wwPDB X-ray Structure Validation Summary Report (i)

Oct 6, 2024 – 12:35 AM EDT

PDB ID	:	1MX0
Title	:	Structure of topoisomerase subunit
Authors	:	Corbett, K.D.; Berger, J.M.
Deposited on	:	2002-10-01
Resolution	:	2.30 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:

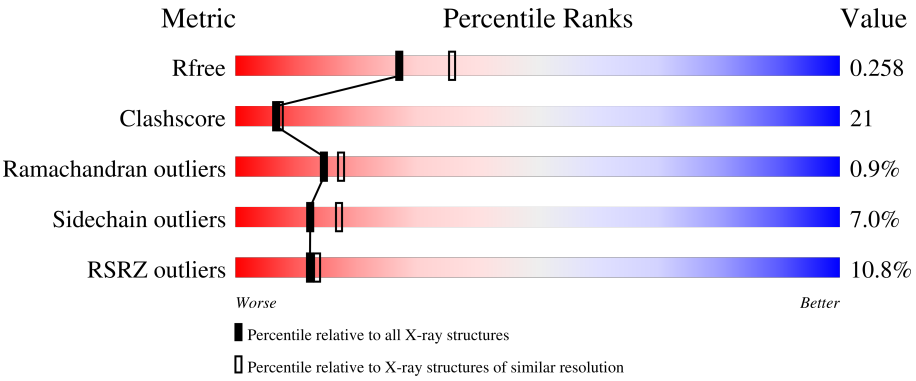
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	472	4% 63% 31%
1	B	472	2% 64% 30%
1	C	472	2% 67% 29%
1	D	472	2% 71% 24%
1	E	472	3% 63% 30%

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Mol	Chain	Length	Quality of chain
1	F	472	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 23057 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 Type II DNA topoisomerase VI subunit B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	Se	0	0	0
			3704	2384	620	694	1	5			
1	B	455	Total	C	N	O	S	Se	0	0	0
			3651	2352	608	685	1	5			
1	C	466	Total	C	N	O	S	Se	0	0	0
			3738	2404	626	702	1	5			
1	D	461	Total	C	N	O	S	Se	0	0	0
			3687	2374	615	692	1	5			
1	E	456	Total	C	N	O	S	Se	0	0	0
			3677	2368	614	689	1	5			
1	F	454	Total	C	N	O	S	Se	0	0	0
			3596	2316	598	676	1	5			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP O05207
A	0	ALA	-	expression tag	UNP O05207
A	107	MSE	MET	modified residue	UNP O05207
A	121	MSE	MET	modified residue	UNP O05207
A	303	TYR	ASP	SEE REMARK 999	UNP O05207
A	409	MSE	MET	modified residue	UNP O05207
A	412	MSE	MET	modified residue	UNP O05207
A	435	ASP	ASN	SEE REMARK 999	UNP O05207
A	445	MSE	MET	modified residue	UNP O05207
B	-1	GLY	-	expression tag	UNP O05207
B	0	ALA	-	expression tag	UNP O05207
B	107	MSE	MET	modified residue	UNP O05207
B	121	MSE	MET	modified residue	UNP O05207
B	303	TYR	ASP	SEE REMARK 999	UNP O05207
B	409	MSE	MET	modified residue	UNP O05207
B	412	MSE	MET	modified residue	UNP O05207
B	435	ASP	ASN	SEE REMARK 999	UNP O05207

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Chain	Residue	Modelled	Actual	Comment	Reference
B	445	MSE	MET	modified residue	UNP O05207
C	-1	GLY	-	expression tag	UNP O05207
C	0	ALA	-	expression tag	UNP O05207
C	107	MSE	MET	modified residue	UNP O05207
C	121	MSE	MET	modified residue	UNP O05207
C	303	TYR	ASP	SEE REMARK 999	UNP O05207
C	409	MSE	MET	modified residue	UNP O05207
C	412	MSE	MET	modified residue	UNP O05207
C	435	ASP	ASN	SEE REMARK 999	UNP O05207
C	445	MSE	MET	modified residue	UNP O05207
D	-1	GLY	-	expression tag	UNP O05207
D	0	ALA	-	expression tag	UNP O05207
D	107	MSE	MET	modified residue	UNP O05207
D	121	MSE	MET	modified residue	UNP O05207
D	303	TYR	ASP	SEE REMARK 999	UNP O05207
D	409	MSE	MET	modified residue	UNP O05207
D	412	MSE	MET	modified residue	UNP O05207
D	435	ASP	ASN	SEE REMARK 999	UNP O05207
D	445	MSE	MET	modified residue	UNP O05207
E	-1	GLY	-	expression tag	UNP O05207
E	0	ALA	-	expression tag	UNP O05207
E	107	MSE	MET	modified residue	UNP O05207
E	121	MSE	MET	modified residue	UNP O05207
E	303	TYR	ASP	SEE REMARK 999	UNP O05207
E	409	MSE	MET	modified residue	UNP O05207
E	412	MSE	MET	modified residue	UNP O05207
E	435	ASP	ASN	SEE REMARK 999	UNP O05207
E	445	MSE	MET	modified residue	UNP O05207
F	-1	GLY	-	expression tag	UNP O05207
F	0	ALA	-	expression tag	UNP O05207
F	107	MSE	MET	modified residue	UNP O05207
F	121	MSE	MET	modified residue	UNP O05207
F	303	TYR	ASP	SEE REMARK 999	UNP O05207
F	409	MSE	MET	modified residue	UNP O05207
F	412	MSE	MET	modified residue	UNP O05207
F	435	ASP	ASN	SEE REMARK 999	UNP O05207
F	445	MSE	MET	modified residue	UNP O05207

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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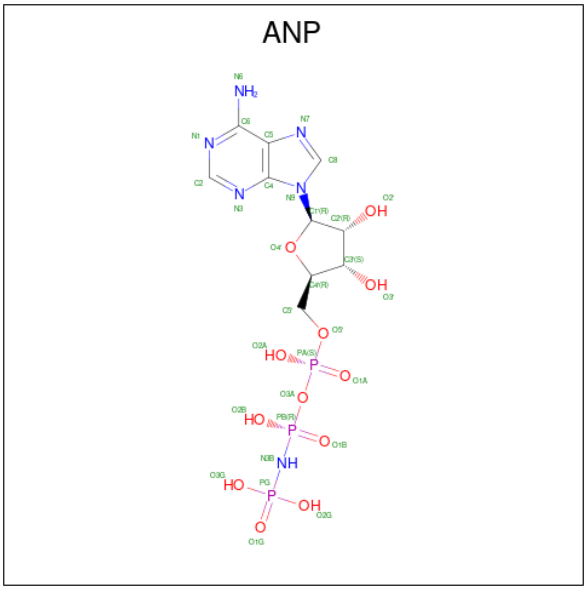
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 31 10 6 12 3	0	0
3	B	1	Total C N O P 31 10 6 12 3	0	0
3	C	1	Total C N O P 31 10 6 12 3	0	0
3	D	1	Total C N O P 31 10 6 12 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Na	0	0
			1	1		

- Molecule 5 is water.

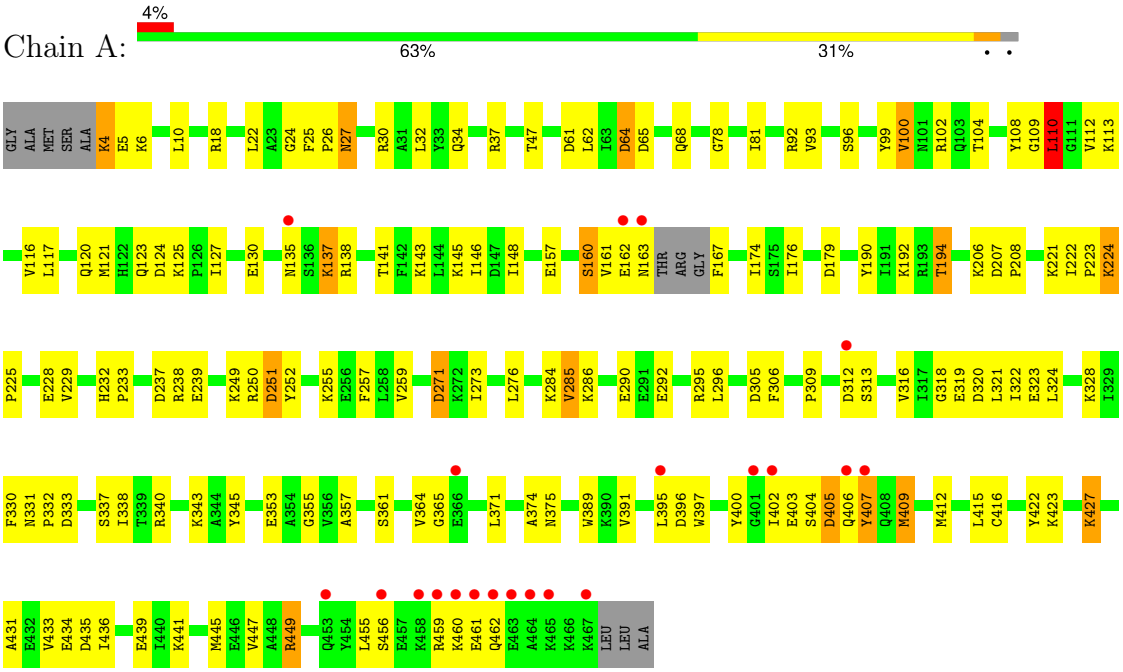
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	160	Total	O	0	0
			160	160		
5	B	145	Total	O	0	0
			145	145		
5	C	140	Total	O	0	0
			140	140		
5	D	160	Total	O	0	0
			160	160		
5	E	125	Total	O	0	0
			125	125		
5	F	81	Total	O	0	0
			81	81		

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.

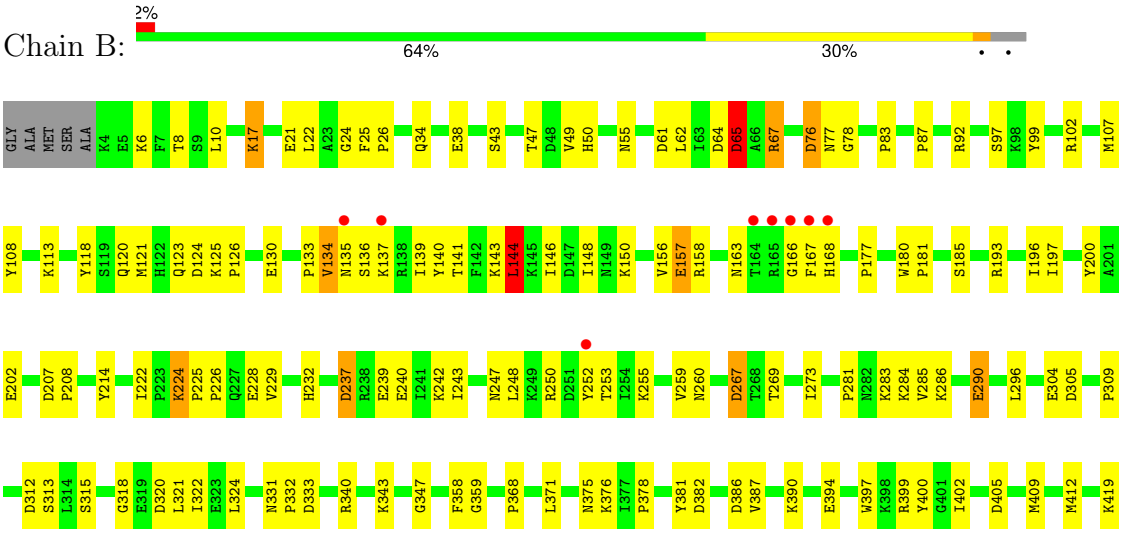
• Molecule 1: Type II DNA topoisomerase VI subunit B

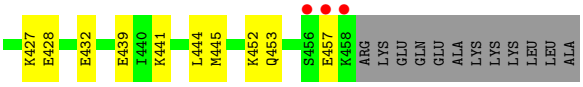
Chain A:



• Molecule 1: Type II DNA topoisomerase VI subunit B

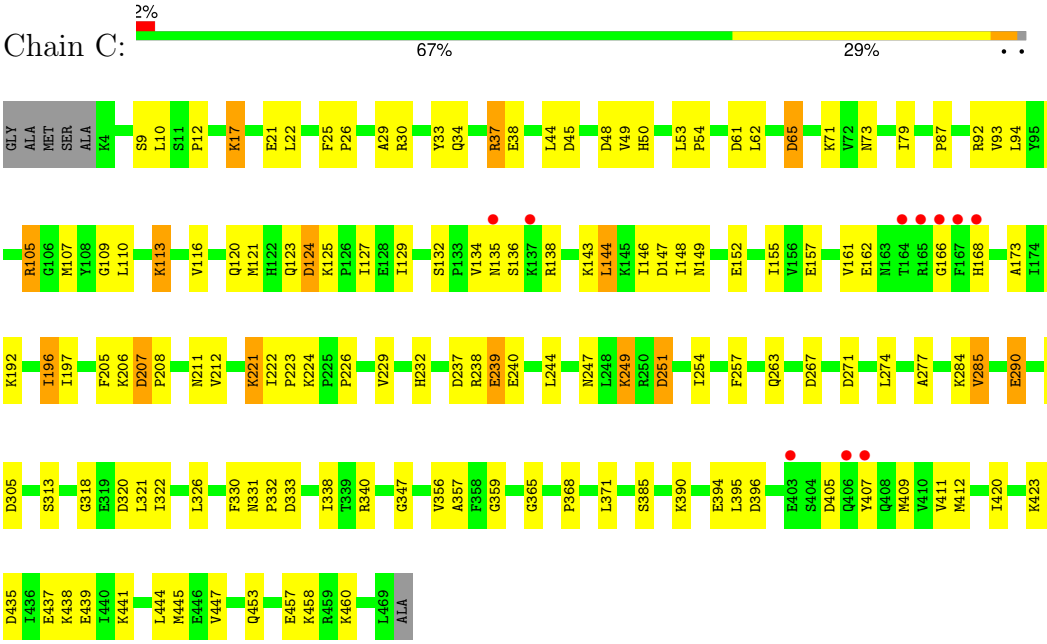
Chain B:





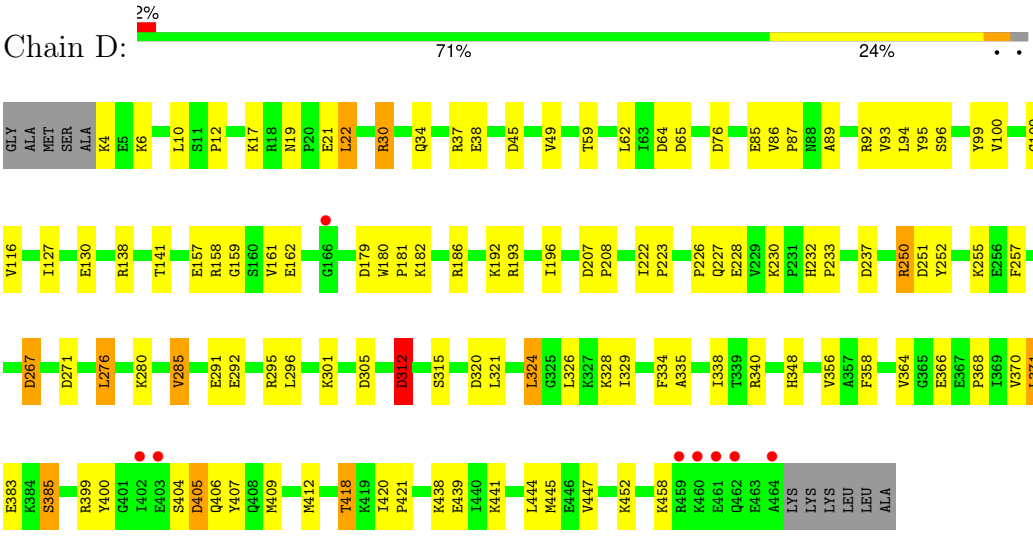
• Molecule 1: Type II DNA topoisomerase VI subunit B

Chain C:



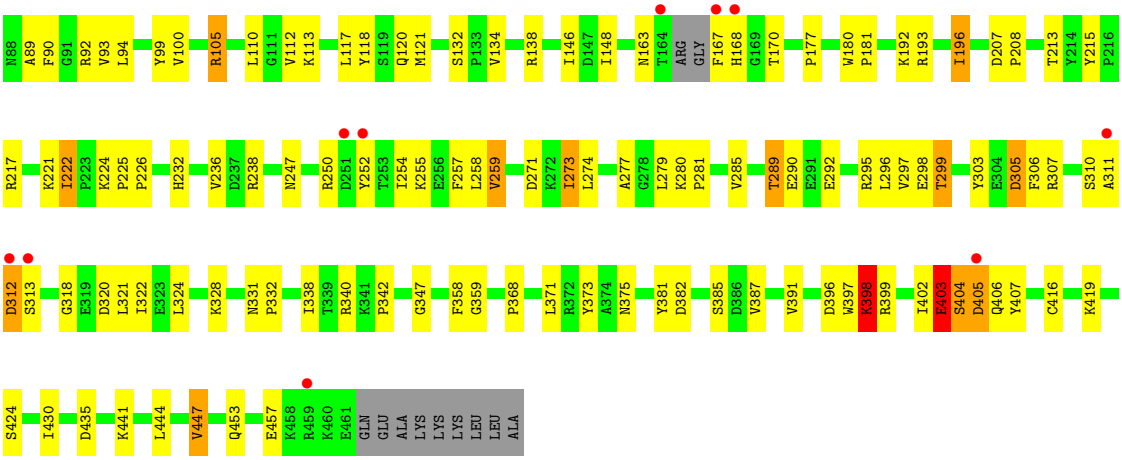
• Molecule 1: Type II DNA topoisomerase VI subunit B

Chain D:



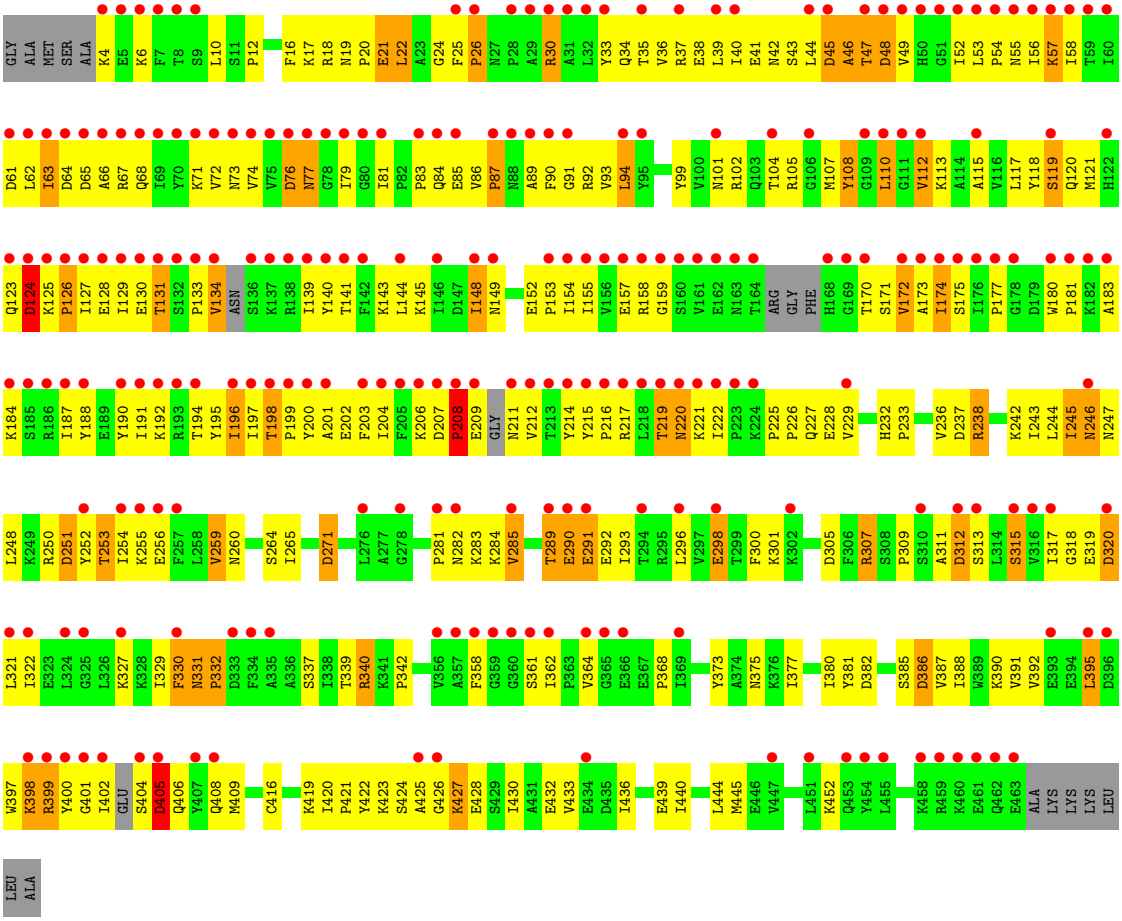
• Molecule 1: Type II DNA topoisomerase VI subunit B

Chain E:



• Molecule 1: Type II DNA topoisomerase VI subunit B

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	146.66Å 219.19Å 106.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-2.30) 97.9 (20.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.214 , 0.263 0.216 , 0.258	Depositor DCC
R_{free} test set	12535 reflections (8.36%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	23057	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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: ANP, NA, 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	0.62	0/3779	0.81	13/5104 (0.3%)
1	B	0.64	0/3727	0.81	13/5038 (0.3%)
1	C	0.60	0/3814	0.79	16/5152 (0.3%)
1	D	0.62	0/3763	0.81	11/5087 (0.2%)
1	E	0.60	0/3752	0.81	14/5067 (0.3%)
1	F	0.48	1/3666 (0.0%)	0.80	16/4955 (0.3%)
All	All	0.59	1/22501 (0.0%)	0.81	83/30403 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	108	TYR	CB-CG	-5.04	1.44	1.51

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	105	ARG	NE-CZ-NH2	-9.59	115.50	120.30
1	C	105	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	D	271	ASP	CB-CG-OD2	6.95	124.56	118.30
1	D	382	ASP	CB-CG-OD2	6.85	124.46	118.30
1	A	251	ASP	CB-CG-OD2	6.82	124.44	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3704	0	3760	155	0
1	B	3651	0	3704	120	0
1	C	3738	0	3792	136	0
1	D	3687	0	3735	98	0
1	E	3677	0	3746	136	0
1	F	3596	0	3605	330	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	31	0	13	0	0
3	B	31	0	13	1	0
3	C	31	0	13	0	0
3	D	31	0	13	1	0
3	E	31	0	13	1	0
3	F	31	0	13	4	0
4	D	1	0	0	0	0
5	A	160	0	0	22	0
5	B	145	0	0	19	0
5	C	140	0	0	17	0
5	D	160	0	0	22	0
5	E	125	0	0	18	0
5	F	81	0	0	34	0
All	All	23057	0	22420	941	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 21.

The worst 5 of 941 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:C:107:MSE:SE	1:C:107:MSE:CE	2.16	1.43
1:C:127:ILE:HD11	1:C:144:LEU:CD1	1.56	1.34
1:A:4:LYS:HD2	1:A:4:LYS:O	1.16	1.33
1:C:127:ILE:CD1	1:C:144:LEU:HD11	1.64	1.27
1:E:402:ILE:HG22	1:E:403:GLU:O	1.30	1.25

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	457/472 (97%)	440 (96%)	17 (4%)	0	100 100
1	B	453/472 (96%)	426 (94%)	24 (5%)	3 (1%)	19 23
1	C	464/472 (98%)	448 (97%)	15 (3%)	1 (0%)	44 55
1	D	459/472 (97%)	440 (96%)	19 (4%)	0	100 100
1	E	452/472 (96%)	427 (94%)	22 (5%)	3 (1%)	19 23
1	F	444/472 (94%)	379 (85%)	48 (11%)	17 (4%)	2 1
All	All	2729/2832 (96%)	2560 (94%)	145 (5%)	24 (1%)	14 17

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	208	PRO
1	F	245	ILE
1	F	246	ASN
1	F	332	PRO
1	F	399	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	407/412 (99%)	382 (94%)	25 (6%)	15 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	402/412 (98%)	380 (94%)	22 (6%)	18 26
1	C	410/412 (100%)	383 (93%)	27 (7%)	14 19
1	D	404/412 (98%)	384 (95%)	20 (5%)	20 30
1	E	407/412 (99%)	378 (93%)	29 (7%)	12 17
1	F	389/412 (94%)	343 (88%)	46 (12%)	4 5
All	All	2419/2472 (98%)	2250 (93%)	169 (7%)	12 17

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	338	ILE
1	F	175	SER
1	E	403	GLU
1	F	76	ASP
1	F	244	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	220	ASN
1	F	227	GLN
1	C	247	ASN
1	C	123	GLN
1	F	331	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 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	ANP	D	930	2	29,33,33	2.31	8 (27%)	31,52,52	1.43	4 (12%)
3	ANP	C	920	2	29,33,33	2.33	8 (27%)	31,52,52	1.42	5 (16%)
3	ANP	B	910	2	29,33,33	2.19	9 (31%)	31,52,52	1.58	4 (12%)
3	ANP	E	940	2	29,33,33	2.19	10 (34%)	31,52,52	1.36	4 (12%)
3	ANP	A	900	2	29,33,33	2.12	6 (20%)	31,52,52	1.25	3 (9%)
3	ANP	F	950	2	29,33,33	2.32	9 (31%)	31,52,52	1.91	5 (16%)

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
3	ANP	D	930	2	-	4/14/38/38	0/3/3/3
3	ANP	C	920	2	-	4/14/38/38	0/3/3/3
3	ANP	B	910	2	-	4/14/38/38	0/3/3/3
3	ANP	E	940	2	-	3/14/38/38	0/3/3/3
3	ANP	A	900	2	-	4/14/38/38	0/3/3/3
3	ANP	F	950	2	-	4/14/38/38	0/3/3/3

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	920	ANP	PB-O3A	-7.83	1.49	1.59
3	F	950	ANP	PA-O3A	-7.75	1.51	1.59
3	D	930	ANP	PA-O3A	-7.06	1.51	1.59
3	C	920	ANP	PA-O3A	-6.70	1.52	1.59
3	A	900	ANP	PA-O3A	-6.67	1.52	1.59

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	950	ANP	O4'-C1'-N9	5.68	116.28	108.75
3	F	950	ANP	C4'-O4'-C1'	4.94	114.45	109.92
3	B	910	ANP	C4'-O4'-C1'	4.68	114.21	109.92
3	F	950	ANP	O1G-PG-N3B	-4.49	105.16	111.77
3	E	940	ANP	C4'-O4'-C1'	4.30	113.86	109.92

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	900	ANP	PB-N3B-PG-O1G
3	A	900	ANP	PG-N3B-PB-O1B
3	A	900	ANP	PA-O3A-PB-O1B
3	B	910	ANP	PB-N3B-PG-O1G
3	B	910	ANP	PG-N3B-PB-O1B

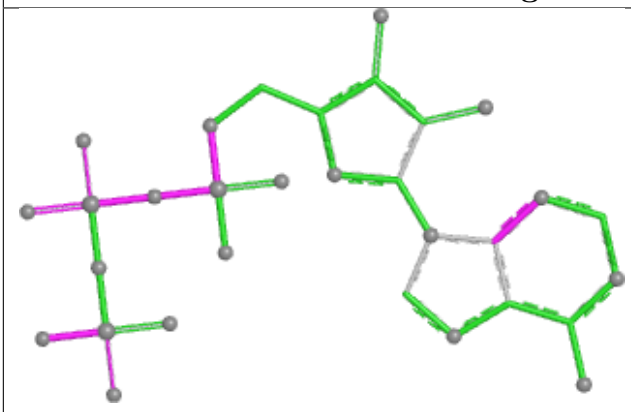
There are no ring outliers.

4 monomers are involved in 7 short contacts:

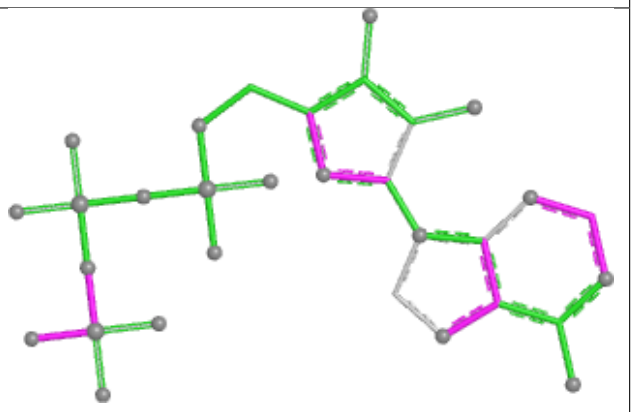
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	930	ANP	1	0
3	B	910	ANP	1	0
3	E	940	ANP	1	0
3	F	950	ANP	4	0

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.

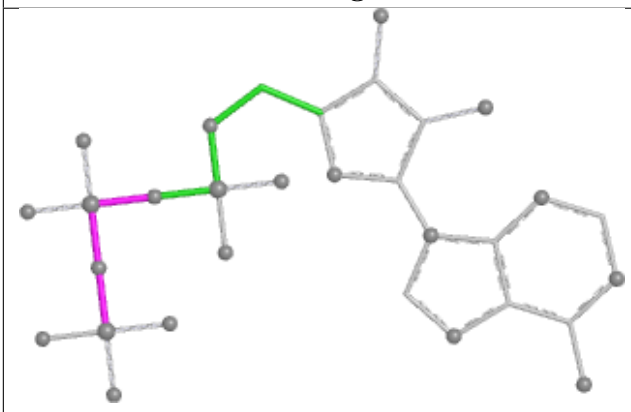
Ligand ANP D 930



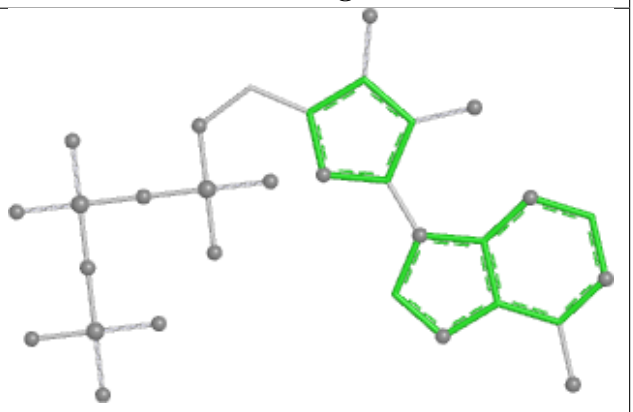
Bond lengths



Bond angles

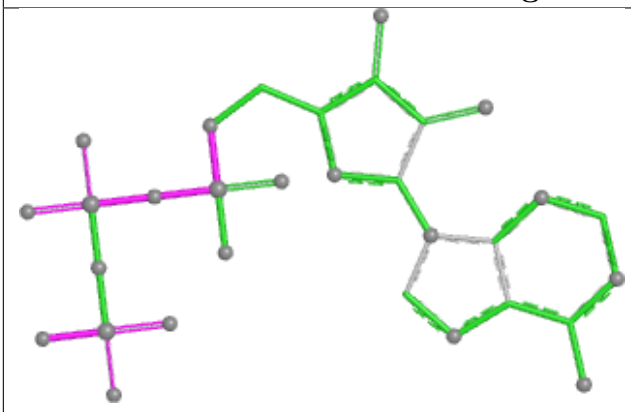


Torsions

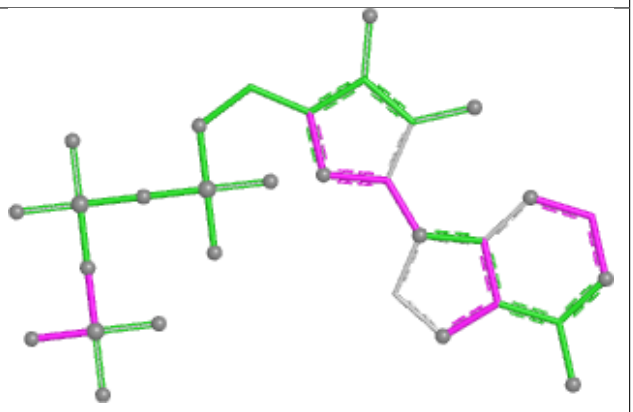


Rings

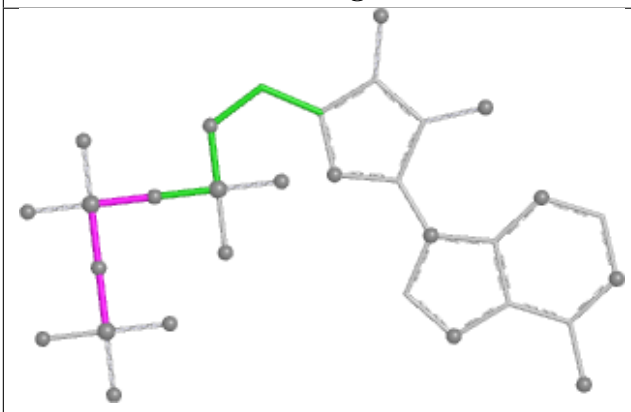
Ligand ANP C 920



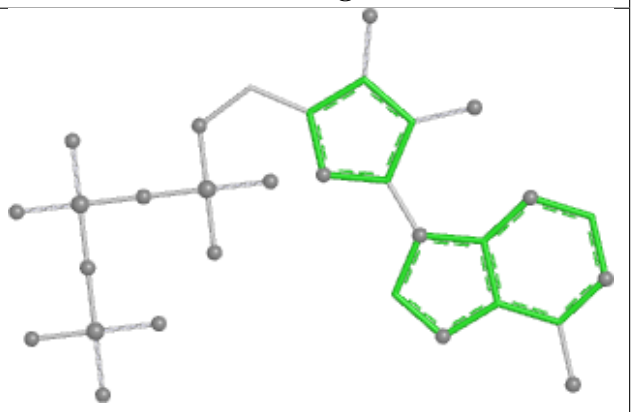
Bond lengths



Bond angles

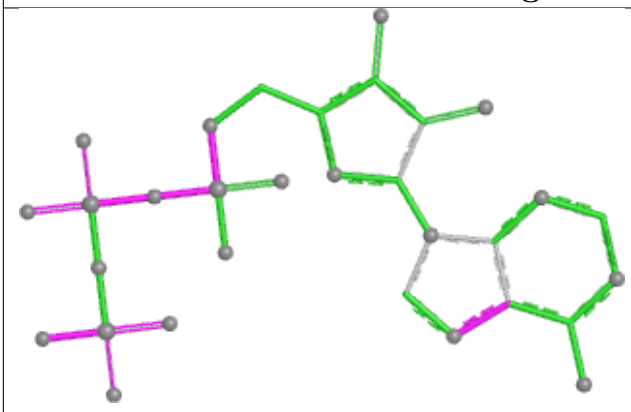


Torsions

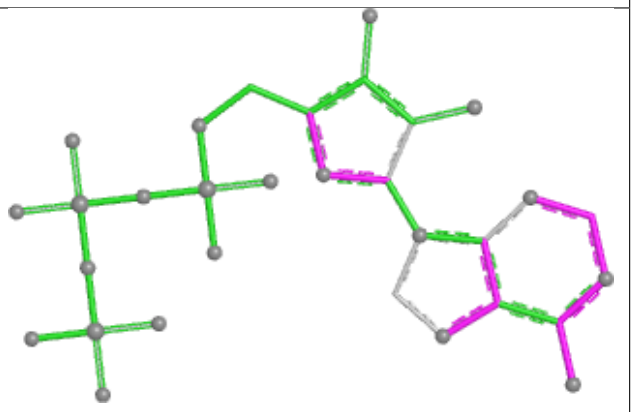


Rings

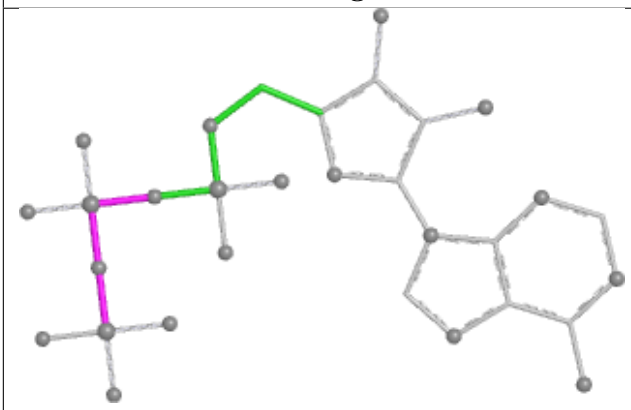
Ligand ANP B 910



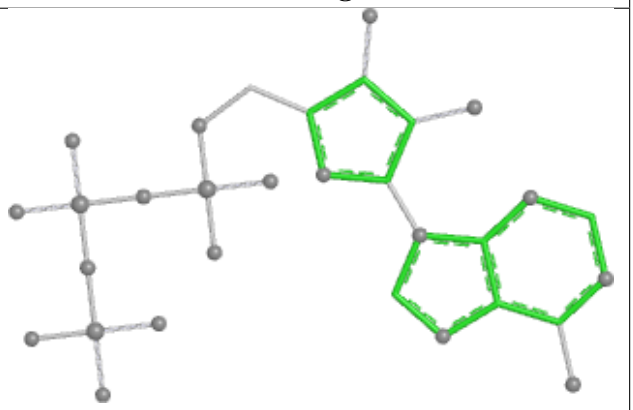
Bond lengths



Bond angles

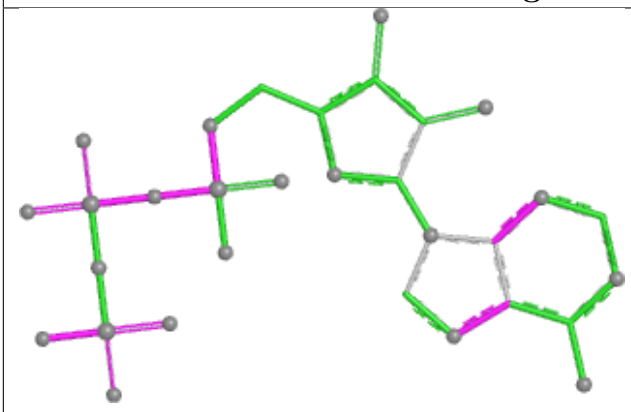


Torsions

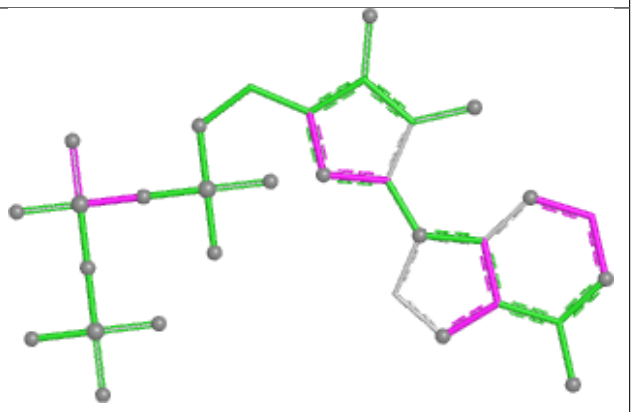


Rings

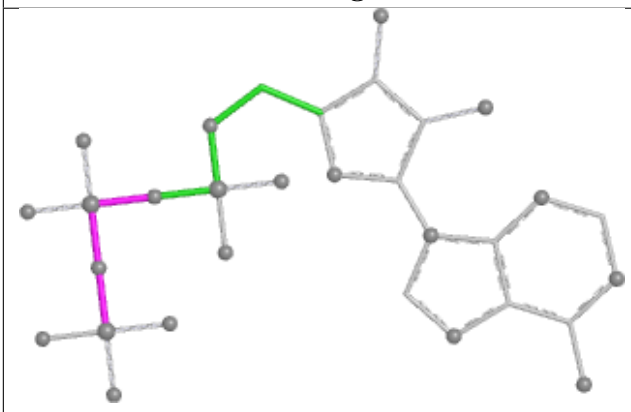
Ligand ANP E 940



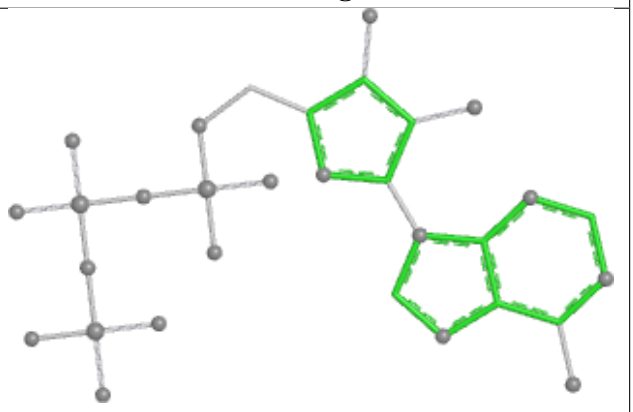
Bond lengths



Bond angles

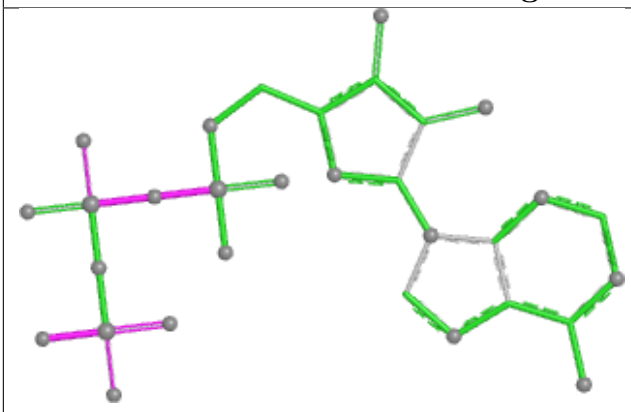


Torsions

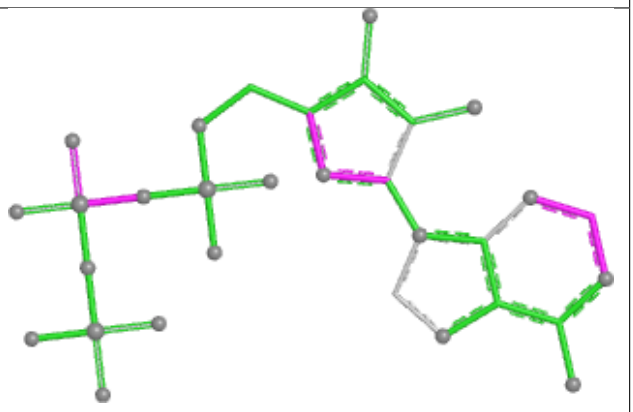


Rings

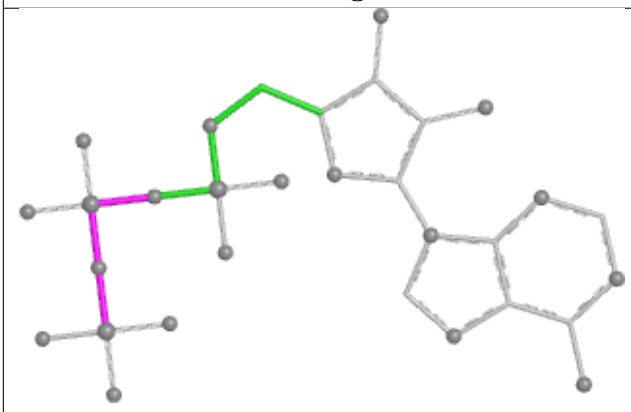
Ligand ANP A 900



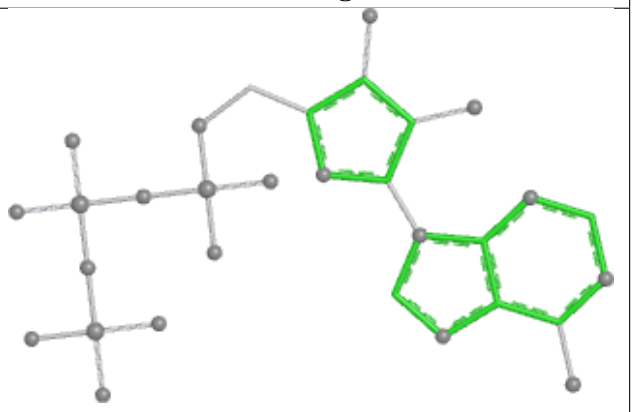
Bond lengths



Bond angles

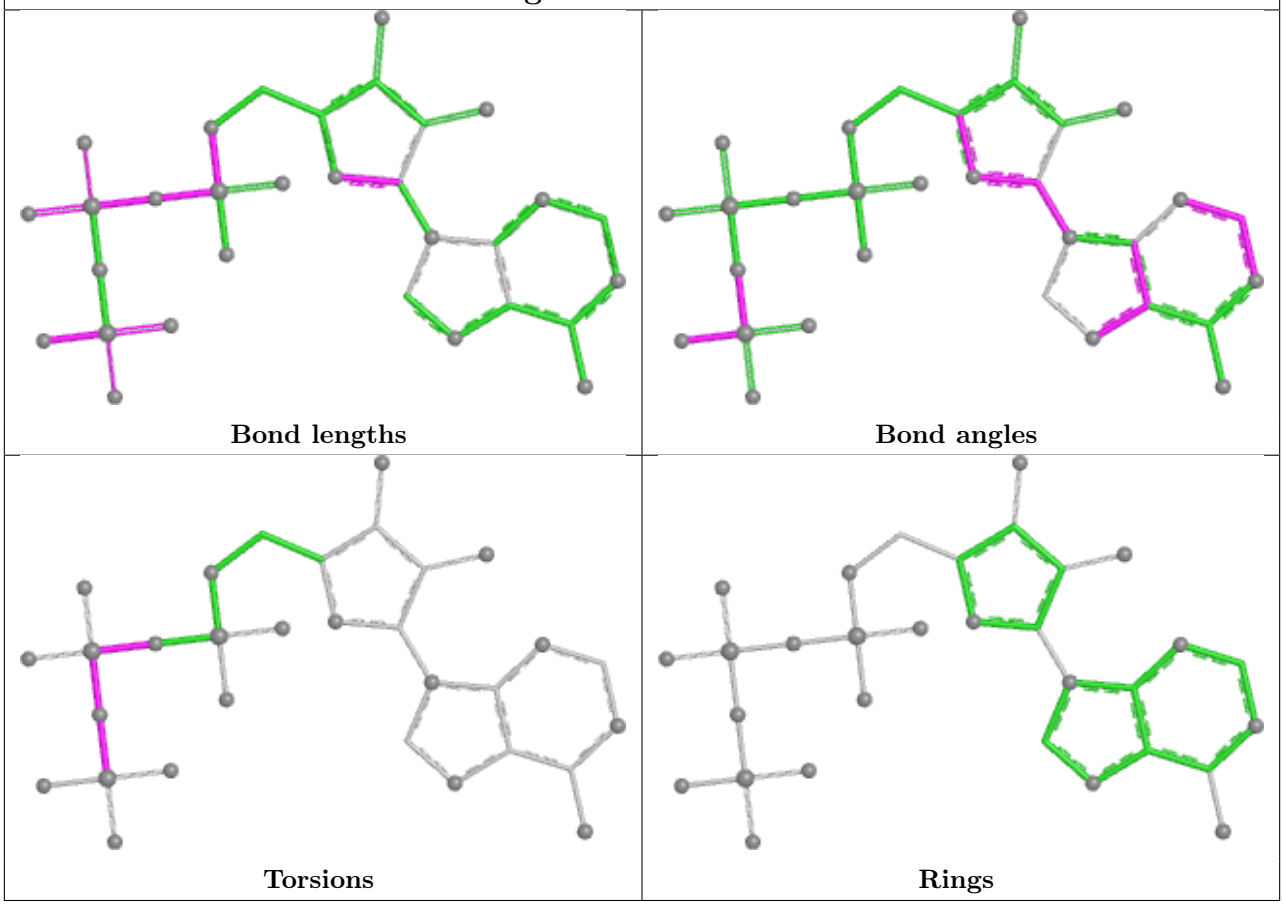


Torsions



Rings

Ligand ANP F 950



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	456/472 (96%)	-0.10	21 (4%)	38	39	4, 16, 48, 94	0
1	B	450/472 (95%)	-0.25	11 (2%)	59	61	4, 16, 40, 56	0
1	C	461/472 (97%)	-0.21	10 (2%)	62	63	7, 18, 39, 52	0
1	D	456/472 (96%)	-0.36	8 (1%)	67	68	4, 15, 37, 71	0
1	E	451/472 (95%)	-0.02	12 (2%)	56	57	4, 18, 50, 72	0
1	F	449/472 (95%)	2.27	233 (51%)	0	0	18, 46, 72, 98	0
All	All	2723/2832 (96%)	0.22	295 (10%)	12	13	4, 19, 59, 98	0

The worst 5 of 295 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	212	VAL	7.7
1	F	217	ARG	7.2
1	F	211	ASN	7.2
1	F	162	GLU	7.0
1	F	159	GLY	6.5

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

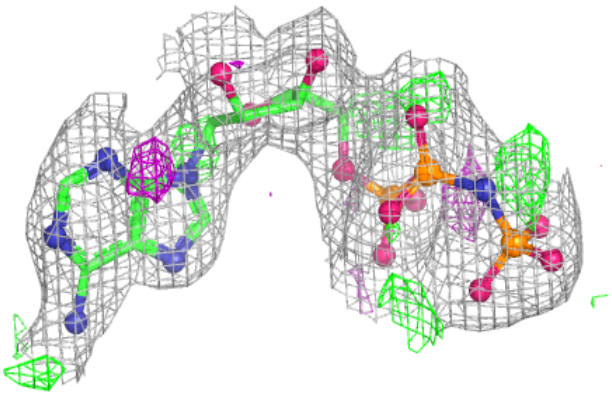
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

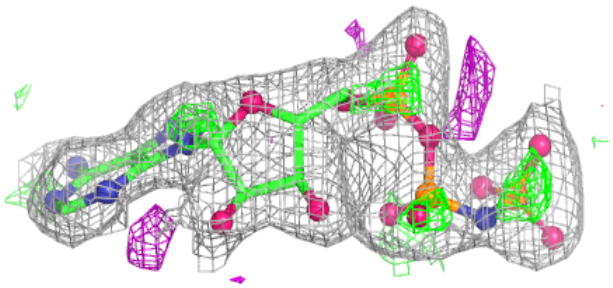
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	F	501	1/1	0.76	0.16	80,80,80,80	0
4	NA	D	901	1/1	0.84	0.21	78,78,78,78	0
3	ANP	F	950	31/31	0.89	0.17	59,76,78,78	0
2	MG	E	501	1/1	0.90	0.11	51,51,51,51	0
3	ANP	B	910	31/31	0.97	0.09	38,43,46,47	0
3	ANP	C	920	31/31	0.97	0.09	42,48,52,52	0
3	ANP	E	940	31/31	0.97	0.10	43,47,49,49	0
2	MG	B	501	1/1	0.97	0.11	42,42,42,42	0
2	MG	C	501	1/1	0.97	0.05	49,49,49,49	0
2	MG	D	501	1/1	0.98	0.06	45,45,45,45	0
3	ANP	A	900	31/31	0.98	0.09	40,45,47,47	0
3	ANP	D	930	31/31	0.98	0.09	41,45,48,48	0
2	MG	A	501	1/1	0.99	0.08	43,43,43,43	0

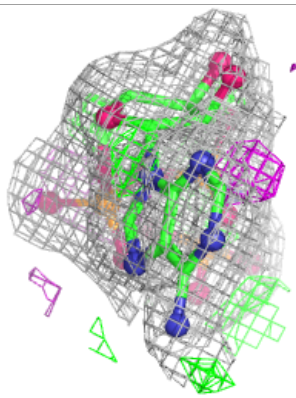
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP F 950:

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

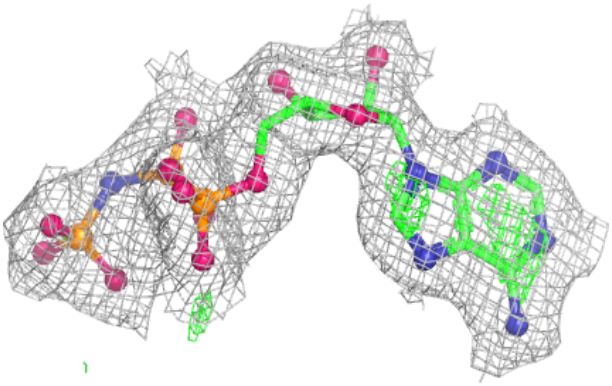


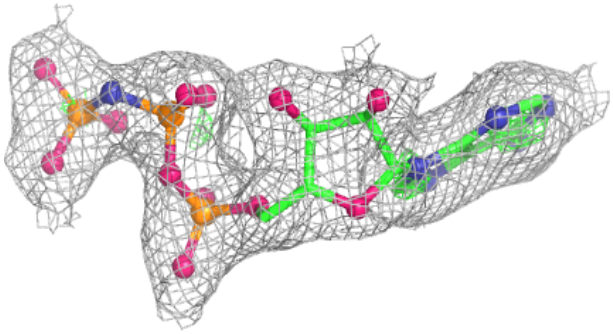


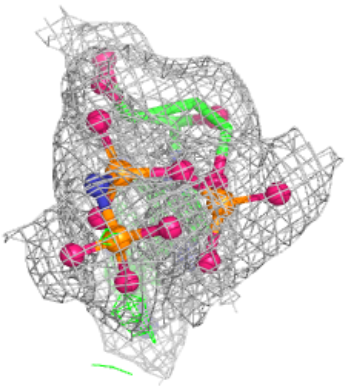


Electron density around ANP B 910:

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

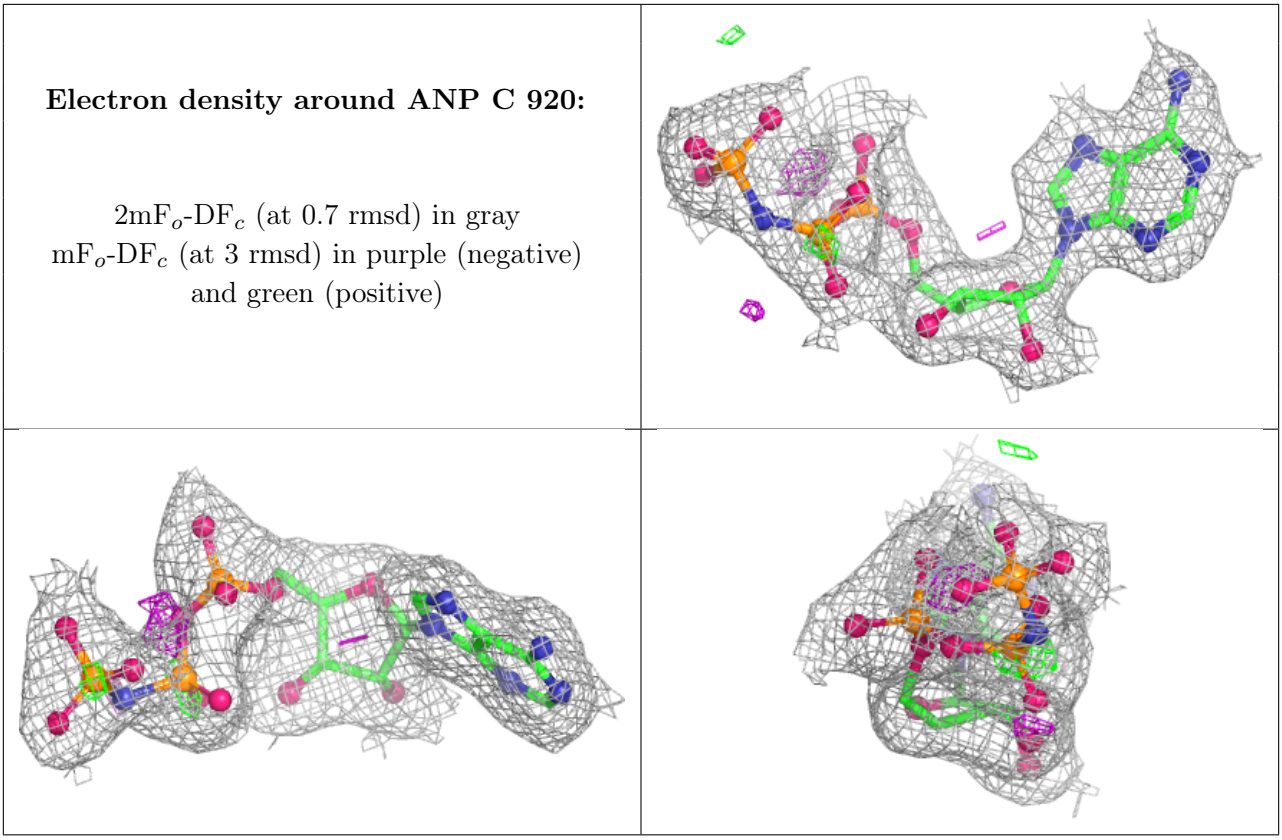






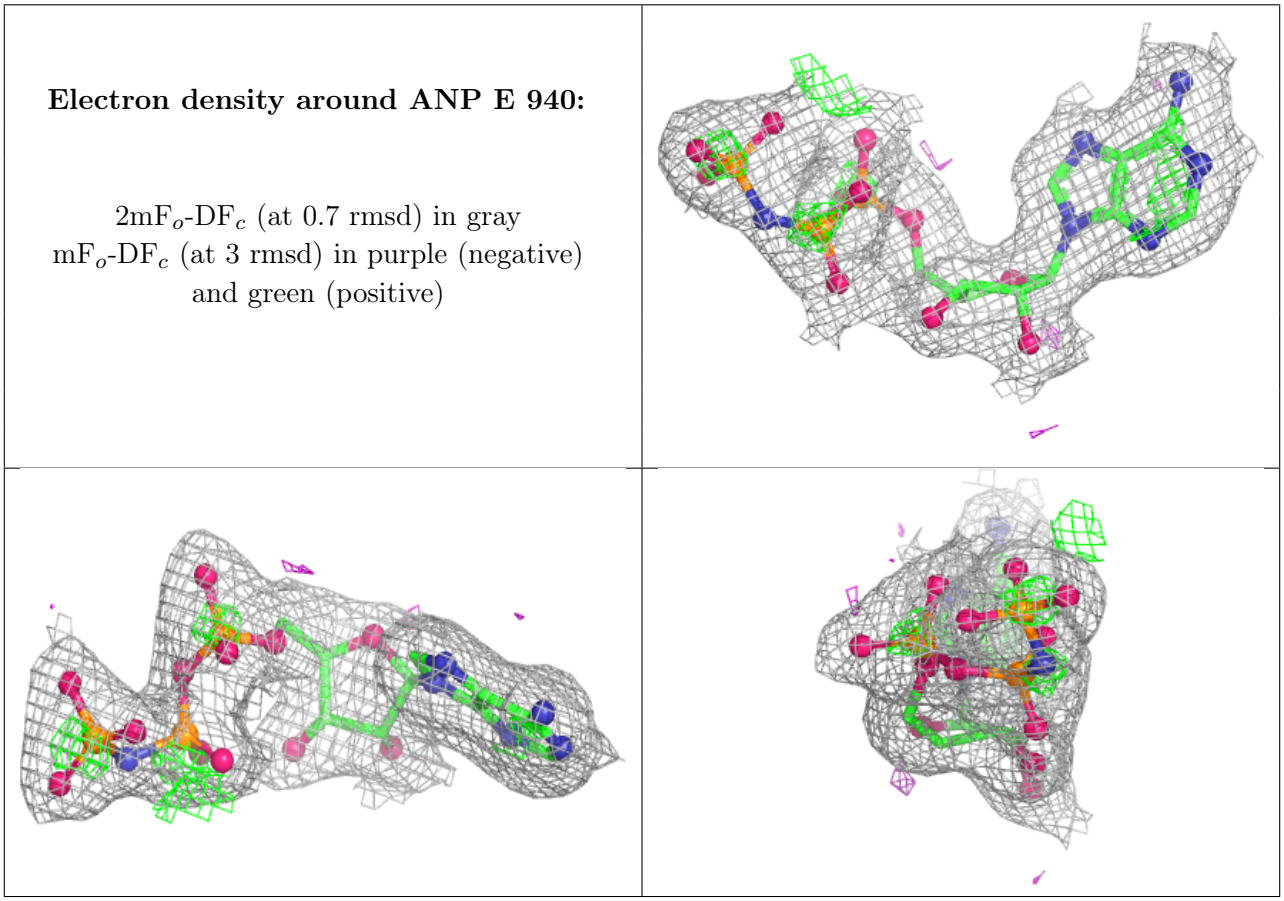
Electron density around ANP C 920:

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



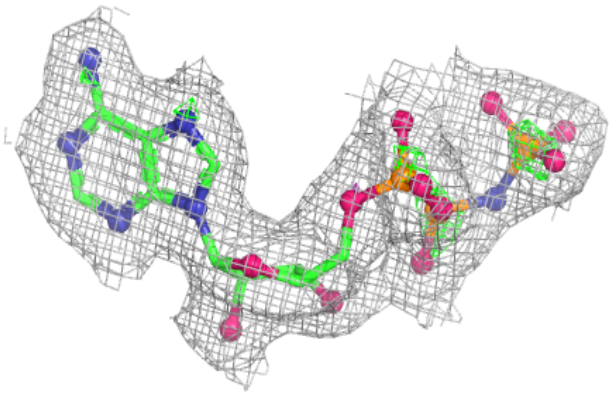
Electron density around ANP E 940:

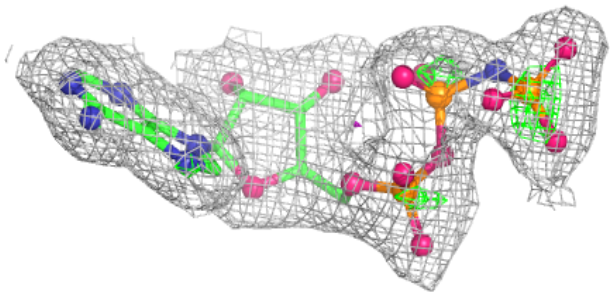
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

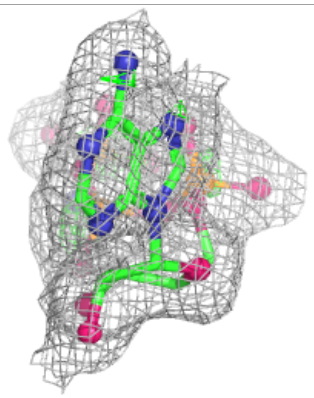


Electron density around ANP A 900:

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

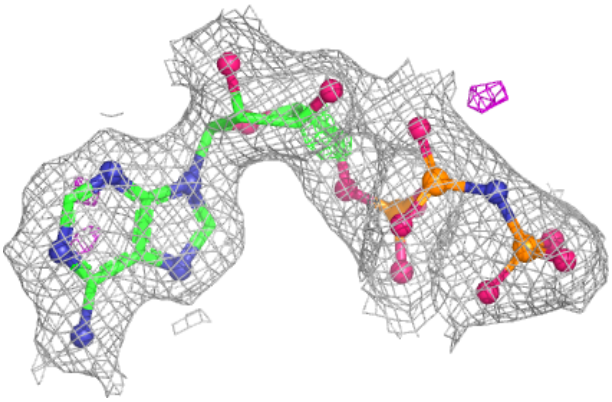


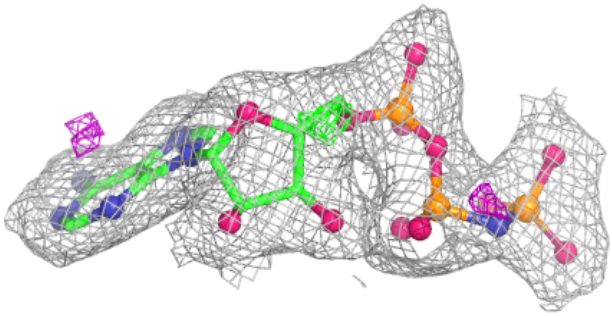


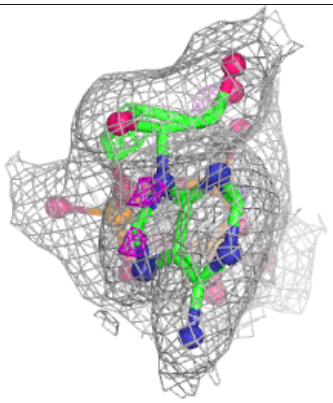


Electron density around ANP D 930:

$2mF_o$-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.