wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2026 – 04:43 AM EDT

PDB ID	:	8UK9 / pdb_00008uk9
Title	:	Structure of T4 Bacteriophage clamp loader mutant D110C bound to the T4 clamp, primer-template DNA, and ATP analog
Authors	:	Marcus, K.; Ghaffari-Kashani, S.; Gee, C.L.
Deposited on	:	2023-10-12
Resolution	:	3.10 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 (i) 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 (i)) were used in the production of this report:

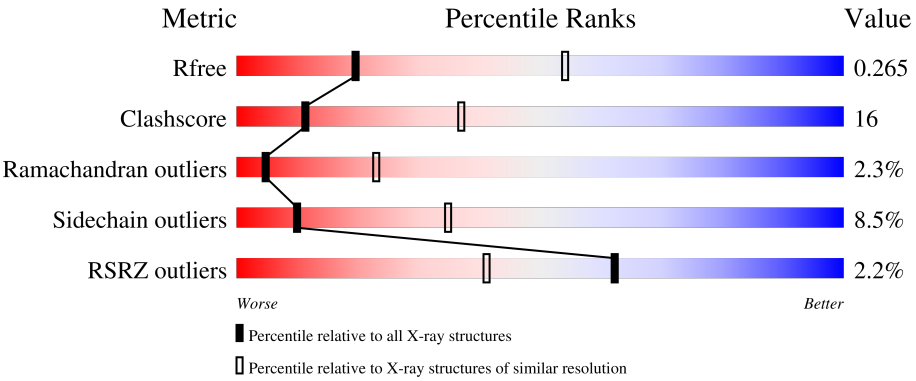
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 <=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	187	3% 50% 36% 10%
1	Q	187	% 52% 34% 11%
2	B	320	2% 66% 30%
2	C	320	67% 29%
2	D	320	59% 37%

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Mol	Chain	Length	Quality of chain
2	E	320	5% 52% 40% 7%
2	K	320	2% 62% 34%
2	L	320	2% 64% 32%
2	M	320	% 60% 35%
2	N	320	7% 52% 36% 7% 5%
3	F	228	4% 54% 39% 7%
3	G	228	4% 73% 24%
3	H	228	% 72% 27%
3	R	228	2% 68% 31%
3	S	228	% 60% 38%
3	T	228	3% 64% 31%
4	I	24	33% 67%
4	O	24	29% 71%
5	J	20	5% 40% 60%
5	P	20	5% 55% 45%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	AF3	B	901	-	-	X	-
6	AF3	K	402	-	-	X	-
6	AF3	L	402	-	-	X	-
6	AF3	M	402	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 35422 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 Sliding-clamp-loader small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	1	0
			1474	951	242	275	6			
1	Q	183	Total	C	N	O	S	0	0	0
			1469	947	244	272	6			

- Molecule 2 is a protein called Sliding-clamp-loader large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	319	Total	C	N	O	S	0	0	0
			2507	1586	431	472	18			
2	C	320	Total	C	N	O	S	0	0	0
			2513	1589	432	474	18			
2	D	318	Total	C	N	O	S	0	0	0
			2499	1581	430	471	17			
2	E	318	Total	C	N	O	S	0	0	0
			2499	1581	430	471	17			
2	K	319	Total	C	N	O	S	0	0	0
			2507	1586	431	472	18			
2	L	320	Total	C	N	O	S	0	0	0
			2513	1589	432	474	18			
2	M	317	Total	C	N	O	S	0	0	0
			2492	1578	426	470	18			
2	N	305	Total	C	N	O	S	0	0	0
			2407	1526	413	451	17			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP P04526
B	110	CYS	ASP	engineered mutation	UNP P04526
C	0	SER	-	expression tag	UNP P04526
C	110	CYS	ASP	engineered mutation	UNP P04526
D	0	SER	-	expression tag	UNP P04526

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Chain	Residue	Modelled	Actual	Comment	Reference
D	110	CYS	ASP	engineered mutation	UNP P04526
E	0	SER	-	expression tag	UNP P04526
E	110	CYS	ASP	engineered mutation	UNP P04526
K	0	SER	-	expression tag	UNP P04526
K	110	CYS	ASP	engineered mutation	UNP P04526
L	0	SER	-	expression tag	UNP P04526
L	110	CYS	ASP	engineered mutation	UNP P04526
M	0	SER	-	expression tag	UNP P04526
M	110	CYS	ASP	engineered mutation	UNP P04526
N	0	SER	-	expression tag	UNP P04526
N	110	CYS	ASP	engineered mutation	UNP P04526

- Molecule 3 is a protein called Sliding clamp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	228	Total	C	N	O	S	0	0	0
			1750	1113	288	343	6			
3	G	228	Total	C	N	O	S	0	0	0
			1750	1113	288	343	6			
3	H	228	Total	C	N	O	S	0	0	0
			1750	1113	288	343	6			
3	R	228	Total	C	N	O	S	0	0	0
			1750	1113	288	343	6			
3	S	228	Total	C	N	O	S	0	0	0
			1750	1113	288	343	6			
3	T	228	Total	C	N	O	S	0	0	0
			1750	1113	288	343	6			

- Molecule 4 is a DNA chain called DNA template.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	24	Total	C	N	O	P	0	0	0
			489	236	76	153	24			
4	O	24	Total	C	N	O	P	0	0	0
			489	236	76	153	24			

- Molecule 5 is a DNA chain called DNA primer.

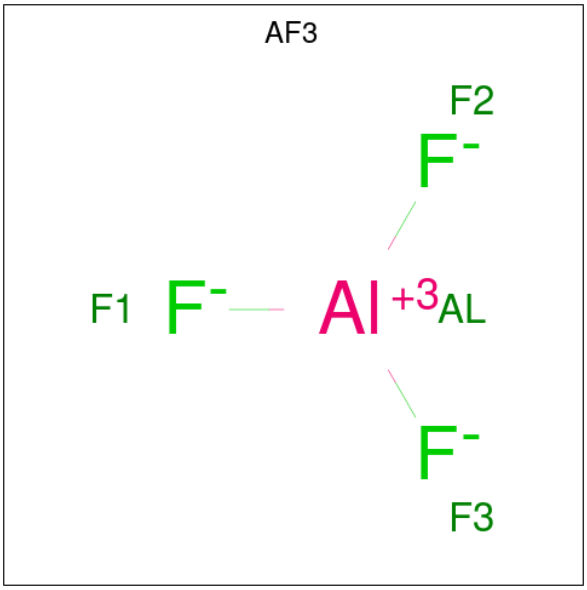
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	20	Total	C	N	O	P	0	0	0
			408	195	81	113	19			

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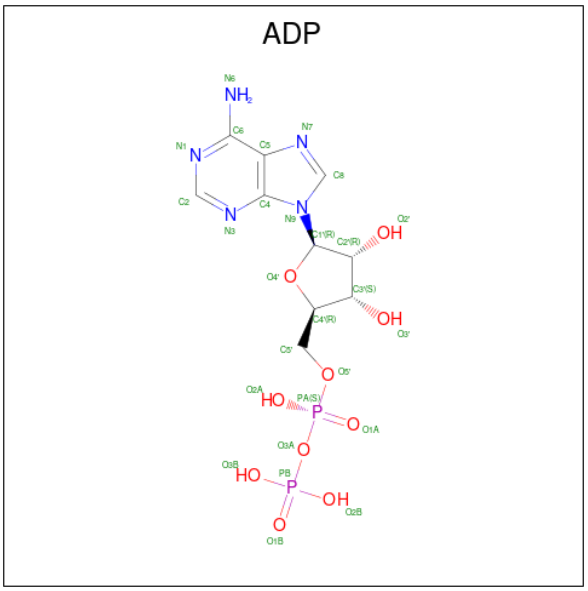
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	P	20	Total	C	N	O	P	0	0	0
			408	195	81	113	19			

- Molecule 6 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	Al	F		0	0
			4	1	3			
6	C	1	Total	Al	F		0	0
			4	1	3			
6	D	1	Total	Al	F		0	0
			4	1	3			
6	K	1	Total	Al	F		0	0
			4	1	3			
6	L	1	Total	Al	F		0	0
			4	1	3			
6	M	1	Total	Al	F		0	0
			4	1	3			

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		
8	E	1	Total	Mg	0	0
			1	1		

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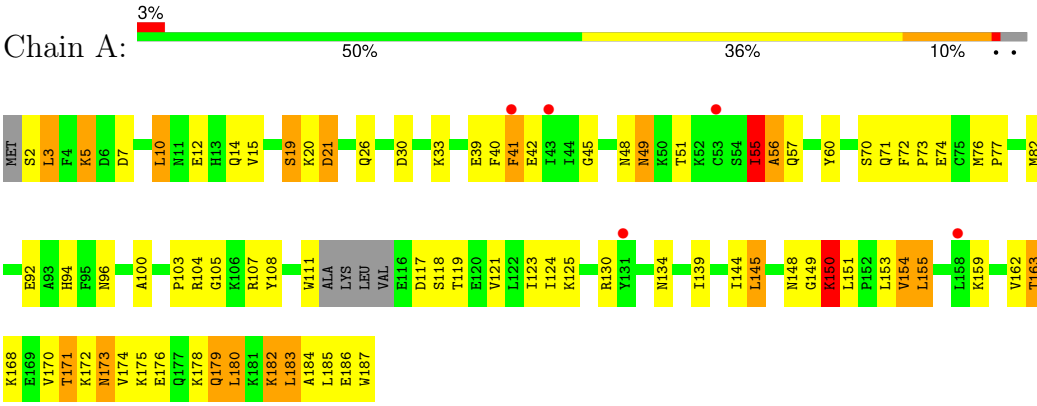
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	K	1	Total Mg 1 1	0	0
8	L	1	Total Mg 1 1	0	0
8	M	1	Total Mg 1 1	0	0
8	N	1	Total Mg 1 1	0	0

3 Residue-property plots (i)

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.

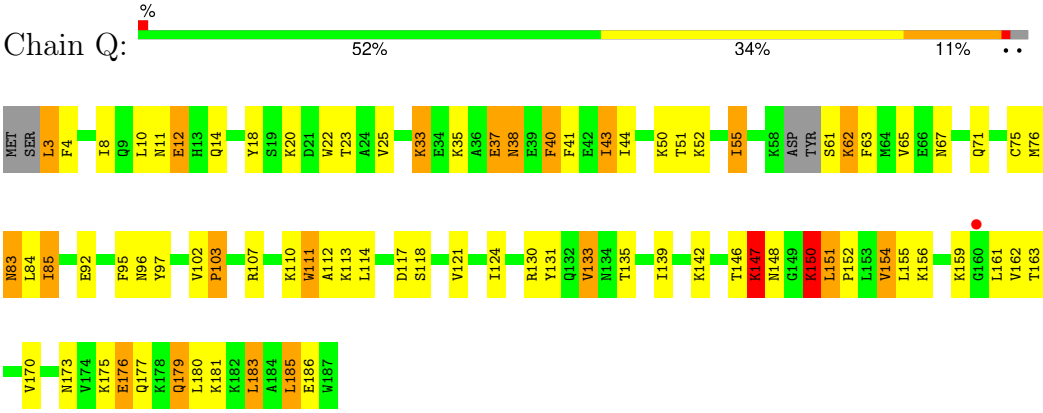
• Molecule 1: Sliding-clamp-loader small subunit

Chain A:



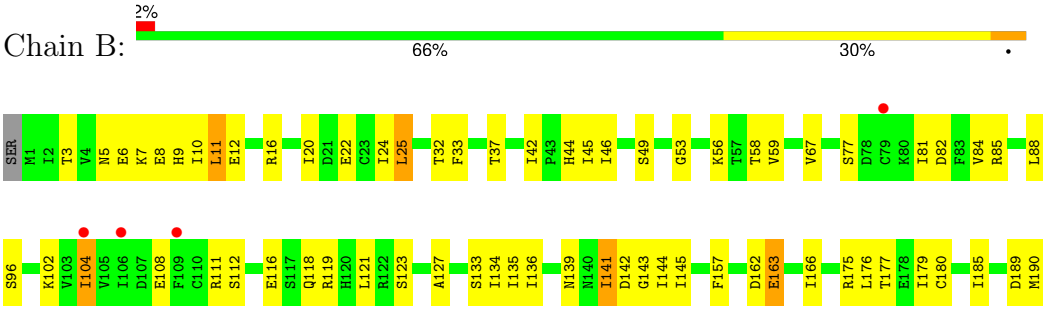
• Molecule 1: Sliding-clamp-loader small subunit

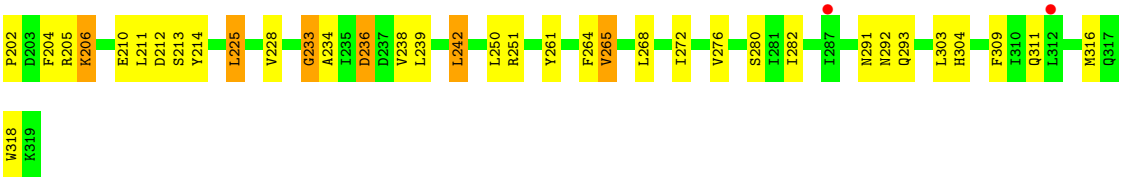
Chain Q:



• Molecule 2: Sliding-clamp-loader large subunit

Chain B:

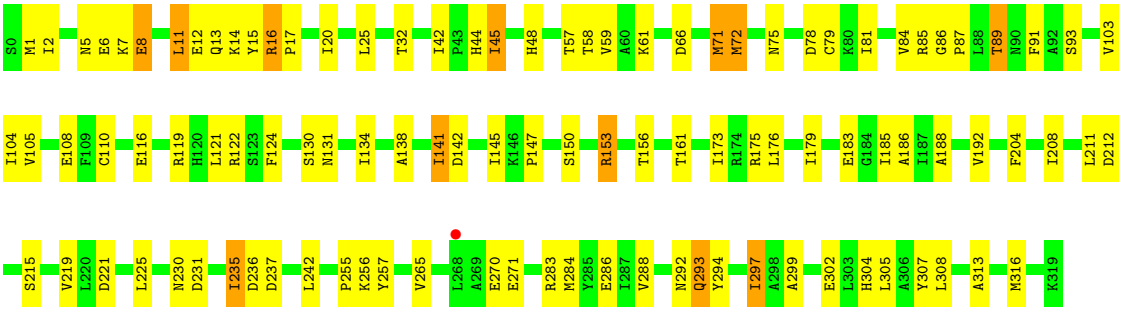




• Molecule 2: Sliding-clamp-loader large subunit

Chain C:

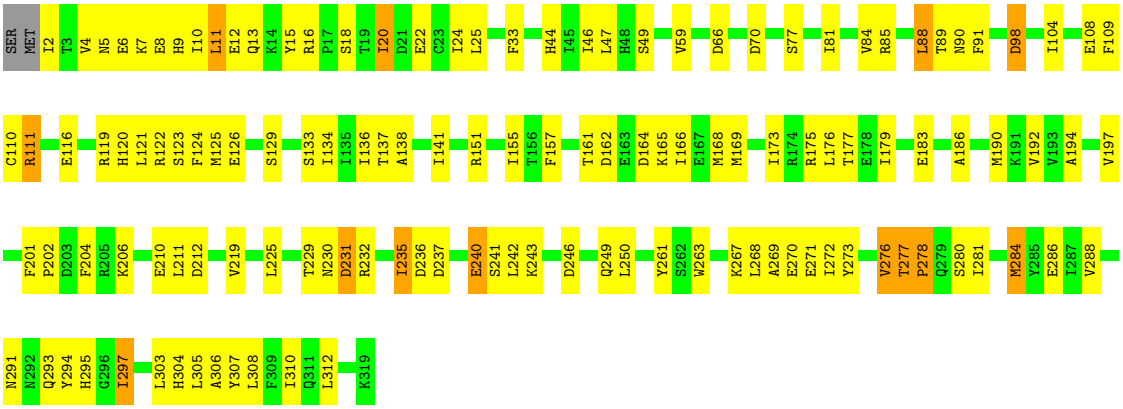




• Molecule 2: Sliding-clamp-loader large subunit

Chain D:

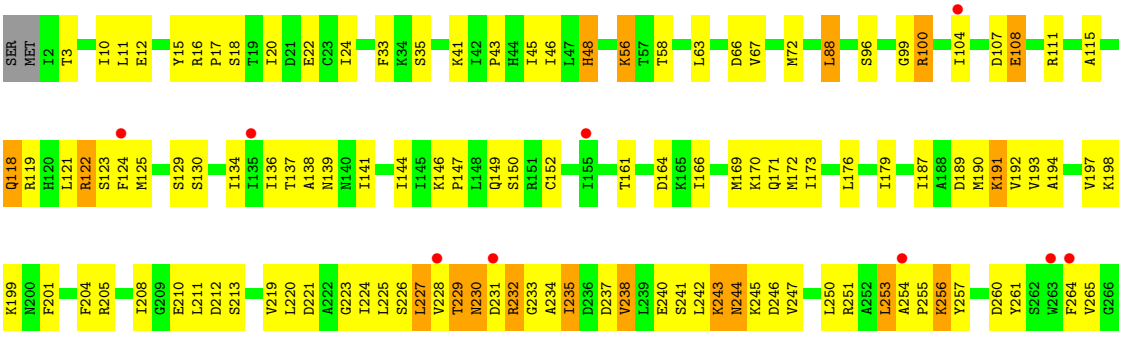


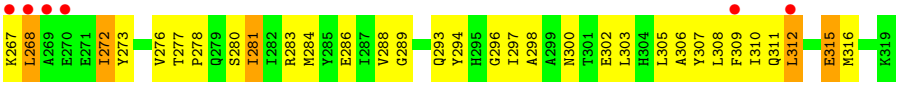


• Molecule 2: Sliding-clamp-loader large subunit

Chain E:

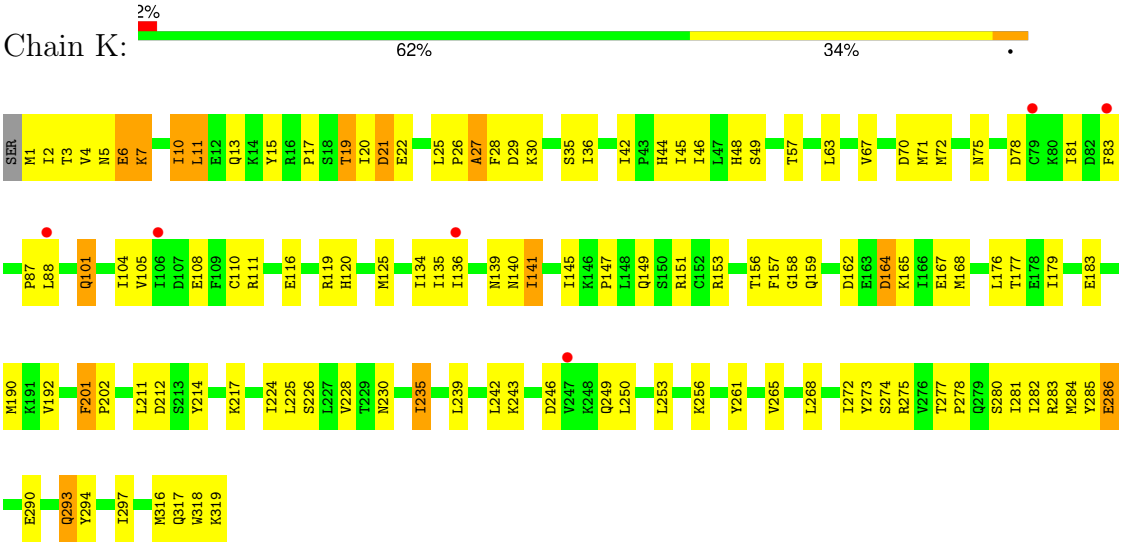






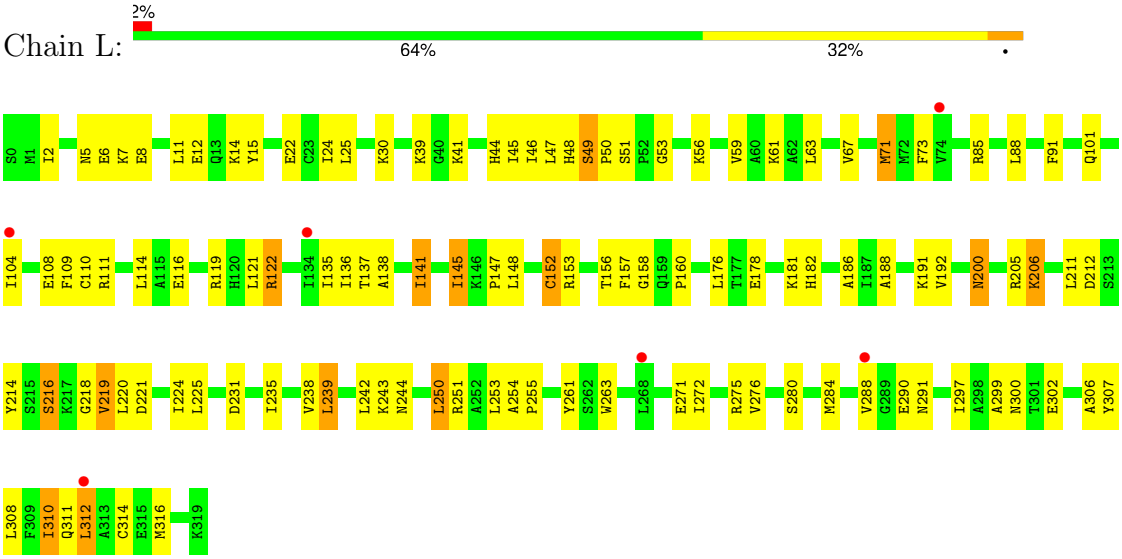
• Molecule 2: Sliding-clamp-loader large subunit

Chain K:



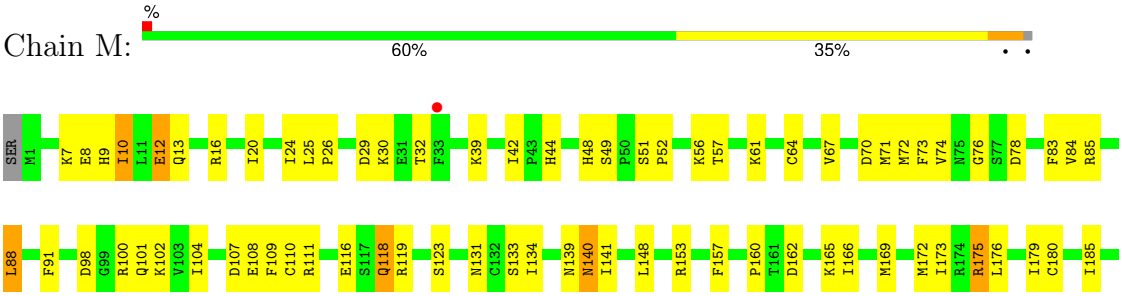
• Molecule 2: Sliding-clamp-loader large subunit

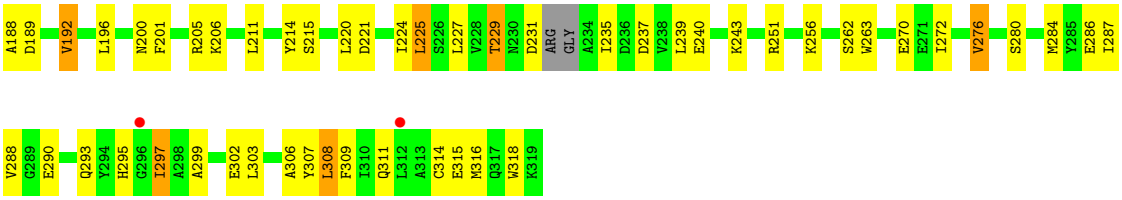
Chain L:



• Molecule 2: Sliding-clamp-loader large subunit

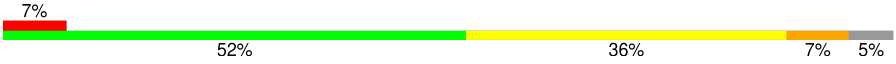
Chain M:

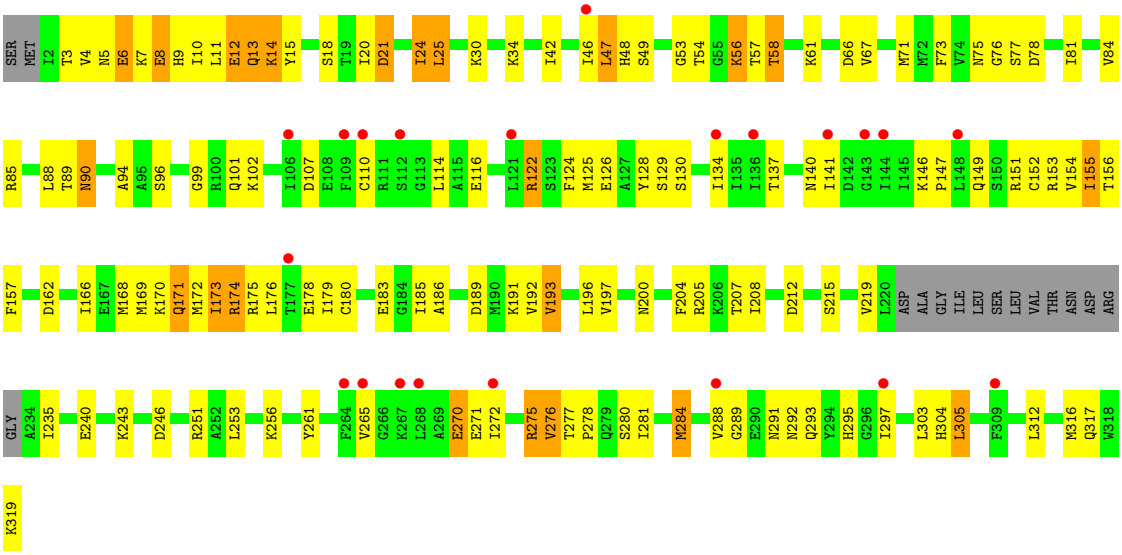




• Molecule 2: Sliding-clamp-loader large subunit

Chain N:

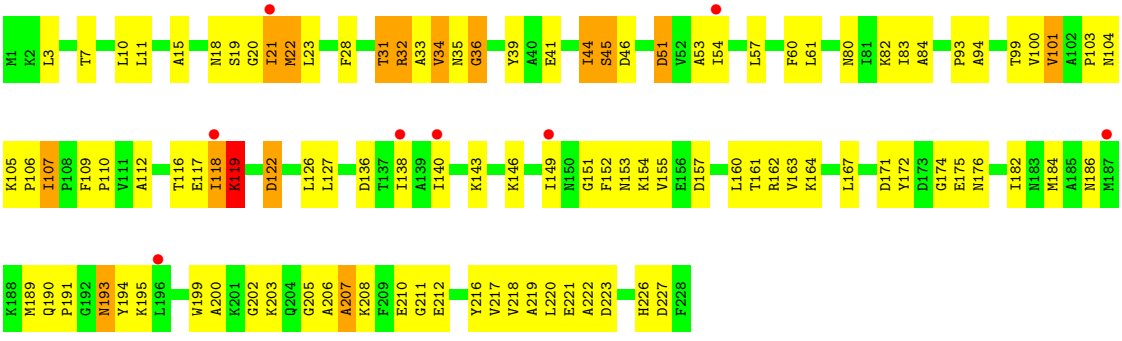




• Molecule 3: Sliding clamp

Chain F:

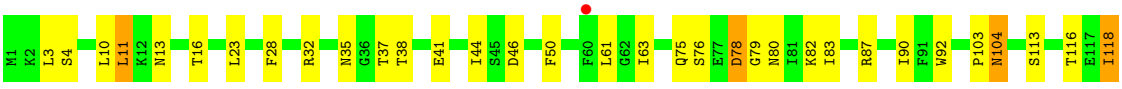


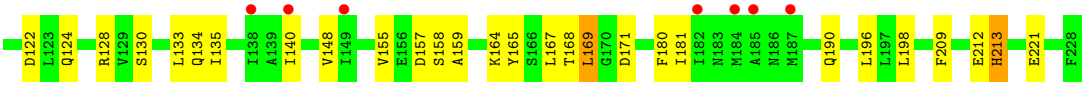


• Molecule 3: Sliding clamp

Chain G:



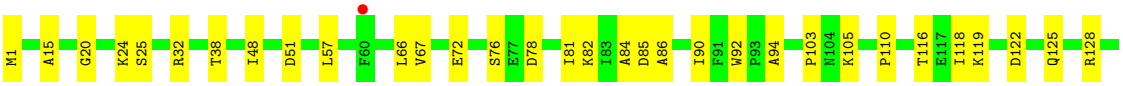


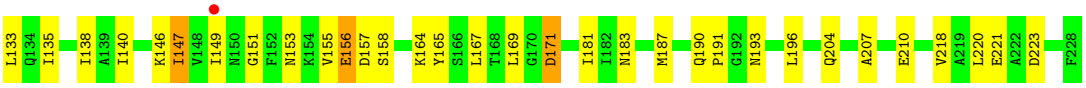


• Molecule 3: Sliding clamp

Chain H:



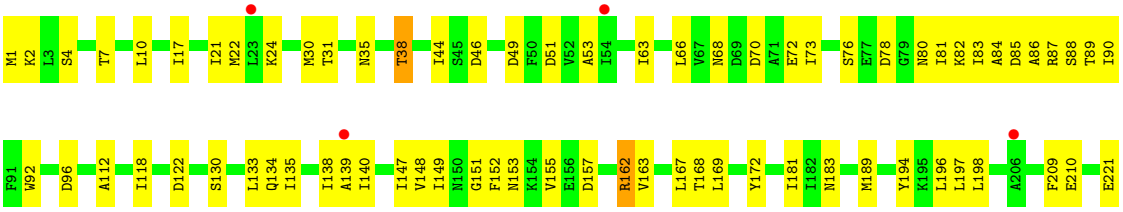




• Molecule 3: Sliding clamp

Chain R:

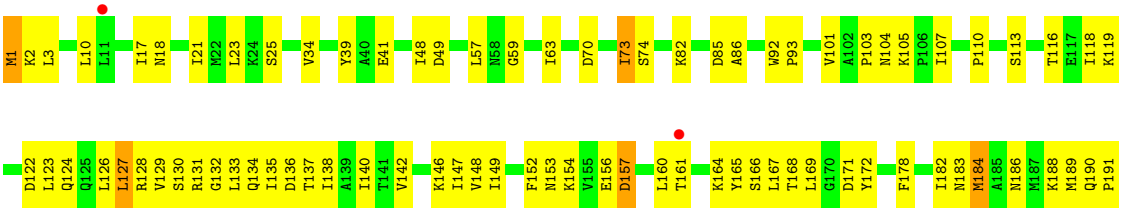




• Molecule 3: Sliding clamp

Chain S:



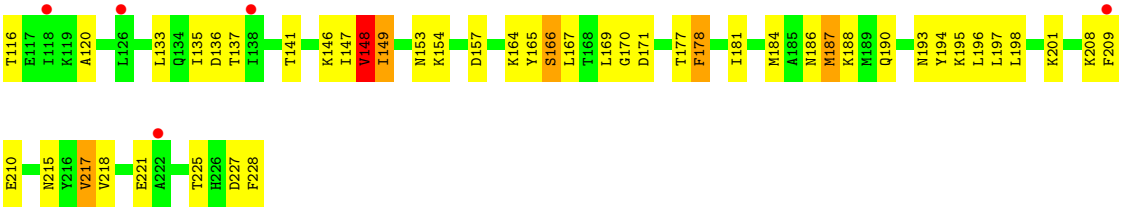


• Molecule 3: Sliding clamp

Chain T:

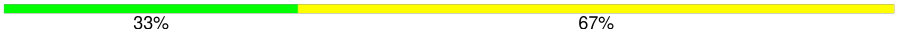


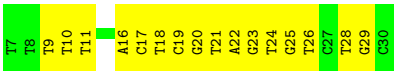




• Molecule 4: DNA template

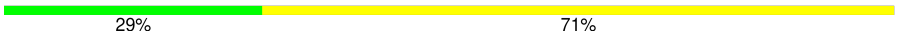
Chain I:





• Molecule 4: DNA template

Chain O:





• Molecule 5: DNA primer

Chain J:

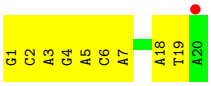




• Molecule 5: DNA primer

Chain P:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.24Å 231.99Å 264.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.13 – 3.10 48.13 – 3.10	Depositor EDS
% Data completeness (in resolution range)	71.3 (48.13-3.10) 71.3 (48.13-3.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.253 , 0.265 0.253 , 0.265	Depositor DCC
R_{free} test set	2000 reflections (1.87%)	wwPDB-VP
Wilson B-factor (Å^2)	95.1	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	35422	wwPDB-VP
Average B, all atoms (Å^2)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, ADP, AF3

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	0.13	0/1505	0.42	0/2025
1	Q	0.16	0/1495	0.43	0/2011
2	B	0.20	0/2551	0.35	1/3438 (0.0%)
2	C	0.11	0/2557	0.32	0/3446
2	D	0.12	0/2543	0.34	0/3428
2	E	0.29	0/2543	0.47	0/3428
2	K	0.12	0/2551	0.36	0/3438
2	L	0.11	0/2557	0.31	0/3446
2	M	0.12	0/2535	0.33	0/3416
2	N	0.12	0/2450	0.38	2/3300 (0.1%)
3	F	0.13	0/1779	0.40	0/2410
3	G	0.09	0/1779	0.28	0/2410
3	H	0.09	0/1779	0.28	0/2410
3	R	0.10	0/1779	0.31	0/2410
3	S	0.10	0/1779	0.29	0/2410
3	T	0.13	0/1779	0.36	0/2410
4	I	0.20	0/544	0.47	0/838
4	O	0.18	0/544	0.42	0/838
5	J	0.19	0/459	0.38	0/706
5	P	0.16	0/459	0.34	0/706
All	All	0.15	0/35967	0.36	3/48924 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	K	0	1
3	T	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	143	GLY	N-CA-C	-7.50	106.07	114.40
2	N	235	ILE	N-CA-C	-6.39	106.22	111.91
2	N	99	GLY	N-CA-C	-5.05	108.73	115.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	K	21	ASP	Peptide
3	T	148	VAL	Peptide

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	1474	0	1491	64	0
1	Q	1469	0	1502	60	0
2	B	2507	0	2538	78	0
2	C	2513	0	2543	76	0
2	D	2499	0	2526	104	0
2	E	2499	0	2523	151	0
2	K	2507	0	2539	83	0
2	L	2513	0	2543	84	0
2	M	2492	0	2521	91	0
2	N	2407	0	2434	102	0
3	F	1750	0	1755	78	0
3	G	1750	0	1755	36	0
3	H	1750	0	1755	35	0
3	R	1750	0	1755	54	0
3	S	1750	0	1755	62	0
3	T	1750	0	1755	54	0
4	I	489	0	277	17	0
4	O	489	0	277	17	0
5	J	408	0	225	10	0
5	P	408	0	225	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	4	0	0	4	0
6	C	4	0	0	1	0
6	D	4	0	0	0	0
6	K	4	0	0	2	0
6	L	4	0	0	2	0
6	M	4	0	0	3	0
7	B	27	0	12	8	0
7	C	27	0	12	6	0
7	D	27	0	12	5	0
7	E	27	0	12	6	0
7	K	27	0	12	4	0
7	L	27	0	12	4	0
7	M	27	0	12	8	0
7	N	27	0	12	5	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
8	K	1	0	0	0	0
8	L	1	0	0	0	0
8	M	1	0	0	0	0
8	N	1	0	0	0	0
All	All	35422	0	34790	1131	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 16.

The worst 5 of 1131 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:E:250:LEU:HD22	2:E:309:PHE:HB3	1.41	1.02
3:F:190:GLN:HB3	3:F:191:PRO:HD2	1.46	0.96
2:C:145:ILE:HG13	2:C:147:PRO:HD2	1.52	0.92
2:E:272:ILE:HG21	2:E:284:MET:HE3	1.53	0.89
3:F:153:ASN:H	3:F:164:LYS:HZ3	1.23	0.86

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	179/187 (96%)	142 (79%)	21 (12%)	16 (9%)	0 3
1	Q	179/187 (96%)	140 (78%)	28 (16%)	11 (6%)	1 7
2	B	317/320 (99%)	291 (92%)	19 (6%)	7 (2%)	5 24
2	C	318/320 (99%)	290 (91%)	22 (7%)	6 (2%)	6 27
2	D	316/320 (99%)	287 (91%)	20 (6%)	9 (3%)	4 20
2	E	316/320 (99%)	281 (89%)	26 (8%)	9 (3%)	4 20
2	K	317/320 (99%)	289 (91%)	21 (7%)	7 (2%)	5 24
2	L	318/320 (99%)	286 (90%)	25 (8%)	7 (2%)	5 24
2	M	313/320 (98%)	289 (92%)	23 (7%)	1 (0%)	36 67
2	N	301/320 (94%)	266 (88%)	32 (11%)	3 (1%)	12 41
3	F	226/228 (99%)	181 (80%)	37 (16%)	8 (4%)	3 16
3	G	226/228 (99%)	208 (92%)	14 (6%)	4 (2%)	6 28
3	H	226/228 (99%)	205 (91%)	19 (8%)	2 (1%)	14 44
3	R	226/228 (99%)	207 (92%)	18 (8%)	1 (0%)	30 61
3	S	226/228 (99%)	201 (89%)	23 (10%)	2 (1%)	14 44
3	T	226/228 (99%)	195 (86%)	24 (11%)	7 (3%)	3 18
All	All	4230/4302 (98%)	3758 (89%)	372 (9%)	100 (2%)	5 22

5 of 100 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	PRO
2	B	201	PHE
2	D	11	LEU
2	E	191	LYS
3	F	34	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	160/163 (98%)	132 (82%)	28 (18%)	2	9
1	Q	159/163 (98%)	118 (74%)	41 (26%)	0	2
2	B	277/278 (100%)	261 (94%)	16 (6%)	18	48
2	C	278/278 (100%)	258 (93%)	20 (7%)	13	40
2	D	276/278 (99%)	263 (95%)	13 (5%)	23	55
2	E	276/278 (99%)	248 (90%)	28 (10%)	7	28
2	K	277/278 (100%)	257 (93%)	20 (7%)	13	40
2	L	278/278 (100%)	257 (92%)	21 (8%)	12	39
2	M	276/278 (99%)	253 (92%)	23 (8%)	10	35
2	N	266/278 (96%)	230 (86%)	36 (14%)	4	16
3	F	189/189 (100%)	167 (88%)	22 (12%)	5	22
3	G	189/189 (100%)	178 (94%)	11 (6%)	18	48
3	H	189/189 (100%)	181 (96%)	8 (4%)	26	58
3	R	189/189 (100%)	184 (97%)	5 (3%)	40	68
3	S	189/189 (100%)	181 (96%)	8 (4%)	26	58
3	T	189/189 (100%)	179 (95%)	10 (5%)	20	51
All	All	3657/3684 (99%)	3347 (92%)	310 (8%)	10	35

5 of 310 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	171	GLN
1	Q	185	LEU
2	N	215	SER
1	Q	83	ASN
3	T	5	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	230	ASN
1	Q	148	ASN
2	M	304	HIS
2	N	171	GLN
3	R	75	GLN

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 22 ligands modelled in this entry, 8 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
7	ADP	N	401	8	28,29,29	1.40	4 (14%)	43,45,45	1.91	8 (18%)
7	ADP	M	403	8,6	28,29,29	1.41	5 (17%)	43,45,45	1.93	9 (20%)
6	AF3	D	402	7	0,3,3	-	-	-		
7	ADP	D	403	8,6	28,29,29	1.40	4 (14%)	43,45,45	1.94	8 (18%)
7	ADP	B	902	8,6	28,29,29	1.41	4 (14%)	43,45,45	1.92	9 (20%)
7	ADP	C	403	8,6	28,29,29	1.42	4 (14%)	43,45,45	1.93	8 (18%)
6	AF3	M	402	7	0,3,3	-	-	-		
6	AF3	C	402	7	0,3,3	-	-	-		
6	AF3	B	901	7	0,3,3	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	ADP	K	403	8,6	28,29,29	1.44	5 (17%)	43,45,45	1.86	8 (18%)
7	ADP	L	403	8,6	28,29,29	1.40	4 (14%)	43,45,45	1.90	9 (20%)
6	AF3	K	402	7	0,3,3	-	-	-		
6	AF3	L	402	7	0,3,3	-	-	-		
7	ADP	E	401	8,2	28,29,29	1.41	4 (14%)	43,45,45	1.88	8 (18%)

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
7	ADP	N	401	8	-	5/16/32/32	0/3/3/3
7	ADP	M	403	8,6	-	5/16/32/32	0/3/3/3
7	ADP	D	403	8,6	-	0/16/32/32	0/3/3/3
7	ADP	B	902	8,6	-	2/16/32/32	0/3/3/3
7	ADP	C	403	8,6	-	0/16/32/32	0/3/3/3
7	ADP	K	403	8,6	-	4/16/32/32	0/3/3/3
7	ADP	L	403	8,6	-	5/16/32/32	0/3/3/3
7	ADP	E	401	8,2	-	4/16/32/32	0/3/3/3

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	403	ADP	C5-C4	4.89	1.47	1.39
7	B	902	ADP	C5-C4	4.83	1.47	1.39
7	E	401	ADP	C5-C4	4.78	1.47	1.39
7	D	403	ADP	C5-C4	4.76	1.47	1.39
7	N	401	ADP	C5-C4	4.75	1.47	1.39

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	403	ADP	C5-C4-N3	-6.31	118.02	126.72
7	N	401	ADP	C5-C4-N3	-6.19	118.19	126.72
7	D	403	ADP	C5-C4-N3	-6.17	118.22	126.72
7	M	403	ADP	C5-C4-N3	-6.14	118.27	126.72
7	L	403	ADP	C5-C4-N3	-6.12	118.30	126.72

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	902	ADP	C5'-O5'-PA-O3A
7	E	401	ADP	C5'-O5'-PA-O1A
7	E	401	ADP	C5'-O5'-PA-O2A
7	E	401	ADP	C5'-O5'-PA-O3A
7	K	403	ADP	PA-O3A-PB-O2B

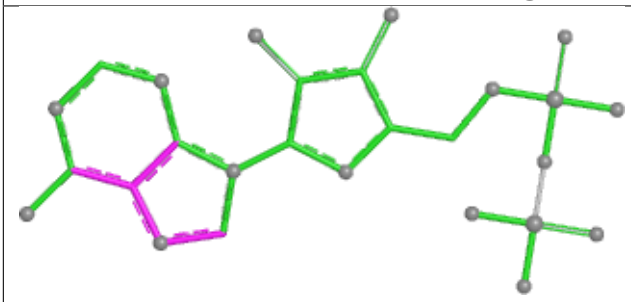
There are no ring outliers.

13 monomers are involved in 53 short contacts:

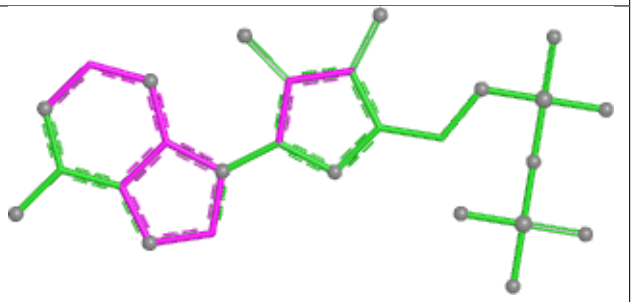
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	N	401	ADP	5	0
7	M	403	ADP	8	0
7	D	403	ADP	5	0
7	B	902	ADP	8	0
7	C	403	ADP	6	0
6	M	402	AF3	3	0
6	C	402	AF3	1	0
6	B	901	AF3	4	0
7	K	403	ADP	4	0
7	L	403	ADP	4	0
6	K	402	AF3	2	0
6	L	402	AF3	2	0
7	E	401	ADP	6	0

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 then 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.

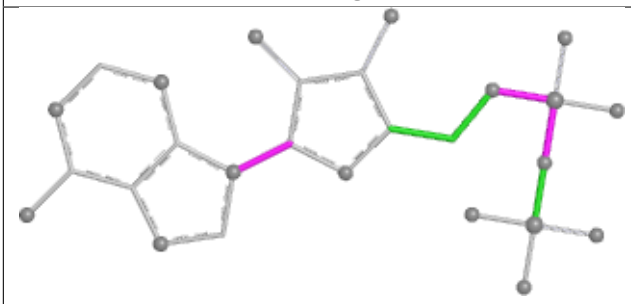
Ligand ADP N 401



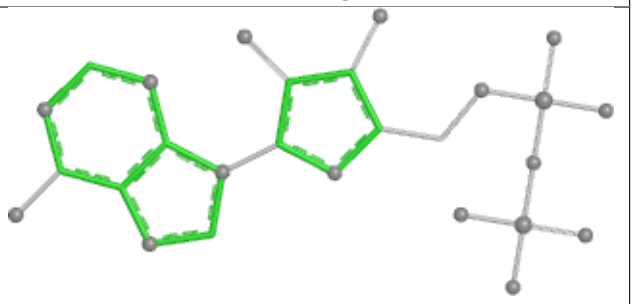
Bond lengths



Bond angles

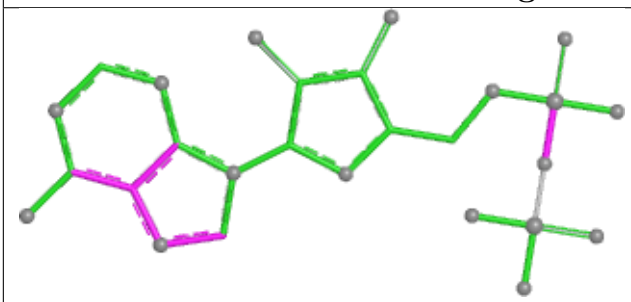


Torsions

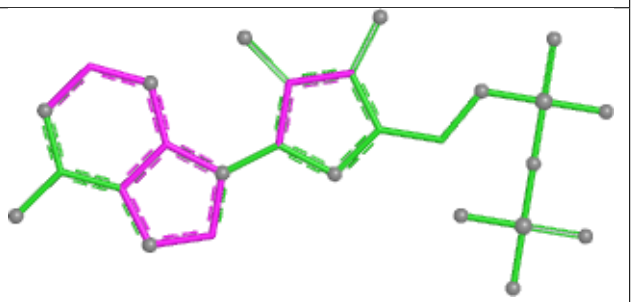


Rings

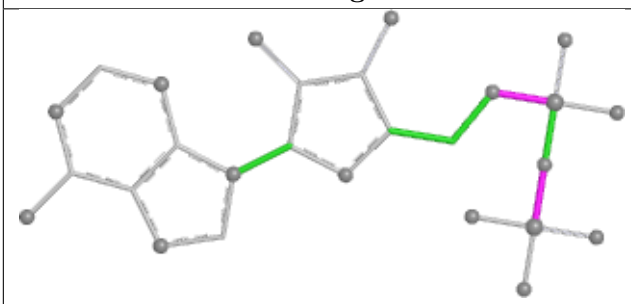
Ligand ADP M 403



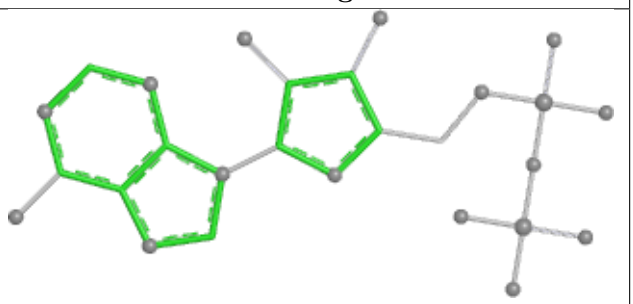
Bond lengths



Bond angles

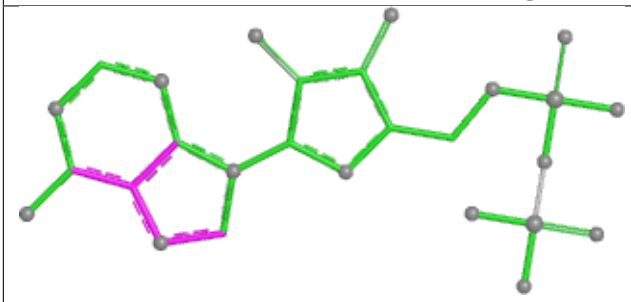


Torsions

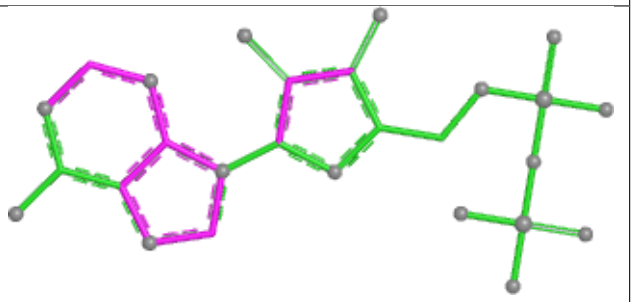


Rings

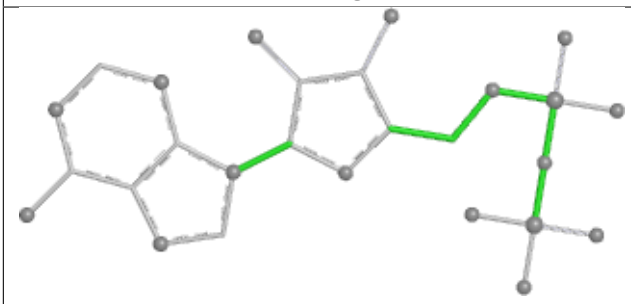
Ligand ADP D 403



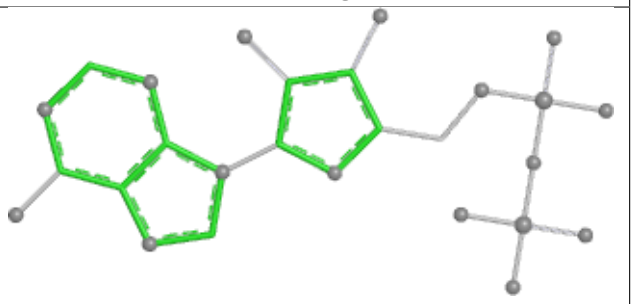
Bond lengths



Bond angles

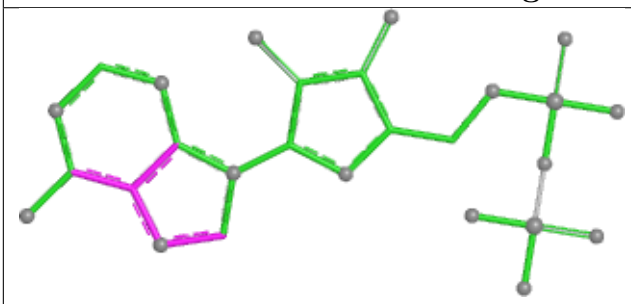


Torsions

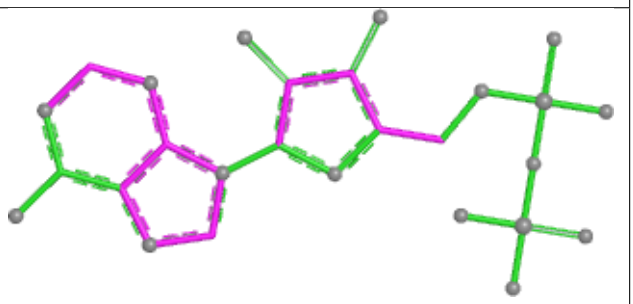


Rings

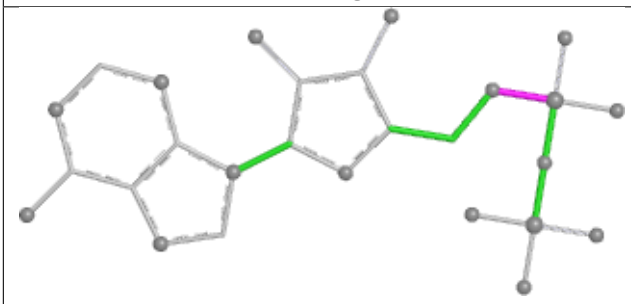
Ligand ADP B 902



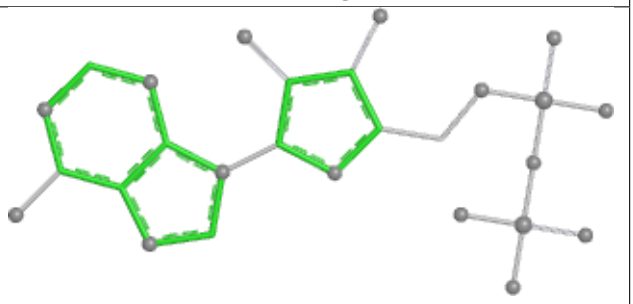
Bond lengths



Bond angles

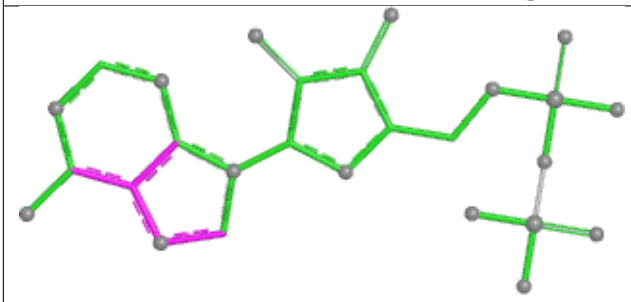


Torsions

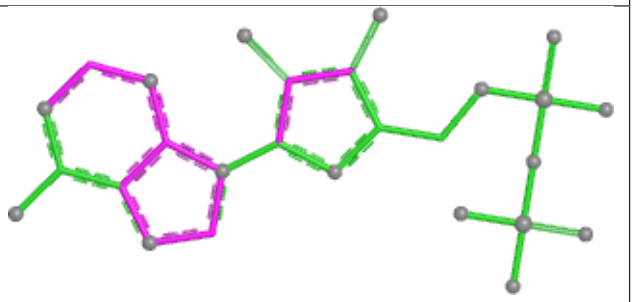


Rings

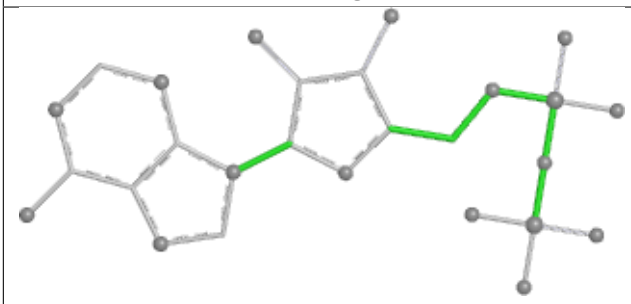
Ligand ADP C 403



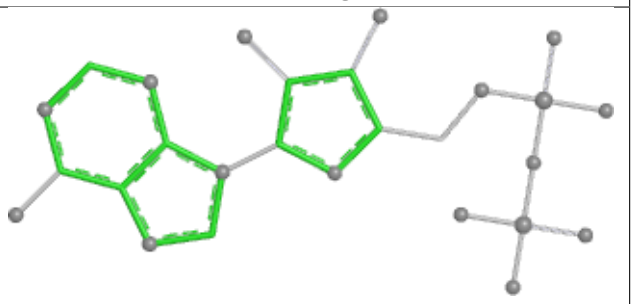
Bond lengths



Bond angles

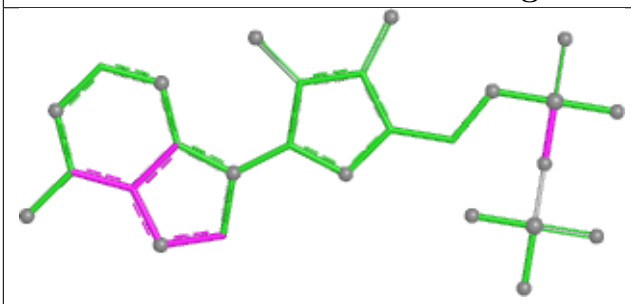


Torsions

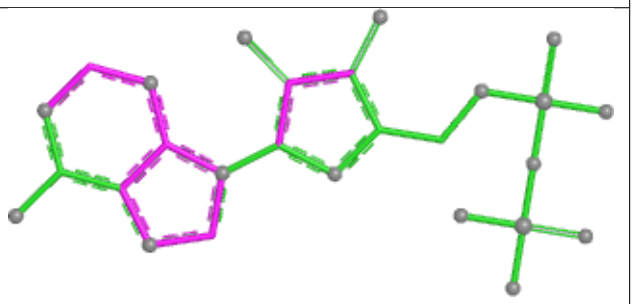


Rings

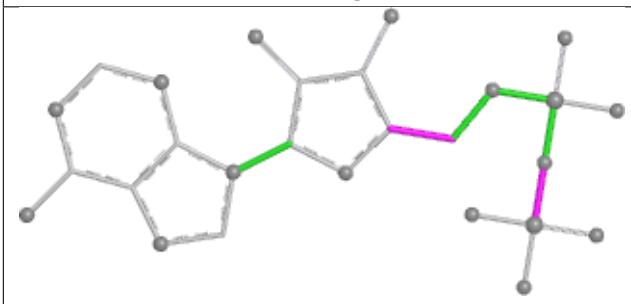
Ligand ADP K 403



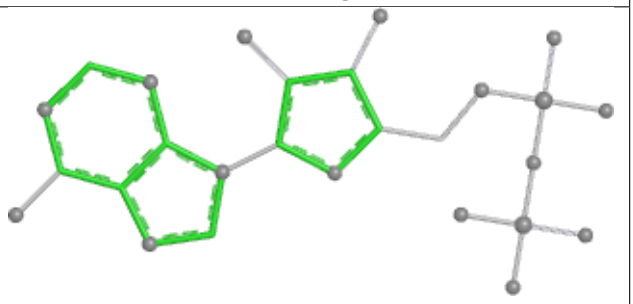
Bond lengths



Bond angles

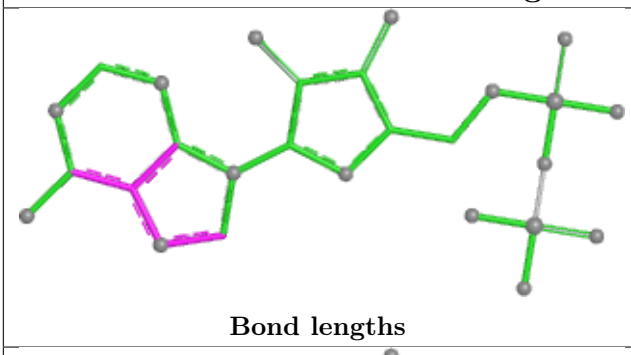


Torsions

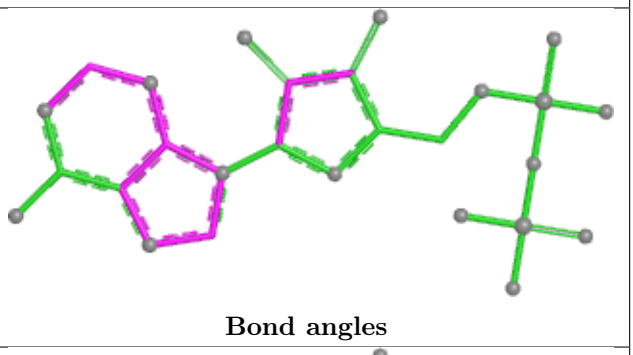


Rings

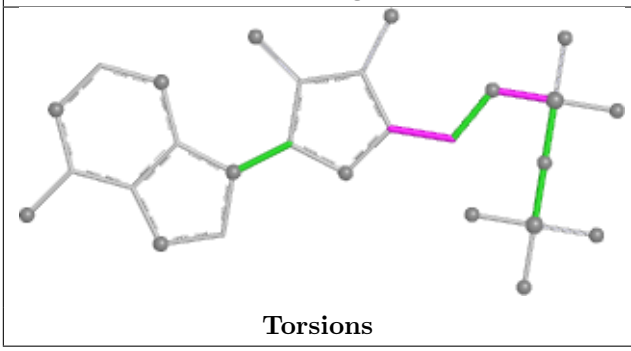
Ligand ADP L 403



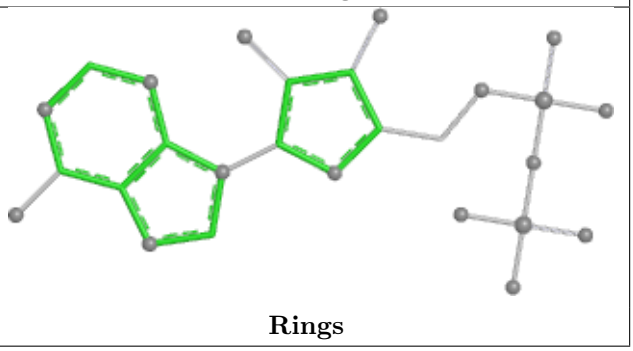
Bond lengths



Bond angles

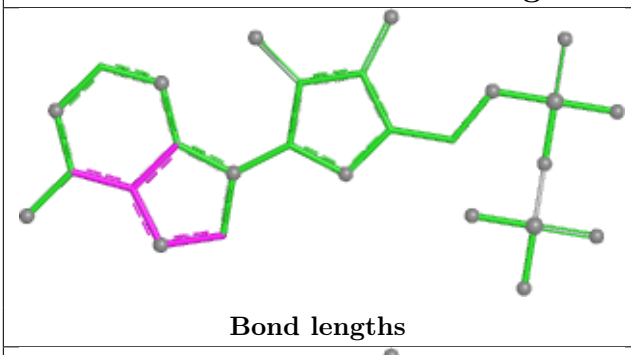


Torsions

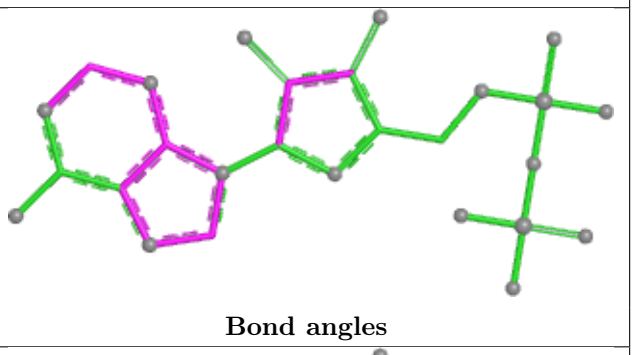


Rings

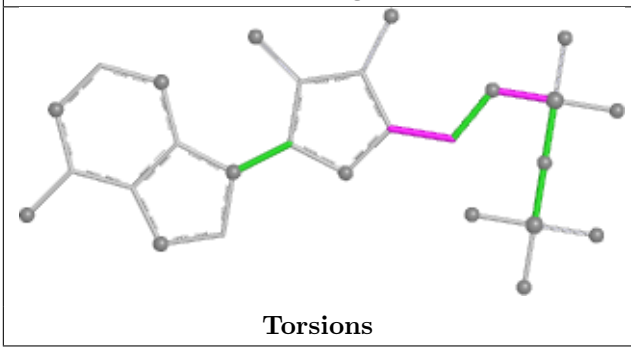
Ligand ADP E 401



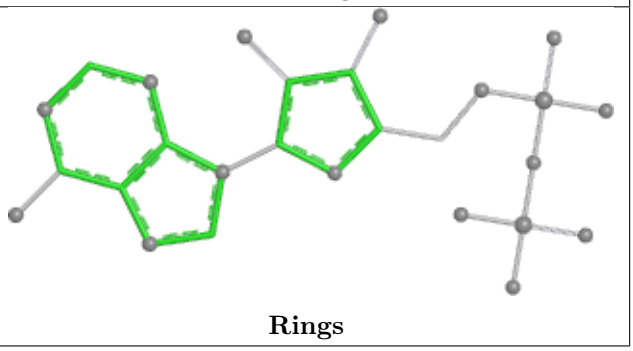
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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, 95^{th} 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	182/187 (97%)	-0.02	5 (2%) 56 35	84, 138, 167, 176	1 (0%)
1	Q	183/187 (97%)	-0.08	1 (0%) 87 73	119, 185, 203, 213	0
2	B	319/320 (99%)	-0.21	6 (1%) 66 45	59, 89, 109, 139	0
2	C	320/320 (100%)	-0.31	1 (0%) 90 80	53, 80, 142, 152	0
2	D	318/320 (99%)	-0.32	0 100 100	53, 86, 168, 191	0
2	E	318/320 (99%)	-0.05	15 (4%) 36 19	60, 119, 168, 188	0
2	K	319/320 (99%)	-0.11	6 (1%) 66 45	102, 138, 186, 199	0
2	L	320/320 (100%)	-0.15	6 (1%) 66 45	89, 116, 197, 206	0
2	M	317/320 (99%)	-0.17	3 (0%) 81 63	80, 119, 192, 202	0
2	N	305/320 (95%)	0.19	21 (6%) 23 12	92, 169, 219, 236	0
3	F	228/228 (100%)	-0.13	8 (3%) 47 27	110, 144, 189, 213	0
3	G	228/228 (100%)	-0.28	8 (3%) 47 27	75, 105, 128, 151	0
3	H	228/228 (100%)	-0.37	2 (0%) 81 63	92, 125, 172, 180	0
3	R	228/228 (100%)	-0.29	4 (1%) 67 47	131, 158, 174, 186	0
3	S	228/228 (100%)	-0.23	3 (1%) 75 56	124, 158, 181, 193	0
3	T	228/228 (100%)	-0.13	6 (2%) 57 36	144, 176, 190, 202	0
4	I	24/24 (100%)	-0.13	0 100 100	80, 160, 248, 304	0
4	O	24/24 (100%)	-0.21	0 100 100	106, 187, 271, 291	0
5	J	20/20 (100%)	-0.03	1 (5%) 34 18	86, 130, 310, 339	0
5	P	20/20 (100%)	0.35	1 (5%) 34 18	132, 214, 282, 306	0
All	All	4357/4390 (99%)	-0.16	97 (2%) 62 41	53, 131, 192, 339	1 (0%)

The worst 5 of 97 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	P	20	DA	7.3
2	E	268	LEU	5.7
2	N	109	PHE	5.6
2	N	268	LEU	5.4
2	E	269	ALA	5.4

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, 95^{th} 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
8	MG	N	402	1/1	0.70	0.17	140,140,140,140	0
8	MG	E	402	1/1	0.72	0.25	79,79,79,79	0
7	ADP	N	401	27/27	0.88	0.08	148,168,177,180	0
6	AF3	K	402	4/4	0.91	0.18	100,100,101,102	0
8	MG	M	401	1/1	0.92	0.20	84,84,84,84	0
6	AF3	L	402	4/4	0.92	0.11	85,85,86,87	0
6	AF3	B	901	4/4	0.95	0.13	66,67,68,68	0
6	AF3	D	402	4/4	0.95	0.12	52,56,62,70	0
6	AF3	M	402	4/4	0.95	0.17	83,84,84,85	0
7	ADP	B	902	27/27	0.95	0.09	69,71,75,76	0
7	ADP	K	403	27/27	0.96	0.08	103,115,122,124	0
7	ADP	M	403	27/27	0.96	0.09	87,96,107,116	0
6	AF3	C	402	4/4	0.96	0.10	54,55,55,55	0
8	MG	D	401	1/1	0.96	0.12	59,59,59,59	0
7	ADP	C	403	27/27	0.96	0.07	54,61,66,67	0
8	MG	K	401	1/1	0.96	0.18	96,96,96,96	0
7	ADP	D	403	27/27	0.96	0.08	56,66,74,80	0
7	ADP	E	401	27/27	0.96	0.06	84,102,106,113	0
8	MG	B	903	1/1	0.97	0.15	64,64,64,64	0

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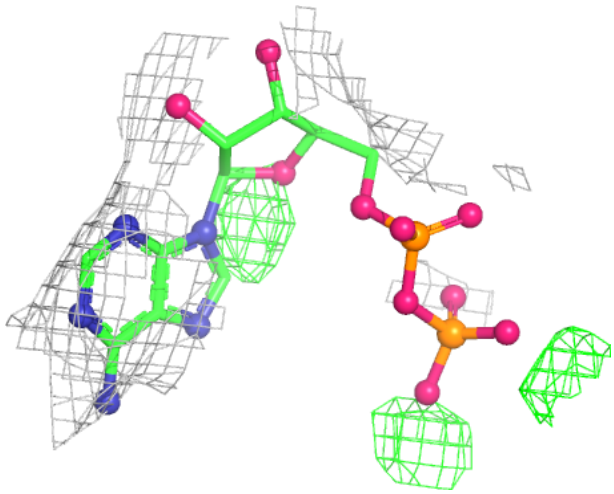
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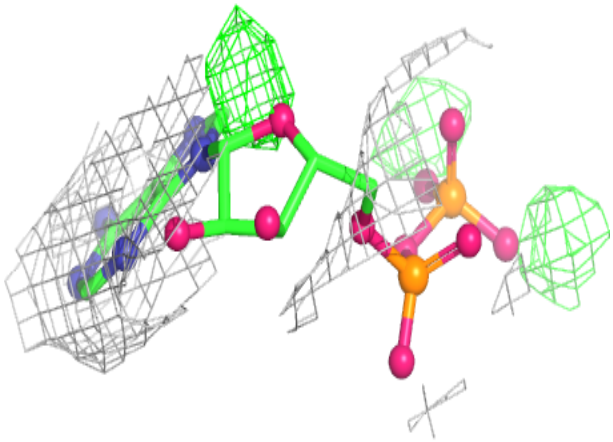
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	ADP	L	403	27/27	0.97	0.07	89,97,102,103	0
8	MG	C	401	1/1	0.98	0.15	48,48,48,48	0
8	MG	L	401	1/1	0.99	0.06	84,84,84,84	0

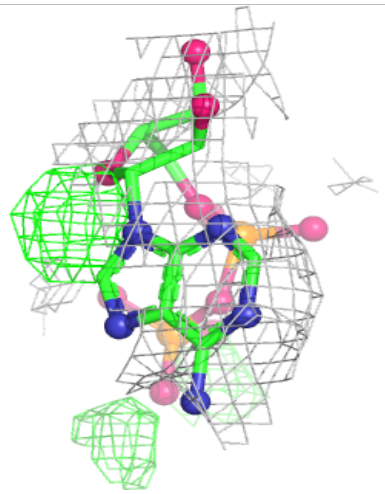
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP N 401:

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

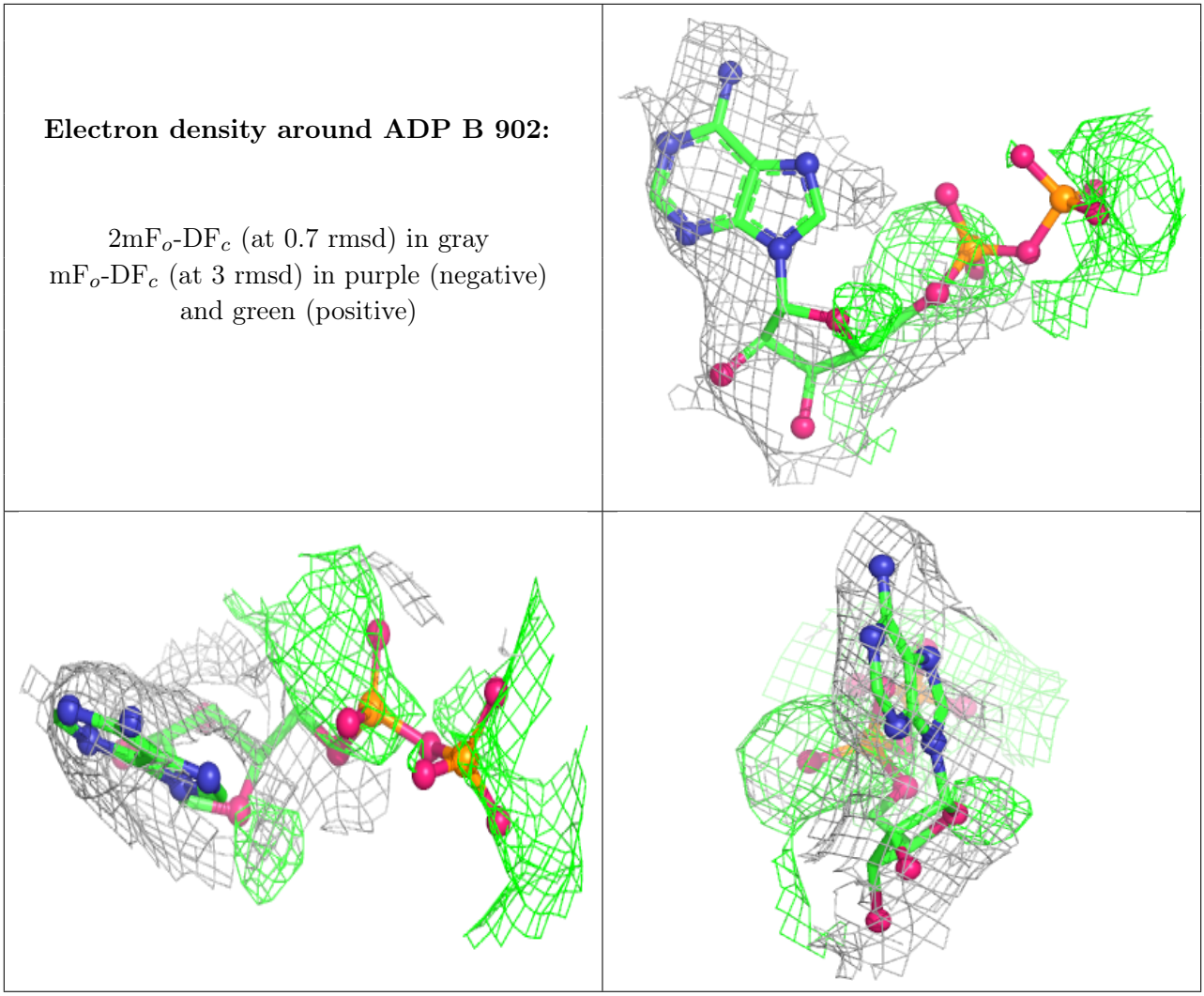






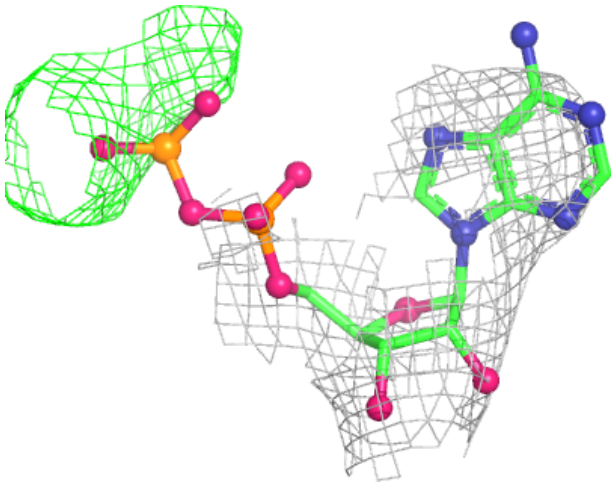
Electron density around ADP B 902:

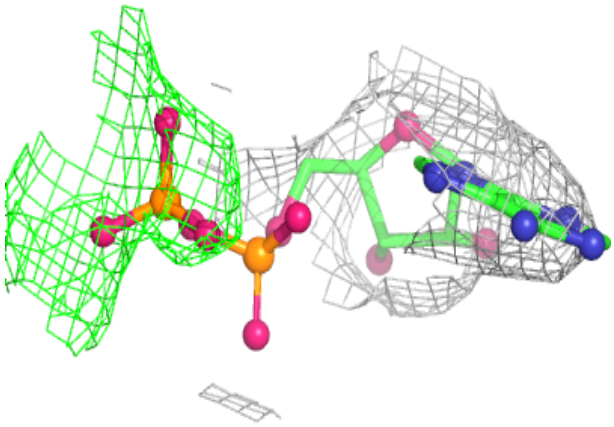
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

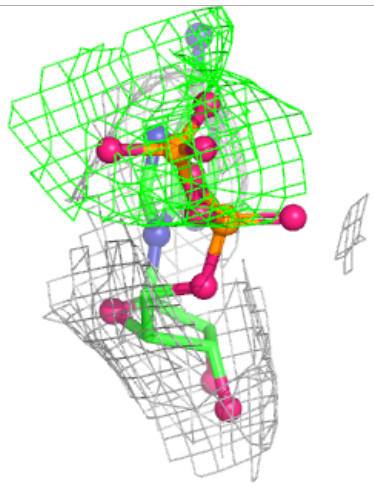


Electron density around ADP K 403:

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

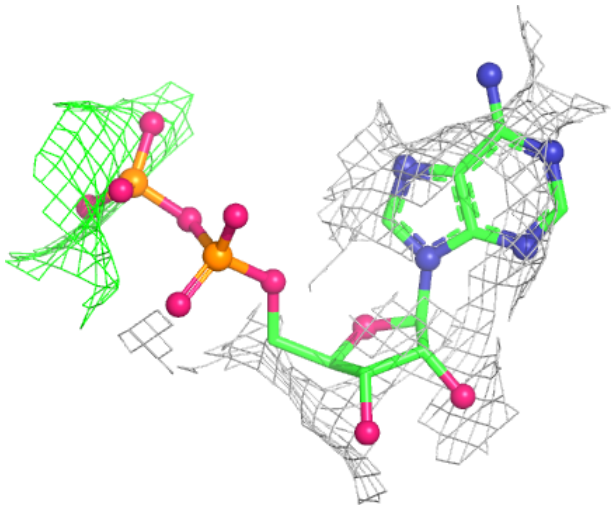


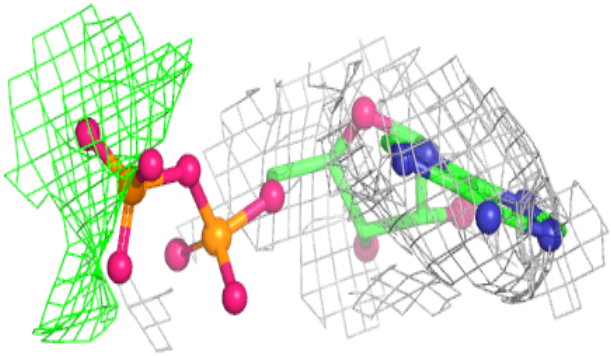


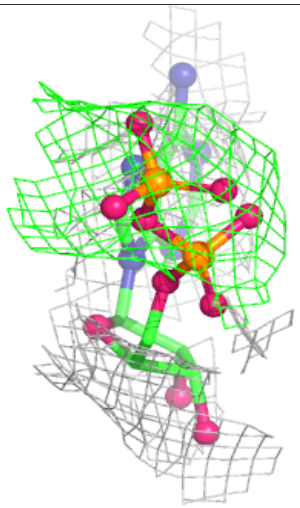


Electron density around ADP M 403:

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

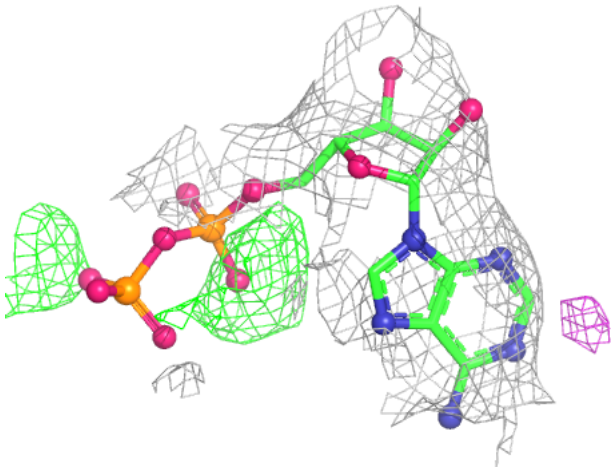


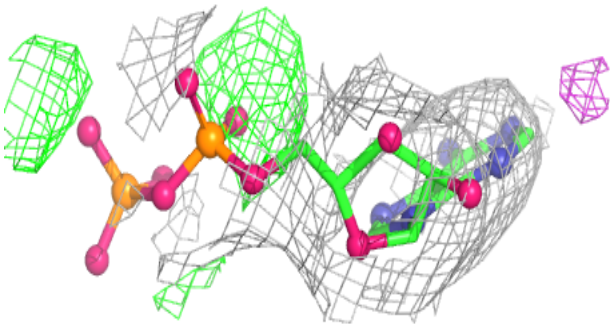


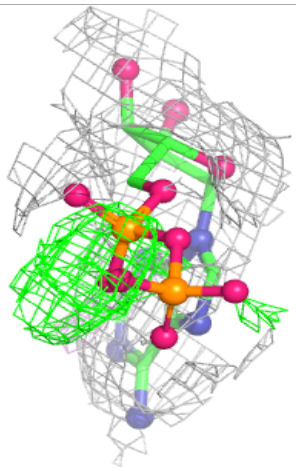


Electron density around ADP C 403:

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

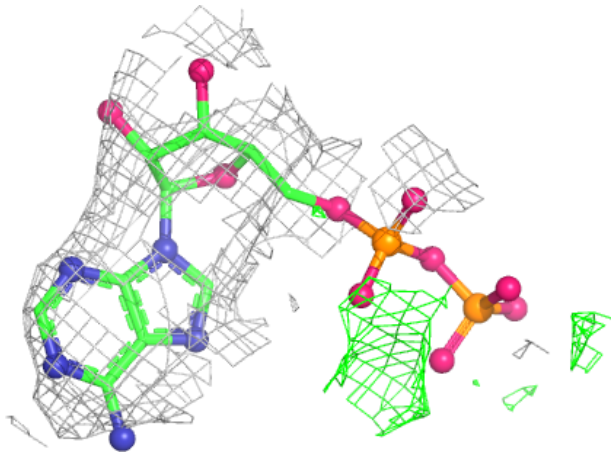


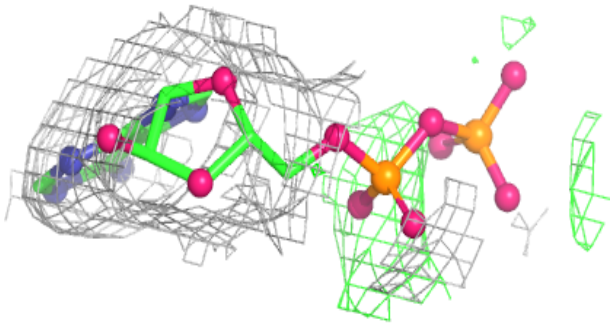


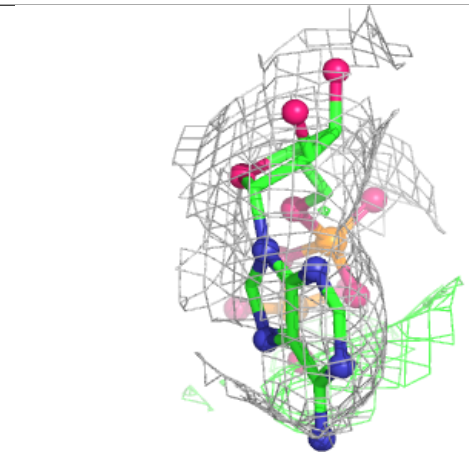


Electron density around ADP D 403:

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

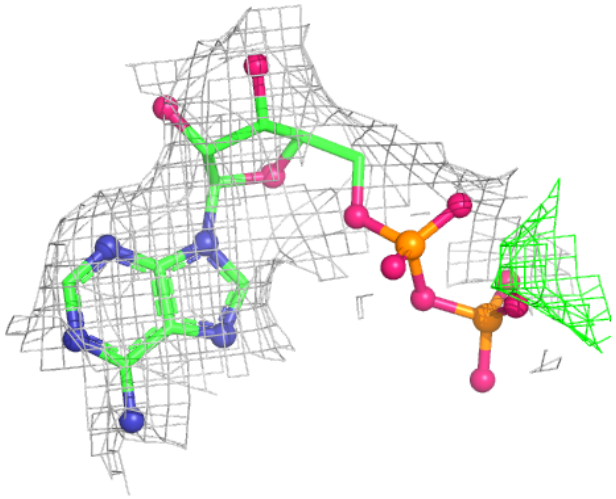


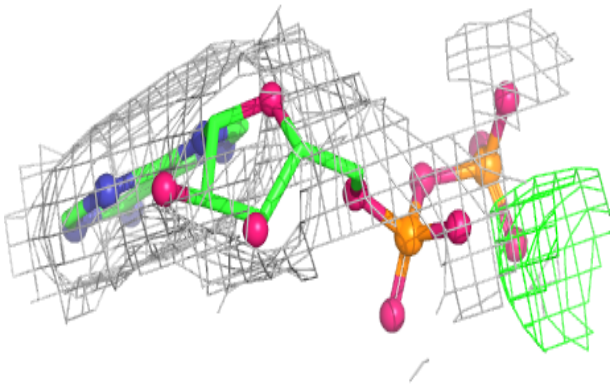


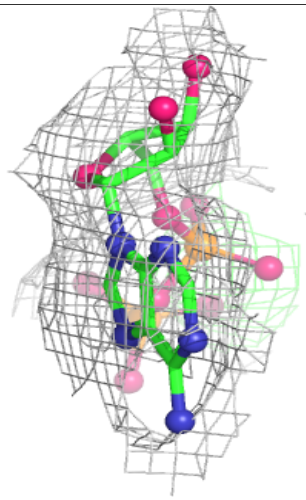


Electron density around ADP E 401:

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

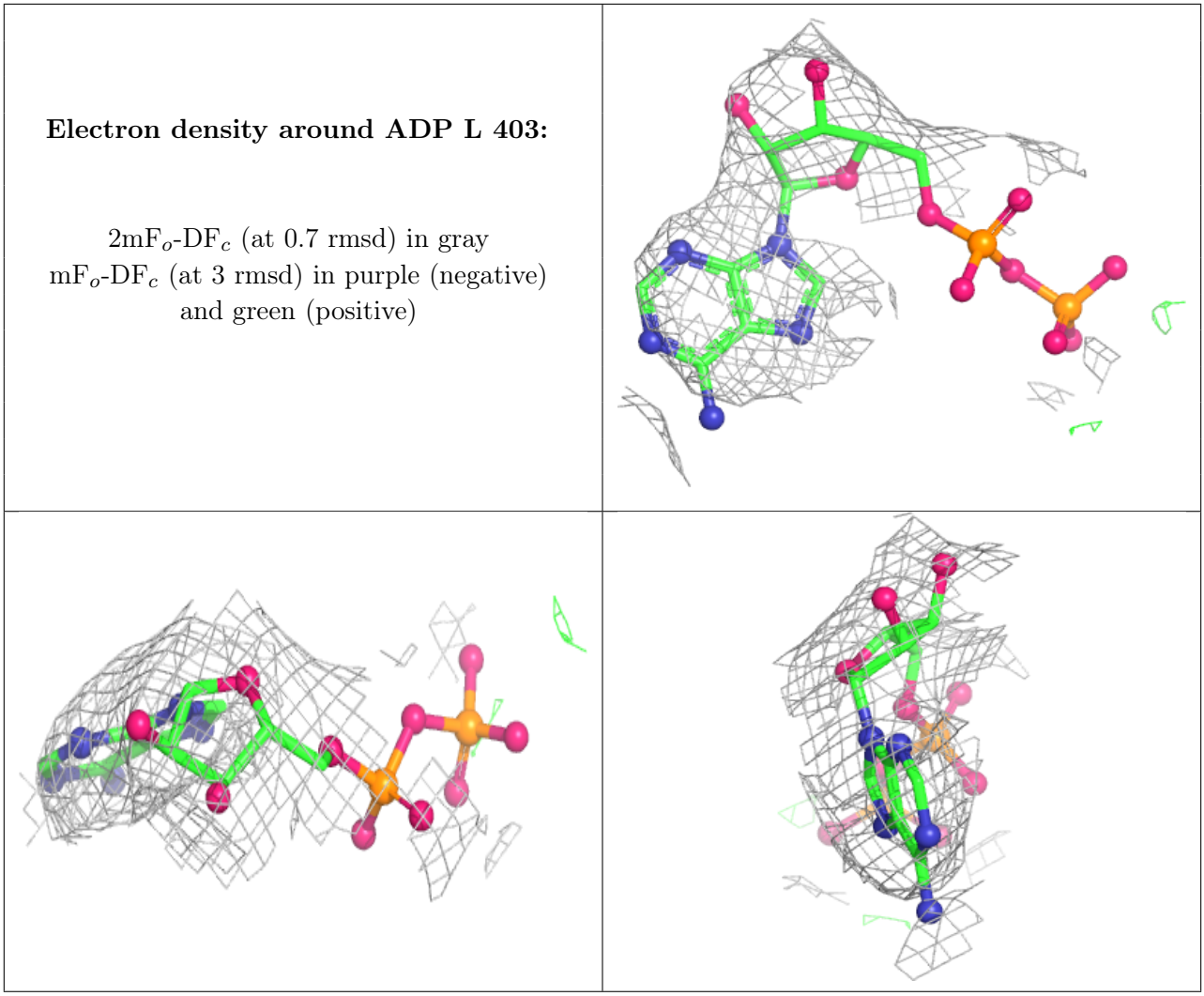






Electron density around ADP L 403:

$2mF_o$-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

There are no such residues in this entry.