wwPDB X-ray Structure Validation Summary Report (i)

Dec 13, 2023 – 09:57 pm GMT

PDB ID	:	2XJA
Title	:	Structure of MurE from M.tuberculosis with dipeptide and ADP
Authors	:	Basavannacharya, C.; Moody, P.R.; Bhakta, S.; Keep, N.
Deposited on	:	2010-07-03
Resolution	:	3.00 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:

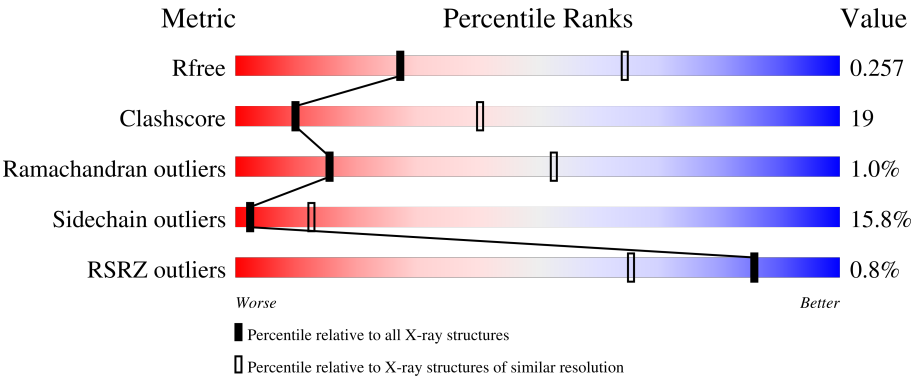
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	535	60% 29% 5% 6%
1	B	535	59% 29% 5% 7%
1	C	535	% 58% 30% • 7%
1	D	535	% 57% 29% 5% 9%

2 Entry composition (i)

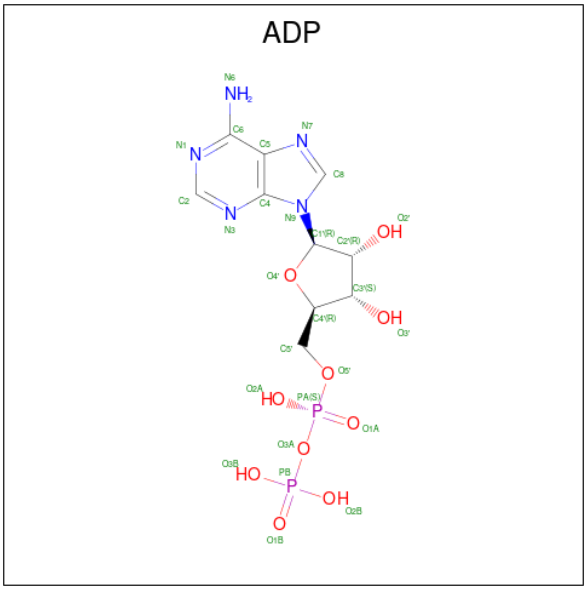
There are 5 unique types of molecules in this entry. The entry contains 14477 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-N-ACETYLMURAMOYL-L-ALANYL-D-GLUTAMATE--2,6-DIAMINOPIMELATE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	502	Total	C	N	O	S	0	0	0
			3567	2220	659	680	8			
1	B	500	Total	C	N	O	S	0	0	0
			3556	2211	660	677	8			
1	C	498	Total	C	N	O	S	0	0	0
			3538	2203	655	672	8			
1	D	488	Total	C	N	O	S	0	0	0
			3462	2159	633	662	8			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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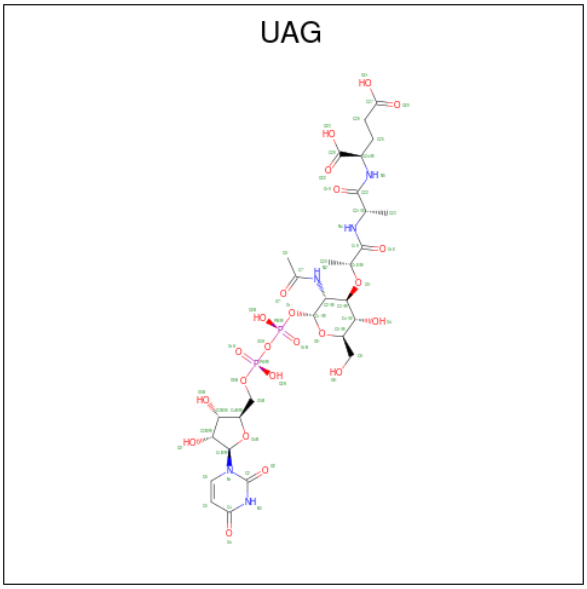
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	3	Total	Mg	0	0
			3	3		
3	C	2	Total	Mg	0	0
			2	2		
3	D	3	Total	Mg	0	0
			3	3		

- Molecule 4 is URIDINE-5'-DIPHOSPHATE-N-ACETYLMURAMOYL-L-ALANINE-D-GLUTAMATE (three-letter code: UAG) (formula: $C_{28}H_{43}N_5O_{23}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			58	28	5	23	2		
4	B	1	Total	C	N	O	P	0	0
			58	28	5	23	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			58	28	5	23	2		
4	D	1	Total	C	N	O	P	0	0
			58	28	5	23	2		

- Molecule 5 is water.

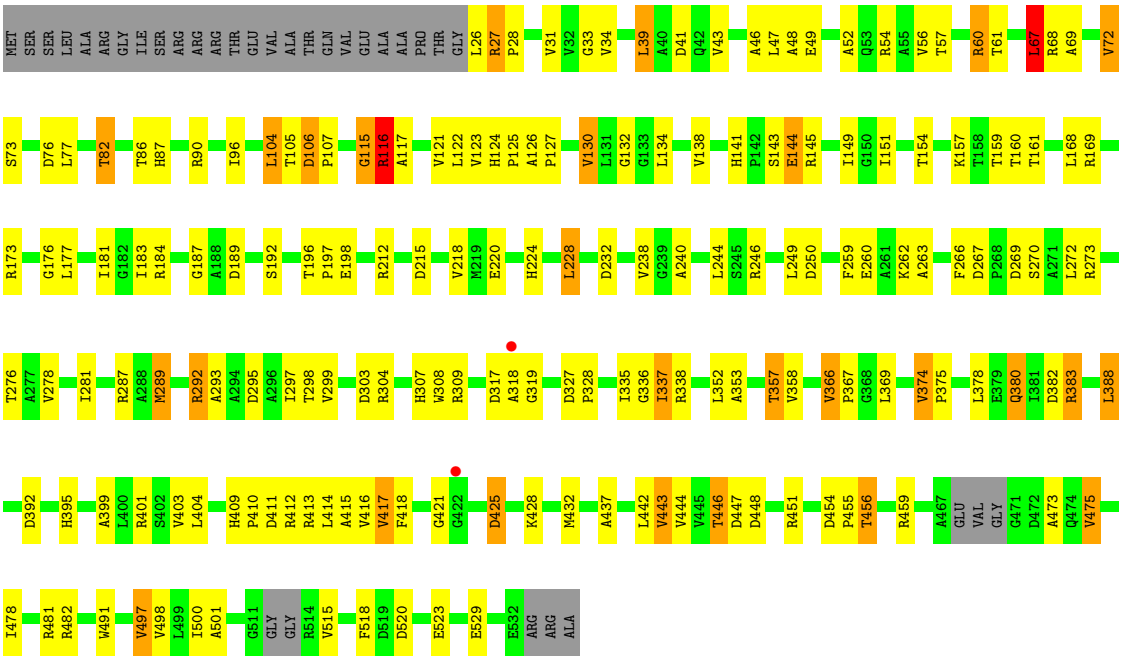
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	1	Total	O	0	0
			1	1		
5	C	1	Total	O	0	0
			1	1		
5	D	1	Total	O	0	0
			1	1		

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.

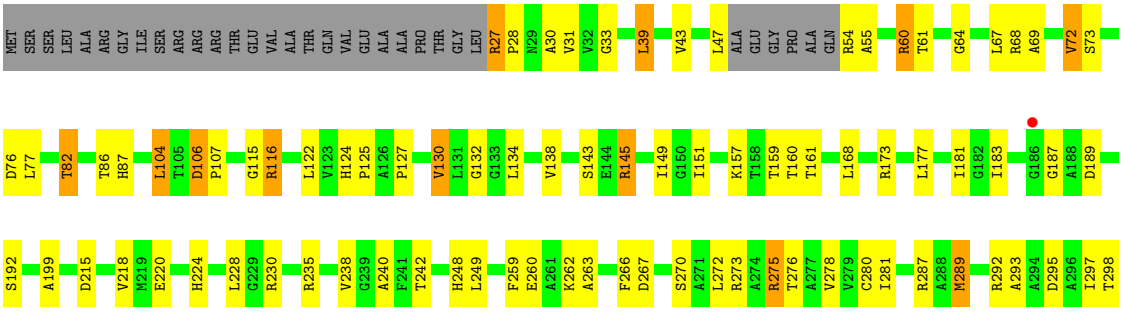
• Molecule 1: UDP-N-ACETYLMURAMOYL-L-ALANYL-D-GLUTAMATE--2,6-DIAMINOPIMELATE LIGASE

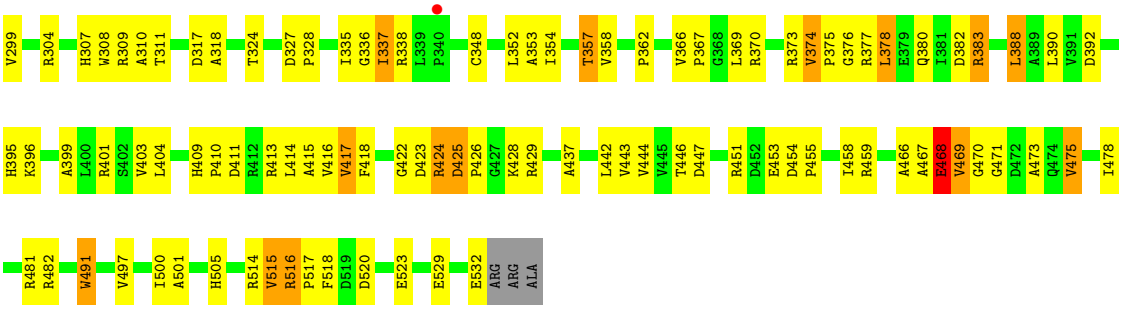
Chain A:



• Molecule 1: UDP-N-ACETYLMURAMOYL-L-ALANYL-D-GLUTAMATE--2,6-DIAMINOPIMELATE LIGASE

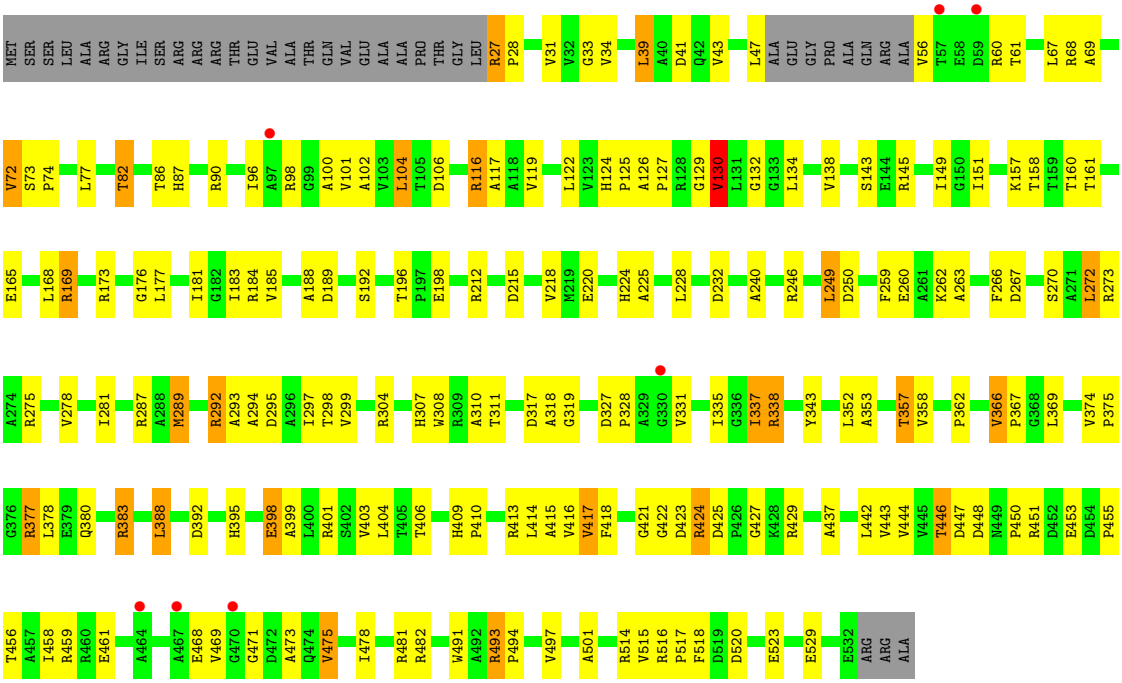
Chain B:





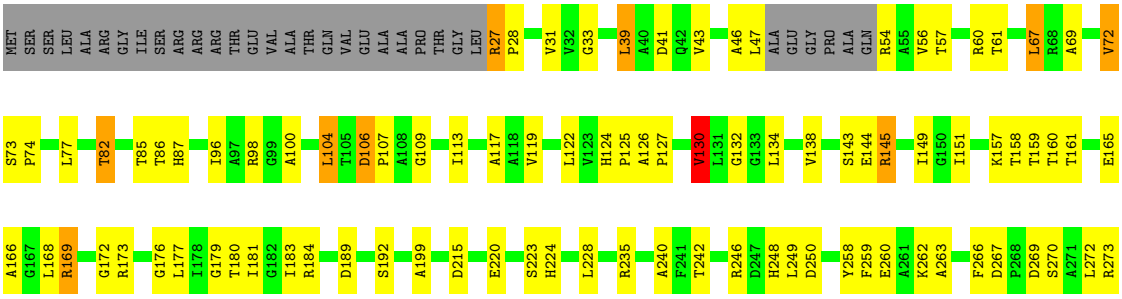
• Molecule 1: UDP-N-ACETYLMURAMOYL-L-ALANYL-D-GLUTAMATE--2,6-DIAMINOPIMELATE LIGASE

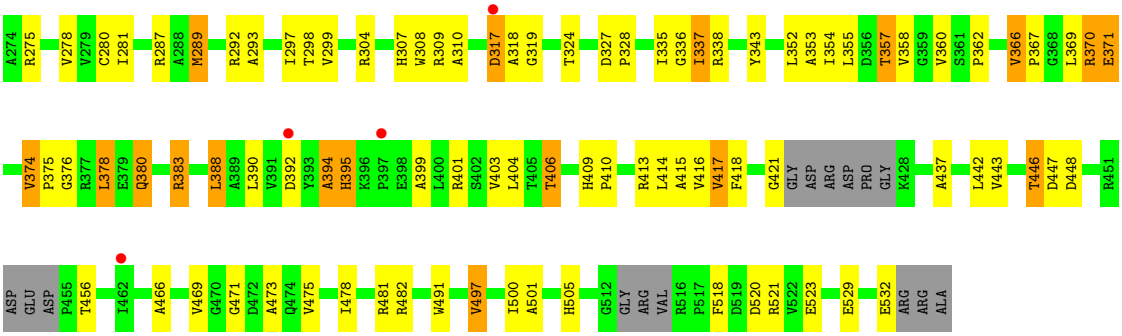
Chain C:



• Molecule 1: UDP-N-ACETYLMURAMOYL-L-ALANYL-D-GLUTAMATE--2,6-DIAMINOPIMELATE LIGASE

Chain D:




A274 R275 V278 V279 C280 I281 R287 A288 M289 R292 A293 I297 T298 V299 R304 H307 W308 R309 A310 D317 A318 G319 T324 D327 P328 I335 G336 I337 R338 Y343 L352 A353 I354 L355 D356 T357 V358 G359 V360 S361 P362 V366 P367 G368 L369 R370 E371
V374 P375 G376 R377 L378 E379 Q380 R383 L388 A389 L390 V391 D392 Y393 A394 H395 K396 P397 E398 A399 L400 R401 S402 V403 L404 T405 T406 H409 P410 R413 L414 A415 V416 V417 F418 G421 GLY ASP ARG ASP PRO GLY K428 A437 L442 V443 T446 D447 D448 R451
ASP GLU ASP P455 T456 I462 A466 V469 G470 G471 D472 A473 Q474 V475 I478 R481 R482 W491 V497 I500 A501 H505 G512 GLY ARG VAL R516 P517 F518 D519 D520 R521 V522 E523 E529 E532 ARG ARG ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	75.04Å 76.32Å 81.99Å 111.32° 91.42° 92.90°	Depositor
Resolution (Å)	76.30 – 3.00 74.86 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.9 (76.30-3.00) 95.9 (74.86-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0077	Depositor
R, R_{free}	0.189 , 0.258 0.189 , 0.257	Depositor DCC
R_{free} test set	1598 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	62.6	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 69.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14477	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: KCX, UAG, MG, ADP

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	0.69	0/3612	0.79	1/4939 (0.0%)
1	B	0.73	1/3601 (0.0%)	0.82	1/4921 (0.0%)
1	C	0.68	0/3583	0.78	2/4898 (0.0%)
1	D	0.69	0/3503	0.78	1/4787 (0.0%)
All	All	0.70	1/14299 (0.0%)	0.79	5/19545 (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
1	A	0	2
1	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	348	CYS	CB-SG	-7.75	1.69	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	67	LEU	CA-CB-CG	5.96	129.00	115.30
1	C	377	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	B	348	CYS	CA-CB-SG	-5.30	104.46	114.00
1	C	427	GLY	N-CA-C	5.20	126.10	113.10
1	D	67	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	GLY	Peptide
1	A	116	ARG	Peptide
1	C	116	ARG	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	3567	0	3524	144	1
1	B	3556	0	3520	144	0
1	C	3538	0	3504	144	0
1	D	3462	0	3424	141	1
2	A	27	0	12	1	0
2	B	27	0	12	2	0
2	C	27	0	12	5	0
2	D	27	0	12	5	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
4	A	58	0	39	5	0
4	B	58	0	39	4	0
4	C	58	0	39	2	0
4	D	58	0	39	7	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	14477	0	14176	547	1

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 19.

The worst 5 of 547 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)
1:A:383:ARG:HG3	1:A:383:ARG:HH11	1.14	1.07
1:C:424:ARG:HG3	1:C:424:ARG:HH11	1.16	1.07
1:A:116:ARG:HG2	1:A:116:ARG:NH1	1.60	1.04
1:D:383:ARG:HG3	1:D:383:ARG:HH11	1.24	1.02
1:B:383:ARG:HG3	1:B:383:ARG:HH11	1.23	1.02

All (1) 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)
1:A:269:ASP:O	1:D:269:ASP:O[1_554]	2.10	0.10

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	495/535 (92%)	453 (92%)	39 (8%)	3 (1%)	25	64
1	B	495/535 (92%)	442 (89%)	46 (9%)	7 (1%)	11	43
1	C	493/535 (92%)	448 (91%)	39 (8%)	6 (1%)	13	48
1	D	477/535 (89%)	439 (92%)	35 (7%)	3 (1%)	25	64
All	All	1960/2140 (92%)	1782 (91%)	159 (8%)	19 (1%)	15	53

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	423	ASP
1	B	469	VAL
1	C	116	ARG
1	B	468	GLU
1	B	514	ARG

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	341/382 (89%)	285 (84%)	56 (16%)	2 11
1	B	340/382 (89%)	290 (85%)	50 (15%)	3 15
1	C	338/382 (88%)	283 (84%)	55 (16%)	2 11
1	D	332/382 (87%)	279 (84%)	53 (16%)	2 12
All	All	1351/1528 (88%)	1137 (84%)	214 (16%)	2 12

5 of 214 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	77	LEU
1	C	395	HIS
1	D	388	LEU
1	C	138	VAL
1	C	272	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	380	GLN
1	D	307	HIS
1	C	307	HIS
1	C	409	HIS
1	B	409	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	$\#\|Z\| > 2$
1	KCX	D	262	1	9,11,12	1.19	1 (11%)	5,12,14	1.43	1 (20%)
1	KCX	C	262	1	9,11,12	1.18	1 (11%)	5,12,14	1.92	1 (20%)
1	KCX	A	262	1	9,11,12	1.28	1 (11%)	5,12,14	1.34	1 (20%)
1	KCX	B	262	1	9,11,12	1.00	1 (11%)	5,12,14	1.96	2 (40%)

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
1	KCX	D	262	1	-	0/9/10/12	-
1	KCX	C	262	1	-	0/9/10/12	-
1	KCX	A	262	1	-	1/9/10/12	-
1	KCX	B	262	1	-	1/9/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	262	KCX	CE-NZ	2.65	1.52	1.46
1	C	262	KCX	OQ1-CX	2.59	1.26	1.21
1	B	262	KCX	OQ1-CX	2.36	1.26	1.21
1	D	262	KCX	CE-NZ	2.13	1.51	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	262	KCX	OQ1-CX-NZ	-4.10	118.61	124.96
1	B	262	KCX	OQ1-CX-NZ	-3.53	119.48	124.96
1	A	262	KCX	OQ1-CX-NZ	-2.67	120.82	124.96
1	B	262	KCX	CE-NZ-CX	-2.37	118.09	121.89
1	D	262	KCX	OQ1-CX-NZ	-2.28	121.42	124.96

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	262	KCX	CG-CD-CE-NZ
1	A	262	KCX	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
2	ADP	C	1533	3	24,29,29	1.15	3 (12%)	29,45,45	1.25	2 (6%)
2	ADP	A	1533	3	24,29,29	1.11	2 (8%)	29,45,45	1.50	6 (20%)
4	UAG	C	1535	3	57,60,60	1.28	4 (7%)	80,88,88	2.18	23 (28%)
4	UAG	B	1536	3	57,60,60	1.19	4 (7%)	80,88,88	2.68	28 (35%)
2	ADP	B	1534	3	24,29,29	1.20	2 (8%)	29,45,45	1.98	8 (27%)
4	UAG	A	1536	3	57,60,60	1.47	6 (10%)	80,88,88	2.80	32 (40%)
4	UAG	D	1536	3	57,60,60	1.19	4 (7%)	80,88,88	2.34	24 (30%)
2	ADP	D	1534	3	24,29,29	1.10	2 (8%)	29,45,45	1.81	9 (31%)

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	ADP	C	1533	3	-	2/12/32/32	0/3/3/3
2	ADP	A	1533	3	-	3/12/32/32	0/3/3/3
4	UAG	C	1535	3	-	9/55/92/92	0/3/3/3
4	UAG	B	1536	3	-	11/55/92/92	0/3/3/3
2	ADP	B	1534	3	-	7/12/32/32	0/3/3/3
4	UAG	A	1536	3	-	8/55/92/92	0/3/3/3
4	UAG	D	1536	3	-	22/55/92/92	0/3/3/3
2	ADP	D	1534	3	-	3/12/32/32	0/3/3/3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1536	UAG	PB-O1B	4.67	1.67	1.50
4	A	1536	UAG	PA-O1A	4.32	1.66	1.50
4	C	1535	UAG	C26-C27	3.69	1.59	1.50
4	D	1536	UAG	C2-N1	3.41	1.43	1.38
4	A	1536	UAG	C26-C27	3.11	1.57	1.50

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1536	UAG	O3A-PB-O1'	-12.06	78.17	102.48
4	A	1536	UAG	O3A-PB-O1'	-11.11	80.08	102.48
4	C	1535	UAG	O3A-PB-O1'	-9.40	83.52	102.48
4	A	1536	UAG	O5'-C1'-O1'	-8.59	100.14	111.36
4	B	1536	UAG	O5'-C1'-O1'	-8.02	100.89	111.36

There are no chirality outliers.

5 of 65 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1533	ADP	C5'-O5'-PA-O2A
2	B	1534	ADP	C5'-O5'-PA-O1A
2	B	1534	ADP	C5'-O5'-PA-O2A
2	B	1534	ADP	O4'-C4'-C5'-O5'
2	D	1534	ADP	PA-O3A-PB-O2B

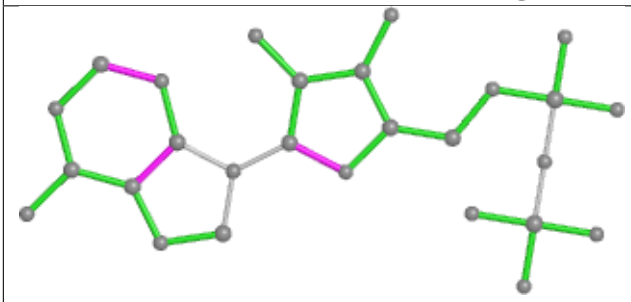
There are no ring outliers.

8 monomers are involved in 31 short contacts:

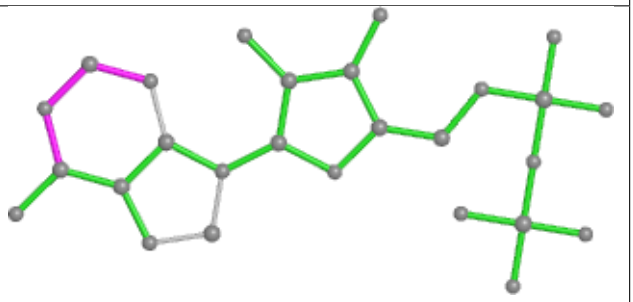
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1533	ADP	5	0
2	A	1533	ADP	1	0
4	C	1535	UAG	2	0
4	B	1536	UAG	4	0
2	B	1534	ADP	2	0
4	A	1536	UAG	5	0
4	D	1536	UAG	7	0
2	D	1534	ADP	5	0

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.

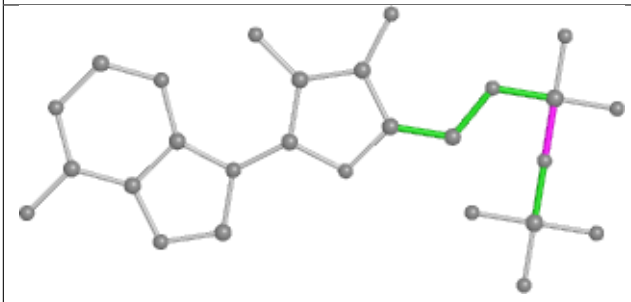
Ligand ADP C 1533



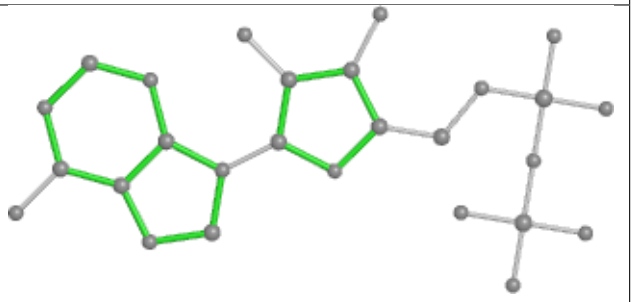
Bond lengths



Bond angles

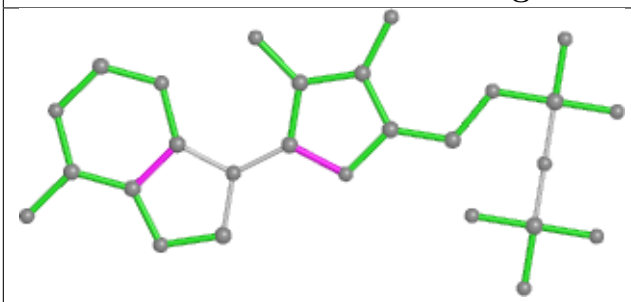


Torsions

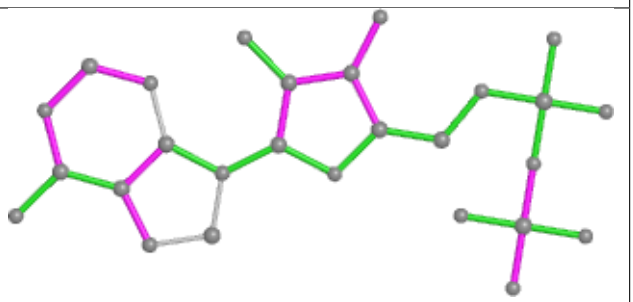


Rings

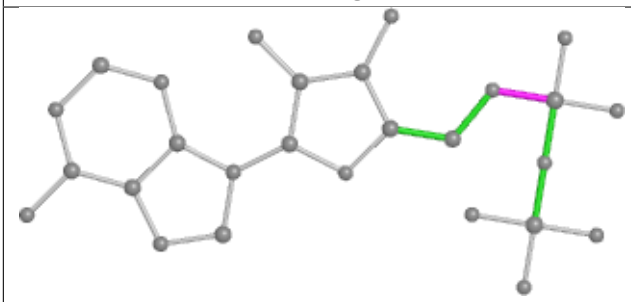
Ligand ADP A 1533



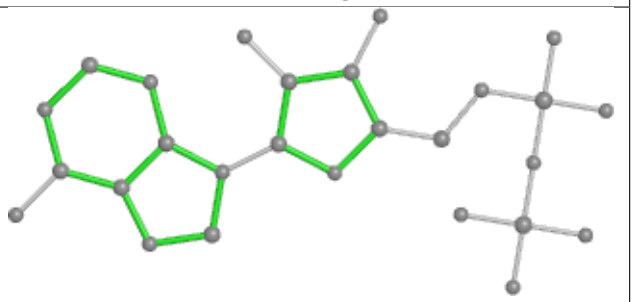
Bond lengths



Bond angles

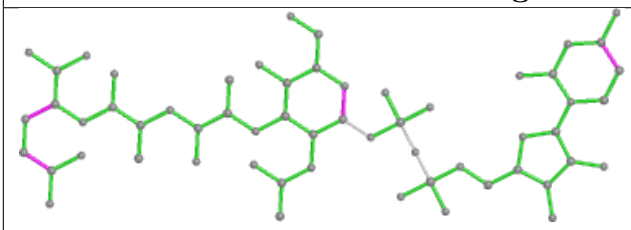


Torsions

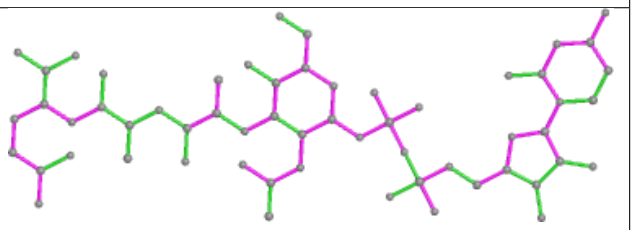


Rings

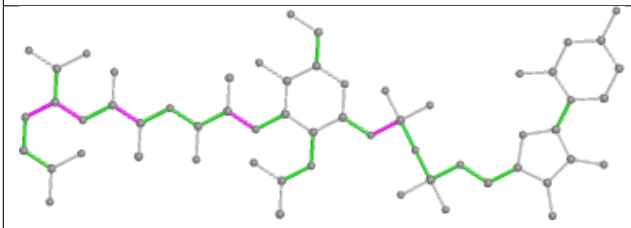
Ligand UAG C 1535



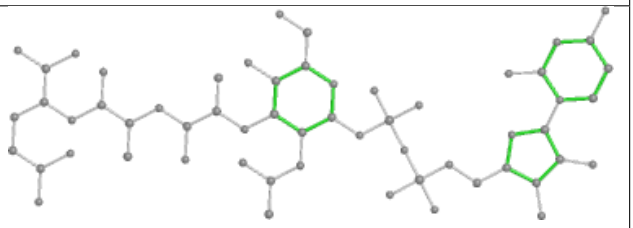
Bond lengths



Bond angles

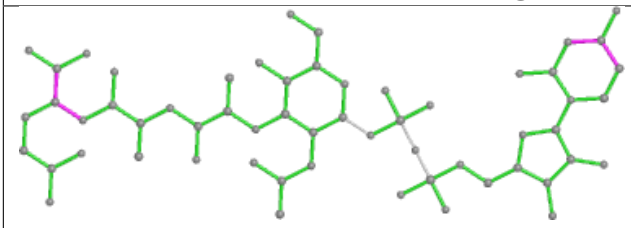


Torsions

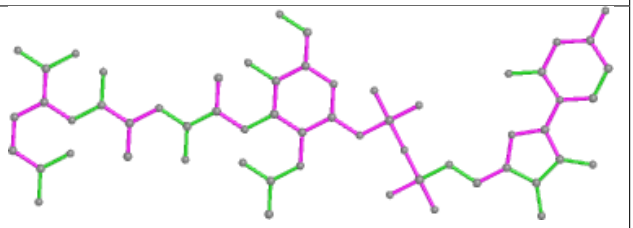


Rings

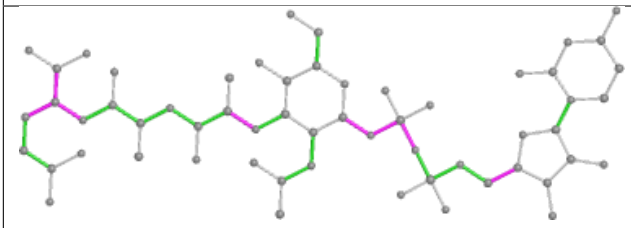
Ligand UAG B 1536



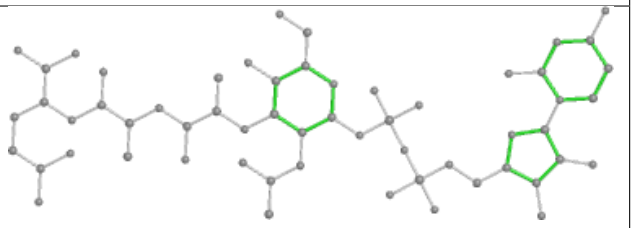
Bond lengths



Bond angles

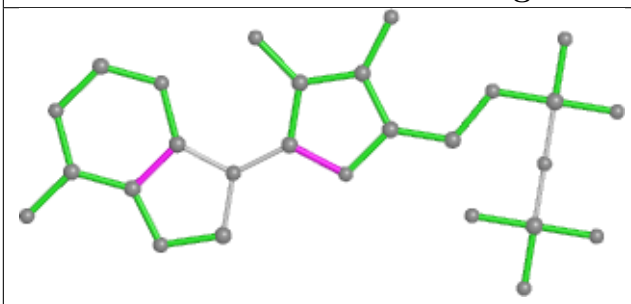


Torsions

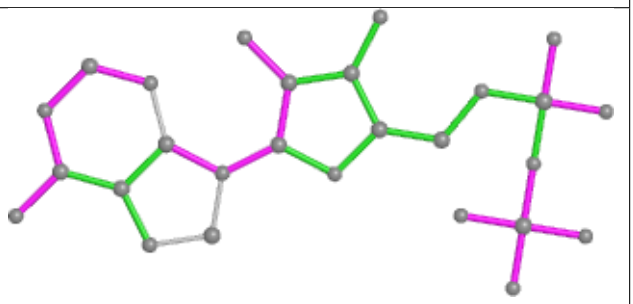


Rings

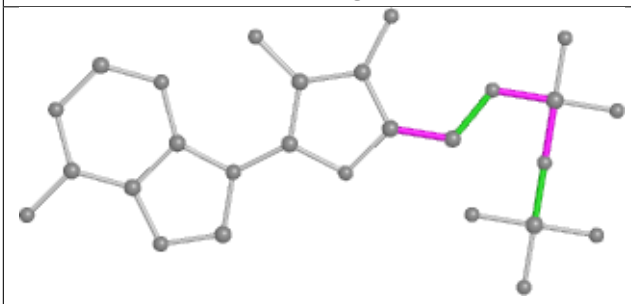
Ligand ADP B 1534



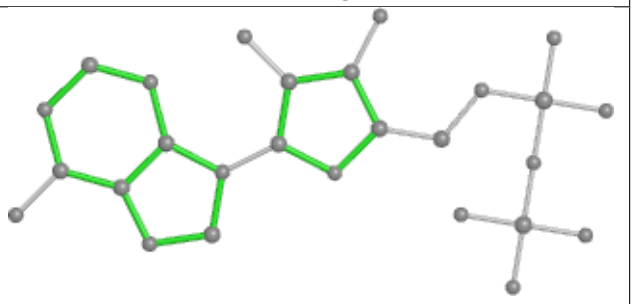
Bond lengths



Bond angles

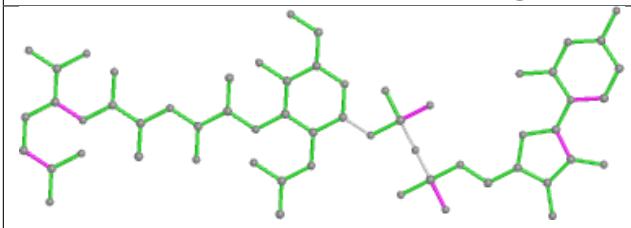


Torsions

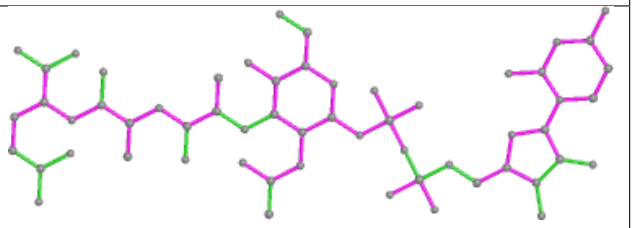


Rings

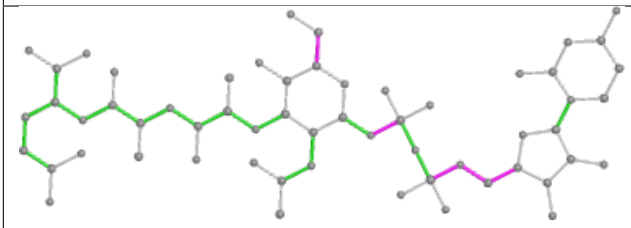
Ligand UAG A 1536



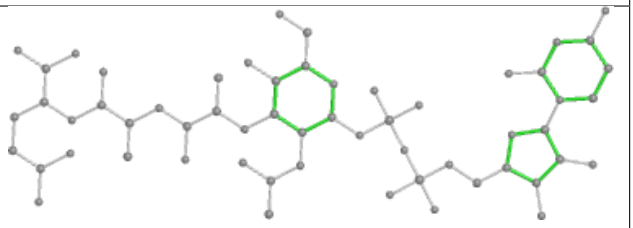
Bond lengths



Bond angles

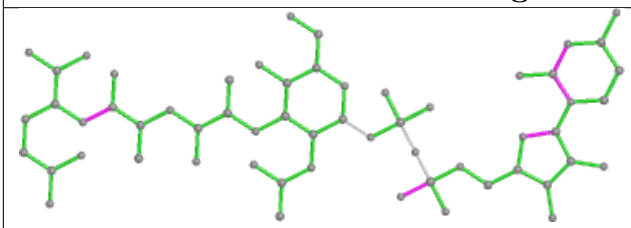


Torsions

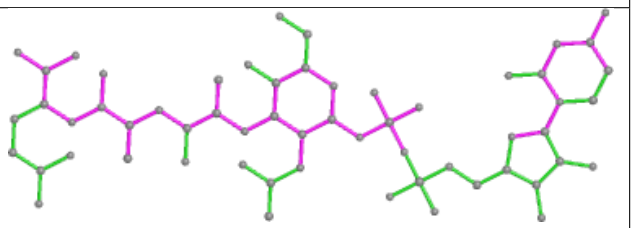


Rings

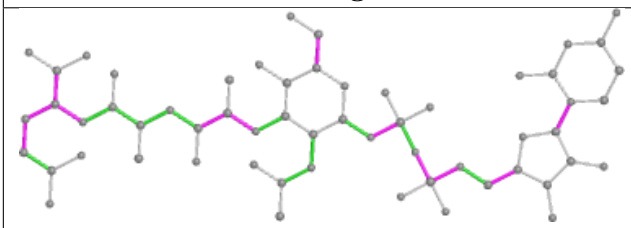
Ligand UAG D 1536



Bond lengths



Bond angles



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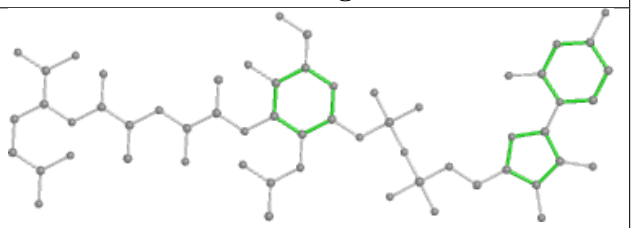
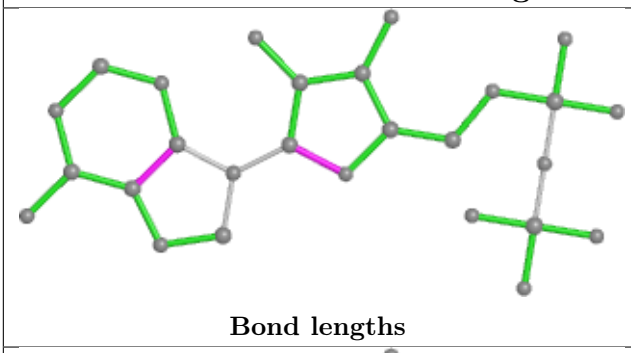
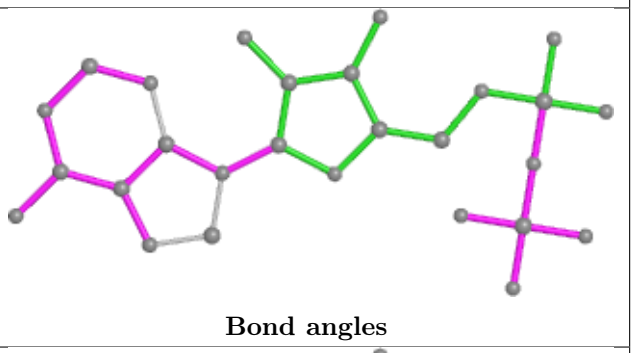


Rings

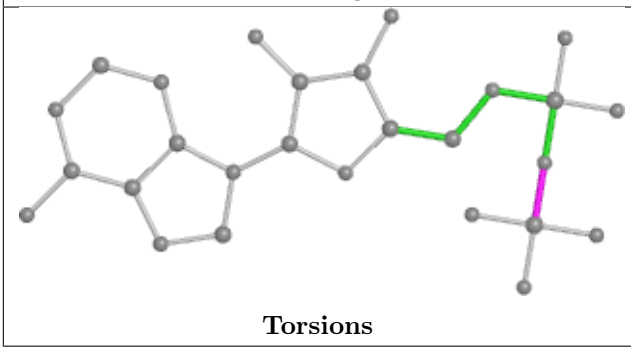
Ligand ADP D 1534



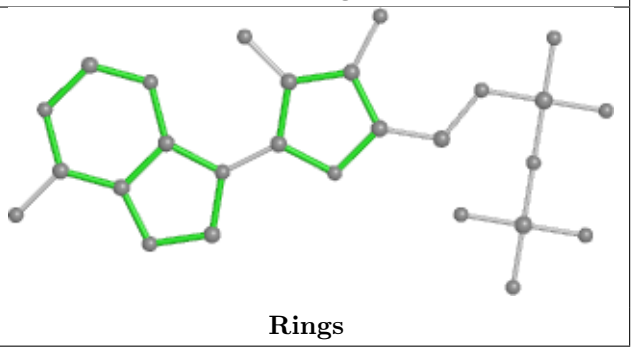
Bond lengths



Bond angles



Torsions



Rings

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, 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	501/535 (93%)	-0.11	2 (0%)	92	79	25, 58, 104, 128	0
1	B	499/535 (93%)	-0.22	2 (0%)	92	79	24, 53, 99, 118	0
1	C	497/535 (92%)	-0.12	7 (1%)	75	49	30, 65, 103, 137	0
1	D	487/535 (91%)	-0.17	4 (0%)	86	65	29, 60, 115, 155	0
All	All	1984/2140 (92%)	-0.15	15 (0%)	86	65	24, 59, 105, 155	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	470	GLY	5.1
1	B	186	GLY	3.8
1	D	392	ASP	3.3
1	C	57	THR	3.2
1	C	59	ASP	3.2

6.2 Non-standard residues in protein, DNA, RNA chains

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
1	KCX	D	262	12/13	0.97	0.17	33,36,42,43	0
1	KCX	B	262	12/13	0.98	0.15	29,32,37,41	0
1	KCX	C	262	12/13	0.98	0.17	35,36,43,45	0
1	KCX	A	262	12/13	0.98	0.18	33,36,39,39	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

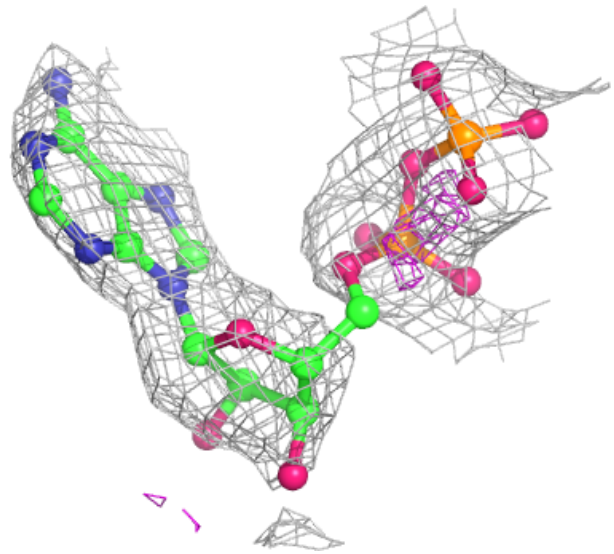
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

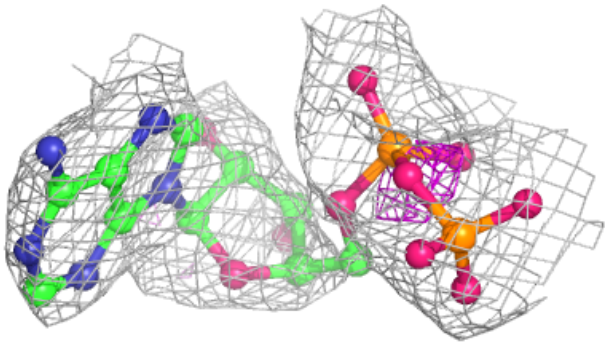
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	1535	1/1	0.69	0.20	37,37,37,37	0
3	MG	C	1536	1/1	0.89	0.19	43,43,43,43	0
2	ADP	A	1533	27/27	0.93	0.27	56,84,93,95	0
3	MG	D	1533	1/1	0.93	0.18	50,50,50,50	0
3	MG	A	1534	1/1	0.94	0.07	48,48,48,48	0
4	UAG	D	1536	58/58	0.94	0.17	48,56,69,74	0
3	MG	B	1533	1/1	0.95	0.30	30,30,30,30	0
3	MG	B	1535	1/1	0.95	0.07	46,46,46,46	0
3	MG	D	1537	1/1	0.95	0.32	53,53,53,53	0
4	UAG	A	1536	58/58	0.95	0.17	36,45,53,62	0
4	UAG	C	1535	58/58	0.95	0.17	44,54,69,74	0
3	MG	B	1537	1/1	0.95	0.18	39,39,39,39	0
4	UAG	B	1536	58/58	0.96	0.16	39,45,52,53	0
2	ADP	B	1534	27/27	0.96	0.17	41,60,69,71	0
3	MG	D	1535	1/1	0.96	0.07	51,51,51,51	0
2	ADP	D	1534	27/27	0.97	0.16	46,55,64,72	0
2	ADP	C	1533	27/27	0.97	0.17	49,59,65,72	0
3	MG	C	1534	1/1	0.99	0.05	60,60,60,60	0

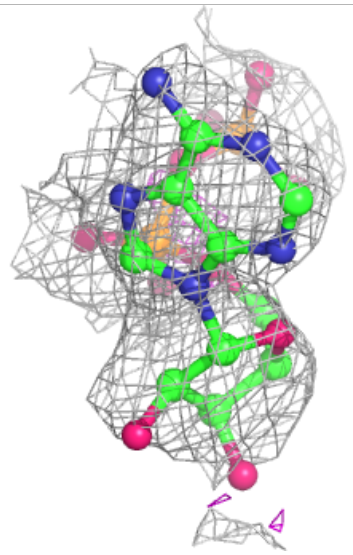
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 1533:

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

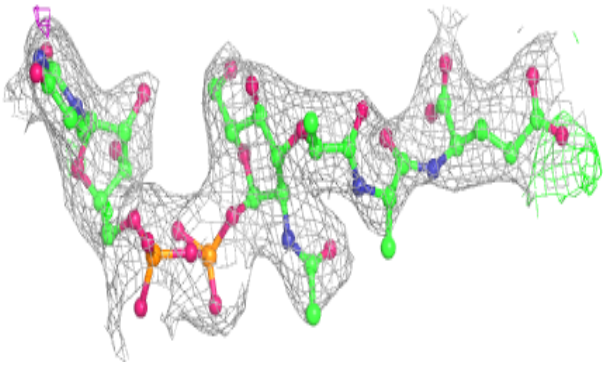


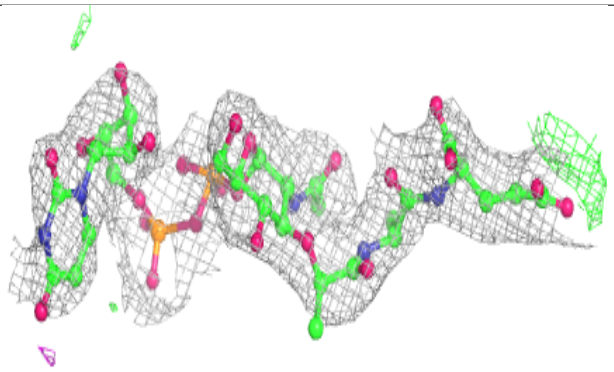


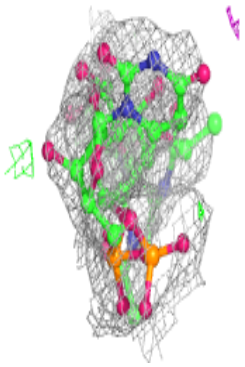


Electron density around UAG D 1536:

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

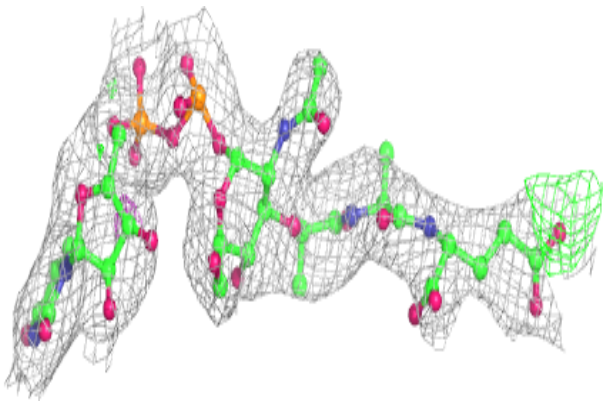


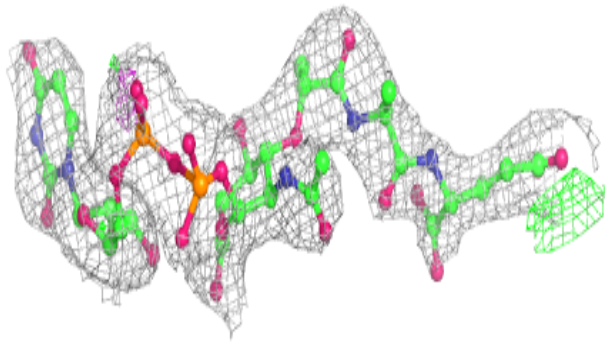


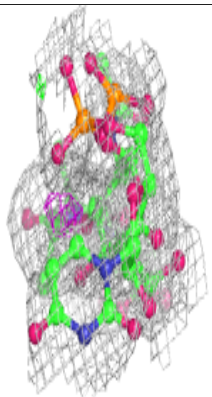


Electron density around UAG A 1536:

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

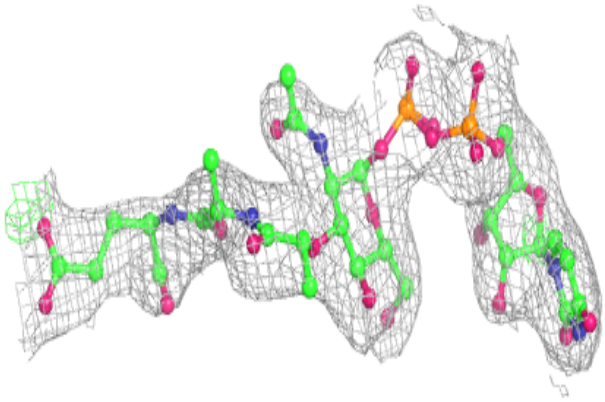


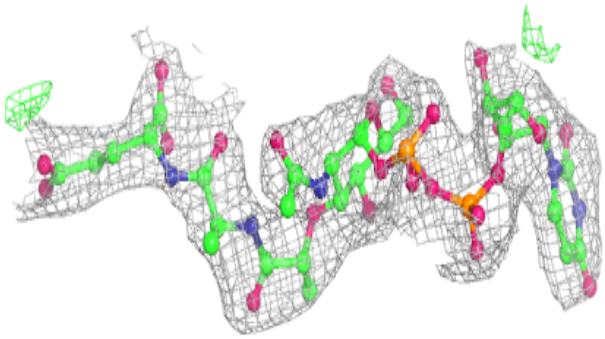


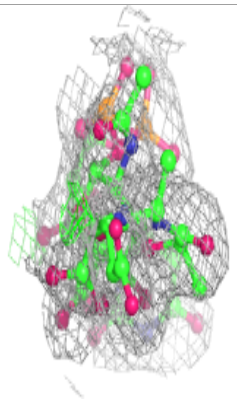


Electron density around UAG C 1535:

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

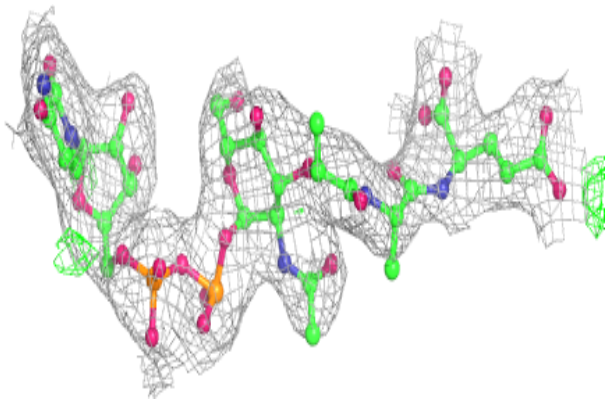


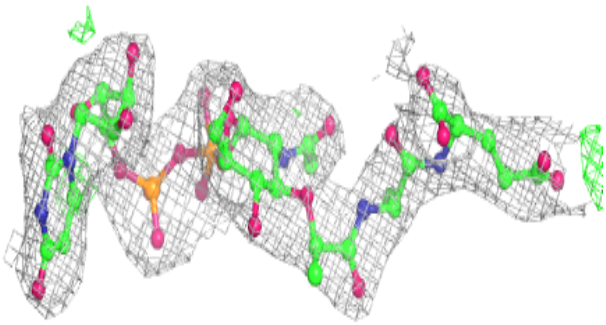


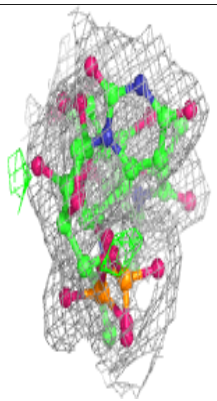


Electron density around UAG B 1536:

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

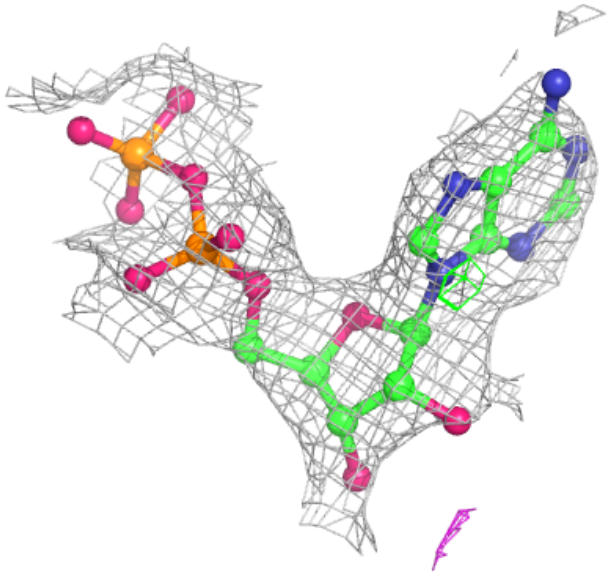


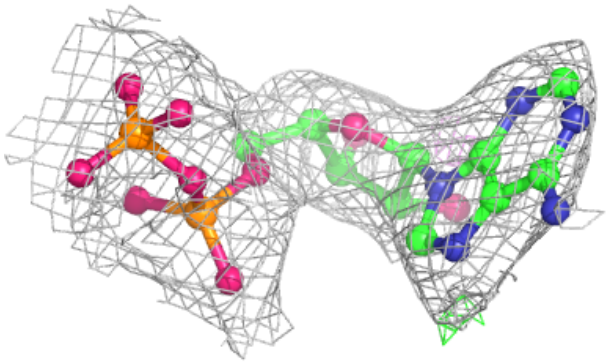


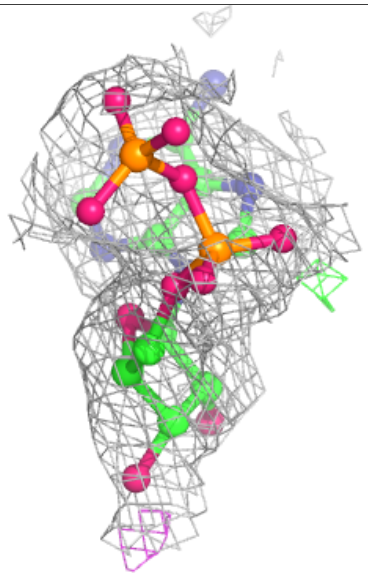


Electron density around ADP B 1534:

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

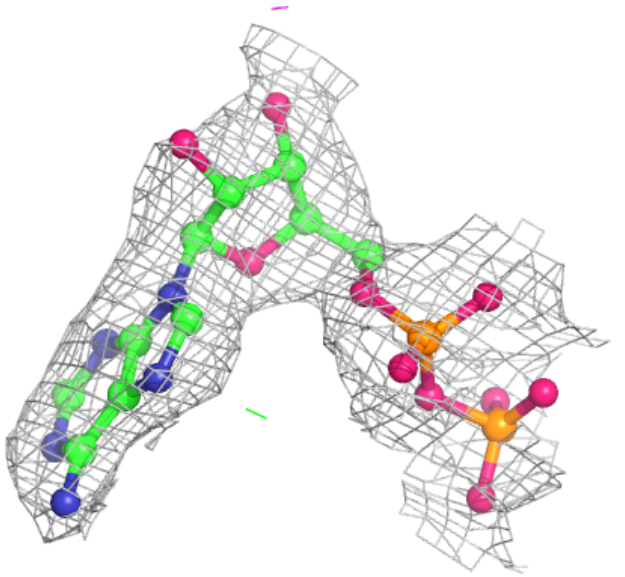


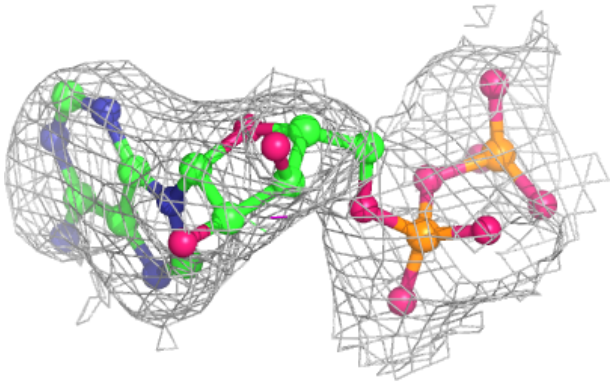


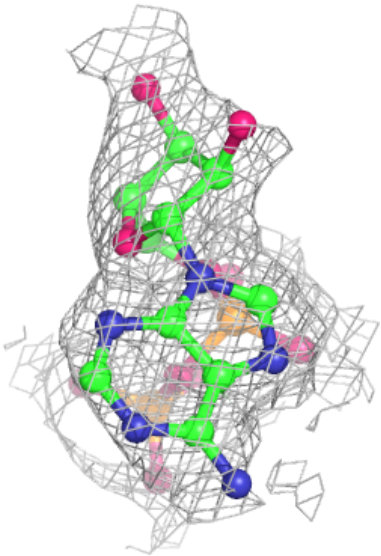


Electron density around ADP D 1534:

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

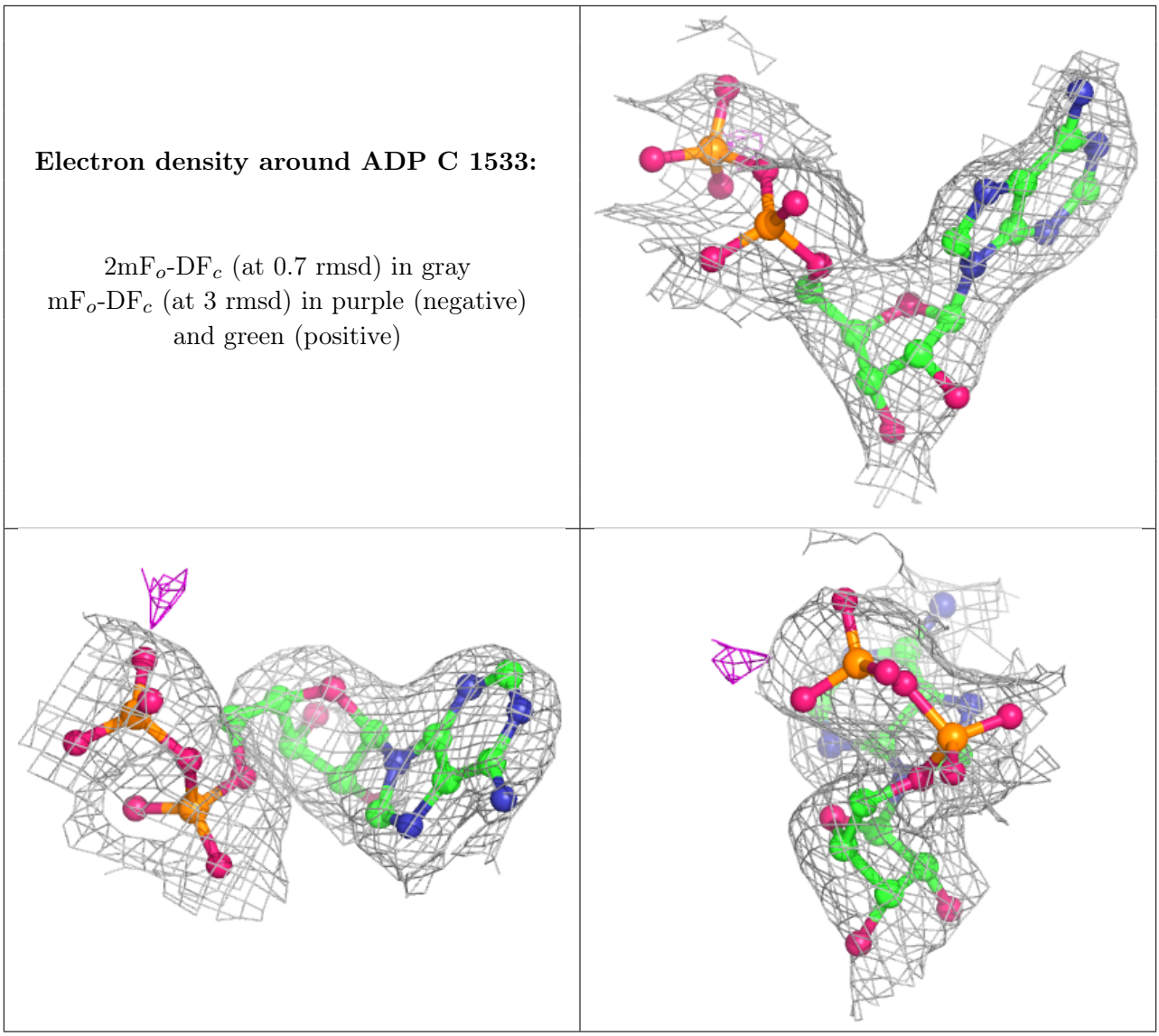






Electron density around ADP C 1533:

$2mF_o$-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.