



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2025 – 10:10 AM EDT

PDB ID : 9N5G / pdb_00009n5g
Title : RNA polymerase II elongation complex with 8-oxoG at +1 site, ATP in both A- and E-site
Authors : Oh, J.; Wang, D.
Deposited on : 2025-02-04
Resolution : 3.15 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

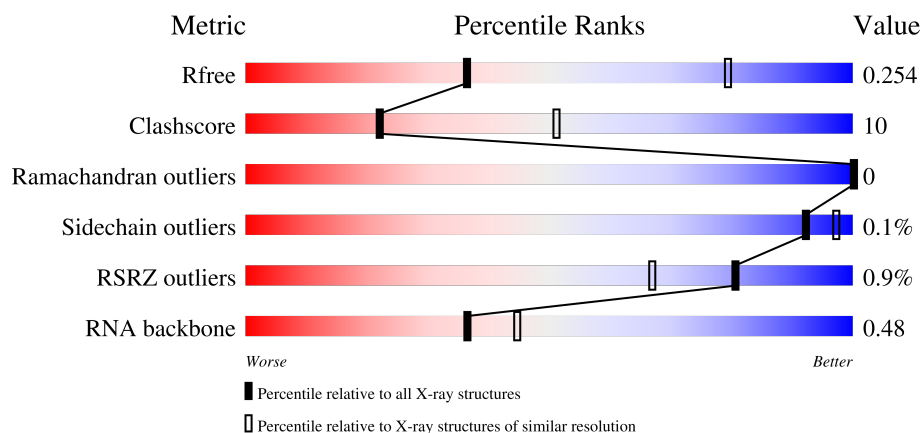
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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}	164625	2168 (3.20-3.12)
Clashscore	180529	2333 (3.20-3.12)
Ramachandran outliers	177936	2266 (3.20-3.12)
Sidechain outliers	177891	2265 (3.20-3.12)
RSRZ outliers	164620	2169 (3.20-3.12)
RNA backbone	3690	1016 (3.42-2.90)

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	R	9	 44% 44% 11%
2	T	29	 31% 52% 17%
3	N	18	 17% 50% 33%
4	A	1733	 61% 19% 20%

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Mol	Chain	Length	Quality of chain
5	B	1224	<p>%</p> <p>70% 21% 8%</p>
6	C	318	<p>64% 20% 16%</p>
7	E	215	<p>%</p> <p>67% 32% 1%</p>
8	F	155	<p>42% 14% 45%</p>
9	H	146	<p>62% 29% 9%</p>
10	I	122	<p>75% 21% 4%</p>
11	J	70	<p>66% 27% 7%</p>
12	K	120	<p>74% 21% 5%</p>
13	L	70	<p>4% 49% 13% 39%</p>

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 28998 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	9	Total	C	N	O	P	0	0	0
			199	88	40	62	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	24	Total	C	N	O	P	0	1	0
			493	235	81	153	24			

- Molecule 3 is a DNA chain called Non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	12	Total	C	N	O	P	0	0	0
			256	119	58	67	12			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1385	Total	C	N	O	S	0	0	0
			10837	6836	1898	2043	60			

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1121	Total	C	N	O	S	0	0	0
			8837	5595	1544	1645	53			

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	213	Total	C	N	O	S	0	0	0
			1734	1102	304	317	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	86	Total	C	N	O	S	0	0	0
			684	437	115	129	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1052	664	173	211	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	118	Total	C	N	O	S	0	0	0
			946	582	170	184	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	43	Total	C	N	O	S	0	0	0
			337	208	66	59	4			

- Molecule 14 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃)

ATP

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

WORLDWIDE
 **PDB**
PROTEIN DATA BANK

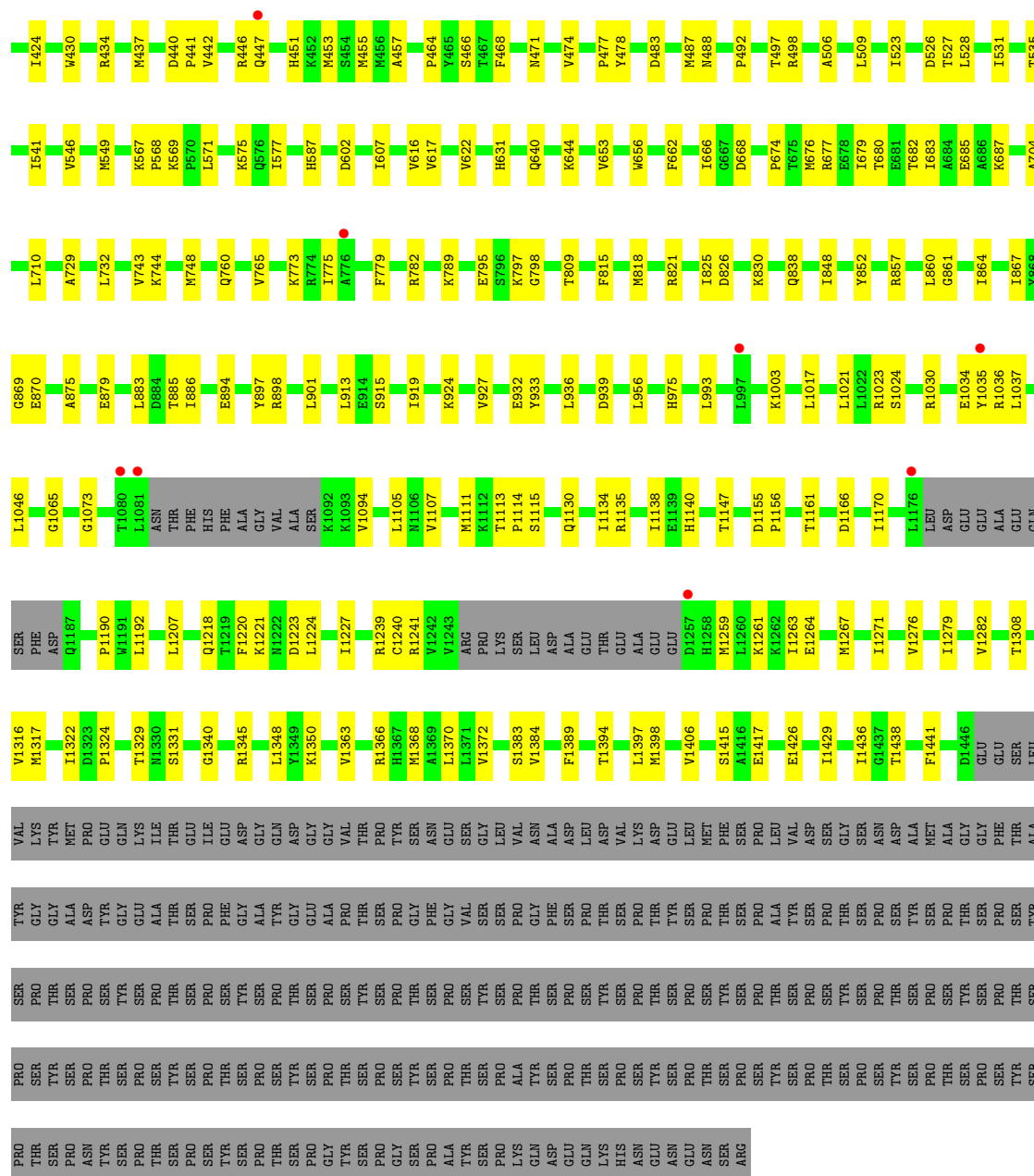
- Molecule 1: RNA

A1	U2	C3	G4	A5	G6		G9
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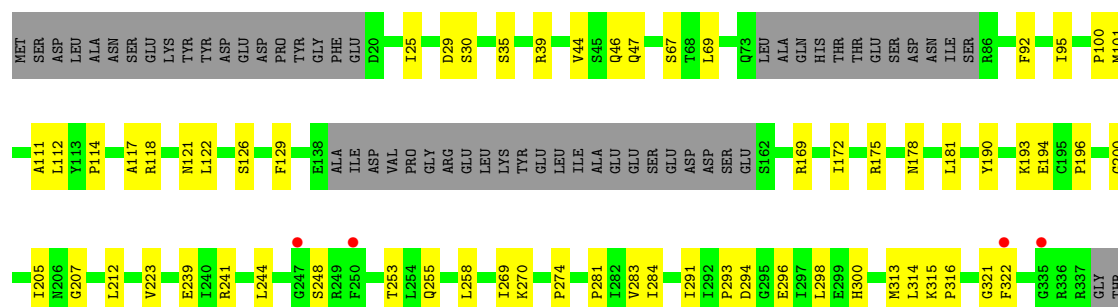
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DT	A3	C5	G10	A13	DA
DC	G4	G6	A11	G14	DA
		A7	G12		DG
		G8			DG
		A9			

[illegible]



• Molecule 5: DNA-directed RNA polymerase II subunit RPB2





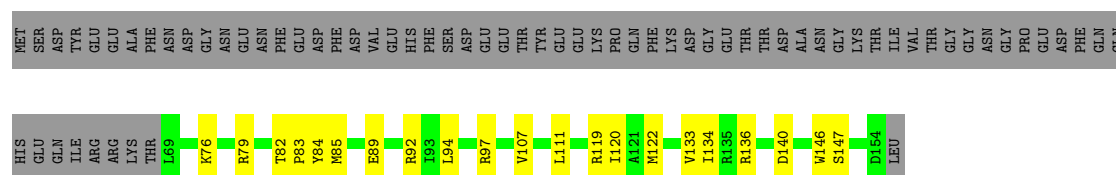
Lys	K146	Met	S2
Val	K147		
Asn	R148		
Phe	K149		
Ala			
Ser	K154		
Gly			
Asp	V158		
Asn	A159		
Thr	K160		
Ala	K161		
Ser	P172		
Asn			
Met	E177		
Leu	F178		
Gly			
Ser	P182		
Asn	D196		
Glu			
Asp	K199		
Val	E210		
Met	P200		
Met	W201		
Thr			
Gly	S204		
Ala			
Glu	C207		
Gln			
Asp	E210		
Pro	Y221		
Tyr	K222		
Ser	R221		
Asn			
Ala	Y229		
Ser	M230		
Gln			
Met	Q242		
Gly			
Asn	R246		
Thr	G247		
Gly	L248		
Ser	D249		
Gly	T250		
Gly	L251		
Tyr	Q252		
Asp	K253		
Asn	K254		
Ala	V255		
Trp	T258		
	L259		
	L262		
	T263		
	Q264		
	M265		
	T266		
	T142		

- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

M83	M84	M85	M86	M87	M88	M89	M90	M91	M92	M93	M94	M95	M96	M97	M98	M99	M100	M101	M102	M103	M104	M105	M106	M107	M108	M109	M110	M111	M112	M113	M114	M115	M116	M117	M118	M119	M120	M121	M122	M123	M124	M125	M126	M127	M128	M129	M130	M131	M132	M133	M134	M135	M136	M137	M138	M139	M140	M141	M142	M143	M144	M145	M146	M147	M148	M149	M150	M151	M152	M153	M154	M155	M156	M157	M158	M159	M160	M161	M162	M163	M164	M165	M166	M167	M168	M169	M170	M171	M172	M173	M174	M175	M176	M177	M178	M179	M180	M181	M182	M183	M184	M185	M186	M187	M188	M189	M190	M191	M192	M193	M194	M195	M196	M197	M198	M199	M200	M201	M202	M203	M204	M205	M206	M207	M208	M209	M210	M211	M212	M213	M214	M215	M216	M217	M218	M219	M220	M221	M222	M223	M224	M225	M226	M227	M228	M229	M230	M231	M232	M233	M234	M235	M236	M237	M238	M239	M240	M241	M242	M243	M244	M245	M246	M247	M248	M249	M250	M251	M252	M253	M254	M255	M256	M257	M258	M259	M260	M261	M262	M263	M264	M265	M266	M267	M268	M269	M270	M271	M272	M273	M274	M275	M276	M277	M278	M279	M280	M281	M282	M283	M284	M285	M286	M287	M288	M289	M290	M291	M292	M293	M294	M295	M296	M297	M298	M299	M300	M301	M302	M303	M304	M305	M306	M307	M308	M309	M310	M311	M312	M313	M314	M315	M316	M317	M318	M319	M320	M321	M322	M323	M324	M325	M326	M327	M328	M329	M330	M331	M332	M333	M334	M335	M336	M337	M338	M339	M340	M341	M342	M343	M344	M345	M346	M347	M348	M349	M350	M351	M352	M353	M354	M355	M356	M357	M358	M359	M360	M361	M362	M363	M364	M365	M366	M367	M368	M369	M370	M371	M372	M373	M374	M375	M376	M377	M378	M379	M380	M381	M382	M383	M384	M385	M386	M387	M388	M389	M390	M391	M392	M393	M394	M395	M396	M397	M398	M399	M400	M401	M402	M403	M404	M405	M406	M407	M408	M409	M410	M411	M412	M413	M414	M415	M416	M417	M418	M419	M420	M421	M422	M423	M424	M425	M426	M427	M428	M429	M430	M431	M432	M433	M434	M435	M436	M437	M438	M439	M440	M441	M442	M443	M444	M445	M446	M447	M448	M449	M450	M451	M452	M453	M454	M455	M456	M457	M458	M459	M460	M461	M462	M463	M464	M465	M466	M467	M468	M469	M470	M471	M472	M473	M474	M475	M476	M477	M478	M479	M480	M481	M482	M483	M484	M485	M486	M487	M488	M489	M490	M491	M492	M493	M494	M495	M496	M497	M498	M499	M500	M501	M502	M503	M504	M505	M506	M507	M508	M509	M510	M511	M512	M513	M514	M515	M516	M517	M518	M519	M520	M521	M522	M523	M524	M525	M526	M527	M528	M529	M530	M531	M532	M533	M534	M535	M536	M537	M538	M539	M540	M541	M542	M543	M544	M545	M546	M547	M548	M549	M550	M551	M552	M553	M554	M555	M556	M557	M558	M559	M560	M561	M562	M563	M564	M565	M566	M567	M568	M569	M570	M571	M572	M573	M574	M575	M576	M577	M578	M579	M580	M581	M582	M583	M584	M585	M586	M587	M588	M589	M590	M591	M592	M593	M594	M595	M596
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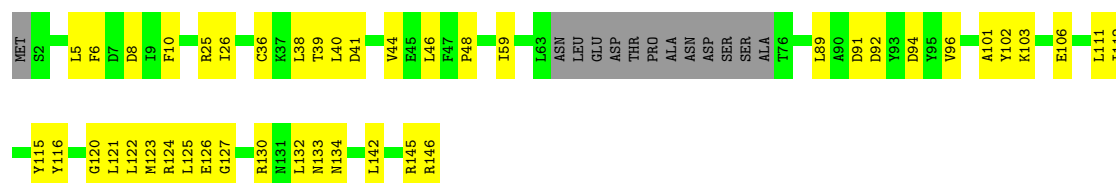
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 



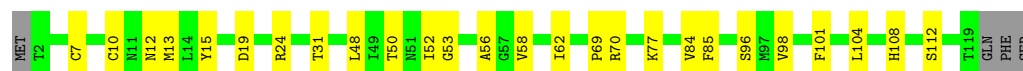
- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 



- Molecule 10: DNA-directed RNA polymerase II subunit RPB9

Chain I: 



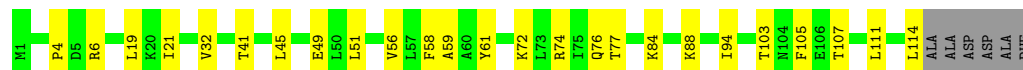
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 



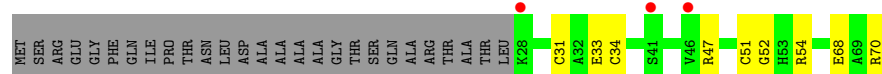
- Molecule 12: DNA-directed RNA polymerase II subunit RPB11

Chain K: 



- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	159.78Å 222.49Å 192.29Å 90.00° 98.10° 90.00°	Depositor
Resolution (Å)	48.06 – 3.15 48.06 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.06-3.15) 99.8 (48.06-3.15)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.220 , 0.254 0.221 , 0.254	Depositor DCC
R_{free} test set	2000 reflections (1.75%)	wwPDB-VP
Wilson B-factor (Å ²)	79.6	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 83.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28998	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 2.58% 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: 8OG, MG, ZN, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	R	0.14	0/223	0.35	0/345
2	T	0.26	0/507	0.53	0/775
3	N	0.25	0/290	0.50	0/447
4	A	0.17	0/11029	0.37	1/14919 (0.0%)
5	B	0.15	0/9008	0.34	0/12158
6	C	0.17	0/2139	0.35	0/2899
7	E	0.14	0/1770	0.36	0/2383
8	F	0.14	0/696	0.33	0/943
9	H	0.15	0/1070	0.39	0/1452
10	I	0.14	0/964	0.34	0/1301
11	J	0.18	0/541	0.38	0/727
12	K	0.15	0/937	0.34	0/1265
13	L	0.16	0/339	0.37	0/450
All	All	0.16	0/29513	0.36	1/40064 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	68	GLN	CB-CA-C	-5.45	103.78	111.95

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	199	0	98	4	0
2	T	493	0	272	17	0
3	N	256	0	133	9	0
4	A	10837	0	10882	241	0
5	B	8837	0	8788	182	0
6	C	2101	0	2056	46	0
7	E	1734	0	1755	53	0
8	F	684	0	692	15	0
9	H	1052	0	1007	28	0
10	I	946	0	887	20	0
11	J	532	0	542	14	0
12	K	919	0	929	20	0
13	L	337	0	353	7	0
14	R	62	0	24	0	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	A	1	0	0	0	0
All	All	28998	0	28418	602	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 10.

The worst 5 of 602 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)
4:A:68:GLN:O	4:A:69:THR:HG22	1.59	1.02
4:A:284:ALA:HB1	4:A:289:ILE:HD11	1.50	0.93
7:E:46:TYR:HD2	7:E:58:MET:HG2	1.36	0.90
5:B:763:GLN:HG2	5:B:765:PRO:HD2	1.55	0.88
4:A:184:SER:HA	4:A:199:LEU:HD21	1.56	0.87

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	1371/1733 (79%)	1331 (97%)	40 (3%)	0	100	100
5	B	1101/1224 (90%)	1076 (98%)	25 (2%)	0	100	100
6	C	265/318 (83%)	261 (98%)	4 (2%)	0	100	100
7	E	211/215 (98%)	204 (97%)	7 (3%)	0	100	100
8	F	84/155 (54%)	83 (99%)	1 (1%)	0	100	100
9	H	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
10	I	116/122 (95%)	116 (100%)	0	0	100	100
11	J	63/70 (90%)	62 (98%)	1 (2%)	0	100	100
12	K	112/120 (93%)	110 (98%)	2 (2%)	0	100	100
13	L	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
All	All	3493/4173 (84%)	3407 (98%)	86 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1195/1520 (79%)	1194 (100%)	1 (0%)	92	97
5	B	953/1061 (90%)	953 (100%)	0	100	100
6	C	235/274 (86%)	235 (100%)	0	100	100
7	E	193/197 (98%)	193 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	F	73/137 (53%)	73 (100%)	0	100	100
9	H	114/128 (89%)	114 (100%)	0	100	100
10	I	109/116 (94%)	108 (99%)	1 (1%)	75	87
11	J	60/65 (92%)	60 (100%)	0	100	100
12	K	99/102 (97%)	99 (100%)	0	100	100
13	L	37/57 (65%)	37 (100%)	0	100	100
All	All	3068/3657 (84%)	3066 (100%)	2 (0%)	92	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	67	CYS
10	I	7	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
7	E	115	ASN
12	K	92	ASN
7	E	146	HIS
10	I	60	GLN
5	B	47	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	8/9 (88%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	U
1	R	9	G

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$
2	8OG	T	19[B]	-	22,25,26	4.11	18 (81%)	26,37,40	1.78	7 (26%)
2	8OG	T	19[A]	-	22,25,26	4.11	18 (81%)	26,37,40	1.75	7 (26%)

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
2	8OG	T	19[B]	-	-	2/7/21/22	0/3/3/3
2	8OG	T	19[A]	-	-	2/7/21/22	0/3/3/3

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	19[A]	8OG	C8-N7	7.32	1.51	1.38
2	T	19[B]	8OG	C8-N7	7.12	1.51	1.38
2	T	19[B]	8OG	C8-N9	6.53	1.52	1.40
2	T	19[A]	8OG	C8-N9	6.26	1.51	1.40
2	T	19[B]	8OG	C2-N3	6.19	1.48	1.33

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	19[A]	8OG	C2-N3-C4	4.79	120.55	112.30
2	T	19[B]	8OG	C2-N3-C4	4.67	120.34	112.30
2	T	19[B]	8OG	N9-C4-N3	3.48	130.48	126.13
2	T	19[B]	8OG	C2-N1-C6	-3.19	119.33	125.11
2	T	19[A]	8OG	C2-N1-C6	-3.10	119.49	125.11

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	19[A]	8OG	O4'-C4'-C5'-O5'
2	T	19[B]	8OG	O4'-C4'-C5'-O5'
2	T	19[A]	8OG	C3'-C4'-C5'-O5'
2	T	19[B]	8OG	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	ATP	R	2101[A]	-	28,33,33	3.84	9 (32%)	34,52,52	2.94	5 (14%)
14	ATP	R	2101[B]	-	28,33,33	3.89	9 (32%)	34,52,52	3.15	4 (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
14	ATP	R	2101[A]	-	-	6/18/38/38	0/3/3/3
14	ATP	R	2101[B]	-	-	5/18/38/38	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	R	2101[B]	ATP	O4'-C1'	11.91	1.56	1.40
14	R	2101[A]	ATP	O4'-C1'	11.66	1.56	1.40
14	R	2101[B]	ATP	C3'-C4'	-9.92	1.27	1.53
14	R	2101[A]	ATP	C3'-C4'	-9.81	1.28	1.53
14	R	2101[B]	ATP	PB-O3A	5.81	1.65	1.59

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	R	2101[B]	ATP	C5-C6-N6	13.37	140.67	120.31
14	R	2101[A]	ATP	C5-C6-N6	12.16	138.84	120.31
14	R	2101[B]	ATP	N6-C6-N1	-9.04	99.01	118.33
14	R	2101[A]	ATP	N6-C6-N1	-8.18	100.86	118.33
14	R	2101[B]	ATP	N3-C2-N1	-6.31	120.10	128.67

There are no chirality outliers.

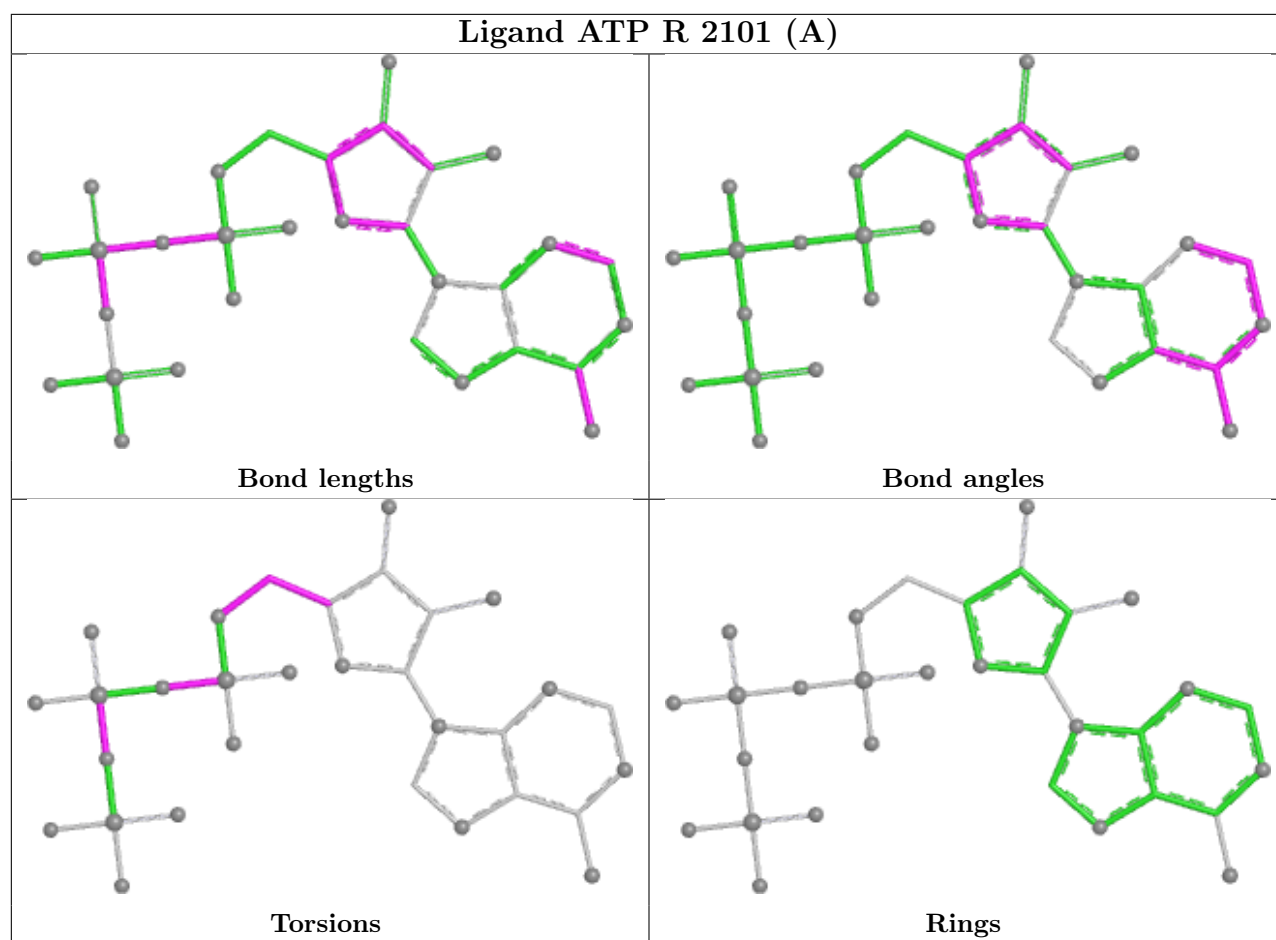
5 of 11 torsion outliers are listed below:

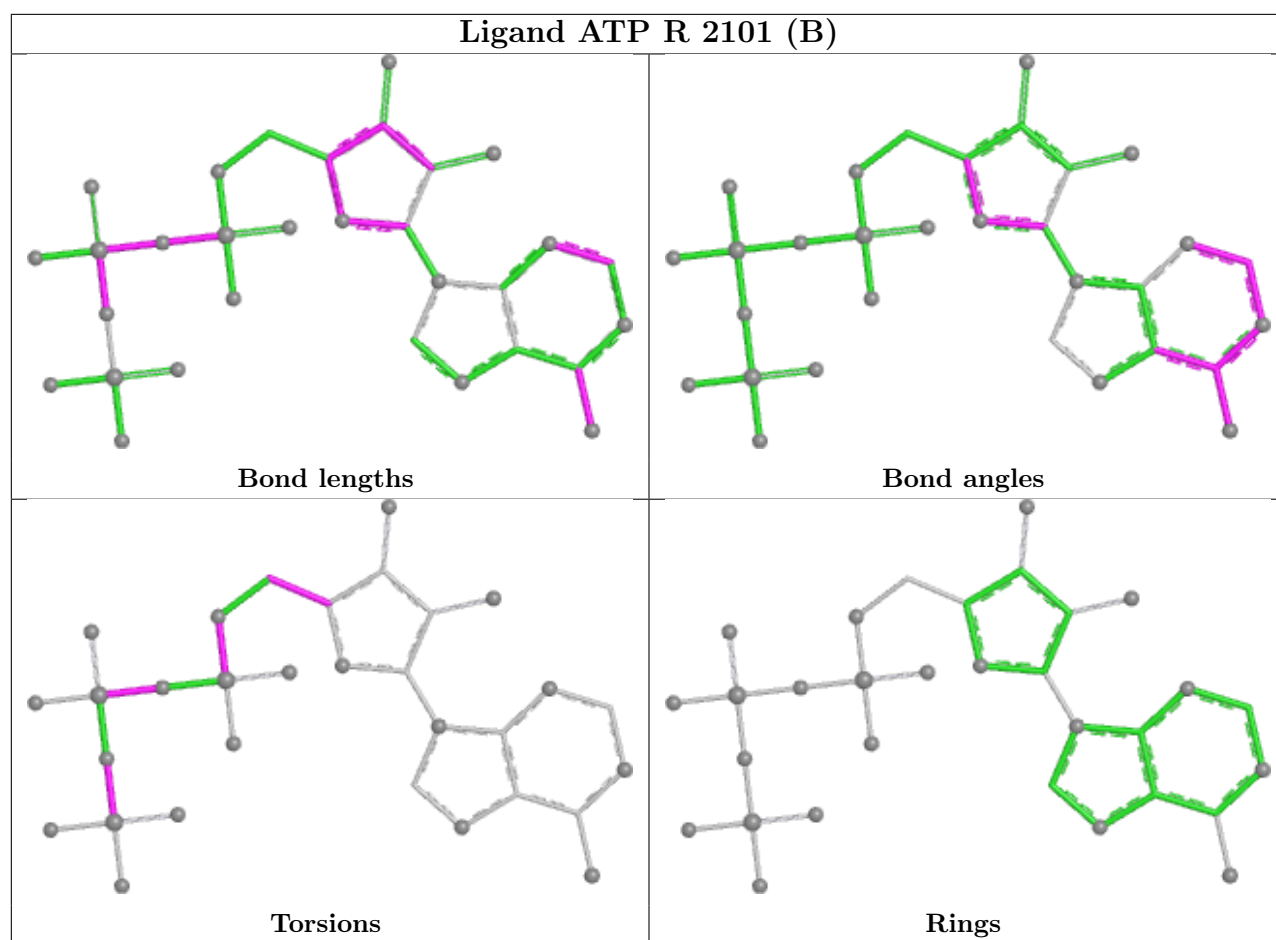
Mol	Chain	Res	Type	Atoms
14	R	2101[A]	ATP	PB-O3A-PA-O5'
14	R	2101[B]	ATP	PB-O3B-PG-O2G
14	R	2101[B]	ATP	C3'-C4'-C5'-O5'
14	R	2101[B]	ATP	O4'-C4'-C5'-O5'
14	R	2101[A]	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	R	9/9 (100%)	-0.06	0 100 100	93, 103, 199, 215	0
2	T	23/29 (79%)	-0.02	0 100 100	88, 160, 258, 264	0
3	N	12/18 (66%)	0.02	0 100 100	151, 188, 267, 275	0
4	A	1385/1733 (79%)	-0.15	14 (1%) 79 65	49, 91, 171, 274	0
5	B	1121/1224 (91%)	-0.13	15 (1%) 74 59	43, 79, 147, 233	0
6	C	267/318 (83%)	-0.35	0 100 100	48, 79, 119, 166	0
7	E	213/215 (99%)	-0.12	2 (0%) 81 67	68, 120, 184, 235	0
8	F	86/155 (55%)	-0.35	0 100 100	61, 96, 146, 212	0
9	H	133/146 (91%)	-0.01	0 100 100	79, 114, 173, 238	0
10	I	118/122 (96%)	-0.10	0 100 100	59, 102, 149, 200	0
11	J	65/70 (92%)	-0.22	0 100 100	55, 71, 109, 142	0
12	K	114/120 (95%)	-0.42	0 100 100	51, 83, 121, 168	0
13	L	43/70 (61%)	0.64	3 (6%) 24 16	59, 151, 198, 273	0
All	All	3589/4229 (84%)	-0.15	34 (0%) 81 67	43, 89, 168, 275	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	714	GLU	5.6
4	A	1257	ASP	3.1
4	A	1081	LEU	3.0
7	E	93	MET	3.0
4	A	447	GLN	2.9

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
2	8OG	T	19[A]	23/24	0.90	0.11	85,97,119,132	12
2	8OG	T	19[B]	23/24	0.90	0.11	85,97,119,132	12

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

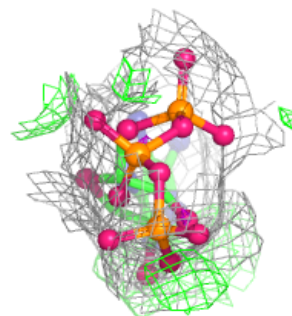
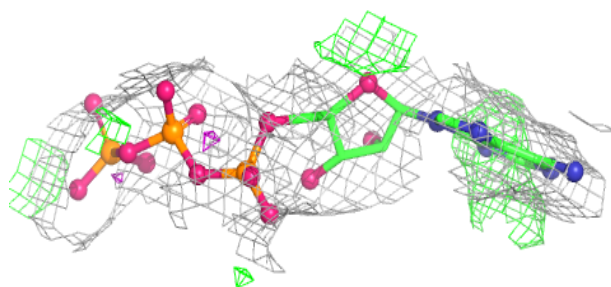
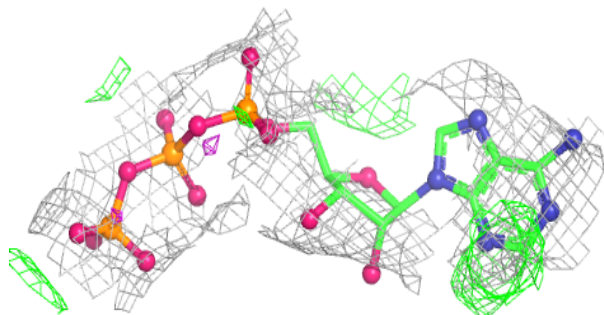
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	ATP	R	2101[A]	31/31	0.55	0.19	102,135,161,164	31
14	ATP	R	2101[B]	31/31	0.55	0.19	115,142,158,159	31
16	MG	A	1803	1/1	0.82	0.23	96,96,96,96	0
15	ZN	A	1801	1/1	0.93	0.06	214,214,214,214	0
15	ZN	L	101	1/1	0.96	0.06	182,182,182,182	0
15	ZN	A	1802	1/1	0.96	0.06	137,137,137,137	0
15	ZN	I	202	1/1	0.97	0.06	97,97,97,97	0
15	ZN	J	101	1/1	0.97	0.05	69,69,69,69	0
15	ZN	B	1301	1/1	0.98	0.04	157,157,157,157	0
15	ZN	I	201	1/1	0.98	0.05	114,114,114,114	0
15	ZN	C	401	1/1	0.99	0.06	105,105,105,105	0

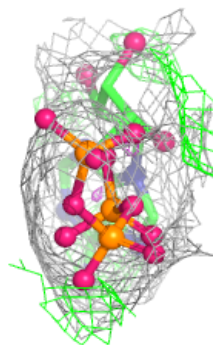
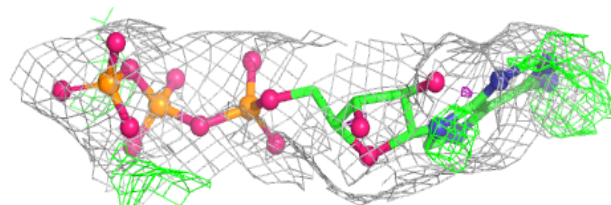
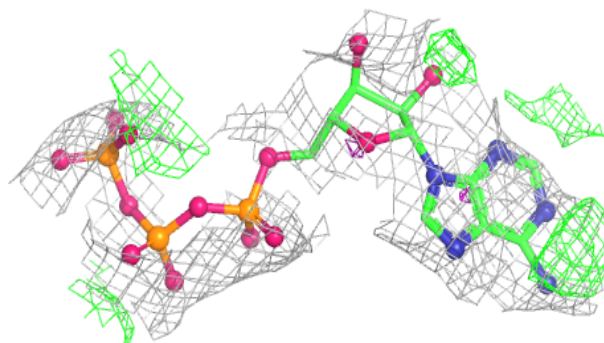
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP R 2101 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ATP R 2101 (B):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.