



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:00 PM UTC

PDB ID : 3GLF / pdb_00003glf
Title : Crystal Structure of the Ecoli Clamp Loader Bound to Primer-Template DNA
Authors : Simonetta, K.R.; Kuriyan, J.
Deposited on : 2009-03-12
Resolution : 3.39 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:

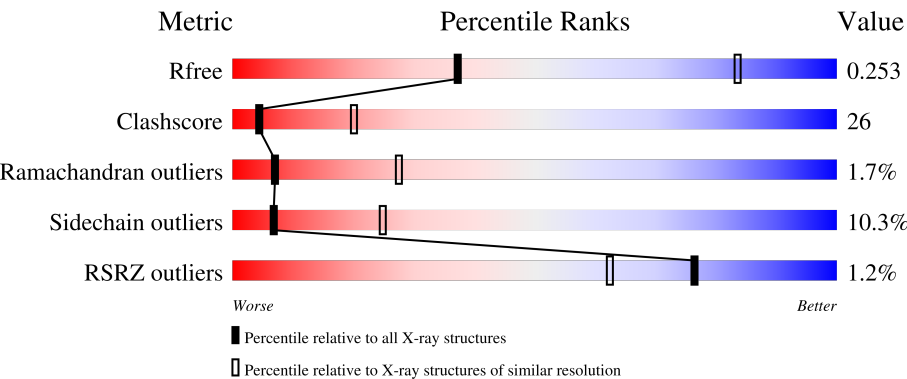
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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	343	5% 44% 46% 7%
1	F	343	% 48% 42% 7%
2	B	395	% 50% 35% 7% 8%
2	C	395	% 48% 34% 10% 8%
2	D	395	% 45% 40% 7% 8%

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Mol	Chain	Length	Quality of chain
2	G	395	% 56% 34% 6%
2	H	395	% 47% 35% 9%
2	I	395	% 44% 40% 6%
3	E	334	59% 35% 5%
3	J	334	62% 30% 7%
4	K	15	13% 53% 27%
4	M	15	13% 47% 33%
5	L	10	10% 80% 10%
5	N	10	30% 50% 20%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 28758 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 polymerase III subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2650	1678	482	480	10			
1	F	333	Total	C	N	O	S	0	0	0
			2650	1678	482	480	10			

- Molecule 2 is a protein called DNA polymerase III subunit tau.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	364	Total	C	N	O	S	0	0	0
			2829	1779	511	523	16			
2	C	365	Total	C	N	O	S	0	0	0
			2838	1784	513	525	16			
2	D	362	Total	C	N	O	S	0	0	0
			2818	1770	510	522	16			
2	G	378	Total	C	N	O	S	0	0	0
			2941	1852	529	543	17			
2	H	365	Total	C	N	O	S	0	0	0
			2838	1784	513	525	16			
2	I	362	Total	C	N	O	S	0	0	0
			2818	1770	510	522	16			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	MET	-	expression tag	UNP P06710
B	-20	GLY	-	expression tag	UNP P06710
B	-19	SER	-	expression tag	UNP P06710
B	-18	SER	-	expression tag	UNP P06710
B	-17	HIS	-	expression tag	UNP P06710
B	-16	HIS	-	expression tag	UNP P06710
B	-15	HIS	-	expression tag	UNP P06710
B	-14	HIS	-	expression tag	UNP P06710

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP P06710
B	-12	HIS	-	expression tag	UNP P06710
B	-11	SER	-	expression tag	UNP P06710
B	-10	SER	-	expression tag	UNP P06710
B	-9	GLY	-	expression tag	UNP P06710
B	-8	LEU	-	expression tag	UNP P06710
B	-7	GLU	-	expression tag	UNP P06710
B	-6	VAL	-	expression tag	UNP P06710
B	-5	LEU	-	expression tag	UNP P06710
B	-4	PHE	-	expression tag	UNP P06710
B	-3	GLN	-	expression tag	UNP P06710
B	-2	GLY	-	expression tag	UNP P06710
B	-1	PRO	-	expression tag	UNP P06710
B	0	HIS	-	expression tag	UNP P06710
C	-21	MET	-	expression tag	UNP P06710
C	-20	GLY	-	expression tag	UNP P06710
C	-19	SER	-	expression tag	UNP P06710
C	-18	SER	-	expression tag	UNP P06710
C	-17	HIS	-	expression tag	UNP P06710
C	-16	HIS	-	expression tag	UNP P06710
C	-15	HIS	-	expression tag	UNP P06710
C	-14	HIS	-	expression tag	UNP P06710
C	-13	HIS	-	expression tag	UNP P06710
C	-12	HIS	-	expression tag	UNP P06710
C	-11	SER	-	expression tag	UNP P06710
C	-10	SER	-	expression tag	UNP P06710
C	-9	GLY	-	expression tag	UNP P06710
C	-8	LEU	-	expression tag	UNP P06710
C	-7	GLU	-	expression tag	UNP P06710
C	-6	VAL	-	expression tag	UNP P06710
C	-5	LEU	-	expression tag	UNP P06710
C	-4	PHE	-	expression tag	UNP P06710
C	-3	GLN	-	expression tag	UNP P06710
C	-2	GLY	-	expression tag	UNP P06710
C	-1	PRO	-	expression tag	UNP P06710
C	0	HIS	-	expression tag	UNP P06710
D	-21	MET	-	expression tag	UNP P06710
D	-20	GLY	-	expression tag	UNP P06710
D	-19	SER	-	expression tag	UNP P06710
D	-18	SER	-	expression tag	UNP P06710
D	-17	HIS	-	expression tag	UNP P06710
D	-16	HIS	-	expression tag	UNP P06710

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	HIS	-	expression tag	UNP P06710
D	-14	HIS	-	expression tag	UNP P06710
D	-13	HIS	-	expression tag	UNP P06710
D	-12	HIS	-	expression tag	UNP P06710
D	-11	SER	-	expression tag	UNP P06710
D	-10	SER	-	expression tag	UNP P06710
D	-9	GLY	-	expression tag	UNP P06710
D	-8	LEU	-	expression tag	UNP P06710
D	-7	GLU	-	expression tag	UNP P06710
D	-6	VAL	-	expression tag	UNP P06710
D	-5	LEU	-	expression tag	UNP P06710
D	-4	PHE	-	expression tag	UNP P06710
D	-3	GLN	-	expression tag	UNP P06710
D	-2	GLY	-	expression tag	UNP P06710
D	-1	PRO	-	expression tag	UNP P06710
D	0	HIS	-	expression tag	UNP P06710
G	-21	MET	-	expression tag	UNP P06710
G	-20	GLY	-	expression tag	UNP P06710
G	-19	SER	-	expression tag	UNP P06710
G	-18	SER	-	expression tag	UNP P06710
G	-17	HIS	-	expression tag	UNP P06710
G	-16	HIS	-	expression tag	UNP P06710
G	-15	HIS	-	expression tag	UNP P06710
G	-14	HIS	-	expression tag	UNP P06710
G	-13	HIS	-	expression tag	UNP P06710
G	-12	HIS	-	expression tag	UNP P06710
G	-11	SER	-	expression tag	UNP P06710
G	-10	SER	-	expression tag	UNP P06710
G	-9	GLY	-	expression tag	UNP P06710
G	-8	LEU	-	expression tag	UNP P06710
G	-7	GLU	-	expression tag	UNP P06710
G	-6	VAL	-	expression tag	UNP P06710
G	-5	LEU	-	expression tag	UNP P06710
G	-4	PHE	-	expression tag	UNP P06710
G	-3	GLN	-	expression tag	UNP P06710
G	-2	GLY	-	expression tag	UNP P06710
G	-1	PRO	-	expression tag	UNP P06710
G	0	HIS	-	expression tag	UNP P06710
H	-21	MET	-	expression tag	UNP P06710
H	-20	GLY	-	expression tag	UNP P06710
H	-19	SER	-	expression tag	UNP P06710
H	-18	SER	-	expression tag	UNP P06710

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-17	HIS	-	expression tag	UNP P06710
H	-16	HIS	-	expression tag	UNP P06710
H	-15	HIS	-	expression tag	UNP P06710
H	-14	HIS	-	expression tag	UNP P06710
H	-13	HIS	-	expression tag	UNP P06710
H	-12	HIS	-	expression tag	UNP P06710
H	-11	SER	-	expression tag	UNP P06710
H	-10	SER	-	expression tag	UNP P06710
H	-9	GLY	-	expression tag	UNP P06710
H	-8	LEU	-	expression tag	UNP P06710
H	-7	GLU	-	expression tag	UNP P06710
H	-6	VAL	-	expression tag	UNP P06710
H	-5	LEU	-	expression tag	UNP P06710
H	-4	PHE	-	expression tag	UNP P06710
H	-3	GLN	-	expression tag	UNP P06710
H	-2	GLY	-	expression tag	UNP P06710
H	-1	PRO	-	expression tag	UNP P06710
H	0	HIS	-	expression tag	UNP P06710
I	-21	MET	-	expression tag	UNP P06710
I	-20	GLY	-	expression tag	UNP P06710
I	-19	SER	-	expression tag	UNP P06710
I	-18	SER	-	expression tag	UNP P06710
I	-17	HIS	-	expression tag	UNP P06710
I	-16	HIS	-	expression tag	UNP P06710
I	-15	HIS	-	expression tag	UNP P06710
I	-14	HIS	-	expression tag	UNP P06710
I	-13	HIS	-	expression tag	UNP P06710
I	-12	HIS	-	expression tag	UNP P06710
I	-11	SER	-	expression tag	UNP P06710
I	-10	SER	-	expression tag	UNP P06710
I	-9	GLY	-	expression tag	UNP P06710
I	-8	LEU	-	expression tag	UNP P06710
I	-7	GLU	-	expression tag	UNP P06710
I	-6	VAL	-	expression tag	UNP P06710
I	-5	LEU	-	expression tag	UNP P06710
I	-4	PHE	-	expression tag	UNP P06710
I	-3	GLN	-	expression tag	UNP P06710
I	-2	GLY	-	expression tag	UNP P06710
I	-1	PRO	-	expression tag	UNP P06710
I	0	HIS	-	expression tag	UNP P06710

- Molecule 3 is a protein called DNA polymerase III subunit delta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	334	Total	C	N	O	S	0	0	0
			2601	1655	468	465	13			
3	J	334	Total	C	N	O	S	0	0	0
			2601	1655	468	465	13			

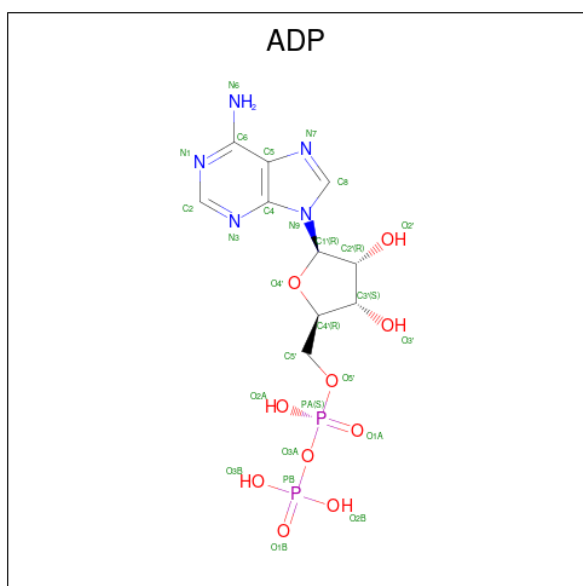
- Molecule 4 is a DNA chain called DNA (5'-D(*TP*TP*TP*TP*TP*TP*AP*TP*AP*GP*GP*CP*CP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	14	Total	C	N	O	P	0	0	0
			287	138	48	87	14			
4	M	14	Total	C	N	O	P	0	0	0
			287	138	48	87	14			

- Molecule 5 is a DNA chain called DNA (5'-D(*CP*TP*GP*GP*CP*CP*TP*AP*TP*A)-3').

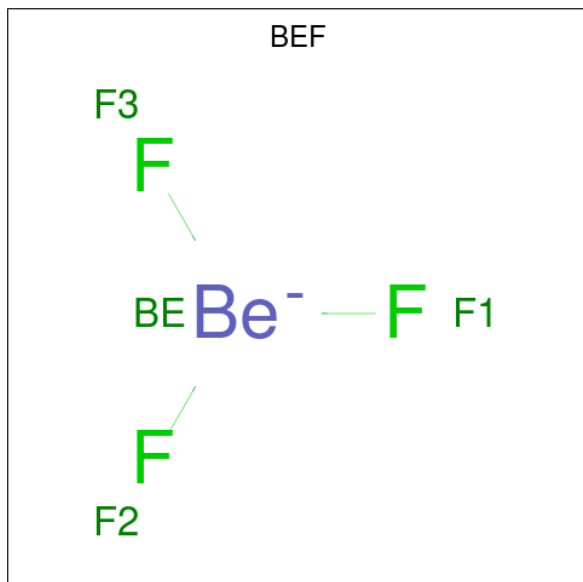
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	10	Total	C	N	O	P	0	0	0
			200	97	35	59	9			
5	N	10	Total	C	N	O	P	0	0	0
			200	97	35	59	9			

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



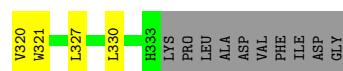
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Be	F	0	0
			4	1	3		
7	C	1	Total	Be	F	0	0
			4	1	3		
7	D	1	Total	Be	F	0	0
			4	1	3		
7	G	1	Total	Be	F	0	0
			4	1	3		
7	H	1	Total	Be	F	0	0
			4	1	3		
7	I	1	Total	Be	F	0	0
			4	1	3		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

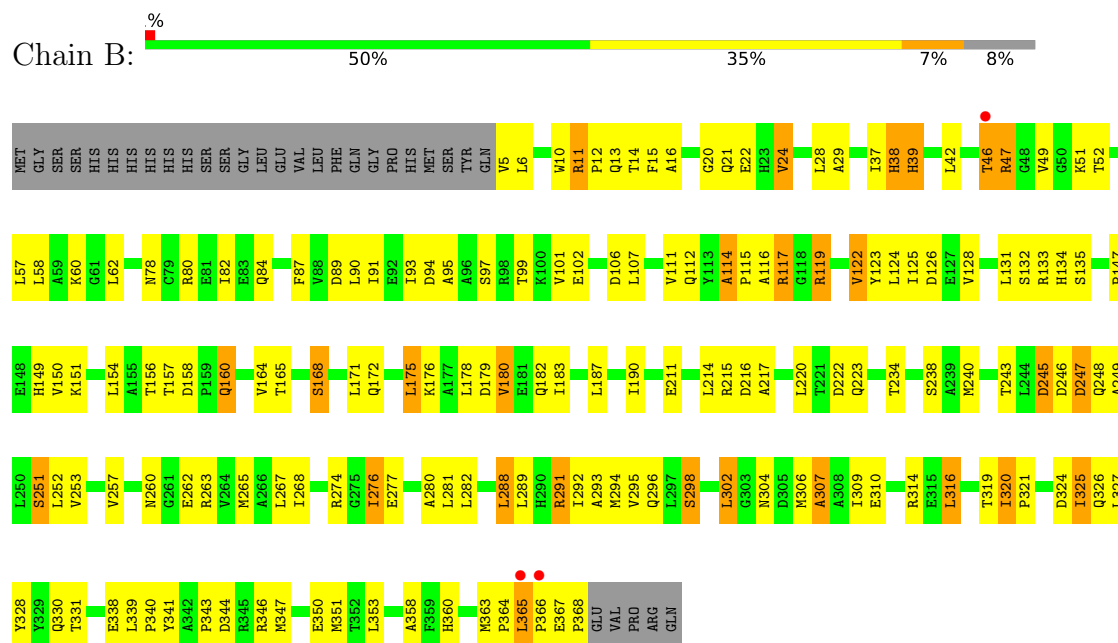
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total 1	Mg 1	0	0
8	C	1	Total 1	Mg 1	0	0
8	D	1	Total 1	Mg 1	0	0
8	G	1	Total 1	Mg 1	0	0
8	H	1	Total 1	Mg 1	0	0
8	I	1	Total 1	Mg 1	0	0

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

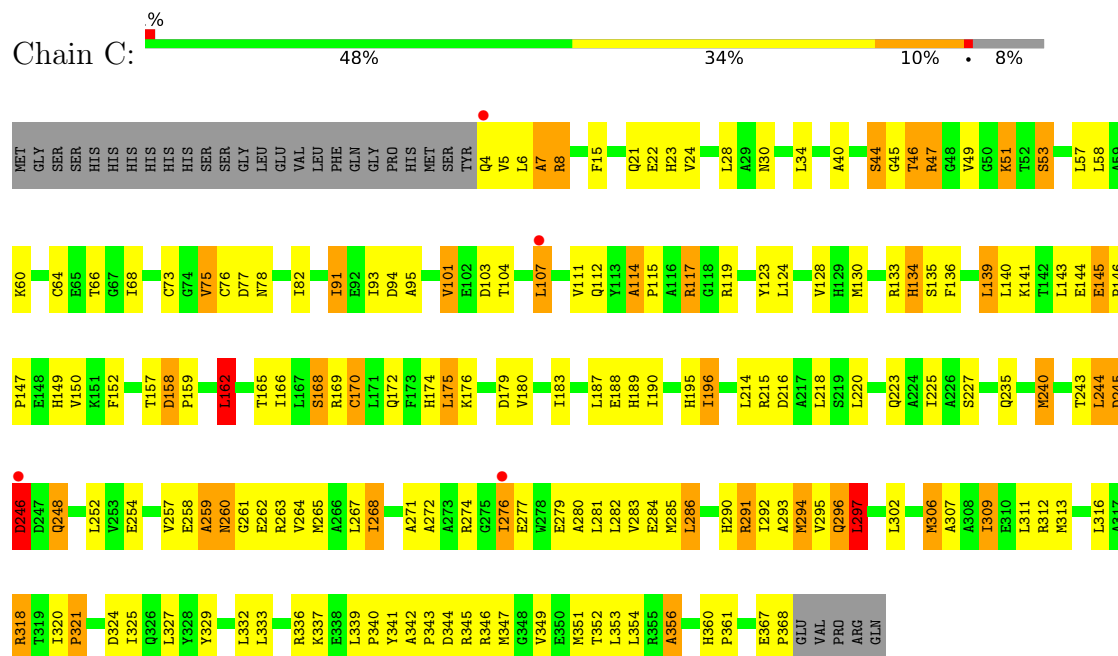
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total 1	Zn 1	0	0
9	C	1	Total 1	Zn 1	0	0
9	D	1	Total 1	Zn 1	0	0
9	E	1	Total 1	Zn 1	0	0
9	G	1	Total 1	Zn 1	0	0
9	H	1	Total 1	Zn 1	0	0
9	I	1	Total 1	Zn 1	0	0
9	J	1	Total 1	Zn 1	0	0



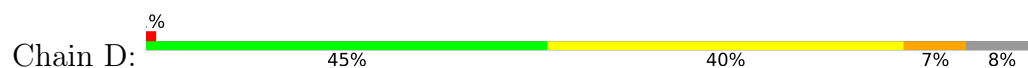
- Molecule 2: DNA polymerase III subunit tau

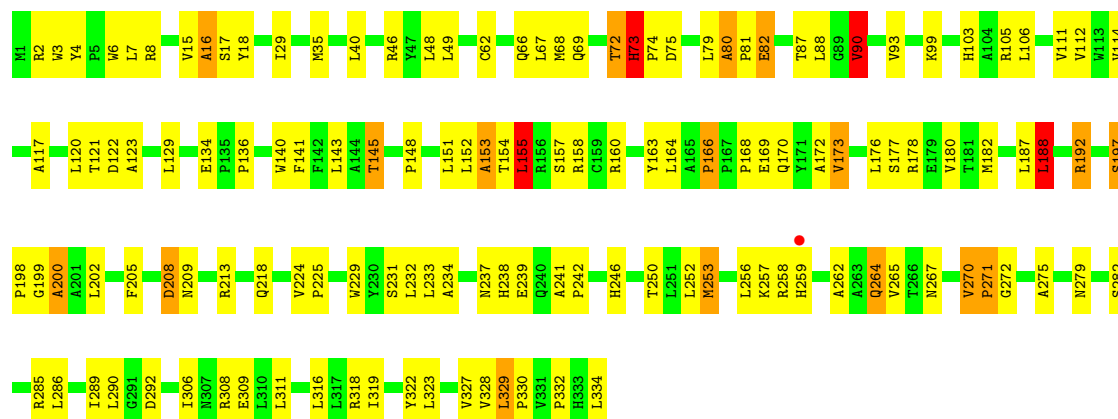


- Molecule 2: DNA polymerase III subunit tau



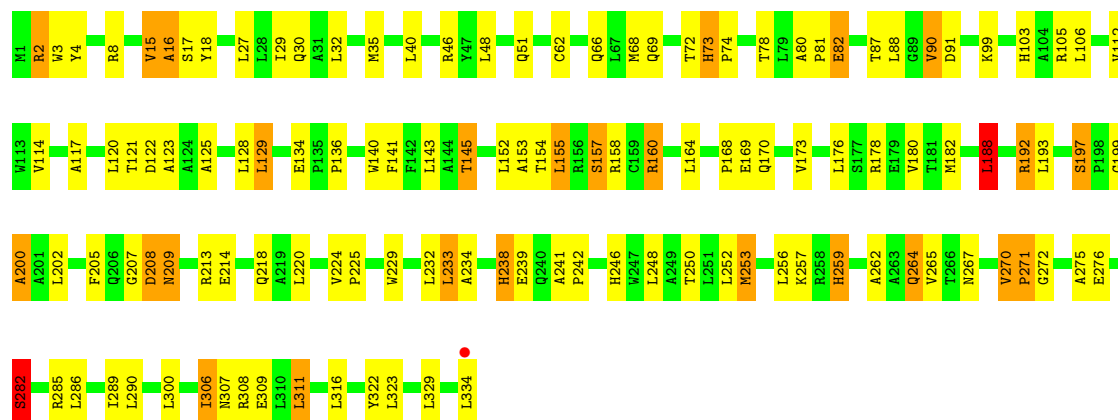
- Molecule 2: DNA polymerase III subunit tau





- Molecule 3: DNA polymerase III subunit delta'

Chain J: 

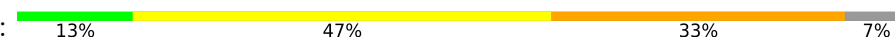


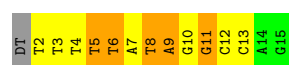
- Molecule 4: DNA (5'-D(*TP*TP*TP*TP*TP*TP*AP*TP*AP*GP*GP*CP*CP*AP*G)-3')

Chain K: 

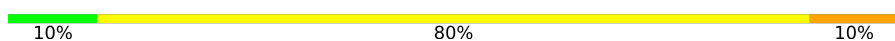


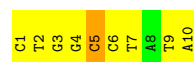
- Molecule 4: DNA (5'-D(*TP*TP*TP*TP*TP*TP*AP*TP*AP*GP*GP*CP*CP*AP*G)-3')

Chain M: 



- Molecule 5: DNA (5'-D(*CP*TP*GP*GP*CP*CP*TP*AP*TP*A)-3')

Chain L: 



- Molecule 5: DNA (5'-D(*CP*TP*GP*GP*CP*CP*TP*AP*TP*A)-3')

Chain N: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.26Å 219.95Å 273.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.97 – 3.39 49.97 – 3.39	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.97-3.39) 97.5 (49.97-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.221 , 0.260 0.213 , 0.253	Depositor DCC
R_{free} test set	4166 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	92.3	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28758	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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: ZN, ADP, BEF, MG

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	0.92	0/2697	1.12	14/3664 (0.4%)
1	F	0.90	1/2697 (0.0%)	1.11	9/3664 (0.2%)
2	B	0.90	1/2876 (0.0%)	1.19	18/3900 (0.5%)
2	C	0.87	0/2885	1.21	19/3912 (0.5%)
2	D	0.96	3/2863 (0.1%)	1.23	16/3879 (0.4%)
2	G	0.91	0/2992	1.21	22/4057 (0.5%)
2	H	1.06	1/2885 (0.0%)	1.29	22/3912 (0.6%)
2	I	1.15	6/2863 (0.2%)	1.31	15/3879 (0.4%)
3	E	1.14	2/2666 (0.1%)	1.30	21/3639 (0.6%)
3	J	1.12	5/2666 (0.2%)	1.25	13/3639 (0.4%)
4	K	0.98	0/320	1.69	4/492 (0.8%)
4	M	0.99	0/320	1.62	6/492 (1.2%)
5	L	0.80	0/223	1.73	2/342 (0.6%)
5	N	0.83	0/223	1.71	4/342 (1.2%)
All	All	0.99	19/29176 (0.1%)	1.25	185/39813 (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
2	B	0	1
2	C	0	1
2	G	0	1
2	H	0	1
2	I	0	1
All	All	0	5

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	306	ILE	CA-CB	-8.75	1.45	1.54
3	J	306	ILE	CA-CB	-7.00	1.47	1.54
2	I	164	VAL	CA-CB	-6.57	1.46	1.54
2	I	101	VAL	CA-CB	-6.50	1.46	1.54
1	F	244	VAL	CA-CB	-6.00	1.47	1.54

The worst 5 of 185 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	329	LEU	CA-C-N	14.53	134.72	119.89
3	E	329	LEU	C-N-CA	14.53	134.72	119.89
3	J	329	LEU	CA-C-N	10.68	130.79	119.89
3	J	329	LEU	C-N-CA	10.68	130.79	119.89
3	J	73	HIS	CA-C-N	10.68	133.19	119.84

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	246	ASP	Peptide
2	C	245	ASP	Peptide
2	G	246	ASP	Peptide
2	H	245	ASP	Peptide
2	I	157	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2650	0	2703	175	0
1	F	2650	0	2703	165	0
2	B	2829	0	2879	163	1
2	C	2838	0	2886	175	1
2	D	2818	0	2863	182	0
2	G	2941	0	2987	148	0
2	H	2838	0	2886	172	2
2	I	2818	0	2863	180	1
3	E	2601	0	2603	120	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	2601	0	2603	126	0
4	K	287	0	161	17	0
4	M	287	0	161	14	0
5	L	200	0	115	5	0
5	N	200	0	115	4	0
6	B	27	0	12	3	0
6	C	27	0	12	3	0
6	D	27	0	12	3	0
6	G	27	0	12	2	0
6	H	27	0	12	4	0
6	I	27	0	12	2	0
7	B	4	0	0	1	0
7	C	4	0	0	0	0
7	D	4	0	0	0	0
7	G	4	0	0	1	0
7	H	4	0	0	0	0
7	I	4	0	0	1	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
8	I	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	E	1	0	0	0	0
9	G	1	0	0	0	0
9	H	1	0	0	0	0
9	I	1	0	0	0	0
9	J	1	0	0	0	0
All	All	28758	0	28600	1517	3

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 26.

The worst 5 of 1517 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:H:351:MET:CE	2:I:290:HIS:HA	1.75	1.15
2:H:351:MET:HE1	2:I:290:HIS:HA	1.16	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:95:GLU:HA	1:F:98:LEU:HD12	1.33	1.08
1:A:95:GLU:HA	1:A:98:LEU:HD12	1.35	1.07
2:I:216:ASP:OD1	3:J:157:SER:HB2	1.57	1.03

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:ARG:NH2	2:I:117:ARG:NE[2_555]	1.99	0.21
3:E:178:ARG:NH2	2:H:195:HIS:O[4_545]	2.02	0.18
2:C:117:ARG:NE	2:H:117:ARG:NH2[2_555]	2.03	0.17

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	
1	A	331/343 (96%)	292 (88%)	34 (10%)	5 (2%)	8	29
1	F	331/343 (96%)	298 (90%)	29 (9%)	4 (1%)	10	34
2	B	362/395 (92%)	323 (89%)	36 (10%)	3 (1%)	16	44
2	C	363/395 (92%)	326 (90%)	31 (8%)	6 (2%)	7	27
2	D	360/395 (91%)	317 (88%)	34 (9%)	9 (2%)	4	21
2	G	376/395 (95%)	340 (90%)	33 (9%)	3 (1%)	16	44
2	H	363/395 (92%)	320 (88%)	37 (10%)	6 (2%)	7	27
2	I	360/395 (91%)	318 (88%)	33 (9%)	9 (2%)	4	21
3	E	332/334 (99%)	300 (90%)	24 (7%)	8 (2%)	4	22
3	J	332/334 (99%)	298 (90%)	28 (8%)	6 (2%)	6	26
All	All	3510/3724 (94%)	3132 (89%)	319 (9%)	59 (2%)	7	27

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	ASN
2	B	307	ALA
2	C	297	LEU
2	D	307	ALA
3	E	153	ALA

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	283/291 (97%)	252 (89%)	31 (11%)	6	22
1	F	283/291 (97%)	251 (89%)	32 (11%)	5	21
2	B	301/329 (92%)	274 (91%)	27 (9%)	9	30
2	C	302/329 (92%)	256 (85%)	46 (15%)	3	11
2	D	299/329 (91%)	277 (93%)	22 (7%)	13	38
2	G	313/329 (95%)	287 (92%)	26 (8%)	10	35
2	H	302/329 (92%)	260 (86%)	42 (14%)	3	14
2	I	299/329 (91%)	272 (91%)	27 (9%)	9	30
3	E	270/270 (100%)	248 (92%)	22 (8%)	11	36
3	J	270/270 (100%)	243 (90%)	27 (10%)	7	26
All	All	2922/3096 (94%)	2620 (90%)	302 (10%)	7	25

5 of 302 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	227	SER
3	J	180	VAL
2	H	268	ILE
2	I	165	THR
3	J	311	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	134	HIS
2	I	84	GLN
2	G	182	GLN
2	H	134	HIS
2	I	269	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 14 are monoatomic - leaving 12 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	$\# Z > 2$
6	ADP	C	402	7,8	28,29,29	1.47	5 (17%)	43,45,45	1.88	10 (23%)
6	ADP	D	404	7,8	28,29,29	1.58	5 (17%)	43,45,45	1.70	12 (27%)
6	ADP	G	406	7,8	28,29,29	1.57	7 (25%)	43,45,45	1.77	12 (27%)
7	BEF	H	409	6	0,3,3	-	-	-	-	-
7	BEF	G	407	6	0,3,3	-	-	-	-	-
6	ADP	B	400	7,8	28,29,29	1.70	6 (21%)	43,45,45	1.75	13 (30%)
7	BEF	D	405	6	0,3,3	-	-	-	-	-
7	BEF	B	401	6	0,3,3	-	-	-	-	-
7	BEF	I	411	6	0,3,3	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BEF	C	403	6	0,3,3	-	-	-		
6	ADP	H	408	7,8	28,29,29	1.61	9 (32%)	43,45,45	1.82	11 (25%)
6	ADP	I	410	7,8	28,29,29	1.98	5 (17%)	43,45,45	1.63	11 (25%)

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
6	ADP	C	402	7,8	-	6/16/32/32	0/3/3/3
6	ADP	D	404	7,8	-	0/16/32/32	0/3/3/3
6	ADP	G	406	7,8	-	0/16/32/32	0/3/3/3
6	ADP	B	400	7,8	-	0/16/32/32	0/3/3/3
6	ADP	H	408	7,8	-	5/16/32/32	0/3/3/3
6	ADP	I	410	7,8	-	1/16/32/32	0/3/3/3

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	400	ADP	C5-C4	5.26	1.48	1.39
6	I	410	ADP	PA-O3A	5.11	1.65	1.59
6	C	402	ADP	C5-C4	4.90	1.47	1.39
6	I	410	ADP	C5-C4	4.54	1.47	1.39
6	G	406	ADP	C5-C4	4.47	1.47	1.39

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	402	ADP	C5-C4-N3	-5.16	119.62	126.72
6	G	406	ADP	C5-C4-N3	-5.10	119.69	126.72
6	H	408	ADP	C5-C4-N3	-5.07	119.73	126.72
6	B	400	ADP	C5-C4-N3	-4.64	120.32	126.72
6	C	402	ADP	N3-C4-N9	4.41	134.67	127.17

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	402	ADP	PA-O3A-PB-O3B
6	C	402	ADP	C5'-O5'-PA-O1A

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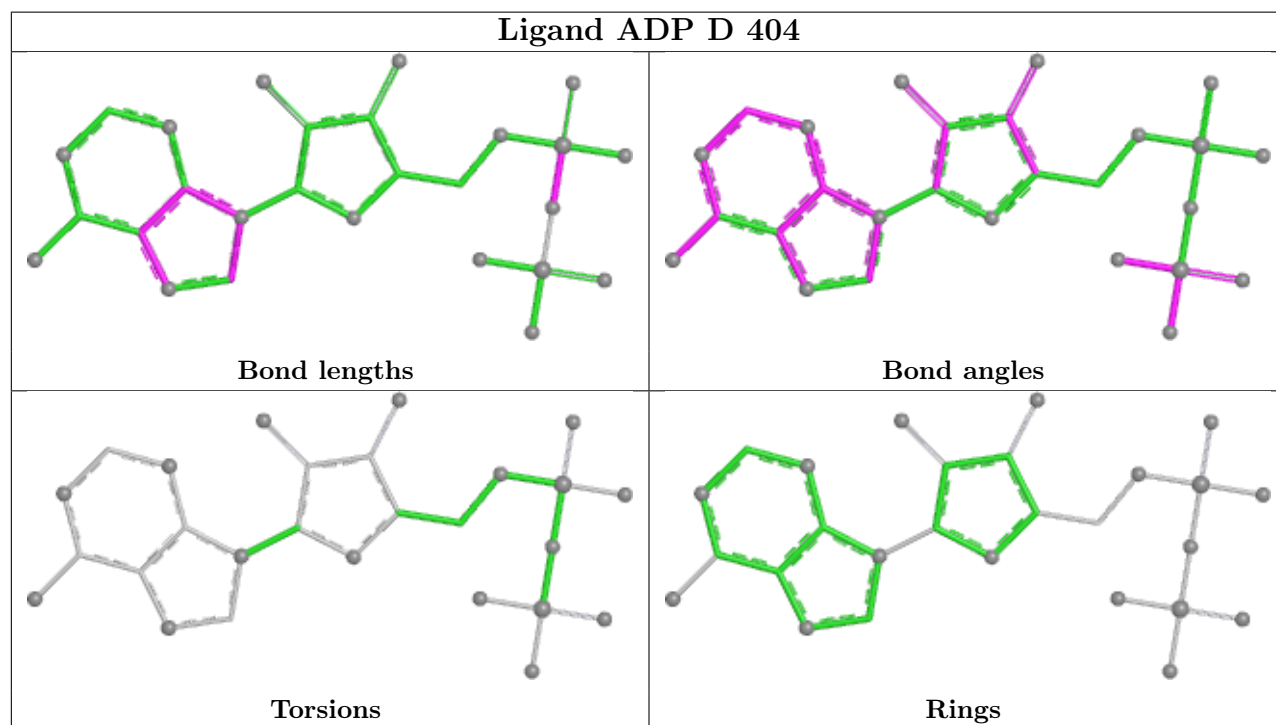
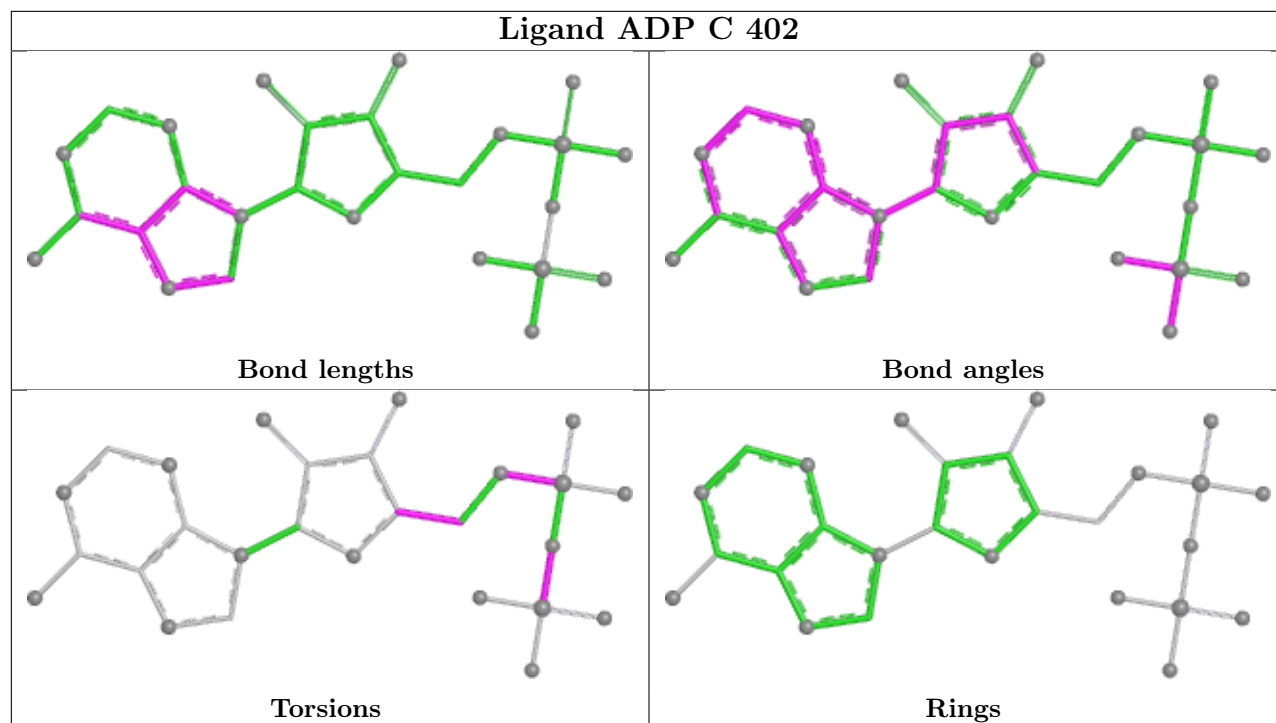
Mol	Chain	Res	Type	Atoms
6	C	402	ADP	C5'-O5'-PA-O2A
6	C	402	ADP	C5'-O5'-PA-O3A
6	H	408	ADP	PA-O3A-PB-O3B

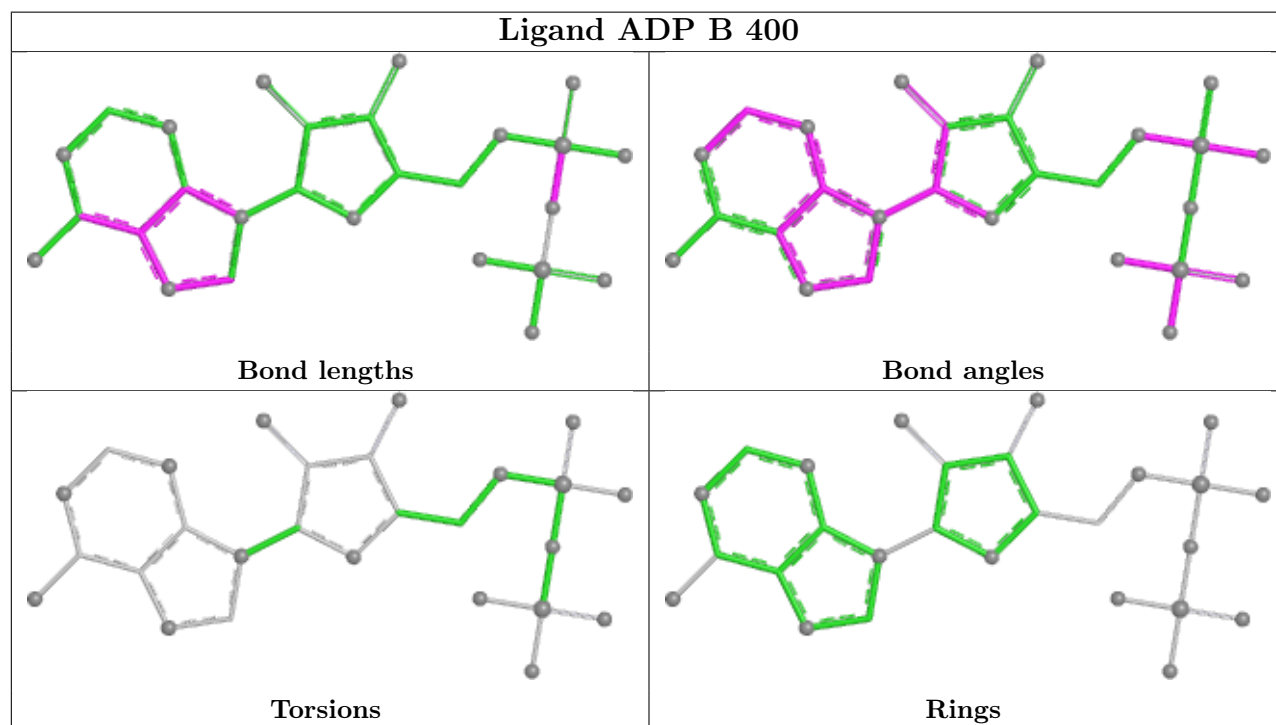
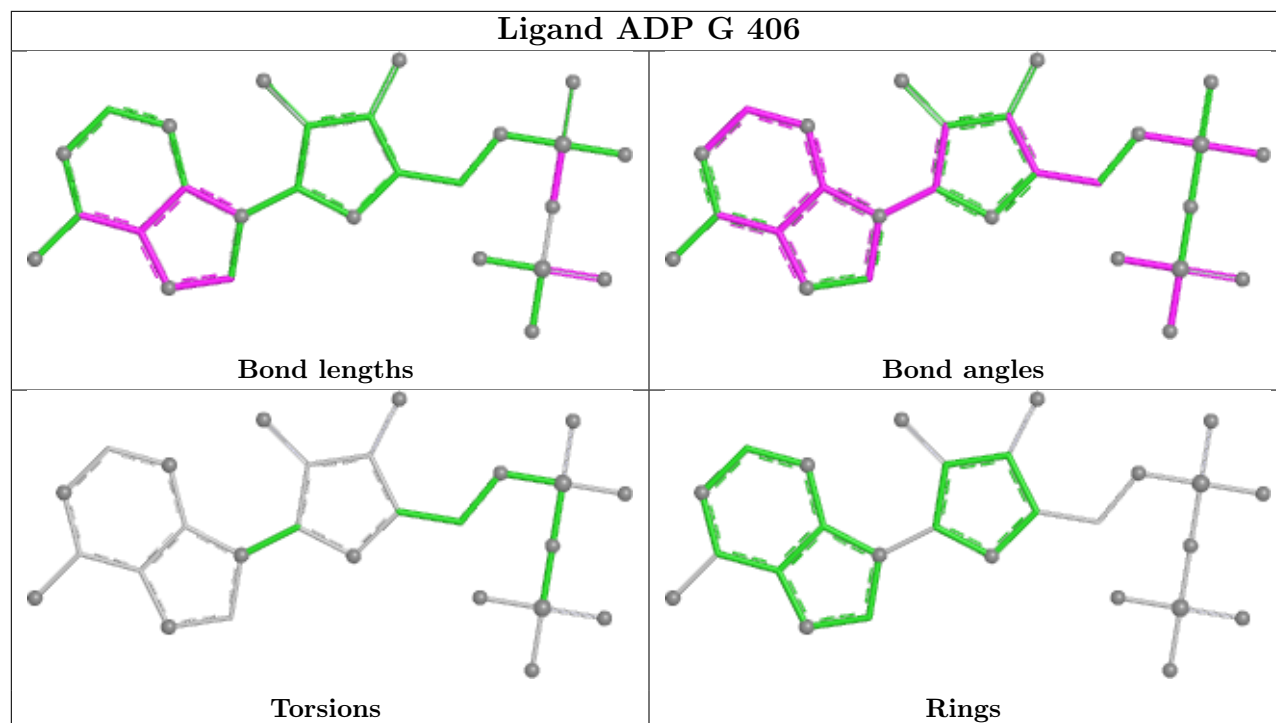
There are no ring outliers.

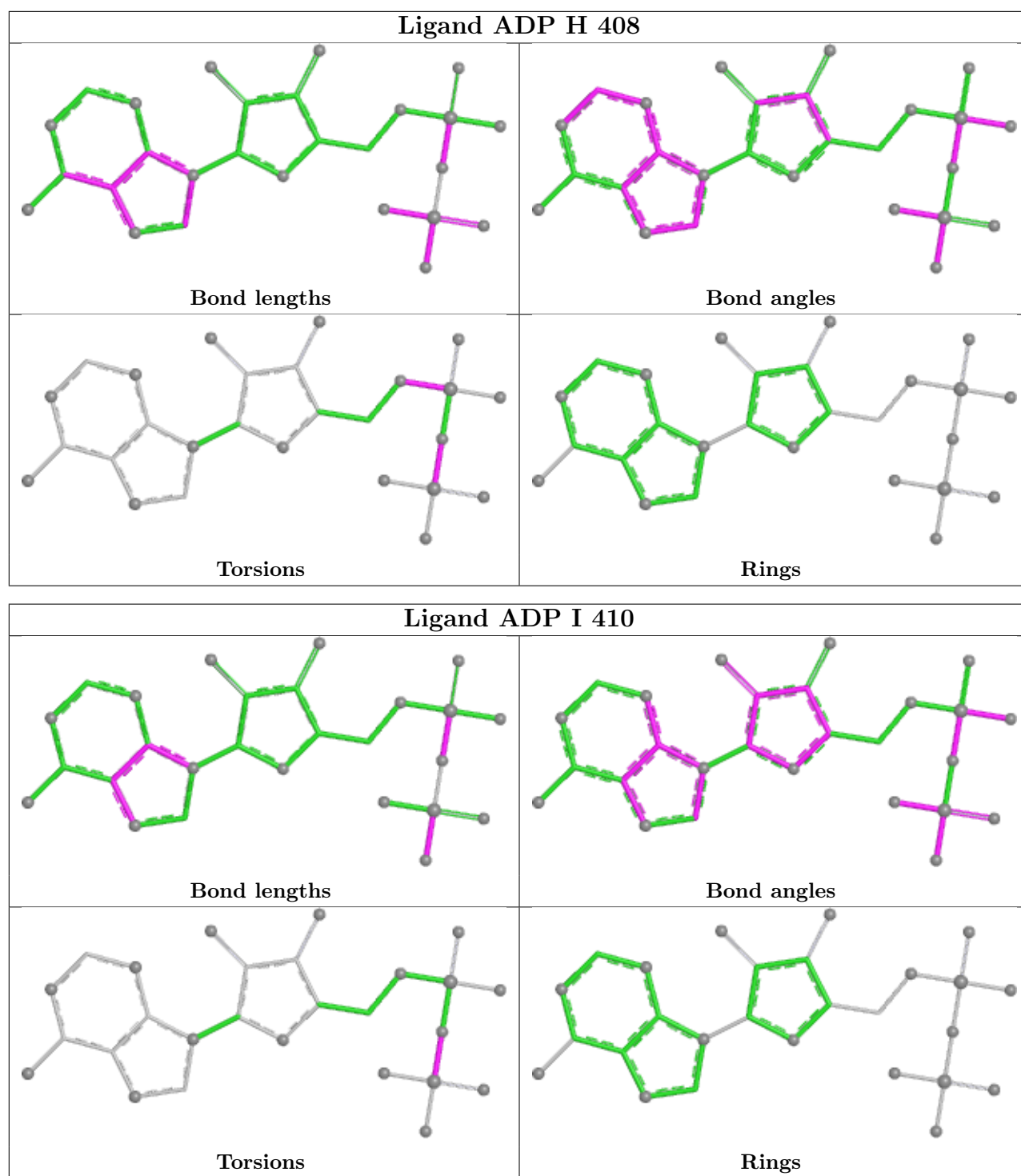
9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	402	ADP	3	0
6	D	404	ADP	3	0
6	G	406	ADP	2	0
7	G	407	BEF	1	0
6	B	400	ADP	3	0
7	B	401	BEF	1	0
7	I	411	BEF	1	0
6	H	408	ADP	4	0
6	I	410	ADP	2	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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	333/343 (97%)	0.22	18 (5%) 31 23	73, 127, 209, 244	0
1	F	333/343 (97%)	0.06	5 (1%) 72 57	67, 127, 197, 222	0
2	B	364/395 (92%)	-0.01	3 (0%) 82 70	76, 119, 164, 189	0
2	C	365/395 (92%)	-0.03	4 (1%) 78 64	68, 114, 180, 208	0
2	D	362/395 (91%)	-0.03	3 (0%) 82 70	69, 106, 156, 198	0
2	G	378/395 (95%)	-0.13	3 (0%) 82 70	76, 101, 146, 182	0
2	H	365/395 (92%)	-0.24	4 (1%) 78 64	58, 88, 125, 165	0
2	I	362/395 (91%)	-0.22	2 (0%) 85 74	56, 80, 125, 184	0
3	E	334/334 (100%)	-0.26	1 (0%) 90 83	67, 86, 134, 175	0
3	J	334/334 (100%)	-0.27	1 (0%) 90 83	63, 84, 133, 172	0
4	K	14/15 (93%)	-0.24	0 100 100	79, 87, 169, 171	0
4	M	14/15 (93%)	-0.21	0 100 100	76, 84, 174, 181	0
5	L	10/10 (100%)	-0.66	0 100 100	85, 88, 95, 105	0
5	N	10/10 (100%)	-0.69	0 100 100	81, 86, 98, 99	0
All	All	3578/3774 (94%)	-0.10	44 (1%) 76 62	56, 101, 175, 244	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	365	LEU	4.9
1	A	55	ILE	4.3
1	F	96	GLN	3.5
1	A	53	PHE	3.3
2	G	358	ALA	3.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

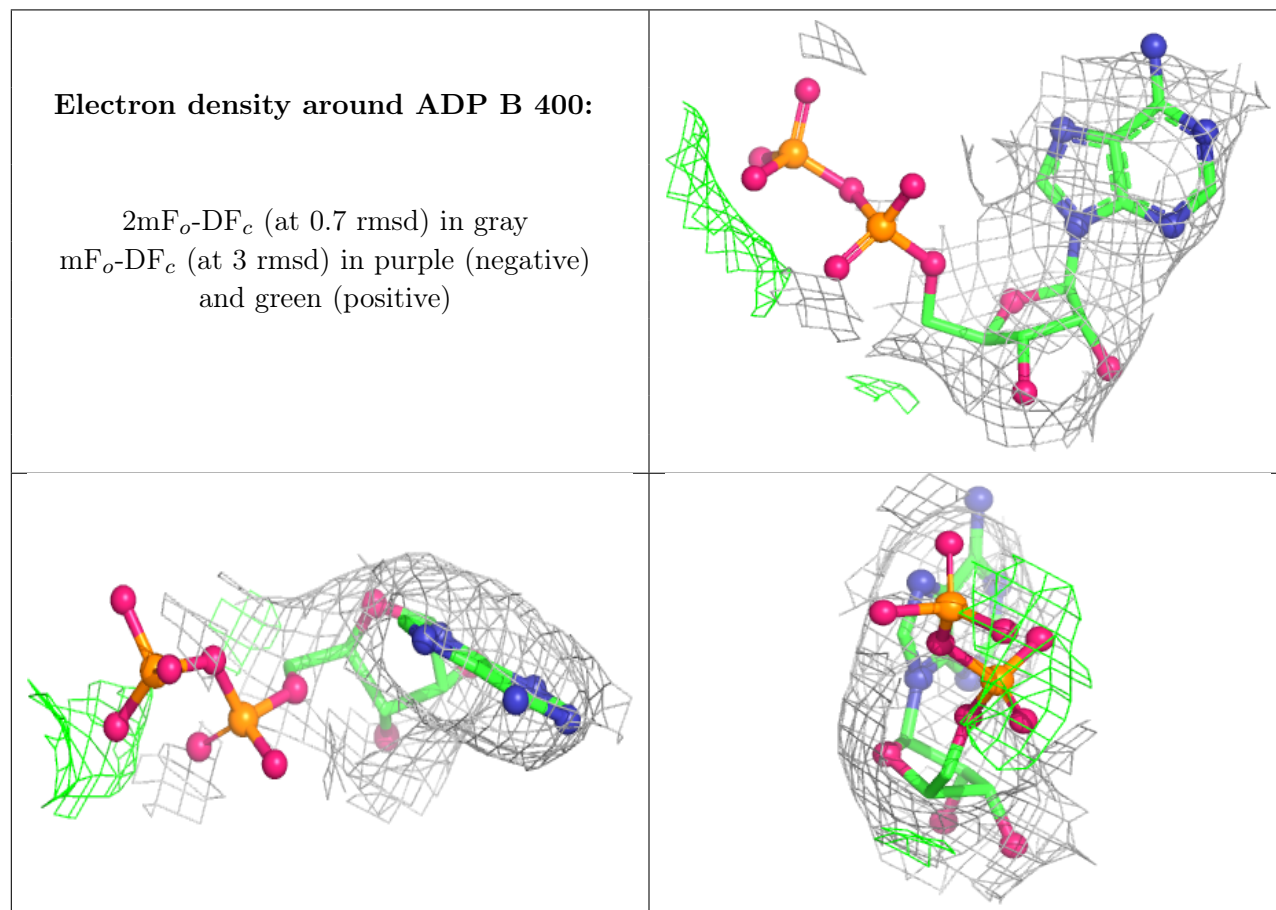
There are no oligosaccharides in this entry.

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.

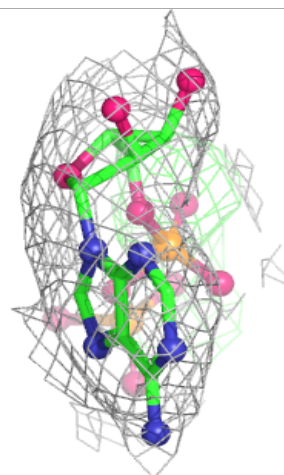
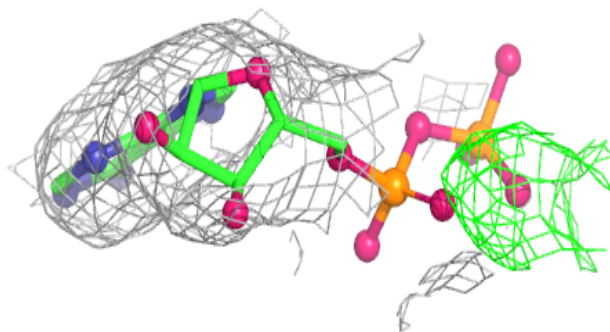
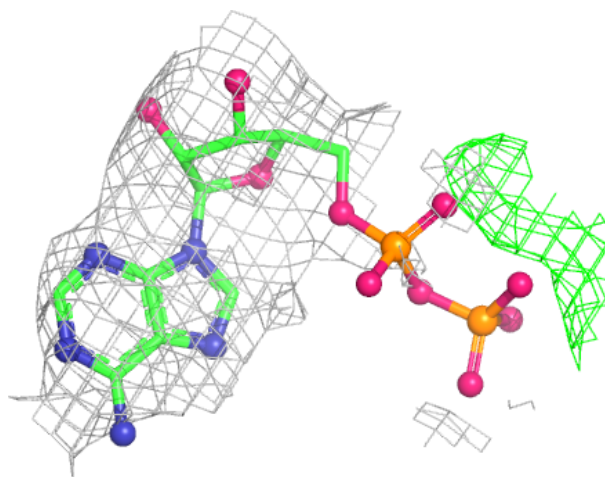
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	MG	B	412	1/1	0.74	0.25	79,79,79,79	0
8	MG	D	414	1/1	0.77	0.29	75,75,75,75	0
8	MG	G	415	1/1	0.80	0.23	79,79,79,79	0
8	MG	C	413	1/1	0.85	0.20	77,77,77,77	0
8	MG	H	416	1/1	0.87	0.19	57,57,57,57	0
7	BEF	H	409	4/4	0.89	0.12	57,57,57,58	0
7	BEF	C	403	4/4	0.89	0.14	77,78,78,79	0
7	BEF	D	405	4/4	0.89	0.12	85,85,86,87	0
8	MG	I	417	1/1	0.90	0.21	58,58,58,58	0
7	BEF	G	407	4/4	0.91	0.12	79,79,80,80	0
7	BEF	B	401	4/4	0.91	0.14	79,80,80,81	0
7	BEF	I	411	4/4	0.91	0.12	62,63,63,64	0
6	ADP	B	400	27/27	0.97	0.06	86,94,99,100	0
6	ADP	C	402	27/27	0.97	0.07	78,86,91,93	0
6	ADP	D	404	27/27	0.97	0.07	80,89,95,96	0
6	ADP	G	406	27/27	0.97	0.08	81,87,92,94	0
6	ADP	H	408	27/27	0.97	0.06	60,62,67,67	0
6	ADP	I	410	27/27	0.97	0.07	62,68,72,73	0
9	ZN	J	425	1/1	0.98	0.04	146,146,146,146	0
9	ZN	G	422	1/1	0.99	0.05	160,160,160,160	0
9	ZN	D	420	1/1	0.99	0.03	133,133,133,133	0
9	ZN	E	421	1/1	1.00	0.02	161,161,161,161	0
9	ZN	C	419	1/1	1.00	0.02	130,130,130,130	0
9	ZN	H	423	1/1	1.00	0.02	112,112,112,112	0
9	ZN	I	424	1/1	1.00	0.01	99,99,99,99	0
9	ZN	B	418	1/1	1.00	0.03	144,144,144,144	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.



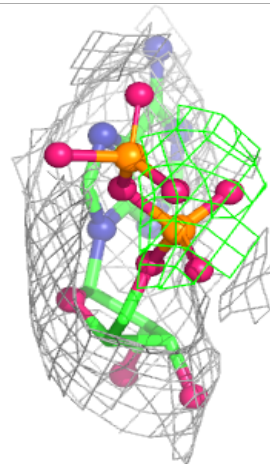
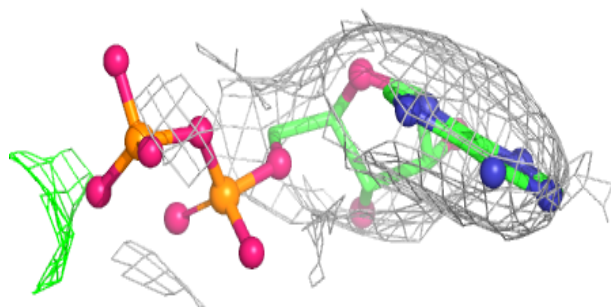
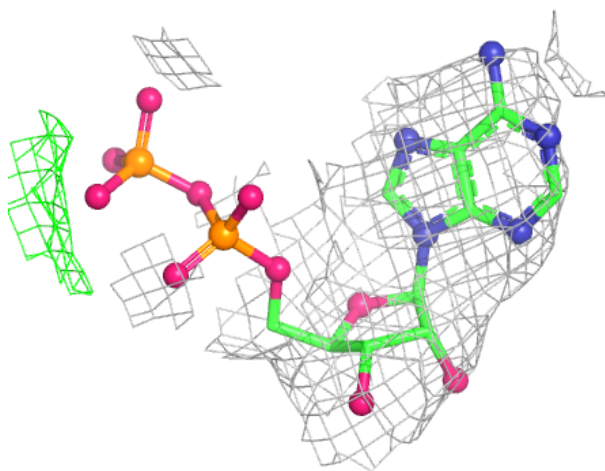
Electron density around ADP C 402:

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



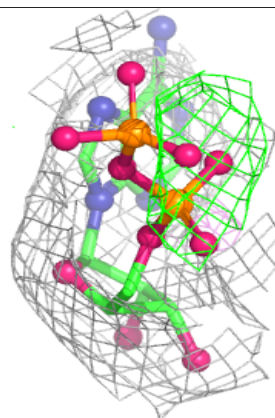
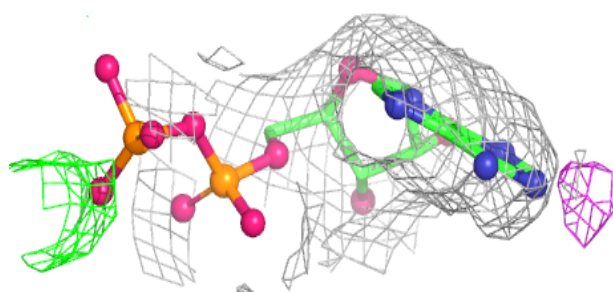
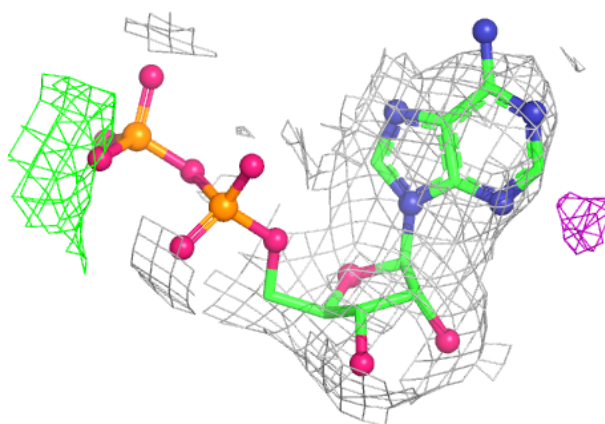
Electron density around ADP D 404:

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

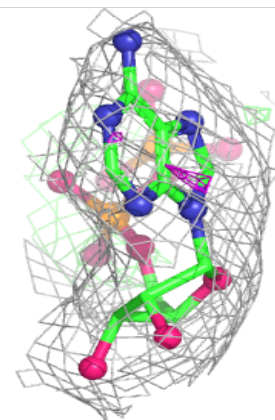
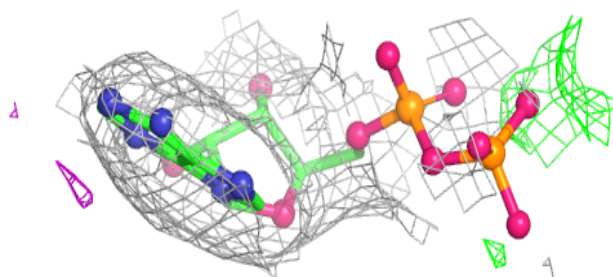
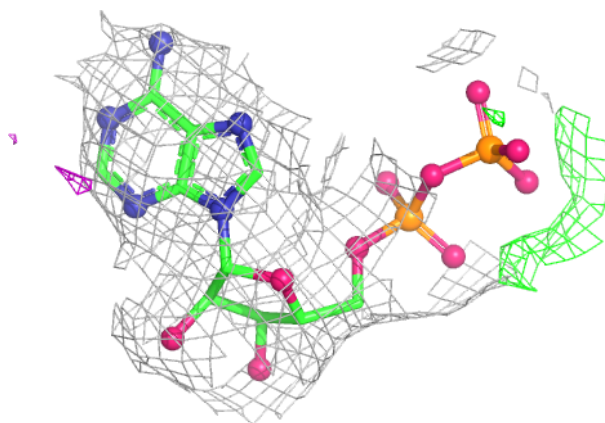


Electron density around ADP G 406:

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

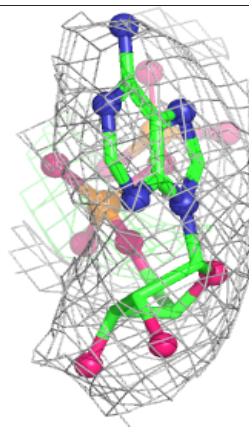
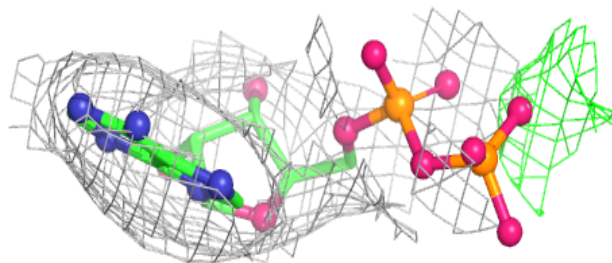
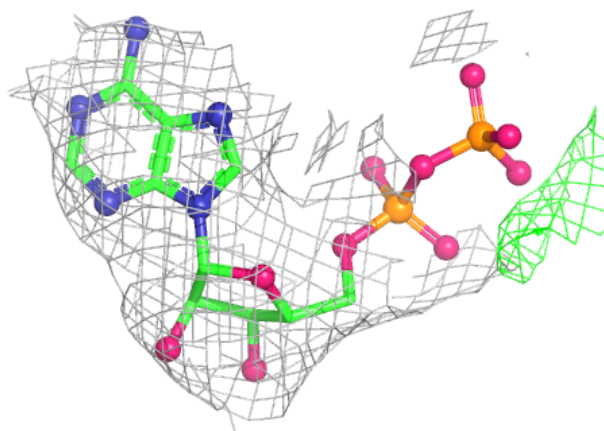
**Electron density around ADP H 408:**

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



Electron density around ADP I 410:

$2mF_o-DF_c$ (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.