	E598	V536	L412	L412	A288	V226	GLU	E40
LEU	K660	T599	N538	L413	L413	G350	F226	GLU	P100
D722	L661	L600	L539	S475	L413	Y351	K227	SER	K41
M662	M661	R601	S540	R475	Q415	A352	K228	GLY	G42
A663	T723	G602	S540	S476	Q415	R353	G290	K164	L43
D724	A663	L603	L541	A477	F417	D354	I292	A230	V44
T664	T664	L603	M542	G478	F417	P293	P293	V165	S105
E665	E665	R604	S543	V479	K418	I355	D294	F166	D106
		R605	C544	S480	T419	L356	G295	S232	G107
		R606	T545	Q481	L420	Q357	E296	G168	V108
D668	I1E	G607	S546	V482	F421	K358	E296	H109	D49
GLU	GLU	D608	V547	L483	R422	F360	I297	H236	S50
GLY	GLY	I609	G548	N484	K423	L361	L298	H110	H110
GLY	GLY	N610	T549	R485	L424	P362	E299	P171	F51
PHE	PHE	P611	D550	Y486	T425	H363	H300	A238	L112
GLU	GLU	E612	P551	T487	K426	I364	D294	E239	M173
ASP	ASP	V613	M552	Y488	D427	T366	G295	R362	M173
VAL	VAL	G614	P553	S489	I428	Q366	E296	I240	Y113
GLU	GLU	M615	L554	S490	F429	L367	P307	R241	P114
T737	T737	E616	L555	T491	R430	E368	X308	R175	F54
F738	E678	W679	T553	Y481	C369	C260	X209	E115	V55
T729	E679								D65

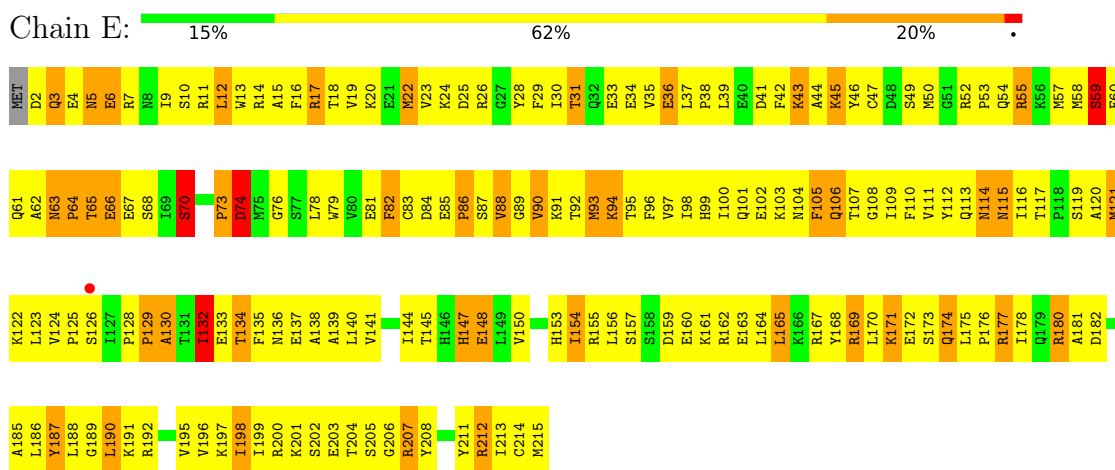


Chain C: 15% 51% 16% 17%

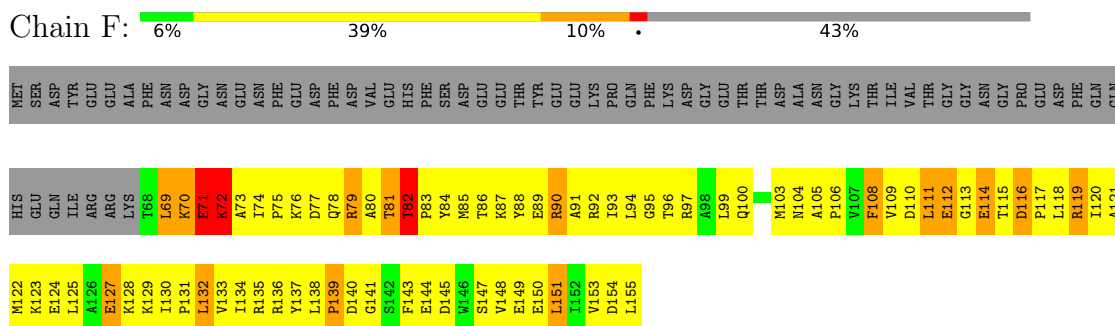




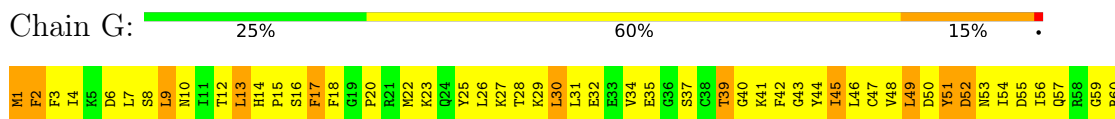
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

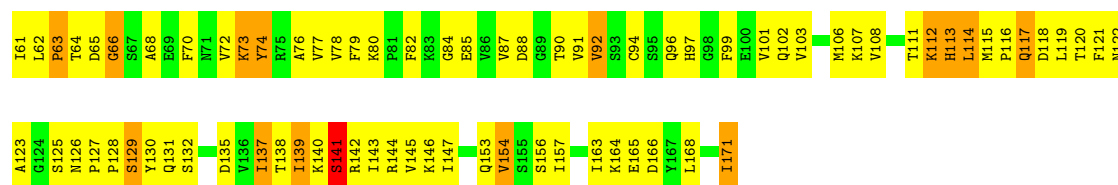


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

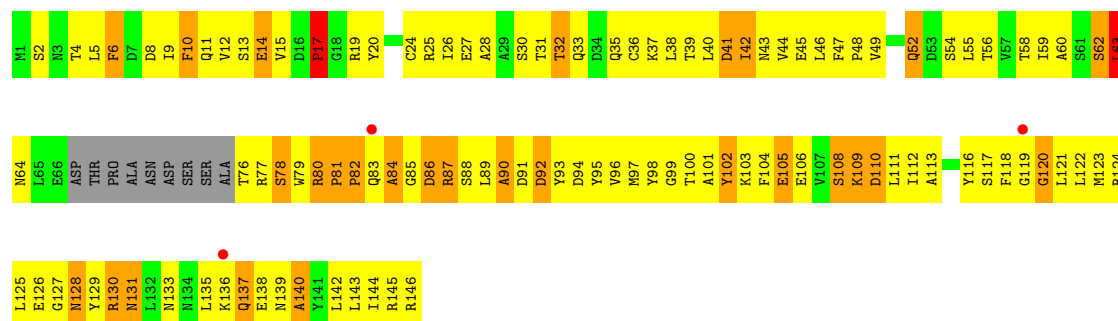
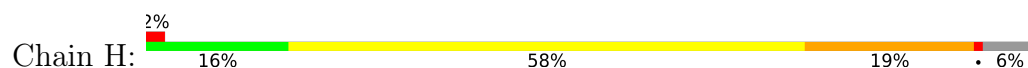


- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

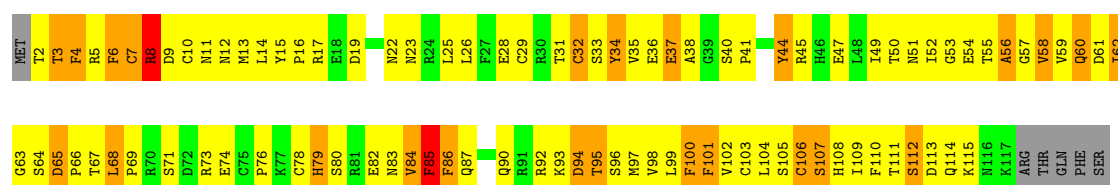
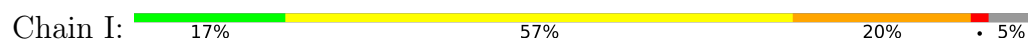




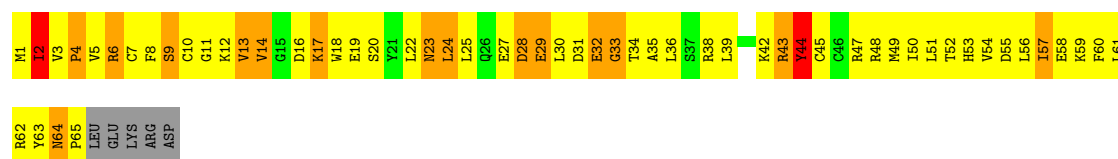
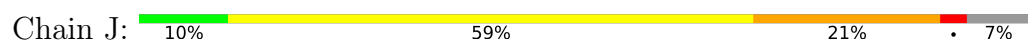
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



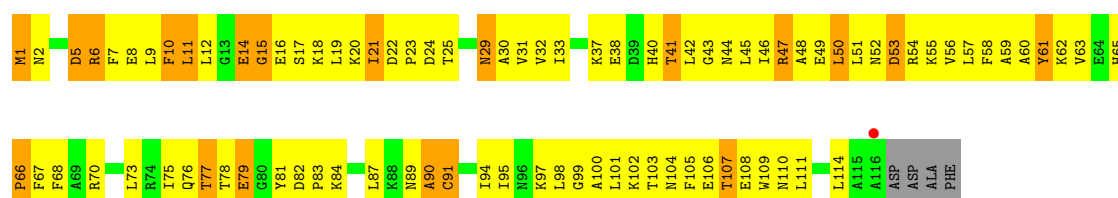
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9



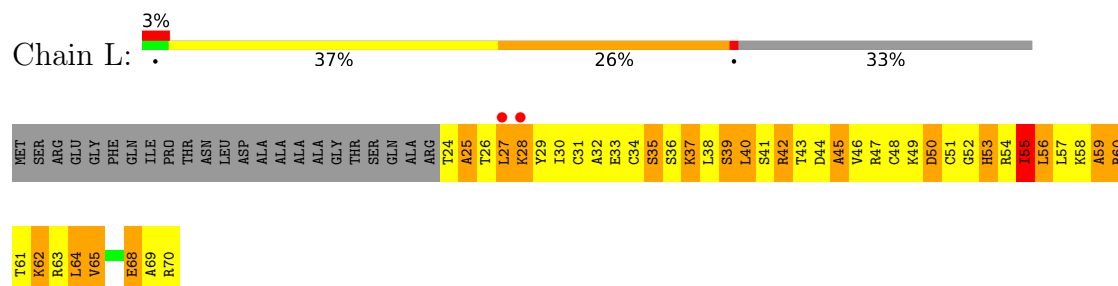
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



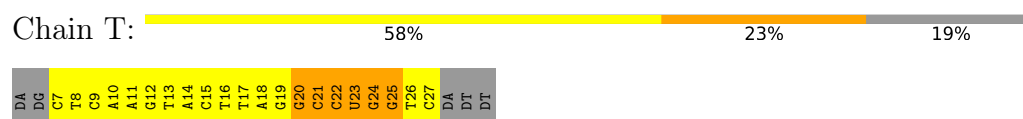
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11



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



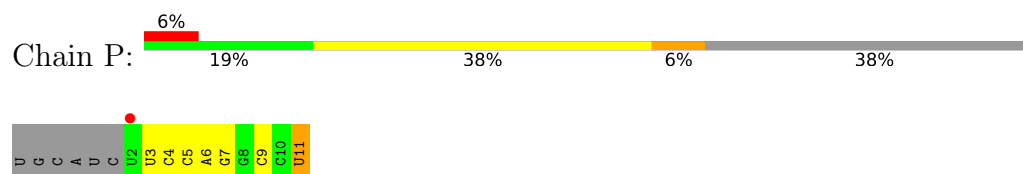
- Molecule 13: DNA (5'-D(*AP*G*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP*(8OG)P*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3')



- 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*CP*U)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	220.65Å 392.00Å 281.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.70 50.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-3.70) 99.9 (50.00-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 3.67Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.225 , 0.258 0.227 , 0.253	Depositor DCC
R_{free} test set	2439 reflections (1.88%)	wwPDB-VP
Wilson B-factor (Å ²)	114.2	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 100.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.029 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.034 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32355	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BRU, MG, 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	0.57	0/11441	1.13	94/15473 (0.6%)
2	B	0.51	0/9116	1.03	47/12291 (0.4%)
3	C	0.52	0/2163	1.05	12/2930 (0.4%)
4	D	0.45	0/1516	0.99	11/2031 (0.5%)
5	E	0.48	0/1788	1.01	11/2406 (0.5%)
6	F	0.66	0/724	1.29	11/977 (1.1%)
7	G	0.54	0/1368	1.03	5/1844 (0.3%)
8	H	0.44	0/1119	1.00	7/1514 (0.5%)
9	I	0.44	0/962	0.98	5/1295 (0.4%)
10	J	0.51	0/541	1.00	1/727 (0.1%)
11	K	0.54	0/947	1.01	1/1279 (0.1%)
12	L	0.45	0/372	0.92	1/495 (0.2%)
13	T	0.35	0/426	0.89	5/650 (0.8%)
14	N	0.31	0/251	0.72	0/386
15	P	0.34	0/227	0.74	0/351
All	All	0.53	0/32961	1.06	211/44649 (0.5%)

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

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

There are no bond length outliers.

The worst 5 of 211 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	PRO	N-CA-C	-12.28	101.91	114.68
1	A	55	ASP	CA-C-N	-11.82	108.78	120.83
1	A	55	ASP	C-N-CA	-11.82	108.78	120.83
5	E	5	ASN	N-CA-C	-11.41	99.32	113.01
2	B	1185	CYS	N-CA-C	-10.38	100.35	113.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1035	TYR	Sidechain
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	11311	1962	0
2	B	8942	0	8986	1564	0
3	C	2125	0	2090	364	0
4	D	1504	0	1518	222	0
5	E	1752	0	1776	297	0
6	F	712	0	738	149	0
7	G	1340	0	1357	226	0
8	H	1101	0	1075	217	0
9	I	944	0	901	169	0
10	J	532	0	542	133	0
11	K	929	0	939	149	0
12	L	370	0	394	93	0
13	T	426	0	236	37	0
14	N	224	0	126	11	0
15	P	205	0	109	8	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	L	1	0	0	0	0
All	All	32355	0	32098	5144	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 80.

The worst 5 of 5144 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:69:LEU:HD13	2:B:429:PHE:CD1	1.39	1.55
2:B:69:LEU:HD13	2:B:429:PHE:CE1	1.66	1.30
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.23	1.20
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.24	1.17
2:B:806:THR:HG22	2:B:808:ALA:H	1.08	1.16

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%)	909 (64%)	310 (22%)	202 (14%)	0	3
2	B	1111/1224 (91%)	694 (62%)	257 (23%)	160 (14%)	0	3
3	C	268/324 (83%)	164 (61%)	66 (25%)	38 (14%)	0	3
4	D	183/221 (83%)	108 (59%)	49 (27%)	26 (14%)	0	3
5	E	212/215 (99%)	134 (63%)	49 (23%)	29 (14%)	0	3
6	F	86/155 (56%)	60 (70%)	20 (23%)	6 (7%)	1	12
7	G	169/171 (99%)	127 (75%)	32 (19%)	10 (6%)	1	15
8	H	133/146 (91%)	72 (54%)	37 (28%)	24 (18%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	114/122 (93%)	73 (64%)	26 (23%)	15 (13%)	0	3
10	J	63/70 (90%)	34 (54%)	13 (21%)	16 (25%)	0	0
11	K	114/120 (95%)	79 (69%)	26 (23%)	9 (8%)	1	10
12	L	45/70 (64%)	19 (42%)	11 (24%)	15 (33%)	0	0
All	All	3919/4571 (86%)	2473 (63%)	896 (23%)	550 (14%)	0	3

5 of 550 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	58	LEU

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	1249/1520 (82%)	1119 (90%)	130 (10%)	7	28
2	B	974/1061 (92%)	871 (89%)	103 (11%)	6	27
3	C	238/280 (85%)	215 (90%)	23 (10%)	8	31
4	D	167/200 (84%)	146 (87%)	21 (13%)	4	21
5	E	196/197 (100%)	177 (90%)	19 (10%)	8	31
6	F	78/137 (57%)	67 (86%)	11 (14%)	3	18
7	G	152/152 (100%)	137 (90%)	15 (10%)	7	30
8	H	121/128 (94%)	114 (94%)	7 (6%)	18	45
9	I	110/116 (95%)	98 (89%)	12 (11%)	6	26
10	J	60/65 (92%)	56 (93%)	4 (7%)	15	42
11	K	99/102 (97%)	86 (87%)	13 (13%)	4	20
12	L	41/57 (72%)	36 (88%)	5 (12%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3485/4015 (87%)	3122 (90%)	363 (10%)	7 28

5 of 363 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1214	PRO
5	E	114	ASN
3	C	62	PHE
4	D	40	HIS
6	F	90	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 153 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	74	GLN
9	I	89	GLN
4	D	143	ASN
7	G	97	HIS
11	K	76	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/16 (56%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	11	U

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	BRU	T	23	13,15	18,21,22	3.94	1 (5%)	25,30,33	0.99	2 (8%)
13	8OG	T	19	13,15	22,25,26	1.03	1 (4%)	26,37,40	1.63	3 (11%)

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	BRU	T	23	13,15	-	1/7/21/22	0/2/2/2
13	8OG	T	19	13,15	-	0/7/21/22	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	23	BRU	BR-C5	-16.68	1.49	1.88
13	T	19	8OG	C8-N7	-3.93	1.31	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	5.81	113.07	106.61
13	T	19	8OG	C5-N7-C8	-3.60	104.51	109.47
13	T	23	BRU	C6-C5-C4	-2.59	118.04	120.67
13	T	19	8OG	C4-C5-N7	2.55	110.73	106.06
13	T	23	BRU	O3'-C3'-C2'	-2.26	103.03	110.88

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	T	23	BRU	C2'-C1'-N1-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T	23	BRU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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%)	-0.28	10 (0%) 84 63	15, 72, 135, 195	0
2	B	1125/1224 (91%)	-0.03	20 (1%) 67 42	11, 88, 154, 194	0
3	C	270/324 (83%)	-0.36	0 100 100	34, 73, 131, 174	0
4	D	187/221 (84%)	-0.09	5 (2%) 56 35	58, 98, 152, 197	0
5	E	214/215 (99%)	-0.17	1 (0%) 87 69	42, 112, 155, 161	0
6	F	88/155 (56%)	-0.49	0 100 100	24, 48, 91, 122	0
7	G	171/171 (100%)	-0.31	0 100 100	48, 74, 117, 128	0
8	H	137/146 (93%)	0.20	3 (2%) 62 39	91, 125, 152, 157	0
9	I	116/122 (95%)	-0.02	0 100 100	65, 121, 152, 153	0
10	J	65/70 (92%)	-0.39	0 100 100	48, 67, 106, 121	0
11	K	116/120 (96%)	-0.53	1 (0%) 81 58	32, 79, 108, 160	0
12	L	47/70 (67%)	0.31	2 (4%) 40 25	73, 124, 147, 159	0
13	T	19/26 (73%)	0.59	0 100 100	128, 194, 200, 200	0
14	N	11/12 (91%)	0.57	0 100 100	186, 198, 200, 200	0
15	P	10/16 (62%)	0.64	1 (10%) 12 13	177, 193, 199, 200	0
All	All	4005/4625 (86%)	-0.18	43 (1%) 78 53	11, 83, 152, 200	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	VAL	4.9
2	B	446	LEU	4.2
1	A	1081	LEU	4.1
2	B	471	LYS	3.8
4	D	1	MET	3.5

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
13	BRU	T	23	20/21	0.58	0.17	153,162,167,170	0
13	8OG	T	19	23/24	0.93	0.10	131,141,154,155	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
16	MG	A	2458	1/1	0.97	0.05	69,69,69,69	0
17	ZN	I	1122	1/1	0.97	0.04	134,134,134,134	0
17	ZN	A	2456	1/1	0.98	0.03	96,96,96,96	0
17	ZN	L	1071	1/1	0.99	0.02	111,111,111,111	0
17	ZN	C	1269	1/1	1.00	0.03	39,39,39,39	0
17	ZN	I	1121	1/1	1.00	0.02	70,70,70,70	0
17	ZN	A	2457	1/1	1.00	0.01	38,38,38,38	0
17	ZN	J	1066	1/1	1.00	0.01	47,47,47,47	0
17	ZN	B	2225	1/1	1.00	0.03	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.