Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2025 – 06:20 PM JST

PDB ID	:	8ZN6 / pdb_00008zn6
Title	:	Crystal Structure of Designed Clock Protein KaiC
Authors	:	Furuike, Y.; Akiyama, S.
Deposited on	:	2024-05-26
Resolution	:	2.94 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

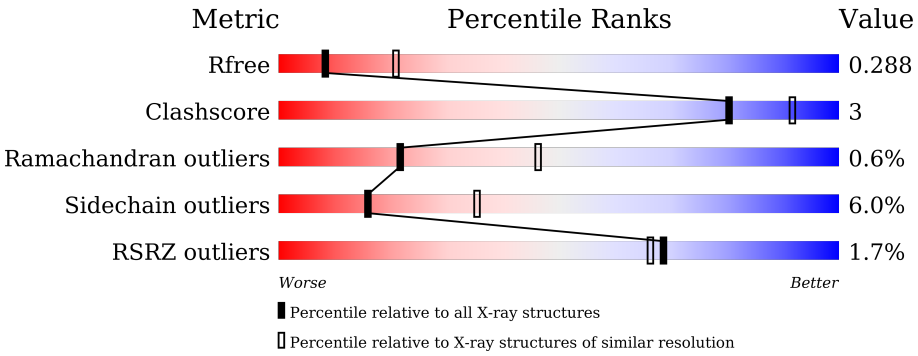
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.94 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	1067 (2.96-2.92)
Clashscore	180529	1122 (2.96-2.92)
Ramachandran outliers	177936	1075 (2.96-2.92)
Sidechain outliers	177891	1075 (2.96-2.92)
RSRZ outliers	164620	1067 (2.96-2.92)

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	515	2% 85% 6% • 8%
1	F	515	% 80% 10% • 9%
1	J	515	2% 82% 8% 10%
1	K	515	2% 82% 7% 11%
2	B	515	% 82% 10% 8%
2	C	515	3% 82% 9% • 9%

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Mol	Chain	Length	Quality of chain
2	D	515	2% 81% 7% • 10%
2	E	515	% 83% 10% 8%
2	G	515	2% 83% 7% • 10%
2	H	515	% 82% 9% • 8%
2	I	515	% 82% 8% • 10%
2	L	515	% 82% 9% • 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 41205 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.

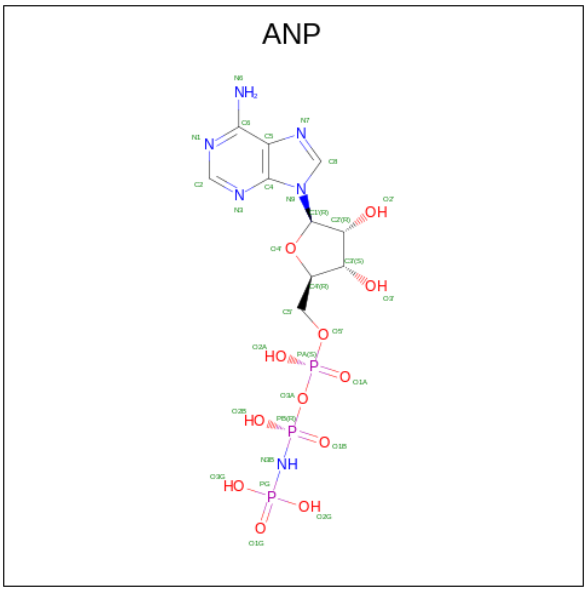
- Molecule 1 is a protein called KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	F	469	Total	C	N	O	P	S	0	0	0
			3437	2172	597	657	1	10			
1	A	475	Total	C	N	O	P	S	0	0	0
			3477	2205	603	658	1	10			
1	K	460	Total	C	N	O	P	S	0	0	0
			3241	2036	566	629	1	9			
1	J	466	Total	C	N	O	P	S	0	0	0
			3316	2090	578	637	1	10			

- Molecule 2 is a protein called KaiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	464	Total	C	N	O	S	0	0	0
			3304	2095	574	626	9			
2	E	476	Total	C	N	O	S	0	0	0
			3446	2180	601	655	10			
2	B	472	Total	C	N	O	S	0	0	0
			3396	2154	586	646	10			
2	C	471	Total	C	N	O	S	0	0	0
			3350	2115	582	641	12			
2	G	466	Total	C	N	O	S	0	0	0
			3376	2144	588	634	10			
2	H	473	Total	C	N	O	S	0	0	0
			3321	2110	584	618	9			
2	L	471	Total	C	N	O	S	0	0	0
			3427	2172	597	647	11			
2	I	466	Total	C	N	O	S	0	0	0
			3296	2091	574	621	10			

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	K	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	K	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	L	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	L	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	I	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	I	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	2	Total Mg 2 2	0	0
4	I	2	Total Mg 2 2	0	0
4	J	1	Total Mg 1 1	0	0

- Molecule 5 is water.

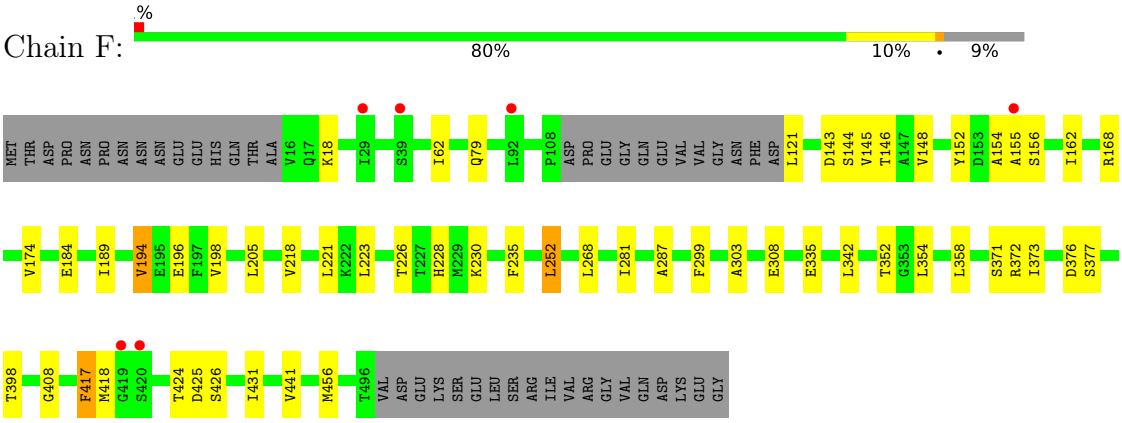
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	5	Total O 5 5	0	0
5	A	5	Total O 5 5	0	0
5	D	5	Total O 5 5	0	0
5	E	6	Total O 6 6	0	0
5	B	3	Total O 3 3	0	0
5	C	4	Total O 4 4	0	0
5	G	4	Total O 4 4	0	0
5	H	8	Total O 8 8	0	0
5	K	2	Total O 2 2	0	0
5	L	5	Total O 5 5	0	0
5	I	4	Total O 4 4	0	0
5	J	3	Total O 3 3	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.

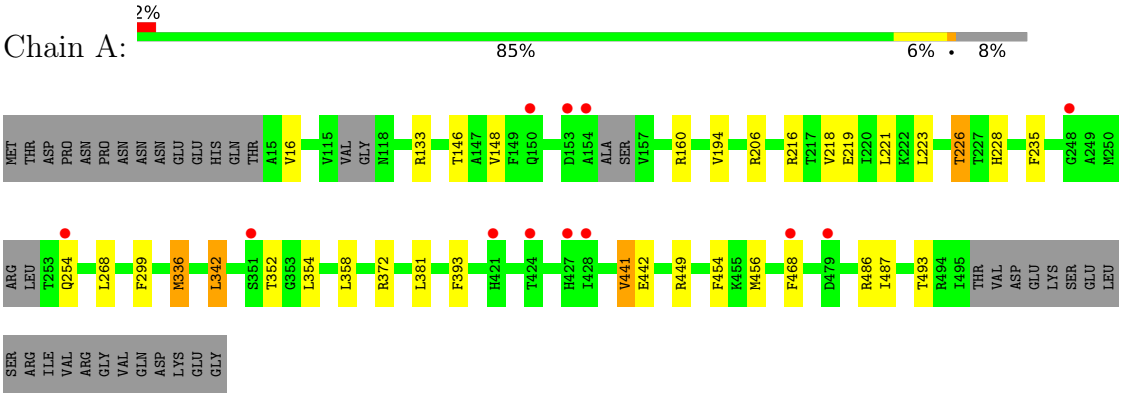
• Molecule 1: KaiC

Chain F:



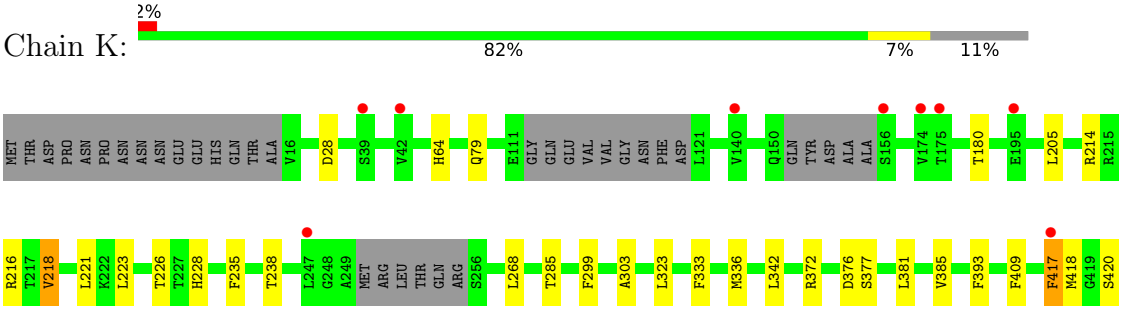
• Molecule 1: KaiC

Chain A:



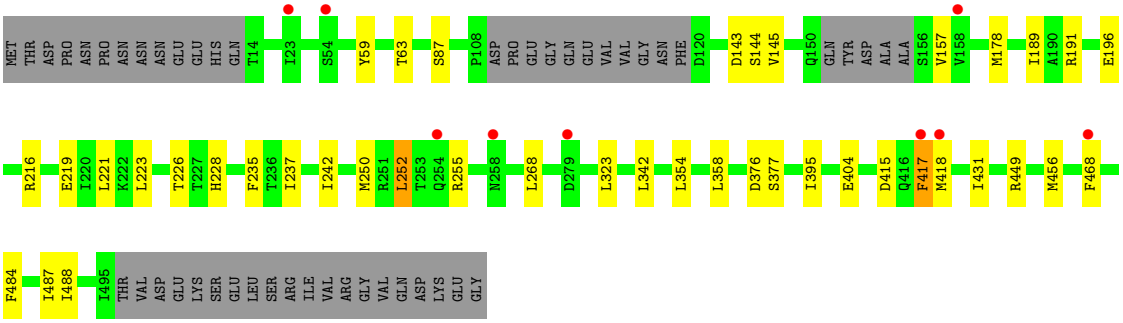
• Molecule 1: KaiC

Chain K:



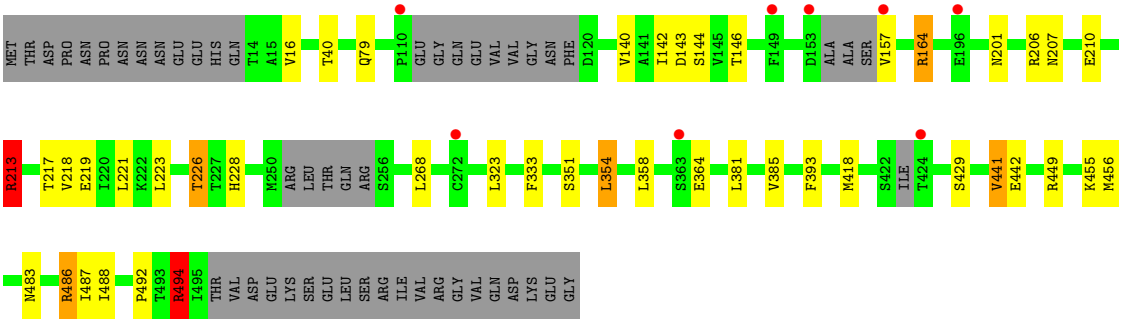
• Molecule 1: KaiC

Chain J:



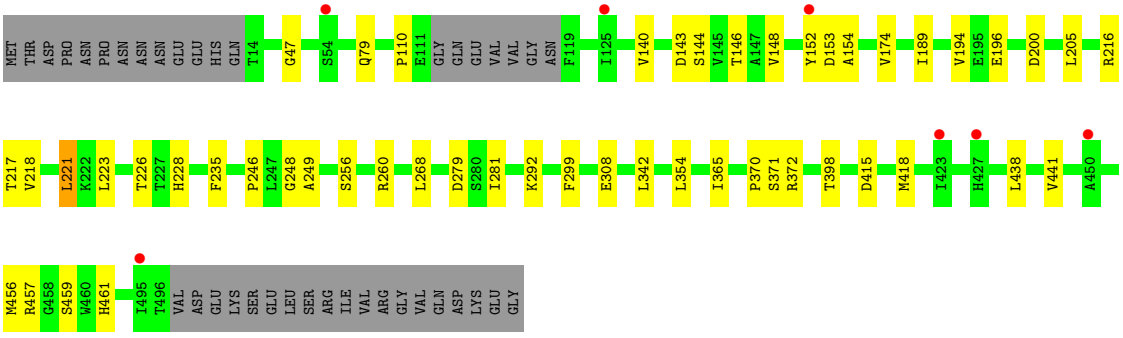
• Molecule 2: KaiC

Chain D:



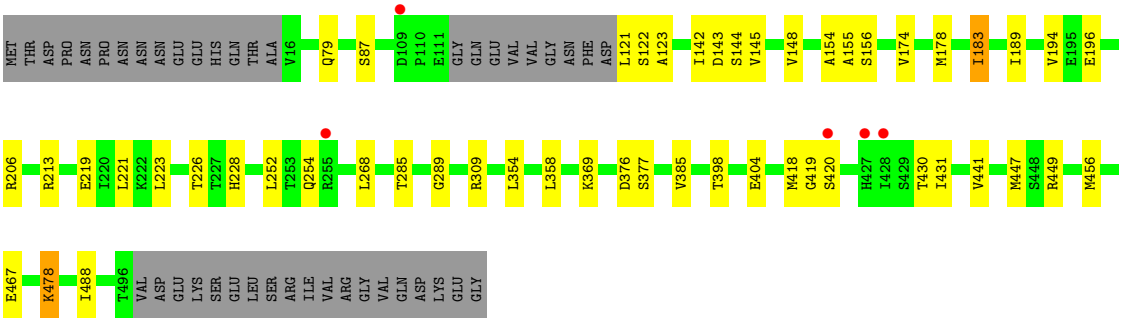
• Molecule 2: KaiC

Chain E:



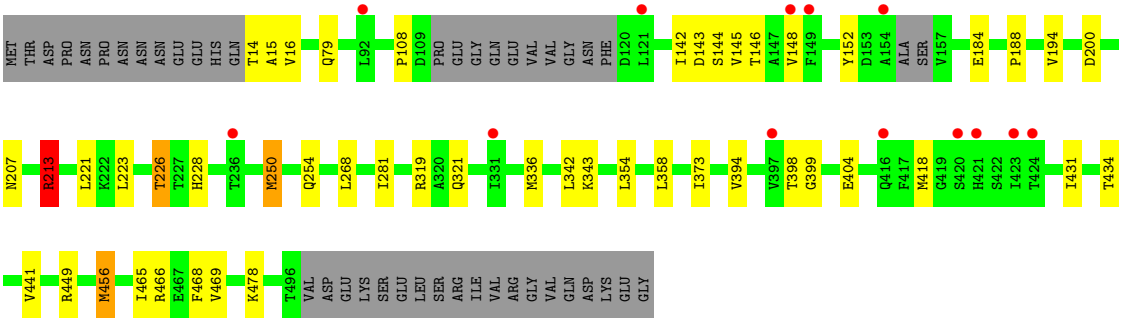
• Molecule 2: KaiC

Chain B:



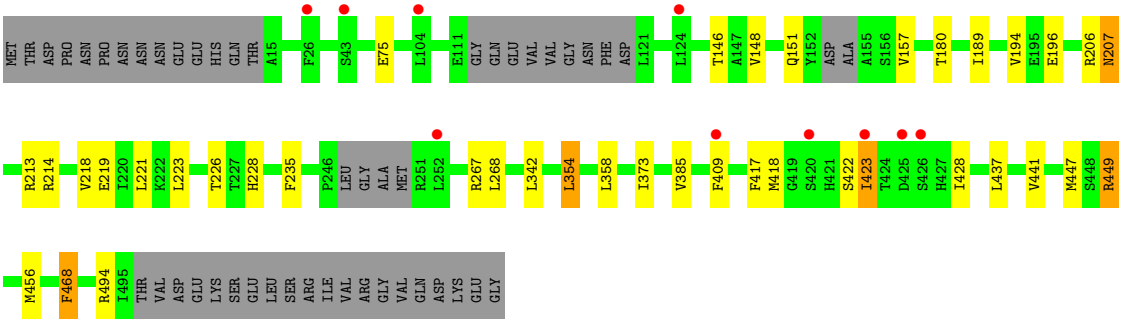
• Molecule 2: KaiC

Chain C:



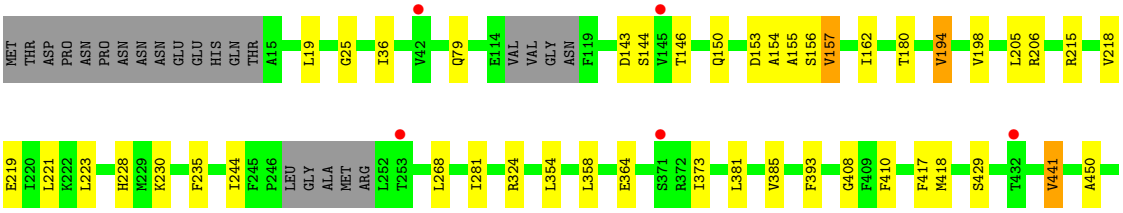
• Molecule 2: KaiC

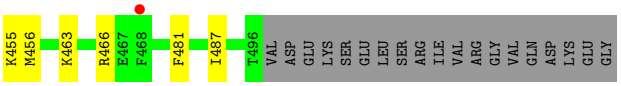
Chain G:



• Molecule 2: KaiC

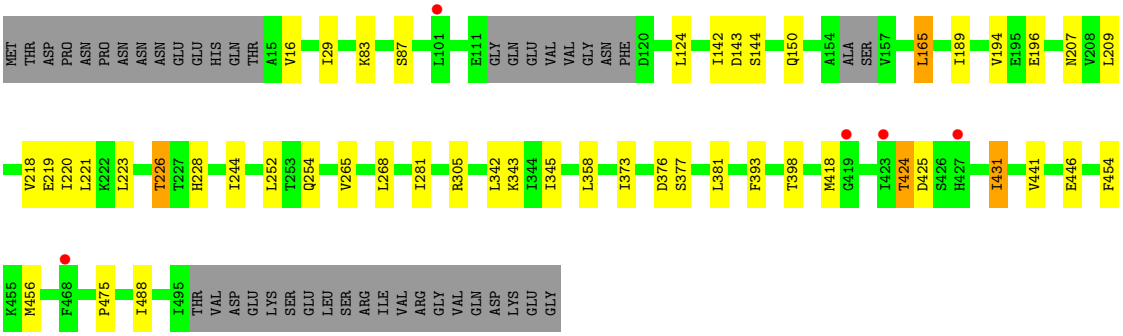
Chain H:





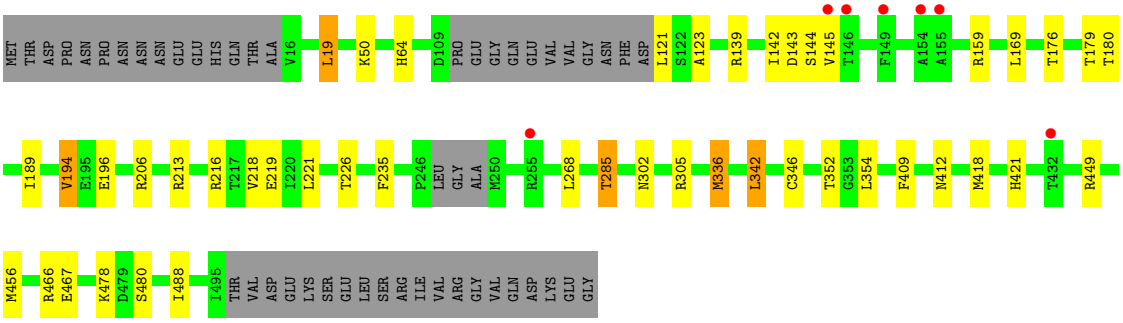
• Molecule 2: KaiC

Chain L:



• Molecule 2: KaiC

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	90.76Å 110.27Å 166.89Å 77.97° 87.25° 82.41°	Depositor
Resolution (Å)	48.74 – 2.94 48.74 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.74-2.94) 99.5 (48.74-2.94)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.239 , 0.292 0.237 , 0.288	Depositor DCC
R_{free} test set	6615 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	79.2	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 75.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	41205	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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, SEP, 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	0.27	0/3527	0.44	0/4784
1	F	0.26	0/3484	0.43	0/4727
1	J	0.27	0/3363	0.44	0/4570
1	K	0.27	0/3287	0.43	0/4467
2	B	0.26	0/3454	0.45	0/4697
2	C	0.27	0/3407	0.44	0/4633
2	D	0.27	0/3362	0.44	0/4571
2	E	0.26	0/3506	0.44	0/4767
2	G	0.26	0/3433	0.44	0/4664
2	H	0.26	0/3379	0.44	0/4604
2	I	0.27	0/3351	0.44	0/4555
2	L	0.27	0/3486	0.44	0/4727
All	All	0.27	0/41039	0.44	0/55766

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	C	0	1
2	D	0	4
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	213	ARG	Sidechain
2	D	164	ARG	Sidechain
2	D	213	ARG	Sidechain
2	D	486	ARG	Sidechain
2	D	494	ARG	Sidechain

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	3477	0	3234	13	0
1	F	3437	0	3225	23	0
1	J	3316	0	2972	14	0
1	K	3241	0	2847	15	0
2	B	3396	0	3162	18	0
2	C	3350	0	3030	21	0
2	D	3304	0	2996	20	0
2	E	3446	0	3184	19	0
2	G	3376	0	3154	10	0
2	H	3321	0	3003	24	0
2	I	3296	0	3006	19	0
2	L	3427	0	3217	19	0
3	A	62	0	26	1	0
3	B	62	0	26	2	0
3	C	62	0	26	1	0
3	D	62	0	26	2	0
3	E	62	0	26	0	0
3	F	62	0	26	0	0
3	G	62	0	26	0	0
3	H	62	0	26	0	0
3	I	62	0	26	1	0
3	J	62	0	26	2	0
3	K	62	0	26	2	0
3	L	62	0	26	1	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	I	2	0	0	0	0
4	J	1	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
5	A	5	0	0	0	0
5	B	3	0	0	0	0
5	C	4	0	0	0	0
5	D	5	0	0	0	0
5	E	6	0	0	0	0
5	F	5	0	0	0	0
5	G	4	0	0	0	0
5	H	8	0	0	0	0
5	I	4	0	0	0	0
5	J	3	0	0	0	0
5	K	2	0	0	0	0
5	L	5	0	0	0	0
All	All	41205	0	37342	199	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 3.

All (199) 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:C:213:ARG:HG2	2:C:213:ARG:HH21	1.29	0.97
2:B:398:THR:HG21	2:B:431:ILE:HG23	1.65	0.79
2:C:398:THR:HG21	2:C:431:ILE:HG23	1.66	0.77
2:B:183:ILE:HD11	2:C:188:PRO:HA	1.66	0.76
2:D:213:ARG:HH11	2:D:213:ARG:HB2	1.57	0.68
1:F:398:THR:HG21	1:F:431:ILE:CG2	2.24	0.67
2:H:218:VAL:HG23	2:H:235:PHE:CD2	2.31	0.65
2:E:189:ILE:HB	2:E:196:GLU:HG2	1.77	0.64
2:G:206:ARG:NH2	2:G:219:GLU:OE2	2.31	0.63
2:L:218:VAL:HG11	2:L:244:ILE:HD13	1.80	0.63
1:A:218:VAL:HG23	1:A:235:PHE:CD2	2.34	0.62
2:C:449:ARG:NH2	3:C:602:ANP:O2'	2.32	0.62
2:B:447:MET:HE2	2:C:465:ILE:HD11	1.84	0.60
1:K:223:LEU:HD12	1:K:228:HIS:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:ALA:O	2:B:156:SER:N	2.34	0.60
1:F:218:VAL:HG23	1:F:235:PHE:CD2	2.38	0.59
2:H:19:LEU:HG	2:H:36:ILE:HG12	1.84	0.58
2:E:223:LEU:HD12	2:E:228:HIS:HB3	1.85	0.57
2:C:398:THR:HG21	2:C:431:ILE:CG2	2.34	0.57
2:H:205:LEU:HD22	2:H:218:VAL:HG22	1.87	0.57
1:J:484:PHE:HB2	1:J:487:ILE:HD11	1.87	0.56
2:G:218:VAL:HG23	2:G:235:PHE:CD2	2.41	0.56
2:D:488:ILE:HG21	2:C:418:MET:HG3	1.88	0.56
2:C:281:ILE:HG13	2:C:398:THR:HG23	1.88	0.55
1:F:205:LEU:HD22	1:F:218:VAL:HG22	1.89	0.55
1:J:237:ILE:HD13	1:J:242:ILE:HD13	1.88	0.55
1:F:281:ILE:HG13	1:F:398:THR:HG23	1.88	0.55
2:E:246:PRO:HB2	2:E:249:ALA:HB3	1.88	0.55
1:F:18:LYS:HE3	1:F:226:THR:HG21	1.89	0.55
2:D:213:ARG:HH11	2:D:213:ARG:CB	2.19	0.55
2:I:206:ARG:NH2	2:I:219:GLU:OE2	2.40	0.55
1:A:449:ARG:NH2	3:A:601:ANP:O2'	2.40	0.55
1:A:206:ARG:NH2	1:A:219:GLU:OE2	2.39	0.54
2:C:394:VAL:HG12	2:C:431:ILE:HD13	1.90	0.54
1:F:223:LEU:HD12	1:F:228:HIS:HB3	1.88	0.54
2:B:206:ARG:NH2	2:B:219:GLU:OE2	2.41	0.54
2:L:29:ILE:HG22	2:L:220:ILE:HD12	1.90	0.53
2:H:281:ILE:HG23	2:H:410:PHE:CE1	2.43	0.53
2:B:309:ARG:NH1	2:B:369:LYS:O	2.41	0.53
2:H:441:VAL:HG11	2:H:487:ILE:HG23	1.91	0.53
1:K:420:SER:HB3	1:K:437:LEU:HD11	1.91	0.53
2:L:281:ILE:HG13	2:L:398:THR:HG23	1.90	0.53
2:C:145:VAL:O	2:C:148:VAL:HG12	2.08	0.52
2:H:429:SER:O	2:H:455:LYS:NZ	2.43	0.52
1:J:216:ARG:HB3	1:J:235:PHE:CE2	2.45	0.52
2:I:218:VAL:HG23	2:I:235:PHE:CD2	2.45	0.52
1:A:442:GLU:HB2	2:B:488:ILE:HD11	1.92	0.52
2:D:213:ARG:HB2	2:D:213:ARG:NH1	2.25	0.51
2:C:342:LEU:HD13	2:C:343:LYS:N	2.26	0.51
2:L:16:VAL:HB	2:L:226:THR:HG23	1.92	0.51
1:J:189:ILE:HB	1:J:196:GLU:HG2	1.92	0.51
2:I:216:ARG:HB3	2:I:235:PHE:CE2	2.45	0.51
2:I:449:ARG:NH1	3:I:602:ANP:O2'	2.44	0.51
1:F:398:THR:HG21	1:F:431:ILE:HG23	1.92	0.50
2:E:218:VAL:HG23	2:E:235:PHE:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:GLY:O	2:B:449:ARG:NH1	2.44	0.50
2:H:154:ALA:HB1	2:H:157:VAL:HG12	1.94	0.50
1:K:484:PHE:HB2	1:K:487:ILE:HD11	1.92	0.50
2:D:213:ARG:HH11	2:D:213:ARG:CG	2.24	0.50
2:E:47:GLY:O	2:E:216:ARG:NH2	2.44	0.50
2:B:354:LEU:HD22	2:B:385:VAL:HG11	1.93	0.50
1:F:424:THR:O	1:F:426:SER:N	2.44	0.50
1:F:145:VAL:O	1:F:148:VAL:HG12	2.12	0.50
1:K:449:ARG:NH2	3:K:602:ANP:O2'	2.45	0.50
1:K:218:VAL:HG23	1:K:235:PHE:CD2	2.48	0.49
2:L:223:LEU:HD12	2:L:228:HIS:HB3	1.93	0.49
1:F:287:ALA:HB2	1:F:417:PHE:HA	1.93	0.49
2:D:40:THR:HA	2:D:201:ASN:HB2	1.93	0.49
2:G:422:SER:O	2:G:423:ILE:C	2.50	0.49
1:F:417:PHE:HB2	1:A:454:PHE:HZ	1.78	0.49
2:D:16:VAL:HB	2:D:226:THR:HG23	1.95	0.49
2:E:205:LEU:HD22	2:E:218:VAL:HG22	1.94	0.49
2:B:121:LEU:O	2:B:123:ALA:N	2.46	0.49
2:I:169:LEU:HD13	2:I:176:THR:HG21	1.94	0.48
2:C:466:ARG:NH1	2:C:478:LYS:O	2.46	0.48
2:G:354:LEU:HD22	2:G:385:VAL:HG11	1.95	0.48
2:D:441:VAL:HG11	2:D:487:ILE:HG23	1.96	0.48
1:K:417:PHE:HB2	2:L:454:PHE:CZ	2.48	0.48
1:K:299:PHE:CZ	1:K:372:ARG:HD3	2.49	0.48
2:D:206:ARG:NH2	2:D:219:GLU:OE2	2.46	0.48
2:D:323:LEU:HD23	2:D:333:PHE:HB2	1.96	0.48
2:B:449:ARG:NH2	3:B:602:ANP:O2'	2.46	0.48
2:G:207:ASN:HD21	2:G:214:ARG:HB3	1.78	0.47
2:G:189:ILE:HB	2:G:196:GLU:HG2	1.95	0.47
2:H:418:MET:HG3	2:I:488:ILE:HG21	1.97	0.47
2:I:346:CYS:HB3	1:J:252:LEU:HB3	1.96	0.47
2:E:260:ARG:HH22	2:E:459:SER:CB	2.28	0.47
1:K:214:ARG:HD2	2:L:219:GLU:OE1	2.15	0.46
1:K:323:LEU:HD23	1:K:333:PHE:HB2	1.97	0.46
1:F:303:ALA:HB2	1:F:372:ARG:HD2	1.97	0.46
1:F:154:ALA:O	1:F:156:SER:N	2.49	0.46
2:H:281:ILE:HG23	2:H:410:PHE:CD1	2.51	0.46
2:L:87:SER:OG	3:L:601:ANP:N6	2.43	0.46
1:J:223:LEU:HD12	1:J:228:HIS:HB3	1.96	0.46
2:L:342:LEU:HD13	2:L:343:LYS:N	2.31	0.46
2:I:50:LYS:HD2	2:I:179:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:SER:HB3	3:B:601:ANP:HN61	1.81	0.46
1:A:299:PHE:CZ	1:A:372:ARG:HD3	2.50	0.46
2:L:424:THR:O	2:L:425:ASP:C	2.54	0.46
2:E:218:VAL:HG23	2:E:235:PHE:CE2	2.51	0.46
2:B:467:GLU:HB3	2:B:478:LYS:HB2	1.97	0.46
1:F:162:ILE:HG22	1:F:198:VAL:HG11	1.98	0.45
1:F:189:ILE:HB	1:F:196:GLU:HG2	1.98	0.45
2:C:14:THR:O	2:C:15:ALA:HB3	2.15	0.45
2:C:143:ASP:HA	2:C:144:SER:HA	1.75	0.45
2:I:121:LEU:O	2:I:123:ALA:N	2.49	0.45
2:D:223:LEU:HD12	2:D:228:HIS:HB3	1.97	0.45
2:D:449:ARG:NH2	3:D:602:ANP:O2'	2.50	0.45
2:D:483:ASN:HB2	2:D:494:ARG:NH2	2.31	0.45
2:B:145:VAL:O	2:B:148:VAL:HG12	2.17	0.45
1:J:449:ARG:NH2	3:J:602:ANP:O2'	2.49	0.45
2:H:162:ILE:HG22	2:H:198:VAL:HG11	1.99	0.45
2:H:381:LEU:HD13	2:H:393:PHE:CE2	2.51	0.45
2:D:442:GLU:O	2:D:492:PRO:HD2	2.16	0.45
2:I:143:ASP:HA	2:I:144:SER:HA	1.79	0.45
2:H:154:ALA:O	2:H:156:SER:N	2.50	0.45
1:A:336:MET:HB2	1:A:342:LEU:HB2	2.00	0.44
2:E:143:ASP:HA	2:E:144:SER:HA	1.72	0.44
2:I:302:ASN:ND2	2:I:305:ARG:HH11	2.15	0.44
2:B:143:ASP:HA	2:B:144:SER:HA	1.71	0.44
2:C:223:LEU:HD12	2:C:228:HIS:HB3	1.99	0.44
1:F:143:ASP:HA	1:F:144:SER:HA	1.71	0.44
1:F:308:GLU:HB3	1:F:371:SER:OG	2.18	0.44
2:B:223:LEU:HD12	2:B:228:HIS:HB3	1.99	0.44
2:C:250:MET:SD	2:C:399:GLY:HA3	2.58	0.44
2:L:381:LEU:HD13	2:L:393:PHE:CE2	2.52	0.44
1:J:143:ASP:HA	1:J:144:SER:HA	1.72	0.44
1:J:376:ASP:HA	1:J:377:SER:HA	1.76	0.44
2:I:466:ARG:HA	2:I:480:SER:HA	1.98	0.44
1:F:376:ASP:HA	1:F:377:SER:HA	1.76	0.44
2:H:143:ASP:HA	2:H:144:SER:HA	1.69	0.44
2:L:189:ILE:HB	2:L:196:GLU:HG2	2.00	0.44
2:D:354:LEU:HD22	2:D:385:VAL:HG11	1.98	0.43
2:E:292:LYS:HG3	2:E:438:LEU:HD12	2.00	0.43
2:C:213:ARG:HG2	2:C:213:ARG:NH2	2.08	0.43
1:J:417:PHE:CD1	1:J:417:PHE:C	2.92	0.43
1:A:223:LEU:HD12	1:A:228:HIS:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:19:LEU:HD22	2:I:139:ARG:NH2	2.33	0.43
2:G:449:ARG:HG3	2:G:468:PHE:O	2.18	0.43
2:H:150:GLN:OE1	2:I:159:ARG:NH1	2.51	0.43
2:H:481:PHE:HB2	2:H:487:ILE:HD13	2.01	0.43
2:C:434:THR:HG23	2:C:456:MET:HG2	1.99	0.43
2:G:447:MET:N	2:H:463:LYS:O	2.42	0.43
1:K:303:ALA:HB2	1:K:372:ARG:HD2	2.01	0.43
2:H:223:LEU:HD12	2:H:228:HIS:HB3	2.00	0.43
2:B:189:ILE:HB	2:B:196:GLU:HG2	2.00	0.43
1:J:59:TYR:CE1	1:J:63:THR:HG21	2.54	0.43
2:G:223:LEU:HD12	2:G:228:HIS:HB3	2.01	0.43
2:B:376:ASP:HA	2:B:377:SER:HA	1.77	0.43
2:I:189:ILE:HB	2:I:196:GLU:HG2	2.00	0.43
1:K:205:LEU:HD22	1:K:218:VAL:HG22	2.01	0.42
1:F:121:LEU:HD23	1:F:121:LEU:HA	1.93	0.42
1:A:16:VAL:HB	1:A:226:THR:HG23	2.00	0.42
2:H:25:GLY:HA3	2:H:244:ILE:O	2.19	0.42
2:L:265:VAL:HG22	2:L:475:PRO:HG3	2.01	0.42
2:L:398:THR:HG21	2:L:431:ILE:HG12	2.01	0.42
2:I:336:MET:HB2	2:I:342:LEU:HB2	1.99	0.42
2:D:381:LEU:HD13	2:D:393:PHE:CE2	2.55	0.42
1:A:381:LEU:HD13	1:A:393:PHE:CE2	2.54	0.42
2:E:299:PHE:CZ	2:E:372:ARG:HD3	2.54	0.42
2:C:336:MET:HB3	2:C:342:LEU:HB2	2.01	0.42
2:H:19:LEU:HD23	2:H:19:LEU:HA	1.94	0.42
1:K:376:ASP:HA	1:K:377:SER:HA	1.81	0.42
2:E:365:ILE:O	2:E:370:PRO:HD3	2.20	0.42
1:F:373:ILE:HG22	1:F:408:GLY:HA2	2.01	0.42
1:K:381:LEU:HD13	1:K:393:PHE:CE2	2.54	0.42
2:D:143:ASP:HA	2:D:144:SER:HA	1.77	0.41
2:H:354:LEU:HD22	2:H:385:VAL:HG11	2.02	0.41
1:A:216:ARG:HB3	1:A:235:PHE:CE2	2.55	0.41
2:H:450:ALA:HA	2:H:466:ARG:O	2.21	0.41
1:F:168:ARG:HD3	2:E:110:PRO:O	2.21	0.41
2:D:213:ARG:HA	2:D:213:ARG:HD3	1.83	0.41
2:C:16:VAL:HB	2:C:226:THR:HG23	2.03	0.41
2:I:418:MET:HG3	1:J:488:ILE:HG12	2.01	0.41
2:G:213:ARG:NH2	2:H:230:LYS:O	2.53	0.41
3:D:602:ANP:HO2'	2:E:461:HIS:CD2	2.39	0.41
2:H:373:ILE:HG22	2:H:408:GLY:HA2	2.02	0.41
1:K:216:ARG:HB2	1:K:235:PHE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:165:LEU:HD23	2:L:165:LEU:HA	1.90	0.41
1:J:395:ILE:HD13	1:J:431:ILE:HD12	2.02	0.41
1:F:252:LEU:HD13	1:F:252:LEU:HA	1.94	0.41
2:D:351:SER:HA	2:E:248:GLY:CA	2.50	0.41
2:E:281:ILE:HG13	2:E:398:THR:HG23	2.02	0.41
1:K:418:MET:HG3	2:L:488:ILE:HG21	2.03	0.41
2:L:143:ASP:HA	2:L:144:SER:HA	1.78	0.41
2:L:376:ASP:HA	2:L:377:SER:HA	1.77	0.41
1:A:441:VAL:HG11	1:A:487:ILE:HG23	2.02	0.40
1:A:486:ARG:NH2	1:A:493:THR:OG1	2.54	0.40
3:K:601:ANP:O3'	2:L:223:LEU:N	2.52	0.40
2:I:285:THR:HG22	2:I:412:ASN:HD22	1.86	0.40
2:I:467:GLU:HB3	2:I:478:LYS:HB2	2.02	0.40
2:E:140:VAL:HG23	2:E:174:VAL:HG11	2.03	0.40
2:E:308:GLU:HB3	2:E:371:SER:OG	2.21	0.40
2:H:206:ARG:NH2	2:H:219:GLU:OE2	2.55	0.40
2:D:429:SER:O	2:D:455:LYS:NZ	2.55	0.40
2:C:213:ARG:HA	2:C:213:ARG:HD3	1.91	0.40
1:J:87:SER:OG	3:J:601:ANP:N6	2.53	0.40
1:F:299:PHE:CZ	1:F:372:ARG:HD3	2.57	0.40
2:E:221:LEU:HD23	2:E:221:LEU:HA	1.97	0.40

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	466/515 (90%)	444 (95%)	21 (4%)	1 (0%)	44	66
1	F	464/515 (90%)	437 (94%)	23 (5%)	4 (1%)	14	35
1	J	459/515 (89%)	436 (95%)	22 (5%)	1 (0%)	44	66
1	K	451/515 (88%)	434 (96%)	15 (3%)	2 (0%)	30	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	468/515 (91%)	441 (94%)	23 (5%)	4 (1%)	14	35
2	C	465/515 (90%)	429 (92%)	33 (7%)	3 (1%)	22	46
2	D	454/515 (88%)	426 (94%)	28 (6%)	0	100	100
2	E	472/515 (92%)	440 (93%)	27 (6%)	5 (1%)	12	30
2	G	458/515 (89%)	438 (96%)	17 (4%)	3 (1%)	19	41
2	H	467/515 (91%)	435 (93%)	28 (6%)	4 (1%)	14	35
2	I	460/515 (89%)	436 (95%)	21 (5%)	3 (1%)	19	41
2	L	465/515 (90%)	433 (93%)	31 (7%)	1 (0%)	44	66
All	All	5549/6180 (90%)	5229 (94%)	289 (5%)	31 (1%)	22	46

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	153	ASP
2	B	155	ALA
2	C	108	PRO
1	F	155	ALA
1	A	194	VAL
2	E	152	TYR
2	E	457	ARG
2	B	122	SER
2	B	420	SER
2	G	151	GLN
2	G	423	ILE
2	H	157	VAL
1	K	64	HIS
1	F	152	TYR
1	F	425	ASP
2	E	256	SER
2	H	153	ASP
1	K	422	SER
2	I	421	HIS
1	J	250	MET
2	C	152	TYR
2	H	155	ALA
2	I	64	HIS
2	E	154	ALA
2	I	194	VAL
2	G	75	GLU

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Mol	Chain	Res	Type
2	L	424	THR
2	C	194	VAL
2	H	194	VAL
1	F	194	VAL
2	B	419	GLY

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	332/442 (75%)	316 (95%)	16 (5%)	21	44
1	F	334/442 (76%)	315 (94%)	19 (6%)	17	37
1	J	300/442 (68%)	280 (93%)	20 (7%)	13	31
1	K	287/442 (65%)	270 (94%)	17 (6%)	16	36
2	B	325/443 (73%)	305 (94%)	20 (6%)	15	34
2	C	309/443 (70%)	287 (93%)	22 (7%)	12	29
2	D	304/443 (69%)	282 (93%)	22 (7%)	12	29
2	E	326/443 (74%)	310 (95%)	16 (5%)	21	43
2	G	323/443 (73%)	299 (93%)	24 (7%)	11	27
2	H	296/443 (67%)	283 (96%)	13 (4%)	24	48
2	I	300/443 (68%)	284 (95%)	16 (5%)	19	40
2	L	330/443 (74%)	308 (93%)	22 (7%)	13	31
All	All	3766/5312 (71%)	3539 (94%)	227 (6%)	16	35

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	62	ILE
1	F	79	GLN
1	F	146	THR
1	F	174	VAL
1	F	184	GLU

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Mol	Chain	Res	Type
1	F	194	VAL
1	F	221	LEU
1	F	230	LYS
1	F	252	LEU
1	F	268	LEU
1	F	335	GLU
1	F	342	LEU
1	F	352	THR
1	F	354	LEU
1	F	358	LEU
1	F	417	PHE
1	F	418	MET
1	F	441	VAL
1	F	456	MET
1	A	133	ARG
1	A	146	THR
1	A	148	VAL
1	A	160	ARG
1	A	221	LEU
1	A	226	THR
1	A	254	GLN
1	A	268	LEU
1	A	336	MET
1	A	342	LEU
1	A	352	THR
1	A	354	LEU
1	A	358	LEU
1	A	441	VAL
1	A	456	MET
1	A	468	PHE
2	D	79	GLN
2	D	140	VAL
2	D	142	ILE
2	D	146	THR
2	D	157	VAL
2	D	164	ARG
2	D	207	ASN
2	D	210	GLU
2	D	213	ARG
2	D	217	THR
2	D	218	VAL
2	D	221	LEU

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Mol	Chain	Res	Type
2	D	226	THR
2	D	268	LEU
2	D	354	LEU
2	D	358	LEU
2	D	364	GLU
2	D	418	MET
2	D	441	VAL
2	D	456	MET
2	D	486	ARG
2	D	494	ARG
2	E	79	GLN
2	E	146	THR
2	E	148	VAL
2	E	194	VAL
2	E	200	ASP
2	E	217	THR
2	E	221	LEU
2	E	226	THR
2	E	268	LEU
2	E	279	ASP
2	E	342	LEU
2	E	354	LEU
2	E	415	ASP
2	E	418	MET
2	E	441	VAL
2	E	456	MET
2	B	79	GLN
2	B	142	ILE
2	B	174	VAL
2	B	178	MET
2	B	183	ILE
2	B	194	VAL
2	B	213	ARG
2	B	221	LEU
2	B	226	THR
2	B	252	LEU
2	B	254	GLN
2	B	268	LEU
2	B	285	THR
2	B	358	LEU
2	B	404	GLU
2	B	418	MET

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Mol	Chain	Res	Type
2	B	430	THR
2	B	441	VAL
2	B	456	MET
2	B	478	LYS
2	C	79	GLN
2	C	142	ILE
2	C	146	THR
2	C	184	GLU
2	C	200	ASP
2	C	207	ASN
2	C	213	ARG
2	C	221	LEU
2	C	226	THR
2	C	250	MET
2	C	254	GLN
2	C	268	LEU
2	C	319	ARG
2	C	321	GLN
2	C	354	LEU
2	C	358	LEU
2	C	373	ILE
2	C	404	GLU
2	C	441	VAL
2	C	456	MET
2	C	468	PHE
2	C	469	VAL
2	G	146	THR
2	G	148	VAL
2	G	157	VAL
2	G	180	THR
2	G	194	VAL
2	G	207	ASN
2	G	221	LEU
2	G	226	THR
2	G	267	ARG
2	G	268	LEU
2	G	342	LEU
2	G	354	LEU
2	G	358	LEU
2	G	373	ILE
2	G	409	PHE
2	G	417	PHE

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Mol	Chain	Res	Type
2	G	418	MET
2	G	428	ILE
2	G	437	LEU
2	G	441	VAL
2	G	449	ARG
2	G	456	MET
2	G	468	PHE
2	G	494	ARG
2	H	79	GLN
2	H	146	THR
2	H	180	THR
2	H	194	VAL
2	H	215	ARG
2	H	221	LEU
2	H	268	LEU
2	H	324	ARG
2	H	358	LEU
2	H	364	GLU
2	H	417	PHE
2	H	441	VAL
2	H	456	MET
1	K	28	ASP
1	K	79	GLN
1	K	180	THR
1	K	218	VAL
1	K	221	LEU
1	K	226	THR
1	K	238	THR
1	K	268	LEU
1	K	285	THR
1	K	336	MET
1	K	342	LEU
1	K	385	VAL
1	K	409	PHE
1	K	417	PHE
1	K	456	MET
1	K	468	PHE
1	K	483	ASN
2	L	83	LYS
2	L	124	LEU
2	L	142	ILE
2	L	150	GLN

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Mol	Chain	Res	Type
2	L	165	LEU
2	L	194	VAL
2	L	207	ASN
2	L	209	LEU
2	L	221	LEU
2	L	226	THR
2	L	252	LEU
2	L	254	GLN
2	L	268	LEU
2	L	305	ARG
2	L	345	ILE
2	L	358	LEU
2	L	373	ILE
2	L	418	MET
2	L	431	ILE
2	L	441	VAL
2	L	446	GLU
2	L	456	MET
2	I	19	LEU
2	I	142	ILE
2	I	145	VAL
2	I	180	THR
2	I	194	VAL
2	I	213	ARG
2	I	221	LEU
2	I	226	THR
2	I	268	LEU
2	I	285	THR
2	I	336	MET
2	I	342	LEU
2	I	352	THR
2	I	354	LEU
2	I	409	PHE
2	I	456	MET
1	J	145	VAL
1	J	157	VAL
1	J	178	MET
1	J	191	ARG
1	J	219	GLU
1	J	221	LEU
1	J	226	THR
1	J	252	LEU

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Mol	Chain	Res	Type
1	J	255	ARG
1	J	268	LEU
1	J	323	LEU
1	J	342	LEU
1	J	354	LEU
1	J	358	LEU
1	J	404	GLU
1	J	415	ASP
1	J	417	PHE
1	J	418	MET
1	J	456	MET
1	J	468	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	31	HIS
1	A	93	GLN
1	A	207	ASN
2	D	207	ASN
2	E	207	ASN
2	E	412	ASN
2	B	31	HIS
2	B	412	ASN
2	C	31	HIS
2	C	207	ASN
2	C	306	ASN
2	C	412	ASN
2	G	31	HIS
2	G	207	ASN
2	G	412	ASN
2	G	452	ASN
2	H	31	HIS
2	H	207	ASN
2	H	452	ASN
1	K	207	ASN
2	L	207	ASN
2	L	306	ASN
2	L	452	ASN
2	I	93	GLN
2	I	207	ASN
2	I	412	ASN

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Mol	Chain	Res	Type
1	J	207	ASN
1	J	412	ASN
1	J	416	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)

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	SEP	F	429	1	8,9,10	0.62	0	8,12,14	0.63	0
1	SEP	J	429	1	8,9,10	0.59	0	8,12,14	0.67	0
1	SEP	A	429	1	8,9,10	0.61	0	8,12,14	0.63	0
1	SEP	K	429	1	8,9,10	0.60	0	8,12,14	0.64	0

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	SEP	F	429	1	-	5/5/8/10	-
1	SEP	J	429	1	-	4/5/8/10	-
1	SEP	A	429	1	-	3/5/8/10	-
1	SEP	K	429	1	-	1/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	429	SEP	N-CA-CB-OG
1	F	429	SEP	CB-OG-P-O1P
1	F	429	SEP	CB-OG-P-O2P
1	F	429	SEP	CB-OG-P-O3P
1	A	429	SEP	CB-OG-P-O2P
1	A	429	SEP	CB-OG-P-O3P
1	K	429	SEP	N-CA-CB-OG
1	J	429	SEP	CB-OG-P-O2P
1	J	429	SEP	CB-OG-P-O3P
1	A	429	SEP	CB-OG-P-O1P
1	J	429	SEP	CB-OG-P-O1P
1	J	429	SEP	CA-CB-OG-P
1	F	429	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 44 ligands modelled in this entry, 20 are monoatomic - leaving 24 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	E	601	4	29,33,33	1.20	5 (17%)	31,52,52	1.11	2 (6%)
3	ANP	D	601	-	29,33,33	1.19	5 (17%)	31,52,52	1.11	2 (6%)
3	ANP	A	602	4	29,33,33	1.19	5 (17%)	31,52,52	1.09	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ANP	I	602	4	29,33,33	1.20	5 (17%)	31,52,52	1.13	2 (6%)
3	ANP	G	601	4	29,33,33	1.19	5 (17%)	31,52,52	1.16	3 (9%)
3	ANP	H	601	4	29,33,33	1.19	5 (17%)	31,52,52	1.11	3 (9%)
3	ANP	F	602	4	29,33,33	1.20	5 (17%)	31,52,52	1.19	2 (6%)
3	ANP	J	601	-	29,33,33	1.20	5 (17%)	31,52,52	1.09	2 (6%)
3	ANP	H	602	4	29,33,33	1.21	5 (17%)	31,52,52	1.14	2 (6%)
3	ANP	L	602	4	29,33,33	1.19	5 (17%)	31,52,52	1.19	3 (9%)
3	ANP	J	602	4	29,33,33	1.22	5 (17%)	31,52,52	1.13	3 (9%)
3	ANP	B	601	-	29,33,33	1.19	5 (17%)	31,52,52	1.09	2 (6%)
3	ANP	K	601	4	29,33,33	1.20	5 (17%)	31,52,52	1.15	3 (9%)
3	ANP	F	601	4	29,33,33	1.22	5 (17%)	31,52,52	1.09	2 (6%)
3	ANP	K	602	4	29,33,33	1.22	5 (17%)	31,52,52	1.13	3 (9%)
3	ANP	G	602	4	29,33,33	1.20	5 (17%)	31,52,52	1.13	3 (9%)
3	ANP	E	602	4	29,33,33	1.21	5 (17%)	31,52,52	1.12	2 (6%)
3	ANP	L	601	4	29,33,33	1.20	5 (17%)	31,52,52	1.10	2 (6%)
3	ANP	A	601	4	29,33,33	1.19	5 (17%)	31,52,52	1.15	2 (6%)
3	ANP	B	602	4	29,33,33	1.19	5 (17%)	31,52,52	1.15	2 (6%)
3	ANP	C	602	4	29,33,33	1.19	5 (17%)	31,52,52	1.08	2 (6%)
3	ANP	I	601	4	29,33,33	1.20	5 (17%)	31,52,52	1.11	2 (6%)
3	ANP	D	602	4	29,33,33	1.18	5 (17%)	31,52,52	1.14	2 (6%)
3	ANP	C	601	-	29,33,33	1.20	5 (17%)	31,52,52	1.14	2 (6%)

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	E	601	4	-	8/14/38/38	0/3/3/3
3	ANP	D	601	-	-	5/14/38/38	0/3/3/3
3	ANP	A	602	4	-	5/14/38/38	0/3/3/3
3	ANP	I	602	4	-	3/14/38/38	0/3/3/3
3	ANP	G	601	4	-	9/14/38/38	0/3/3/3
3	ANP	H	601	4	-	7/14/38/38	0/3/3/3
3	ANP	F	602	4	-	3/14/38/38	0/3/3/3
3	ANP	J	601	-	-	7/14/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	H	602	4	-	6/14/38/38	0/3/3/3
3	ANP	L	602	4	-	3/14/38/38	0/3/3/3
3	ANP	J	602	4	-	6/14/38/38	0/3/3/3
3	ANP	B	601	-	-	5/14/38/38	0/3/3/3
3	ANP	K	601	4	-	4/14/38/38	0/3/3/3
3	ANP	F	601	4	-	4/14/38/38	0/3/3/3
3	ANP	K	602	4	-	6/14/38/38	0/3/3/3
3	ANP	G	602	4	-	6/14/38/38	0/3/3/3
3	ANP	E	602	4	-	3/14/38/38	0/3/3/3
3	ANP	L	601	4	-	8/14/38/38	0/3/3/3
3	ANP	A	601	4	-	3/14/38/38	0/3/3/3
3	ANP	B	602	4	-	6/14/38/38	0/3/3/3
3	ANP	C	602	4	-	1/14/38/38	0/3/3/3
3	ANP	I	601	4	-	5/14/38/38	0/3/3/3
3	ANP	D	602	4	-	5/14/38/38	0/3/3/3
3	ANP	C	601	-	-	2/14/38/38	0/3/3/3

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	601	ANP	PG-O1G	3.30	1.51	1.46
3	L	601	ANP	PG-O1G	3.22	1.51	1.46
3	J	601	ANP	PG-O1G	3.21	1.51	1.46
3	J	602	ANP	PG-O1G	3.21	1.51	1.46
3	G	601	ANP	PG-O1G	3.18	1.51	1.46
3	H	602	ANP	PG-O1G	3.17	1.51	1.46
3	C	601	ANP	PG-O1G	3.17	1.51	1.46
3	K	601	ANP	PG-O1G	3.17	1.51	1.46
3	I	601	ANP	PG-O1G	3.16	1.51	1.46
3	B	601	ANP	PG-O1G	3.15	1.51	1.46
3	F	602	ANP	PG-O1G	3.15	1.51	1.46
3	A	602	ANP	PG-O1G	3.14	1.51	1.46
3	D	601	ANP	PG-O1G	3.14	1.51	1.46
3	K	602	ANP	PG-O1G	3.12	1.51	1.46
3	E	601	ANP	PG-O1G	3.11	1.51	1.46
3	G	602	ANP	PG-O1G	3.10	1.51	1.46
3	E	602	ANP	PG-O1G	3.09	1.51	1.46
3	H	601	ANP	PG-O1G	3.07	1.51	1.46
3	L	602	ANP	PG-O1G	3.03	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	ANP	PG-O1G	3.02	1.50	1.46
3	I	602	ANP	PG-O1G	3.01	1.50	1.46
3	A	601	ANP	PG-O1G	2.99	1.50	1.46
3	E	602	ANP	PB-O1B	2.96	1.50	1.46
3	E	601	ANP	PB-O1B	2.95	1.50	1.46
3	K	601	ANP	PB-O1B	2.95	1.50	1.46
3	C	602	ANP	PG-O1G	2.95	1.50	1.46
3	A	601	ANP	PB-O1B	2.94	1.50	1.46
3	L	602	ANP	PB-O1B	2.93	1.50	1.46
3	D	601	ANP	PB-O1B	2.92	1.50	1.46
3	H	602	ANP	PB-O1B	2.92	1.50	1.46
3	I	602	ANP	PB-O1B	2.92	1.50	1.46
3	D	602	ANP	PB-O1B	2.92	1.50	1.46
3	I	601	ANP	PB-O1B	2.91	1.50	1.46
3	K	602	ANP	PB-O1B	2.90	1.50	1.46
3	J	601	ANP	PB-O1B	2.90	1.50	1.46
3	G	601	ANP	PB-O1B	2.89	1.50	1.46
3	A	602	ANP	PB-O1B	2.89	1.50	1.46
3	B	602	ANP	PB-O1B	2.88	1.50	1.46
3	J	602	ANP	PB-O1B	2.88	1.50	1.46
3	H	601	ANP	PB-O1B	2.88	1.50	1.46
3	F	602	ANP	PB-O1B	2.88	1.50	1.46
3	C	602	ANP	PB-O1B	2.87	1.50	1.46
3	F	601	ANP	PB-O1B	2.87	1.50	1.46
3	C	601	ANP	PB-O1B	2.87	1.50	1.46
3	B	601	ANP	PB-O1B	2.87	1.50	1.46
3	L	601	ANP	PB-O1B	2.87	1.50	1.46
3	G	602	ANP	PB-O1B	2.84	1.50	1.46
3	D	602	ANP	PG-O1G	2.84	1.50	1.46
3	D	602	ANP	PG-O2G	-2.35	1.50	1.56
3	K	602	ANP	PG-O3G	-2.30	1.50	1.56
3	B	602	ANP	PG-O2G	-2.27	1.50	1.56
3	H	601	ANP	PB-O2B	-2.26	1.50	1.56
3	A	601	ANP	PB-O2B	-2.26	1.50	1.56
3	B	601	ANP	PB-O2B	-2.26	1.50	1.56
3	L	602	ANP	PB-O2B	-2.25	1.50	1.56
3	D	601	ANP	PG-O2G	-2.25	1.50	1.56
3	C	601	ANP	PB-O2B	-2.25	1.50	1.56
3	E	601	ANP	PG-O2G	-2.25	1.50	1.56
3	C	602	ANP	PB-O2B	-2.24	1.50	1.56
3	D	601	ANP	PB-O2B	-2.24	1.50	1.56
3	J	602	ANP	PG-O2G	-2.24	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	602	ANP	PG-O2G	-2.24	1.50	1.56
3	A	602	ANP	PB-O2B	-2.24	1.50	1.56
3	E	602	ANP	PB-O2B	-2.24	1.50	1.56
3	G	602	ANP	PB-O2B	-2.23	1.50	1.56
3	L	601	ANP	PB-O2B	-2.23	1.50	1.56
3	J	602	ANP	PB-O2B	-2.23	1.50	1.56
3	J	601	ANP	PB-O2B	-2.22	1.50	1.56
3	H	602	ANP	PG-O3G	-2.22	1.50	1.56
3	C	602	ANP	PG-O2G	-2.22	1.50	1.56
3	B	602	ANP	PB-O2B	-2.22	1.50	1.56
3	F	601	ANP	PB-O2B	-2.22	1.50	1.56
3	G	601	ANP	PB-O2B	-2.22	1.50	1.56
3	H	602	ANP	PB-O2B	-2.22	1.50	1.56
3	I	601	ANP	PB-O2B	-2.21	1.50	1.56
3	K	601	ANP	PB-O2B	-2.21	1.50	1.56
3	E	601	ANP	PB-O2B	-2.21	1.50	1.56
3	F	602	ANP	PG-O2G	-2.21	1.50	1.56
3	F	601	ANP	PG-O2G	-2.21	1.50	1.56
3	K	601	ANP	PG-O2G	-2.20	1.50	1.56
3	F	602	ANP	PB-O2B	-2.20	1.50	1.56
3	L	601	ANP	PG-O2G	-2.20	1.50	1.56
3	A	601	ANP	PG-O3G	-2.19	1.50	1.56
3	K	602	ANP	PB-O2B	-2.19	1.50	1.56
3	D	602	ANP	PB-O2B	-2.19	1.50	1.56
3	H	601	ANP	PG-O3G	-2.19	1.50	1.56
3	C	601	ANP	PG-O2G	-2.19	1.50	1.56
3	I	602	ANP	PG-O3G	-2.19	1.50	1.56
3	L	601	ANP	PG-O3G	-2.19	1.50	1.56
3	F	602	ANP	PG-O3G	-2.18	1.50	1.56
3	C	602	ANP	PG-O3G	-2.18	1.50	1.56
3	L	602	ANP	PG-O2G	-2.18	1.50	1.56
3	H	602	ANP	PG-O2G	-2.18	1.50	1.56
3	E	602	ANP	PG-O3G	-2.18	1.50	1.56
3	G	601	ANP	PG-O2G	-2.17	1.50	1.56
3	I	602	ANP	PB-O2B	-2.17	1.50	1.56
3	J	602	ANP	PG-O3G	-2.17	1.50	1.56
3	L	602	ANP	PG-O3G	-2.17	1.50	1.56
3	I	601	ANP	PG-O3G	-2.16	1.50	1.56
3	H	601	ANP	PG-O2G	-2.16	1.50	1.56
3	G	602	ANP	PG-O2G	-2.16	1.50	1.56
3	K	602	ANP	PG-O2G	-2.16	1.50	1.56
3	G	601	ANP	PG-O3G	-2.16	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	ANP	PG-O2G	-2.16	1.50	1.56
3	E	601	ANP	PG-O3G	-2.16	1.50	1.56
3	B	602	ANP	PG-O3G	-2.15	1.51	1.56
3	A	601	ANP	PG-O2G	-2.15	1.51	1.56
3	F	601	ANP	PG-O3G	-2.15	1.51	1.56
3	A	602	ANP	PG-O2G	-2.15	1.51	1.56
3	D	602	ANP	PG-O3G	-2.14	1.51	1.56
3	C	601	ANP	PG-O3G	-2.14	1.51	1.56
3	B	601	ANP	PG-O2G	-2.14	1.51	1.56
3	B	601	ANP	PG-O3G	-2.13	1.51	1.56
3	G	602	ANP	PG-O3G	-2.11	1.51	1.56
3	K	601	ANP	PG-O3G	-2.10	1.51	1.56
3	J	601	ANP	PG-O2G	-2.10	1.51	1.56
3	D	601	ANP	PG-O3G	-2.09	1.51	1.56
3	I	601	ANP	PG-O2G	-2.08	1.51	1.56
3	J	601	ANP	PG-O3G	-2.08	1.51	1.56
3	A	602	ANP	PG-O3G	-2.07	1.51	1.56

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	ANP	O2B-PB-O1B	4.28	118.90	109.92
3	J	601	ANP	O2B-PB-O1B	4.23	118.79	109.92
3	G	601	ANP	O2B-PB-O1B	4.23	118.78	109.92
3	L	602	ANP	O2B-PB-O1B	4.22	118.77	109.92
3	I	602	ANP	O2B-PB-O1B	4.21	118.75	109.92
3	H	602	ANP	O2B-PB-O1B	4.21	118.75	109.92
3	A	601	ANP	O2B-PB-O1B	4.18	118.68	109.92
3	C	601	ANP	O2B-PB-O1B	4.17	118.66	109.92
3	K	601	ANP	O2B-PB-O1B	4.16	118.64	109.92
3	J	602	ANP	O2B-PB-O1B	4.16	118.64	109.92
3	D	602	ANP	O2B-PB-O1B	4.15	118.61	109.92
3	I	601	ANP	O2B-PB-O1B	4.15	118.61	109.92
3	A	602	ANP	O2B-PB-O1B	4.14	118.61	109.92
3	L	601	ANP	O2B-PB-O1B	4.14	118.60	109.92
3	C	602	ANP	O2B-PB-O1B	4.14	118.59	109.92
3	D	601	ANP	O2B-PB-O1B	4.14	118.59	109.92
3	G	602	ANP	O2B-PB-O1B	4.13	118.57	109.92
3	H	601	ANP	O2B-PB-O1B	4.11	118.54	109.92
3	F	602	ANP	O2B-PB-O1B	4.11	118.54	109.92
3	E	601	ANP	O2B-PB-O1B	4.11	118.53	109.92
3	K	602	ANP	O2B-PB-O1B	4.10	118.53	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	601	ANP	O2B-PB-O1B	4.10	118.51	109.92
3	E	602	ANP	O2B-PB-O1B	4.06	118.44	109.92
3	F	601	ANP	O2B-PB-O1B	4.04	118.39	109.92
3	B	601	ANP	C5-C6-N6	2.48	124.12	120.35
3	L	601	ANP	C5-C6-N6	2.43	124.04	120.35
3	D	601	ANP	C5-C6-N6	2.42	124.03	120.35
3	H	601	ANP	C5-C6-N6	2.37	123.96	120.35
3	C	601	ANP	C5-C6-N6	2.34	123.91	120.35
3	B	602	ANP	C5-C6-N6	2.33	123.89	120.35
3	G	601	ANP	C5-C6-N6	2.31	123.87	120.35
3	K	602	ANP	O3G-PG-O1G	-2.31	107.66	113.45
3	K	601	ANP	C5-C6-N6	2.28	123.81	120.35
3	D	602	ANP	C5-C6-N6	2.27	123.81	120.35
3	J	601	ANP	C5-C6-N6	2.27	123.80	120.35
3	H	602	ANP	C5-C6-N6	2.27	123.80	120.35
3	J	602	ANP	C5-C6-N6	2.25	123.77	120.35
3	E	602	ANP	C5-C6-N6	2.24	123.76	120.35
3	G	602	ANP	C5-C6-N6	2.23	123.74	120.35
3	C	602	ANP	C5-C6-N6	2.22	123.73	120.35
3	L	602	ANP	C5-C6-N6	2.22	123.73	120.35
3	F	601	ANP	C5-C6-N6	2.22	123.73	120.35
3	A	601	ANP	C5-C6-N6	2.20	123.70	120.35
3	A	602	ANP	C5-C6-N6	2.19	123.69	120.35
3	K	602	ANP	C5-C6-N6	2.18	123.66	120.35
3	I	601	ANP	C5-C6-N6	2.17	123.65	120.35
3	E	601	ANP	C5-C6-N6	2.15	123.62	120.35
3	F	602	ANP	C5-C6-N6	2.15	123.62	120.35
3	J	602	ANP	O3G-PG-O1G	-2.14	108.07	113.45
3	G	601	ANP	O2G-PG-O1G	-2.14	108.08	113.45
3	I	602	ANP	C5-C6-N6	2.11	123.56	120.35
3	K	601	ANP	O3G-PG-O1G	-2.08	108.23	113.45
3	L	602	ANP	C3'-C2'-C1'	2.06	104.09	100.98
3	H	601	ANP	O2G-PG-O1G	-2.04	108.31	113.45
3	G	602	ANP	O2G-PG-O1G	-2.03	108.34	113.45

There are no chirality outliers.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	601	ANP	PB-N3B-PG-O1G
3	F	601	ANP	PG-N3B-PB-O1B
3	F	601	ANP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
3	F	601	ANP	PA-O3A-PB-O2B
3	F	602	ANP	PB-N3B-PG-O1G
3	F	602	ANP	PG-N3B-PB-O1B
3	F	602	ANP	PG-N3B-PB-O3A
3	A	601	ANP	PB-N3B-PG-O1G
3	A	601	ANP	PG-N3B-PB-O1B
3	A	602	ANP	PB-N3B-PG-O1G
3	A	602	ANP	PG-N3B-PB-O1B
3	A	602	ANP	PG-N3B-PB-O3A
3	A	602	ANP	PA-O3A-PB-O1B
3	A	602	ANP	PA-O3A-PB-O2B
3	D	601	ANP	PG-N3B-PB-O3A
3	D	601	ANP	C5'-O5'-PA-O2A
3	D	602	ANP	PB-N3B-PG-O1G
3	D	602	ANP	PG-N3B-PB-O1B
3	D	602	ANP	PG-N3B-PB-O3A
3	E	601	ANP	PB-N3B-PG-O1G
3	E	601	ANP	PG-N3B-PB-O1B
3	E	601	ANP	PG-N3B-PB-O3A
3	E	601	ANP	PA-O3A-PB-O1B
3	E	601	ANP	PA-O3A-PB-O2B
3	E	601	ANP	C5'-O5'-PA-O2A
3	E	602	ANP	PB-N3B-PG-O1G
3	E	602	ANP	PG-N3B-PB-O1B
3	E	602	ANP	PG-N3B-PB-O3A
3	B	601	ANP	C5'-O5'-PA-O2A
3	B	602	ANP	PB-N3B-PG-O1G
3	B	602	ANP	PG-N3B-PB-O1B
3	B	602	ANP	PG-N3B-PB-O3A
3	B	602	ANP	C5'-O5'-PA-O2A
3	C	601	ANP	PB-N3B-PG-O1G
3	C	601	ANP	PG-N3B-PB-O1B
3	C	602	ANP	PB-N3B-PG-O1G
3	G	601	ANP	PB-N3B-PG-O1G
3	G	601	ANP	PG-N3B-PB-O1B
3	G	601	ANP	PG-N3B-PB-O3A
3	G	601	ANP	PA-O3A-PB-O1B
3	G	601	ANP	PA-O3A-PB-O2B
3	G	601	ANP	C5'-O5'-PA-O1A
3	G	601	ANP	C5'-O5'-PA-O2A
3	G	602	ANP	PB-N3B-PG-O1G
3	G	602	ANP	PG-N3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
3	G	602	ANP	PG-N3B-PB-O3A
3	H	601	ANP	PB-N3B-PG-O1G
3	H	601	ANP	C5'-O5'-PA-O1A
3	H	601	ANP	C5'-O5'-PA-O2A
3	H	602	ANP	PB-N3B-PG-O1G
3	H	602	ANP	PG-N3B-PB-O1B
3	H	602	ANP	PG-N3B-PB-O3A
3	H	602	ANP	C5'-O5'-PA-O2A
3	K	601	ANP	PB-N3B-PG-O1G
3	K	601	ANP	PG-N3B-PB-O1B
3	K	601	ANP	PG-N3B-PB-O3A
3	K	602	ANP	PB-N3B-PG-O1G
3	K	602	ANP	PG-N3B-PB-O1B
3	K	602	ANP	PG-N3B-PB-O3A
3	K	602	ANP	C5'-O5'-PA-O2A
3	L	601	ANP	PB-N3B-PG-O1G
3	L	601	ANP	PG-N3B-PB-O1B
3	L	601	ANP	C5'-O5'-PA-O3A
3	L	601	ANP	C3'-C4'-C5'-O5'
3	L	602	ANP	PB-N3B-PG-O1G
3	L	602	ANP	PG-N3B-PB-O1B
3	L	602	ANP	PG-N3B-PB-O3A
3	I	601	ANP	PB-N3B-PG-O1G
3	I	601	ANP	PG-N3B-PB-O1B
3	I	601	ANP	PA-O3A-PB-O1B
3	I	601	ANP	PA-O3A-PB-O2B
3	I	602	ANP	PB-N3B-PG-O1G
3	I	602	ANP	PG-N3B-PB-O1B
3	I	602	ANP	PG-N3B-PB-O3A
3	J	601	ANP	PB-N3B-PG-O1G
3	J	601	ANP	PG-N3B-PB-O3A
3	J	601	ANP	C5'-O5'-PA-O3A
3	J	601	ANP	C3'-C4'-C5'-O5'
3	J	602	ANP	PB-N3B-PG-O1G
3	J	602	ANP	PG-N3B-PB-O1B
3	J	602	ANP	PG-N3B-PB-O3A
3	J	602	ANP	C5'-O5'-PA-O2A
3	H	601	ANP	C3'-C4'-C5'-O5'
3	L	601	ANP	O4'-C4'-C5'-O5'
3	J	601	ANP	O4'-C4'-C5'-O5'
3	H	601	ANP	O4'-C4'-C5'-O5'
3	B	601	ANP	PB-O3A-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	D	601	ANP	C5'-O5'-PA-O3A
3	E	601	ANP	C5'-O5'-PA-O3A
3	B	601	ANP	C5'-O5'-PA-O3A
3	B	602	ANP	C5'-O5'-PA-O3A
3	G	601	ANP	C5'-O5'-PA-O3A
3	H	602	ANP	C5'-O5'-PA-O3A
3	K	602	ANP	C5'-O5'-PA-O3A
3	J	602	ANP	C5'-O5'-PA-O3A
3	D	601	ANP	C5'-O5'-PA-O1A
3	E	601	ANP	C5'-O5'-PA-O1A
3	B	601	ANP	C5'-O5'-PA-O1A
3	L	601	ANP	C5'-O5'-PA-O1A
3	L	601	ANP	C5'-O5'-PA-O2A
3	J	601	ANP	C5'-O5'-PA-O1A
3	J	602	ANP	C5'-O5'-PA-O1A
3	B	601	ANP	PG-N3B-PB-O3A
3	L	601	ANP	PA-O3A-PB-O2B
3	G	601	ANP	C3'-C4'-C5'-O5'
3	D	601	ANP	PB-O3A-PA-O2A
3	H	601	ANP	PB-O3A-PA-O2A
3	K	601	ANP	PB-O3A-PA-O2A
3	J	601	ANP	PB-O3A-PA-O2A
3	D	602	ANP	C5'-O5'-PA-O3A
3	G	602	ANP	C5'-O5'-PA-O3A
3	H	601	ANP	C5'-O5'-PA-O3A
3	D	602	ANP	C5'-O5'-PA-O1A
3	B	602	ANP	C5'-O5'-PA-O1A
3	G	602	ANP	C5'-O5'-PA-O1A
3	G	602	ANP	C5'-O5'-PA-O2A
3	H	602	ANP	C5'-O5'-PA-O1A
3	K	602	ANP	C5'-O5'-PA-O1A
3	A	601	ANP	PG-N3B-PB-O3A
3	I	601	ANP	C3'-C4'-C5'-O5'

There are no ring outliers.

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	602	ANP	1	0
3	J	601	ANP	1	0
3	J	602	ANP	1	0
3	B	601	ANP	1	0

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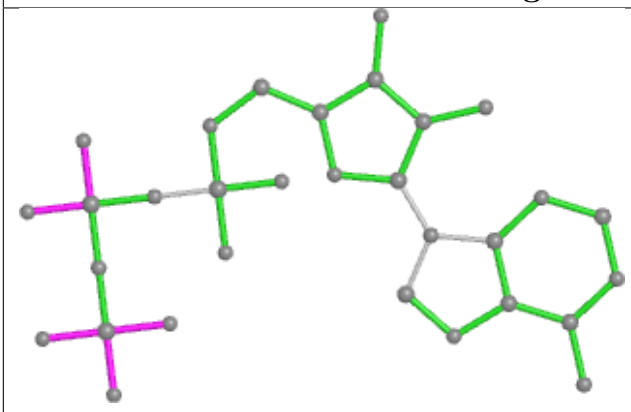
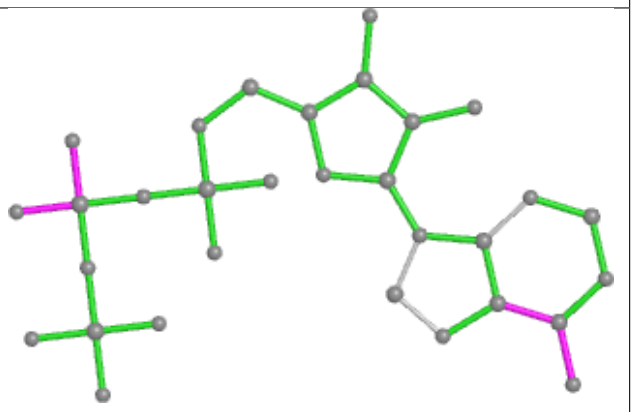
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	601	ANP	1	0
3	K	602	ANP	1	0
3	L	601	ANP	1	0
3	A	601	ANP	1	0
3	B	602	ANP	1	0
3	C	602	ANP	1	0
3	D	602	ANP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

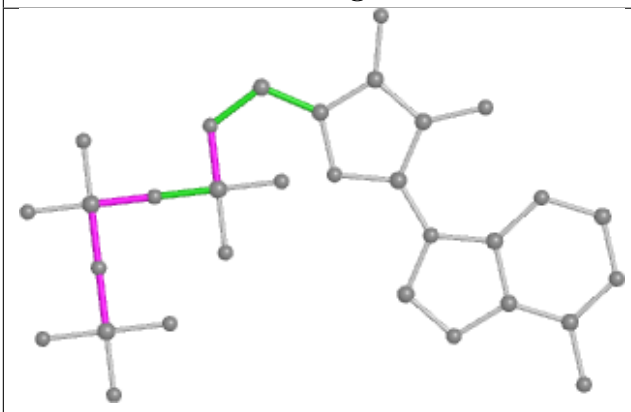
Ligand ANP E 601



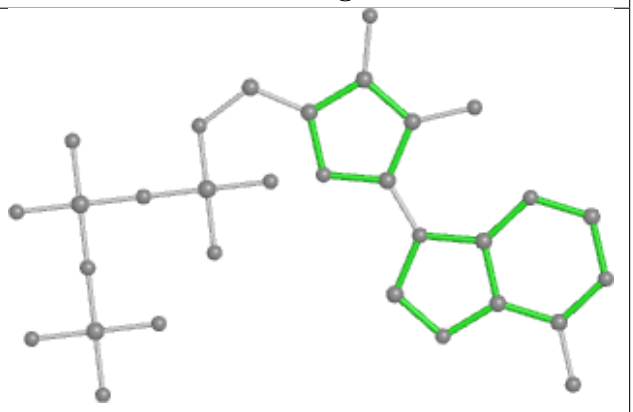
Bond lengths



Bond angles

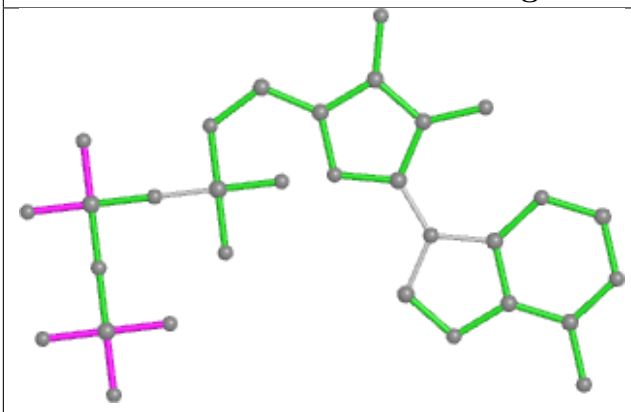


Torsions

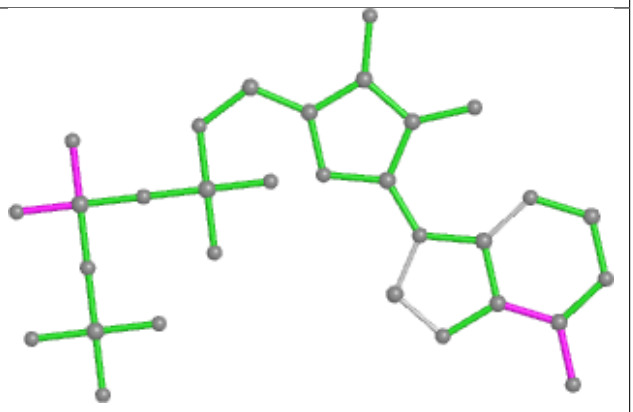


Rings

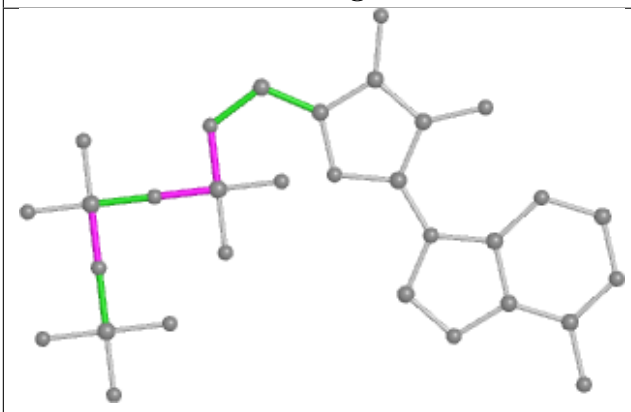
Ligand ANP D 601



Bond lengths



Bond angles



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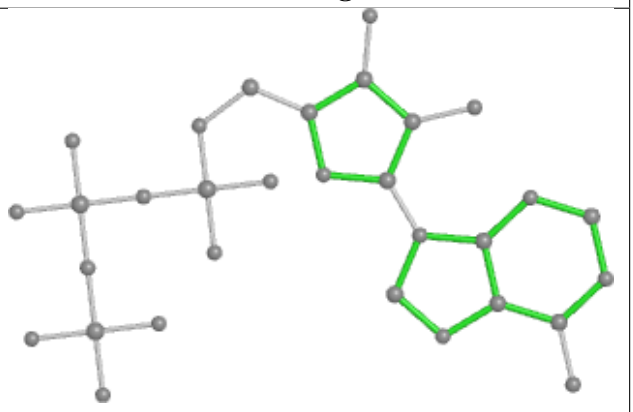
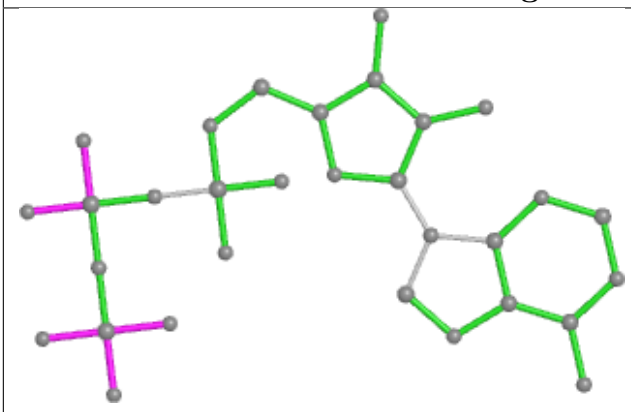
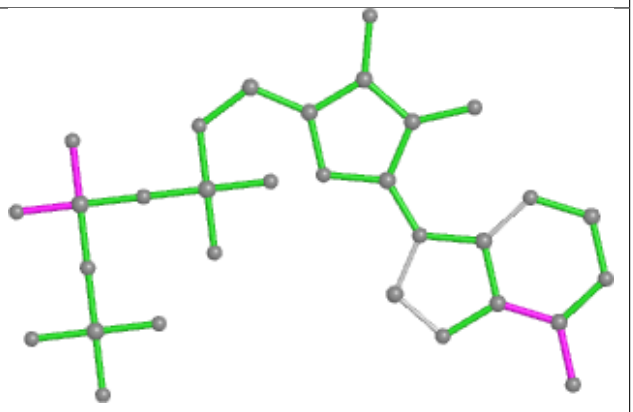


Rings

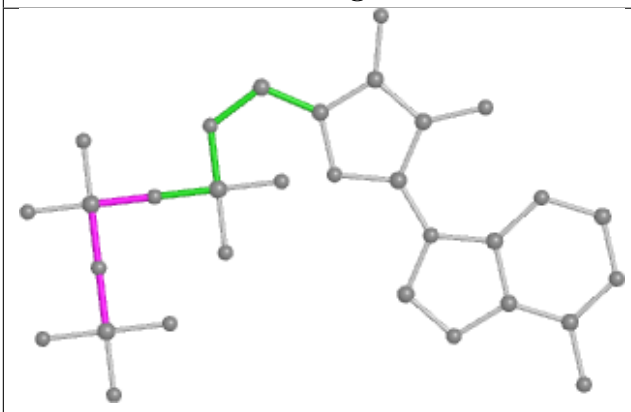
Ligand ANP A 602



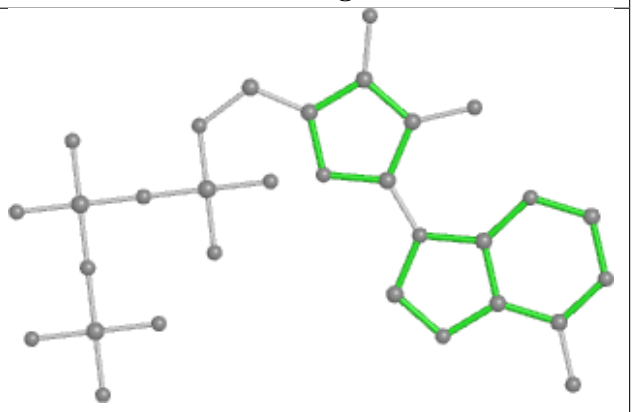
Bond lengths



Bond angles

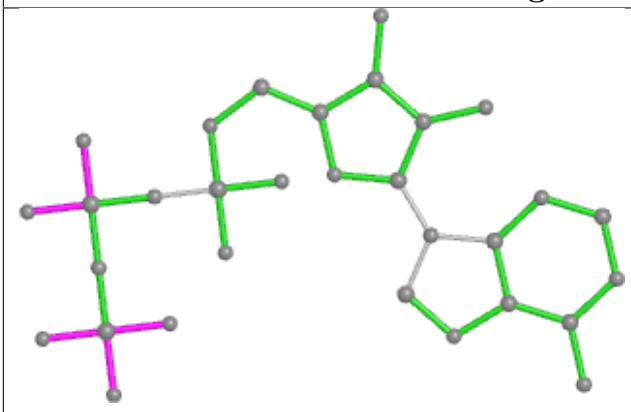


Torsions

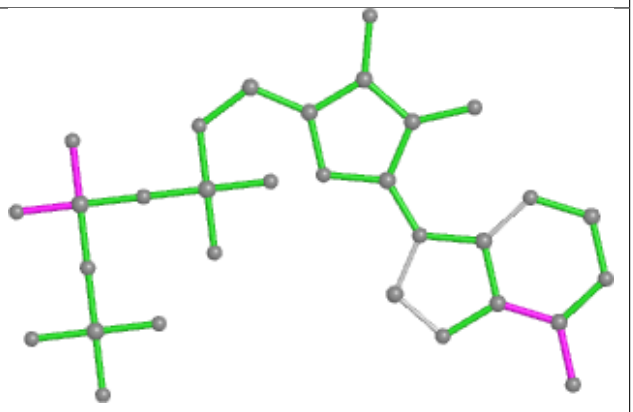


Rings

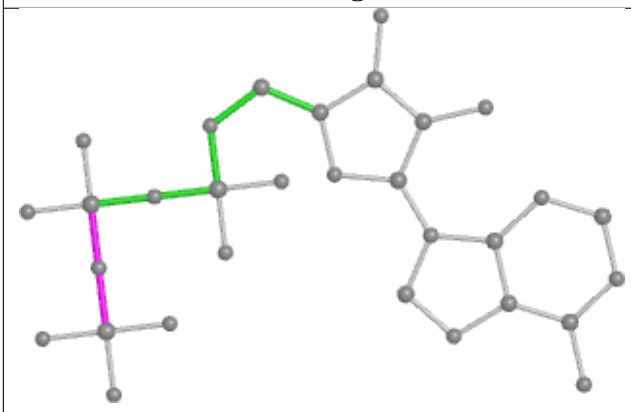
Ligand ANP I 602



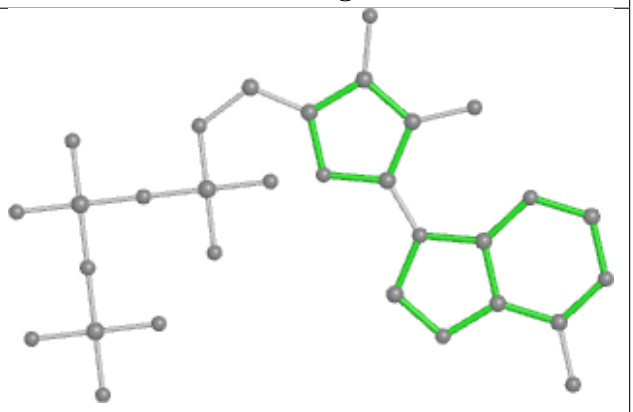
Bond lengths



Bond angles

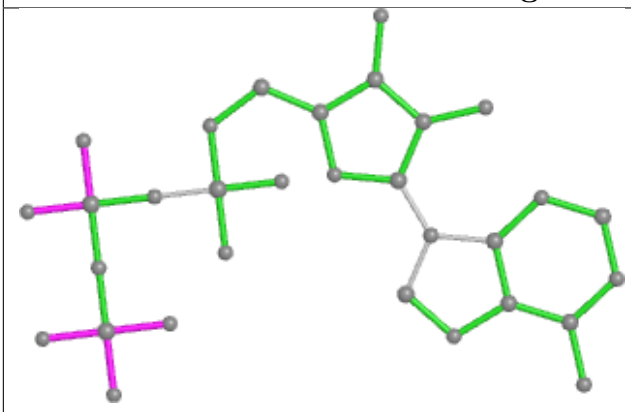


Torsions

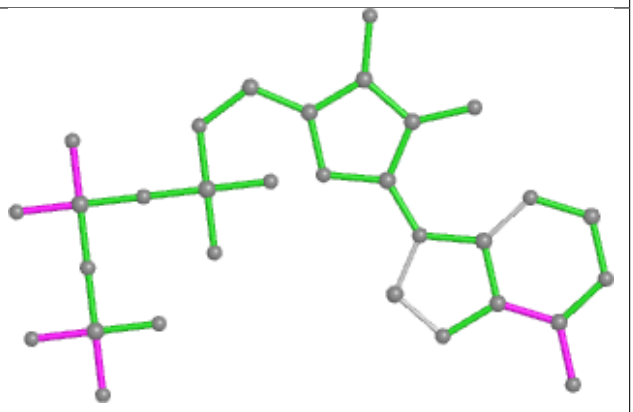


Rings

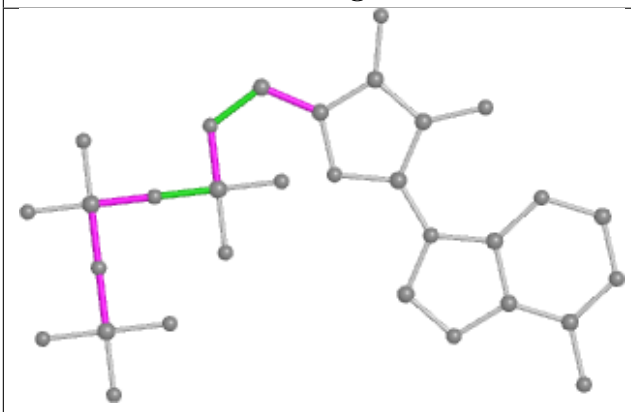
Ligand ANP G 601



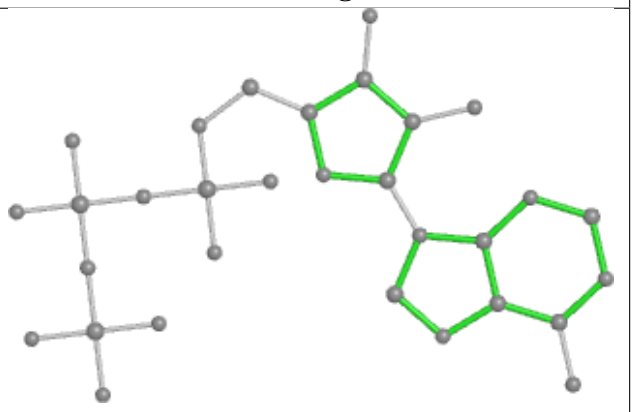
Bond lengths



Bond angles

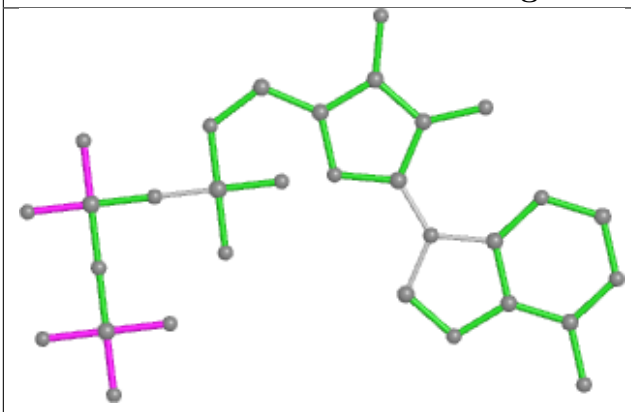


Torsions



Rings

Ligand ANP H 601



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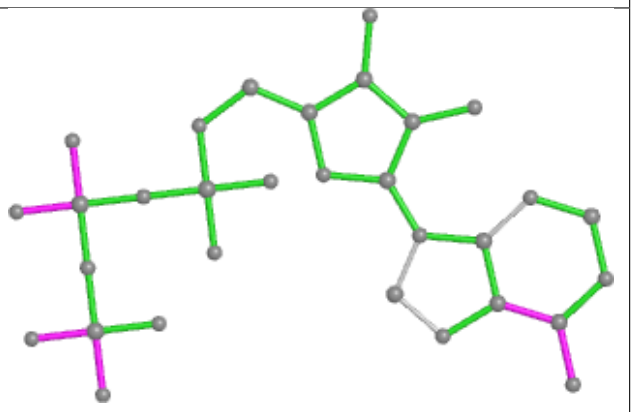

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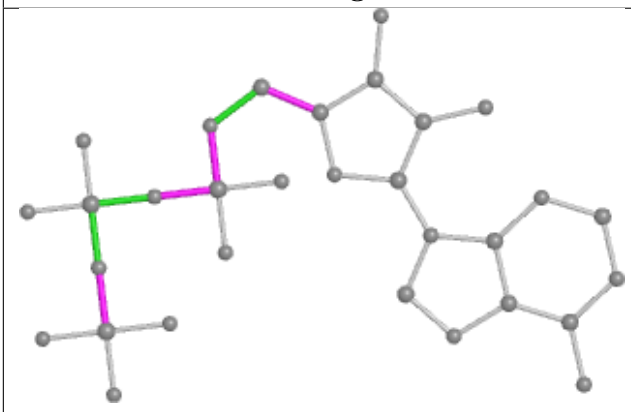

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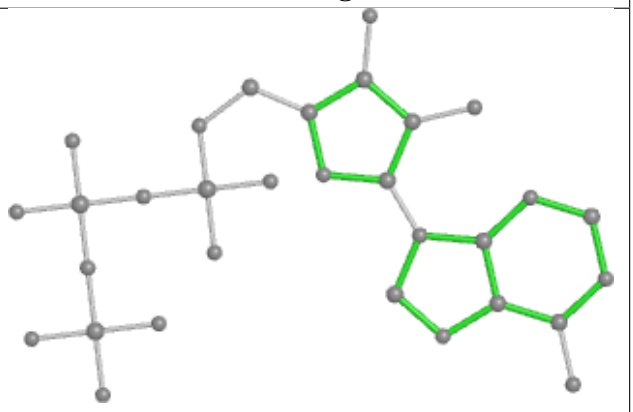

Rings

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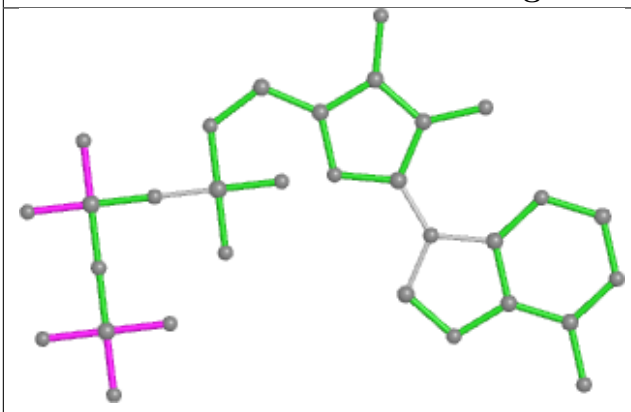

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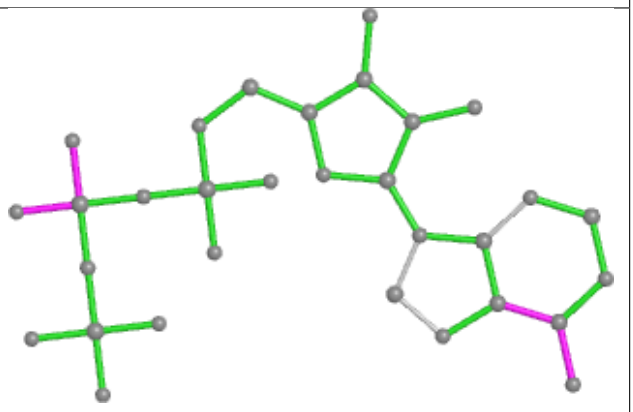

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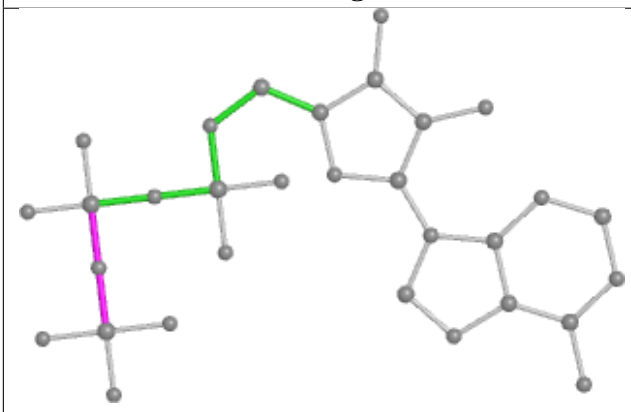

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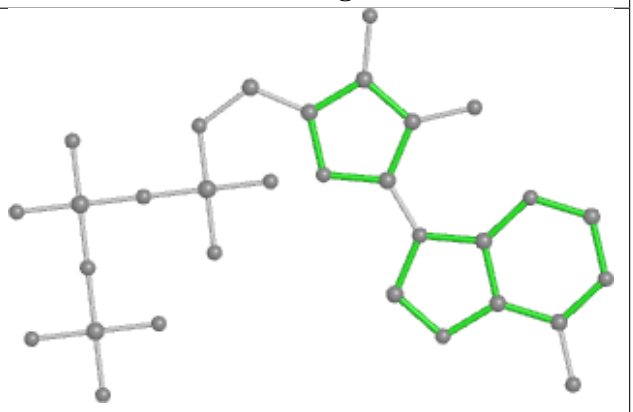

Rings

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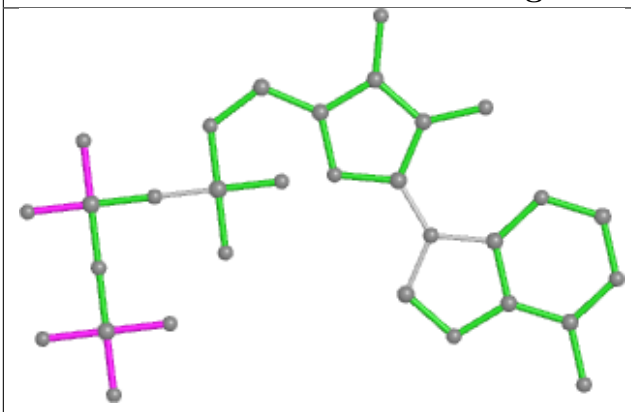

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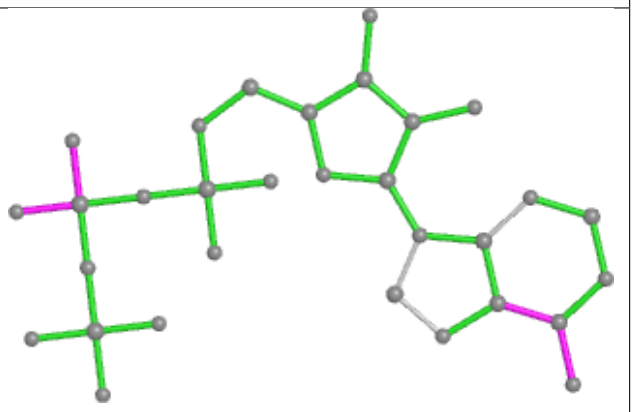

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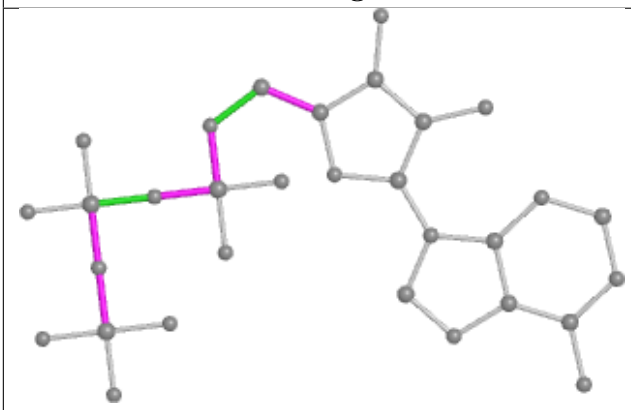

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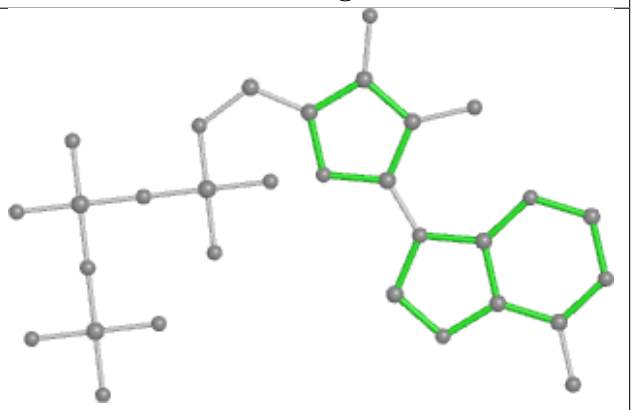

Rings

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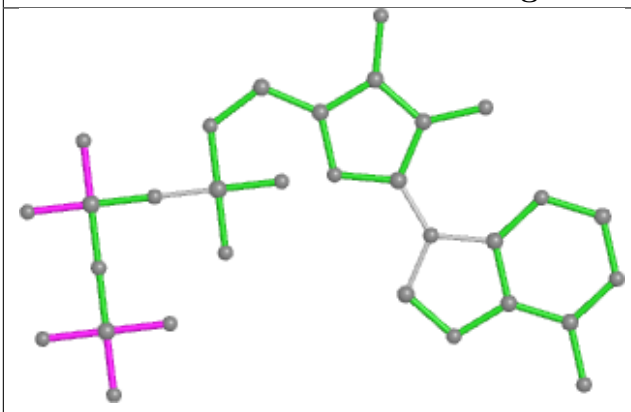

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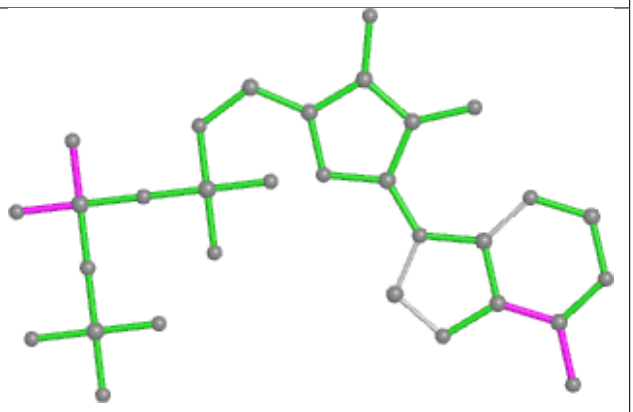

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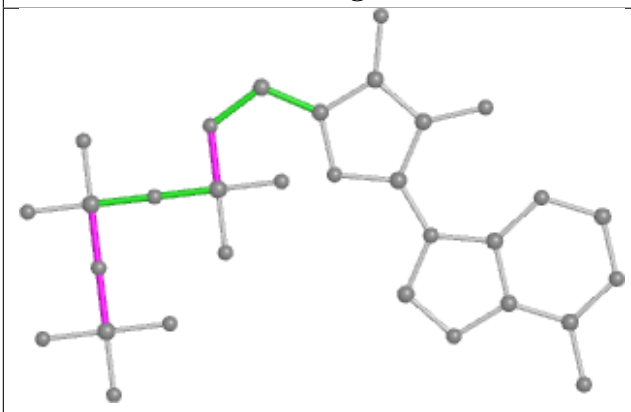

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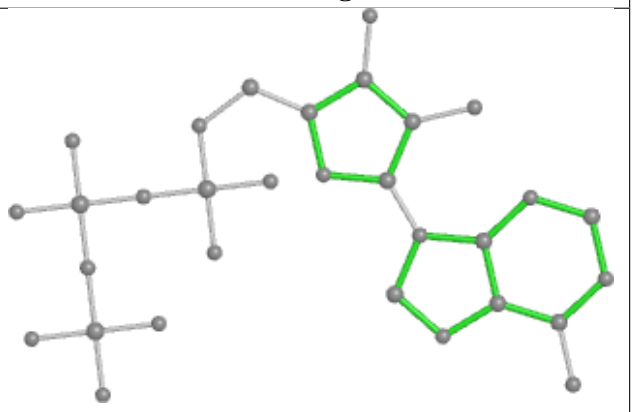

Rings

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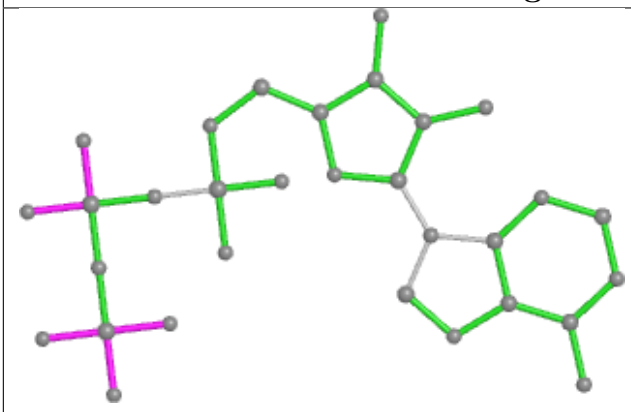

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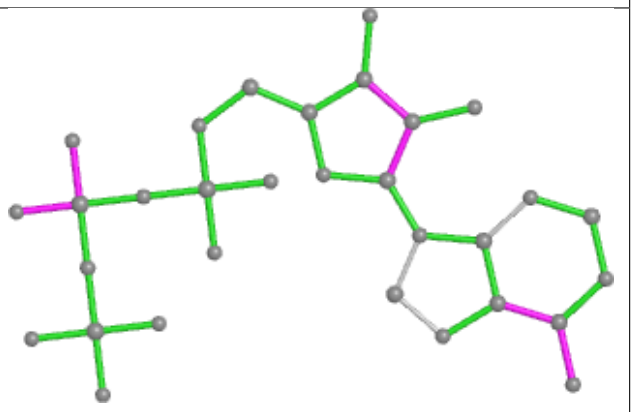

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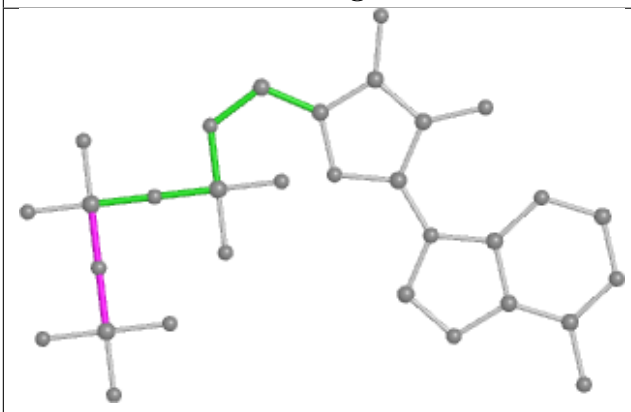

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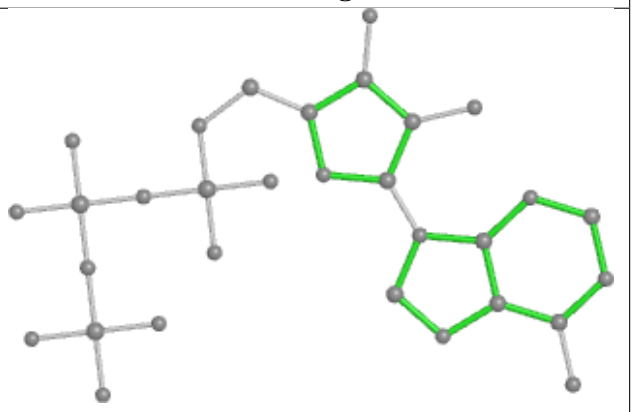

Rings

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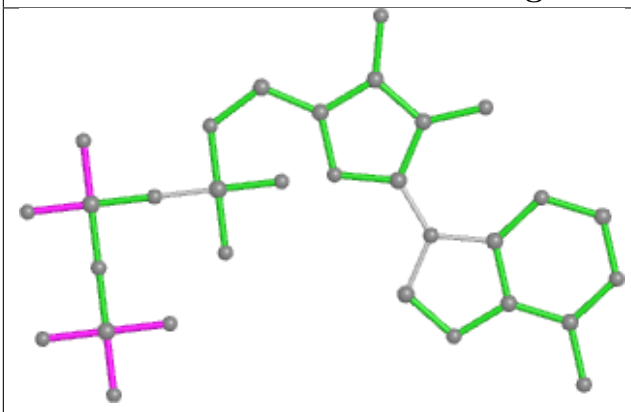

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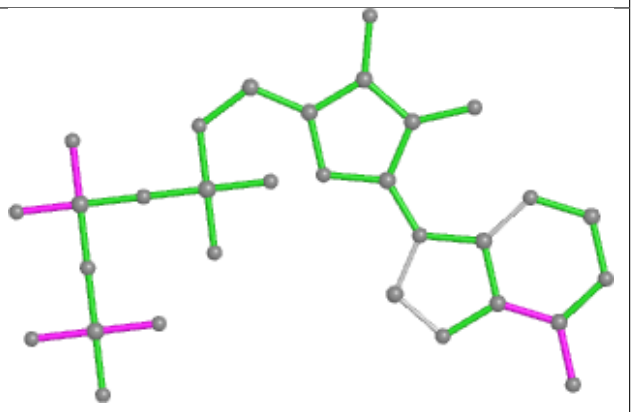

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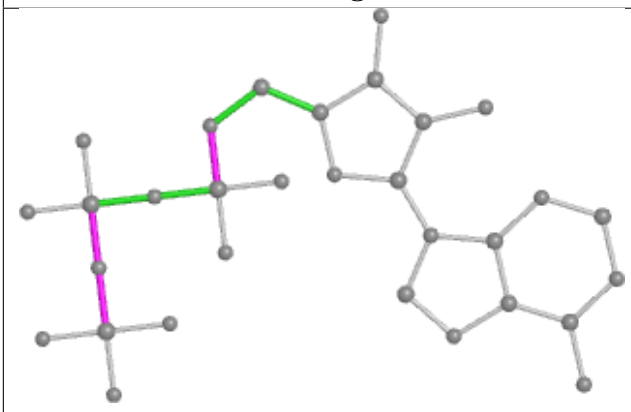

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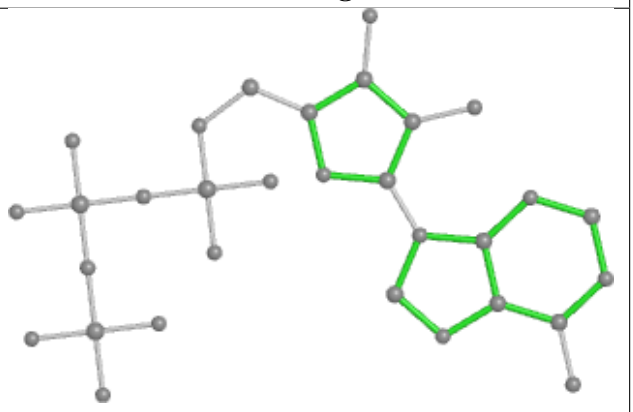

Rings

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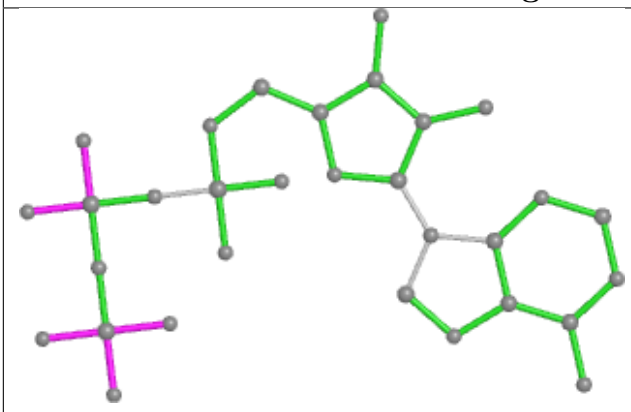

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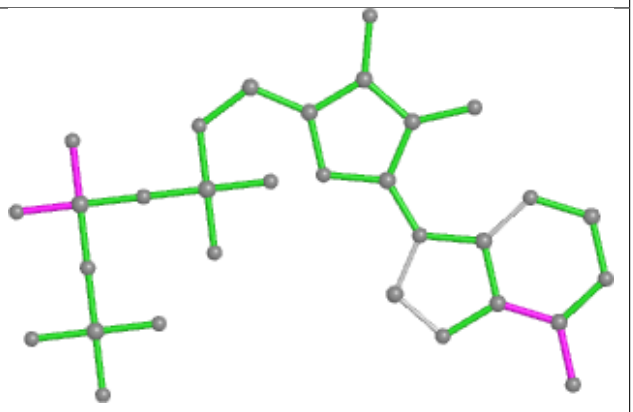

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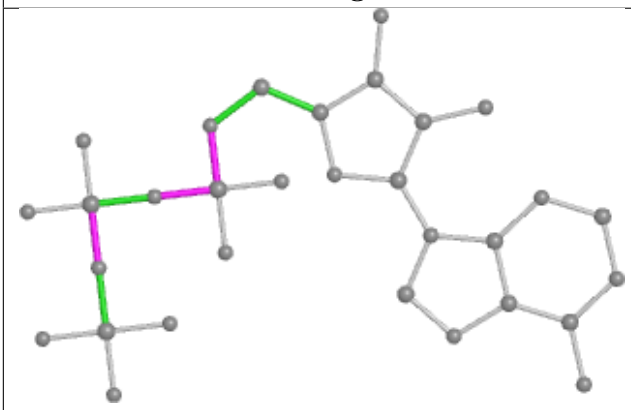

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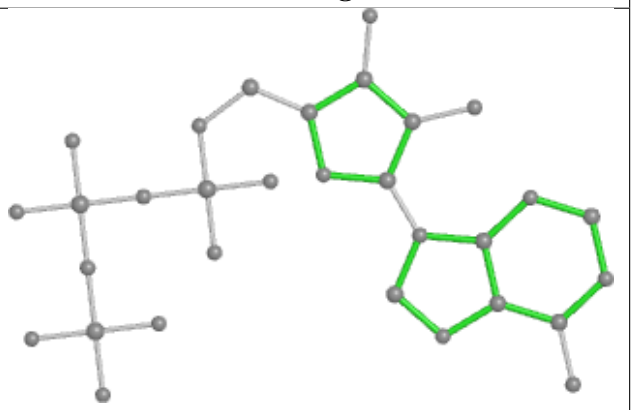

Rings

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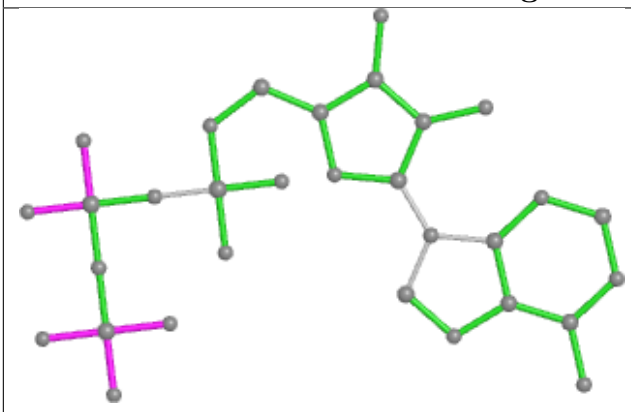

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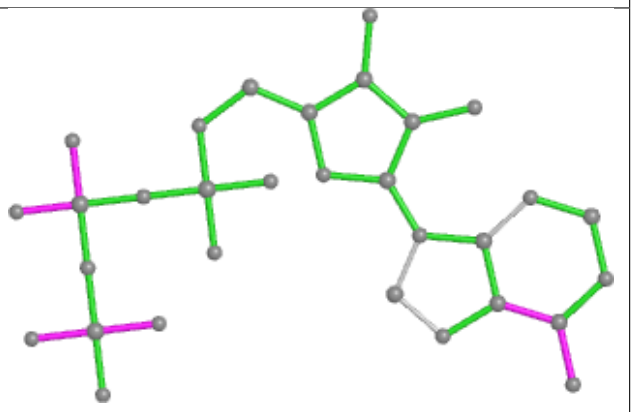

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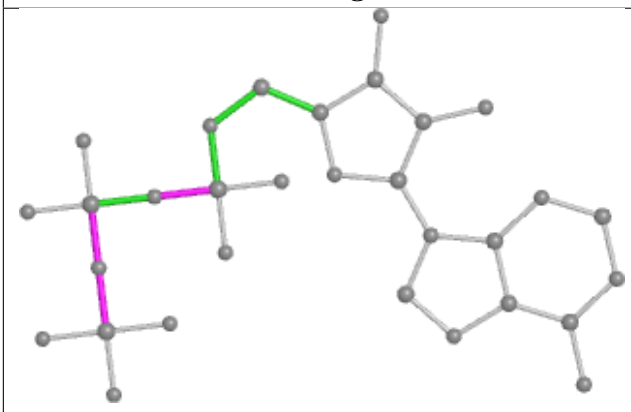

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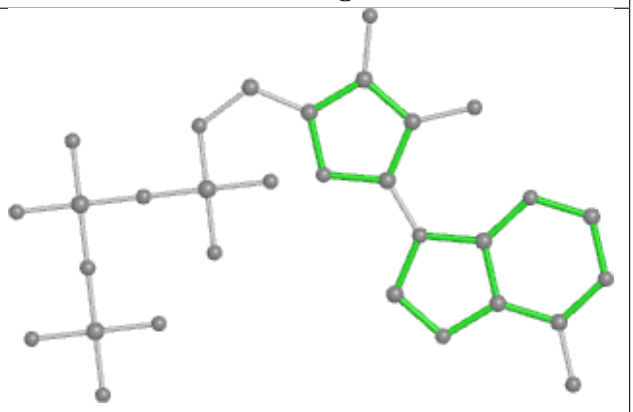

Rings

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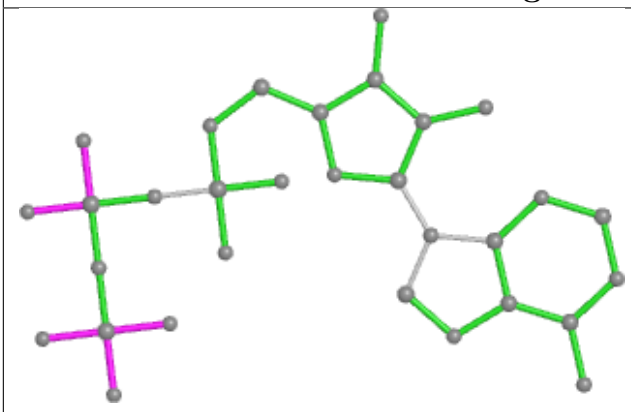

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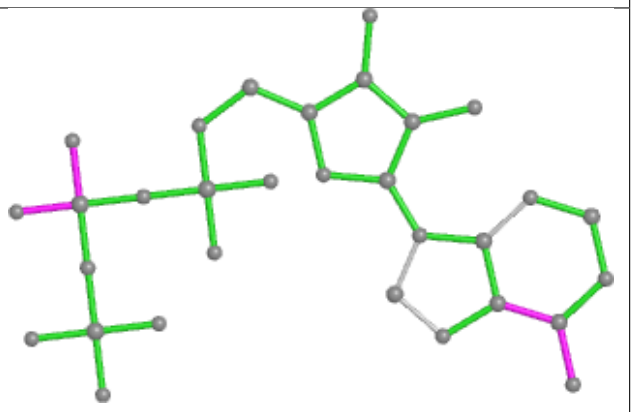

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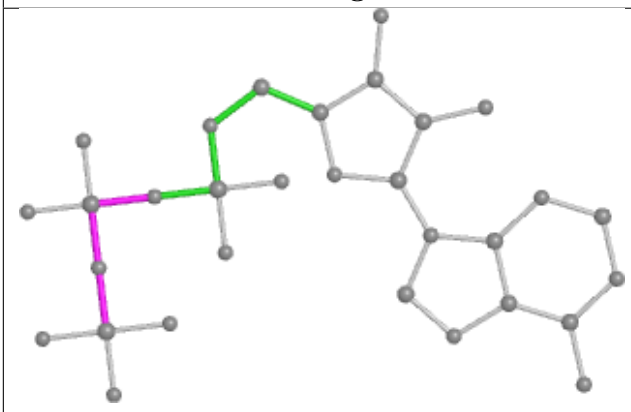

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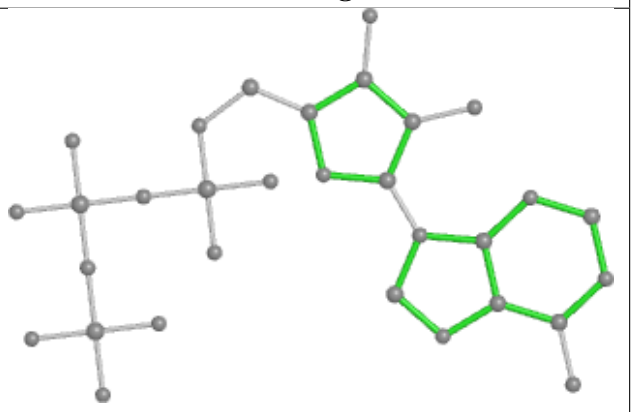

Rings

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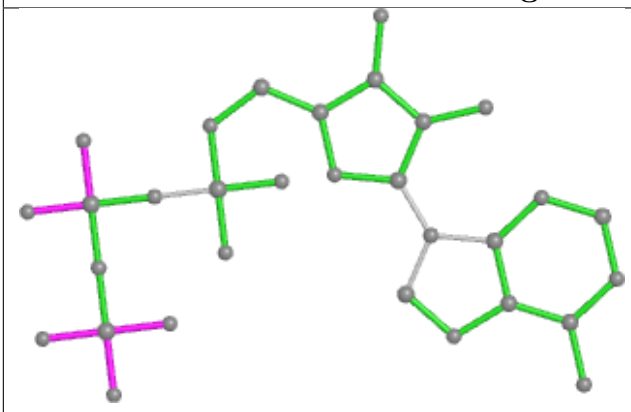

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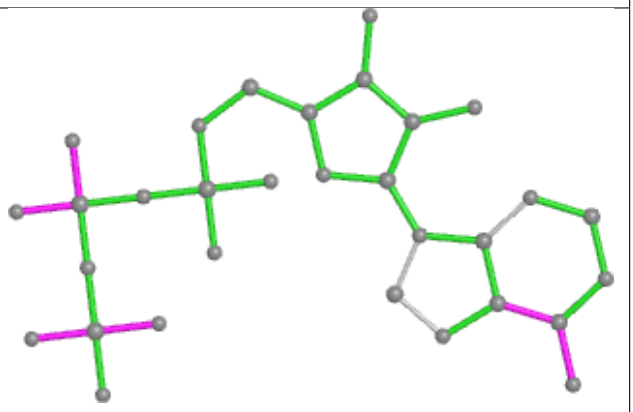

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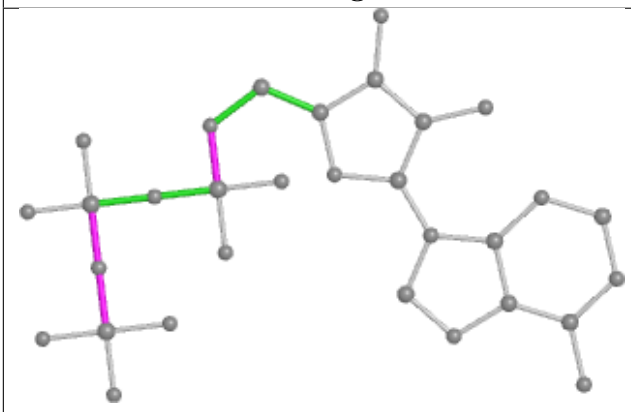

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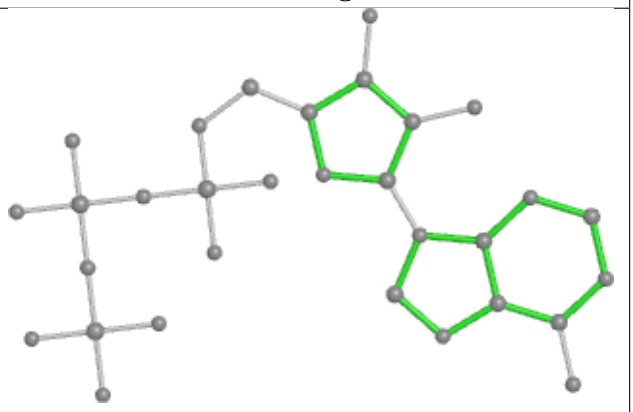

Rings

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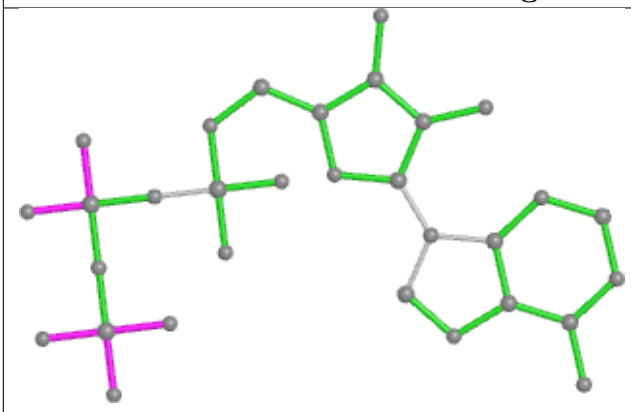

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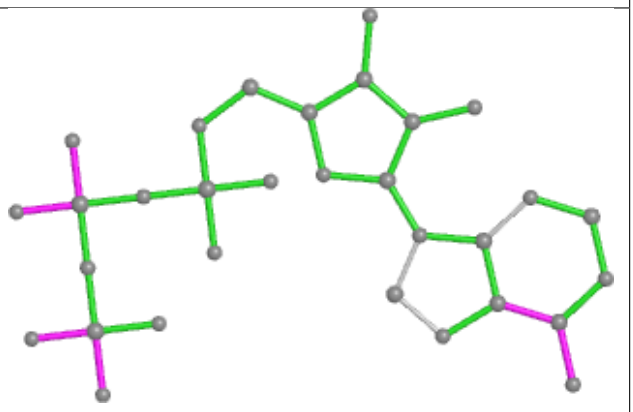

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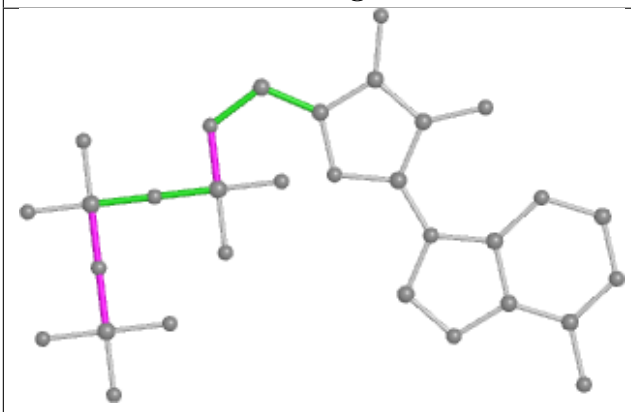

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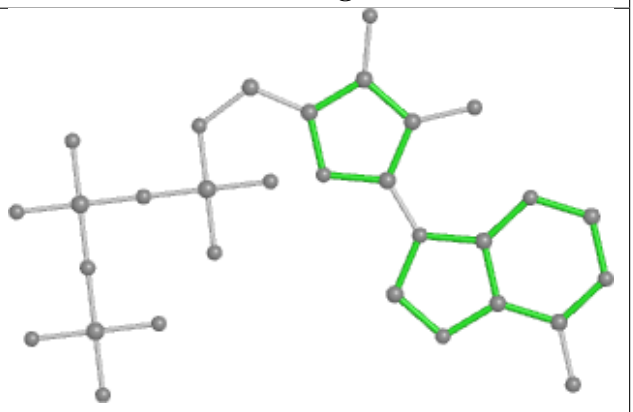
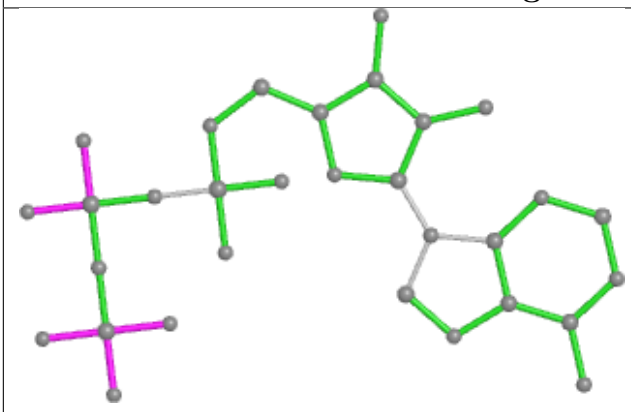


Rings

Ligand ANP E 602



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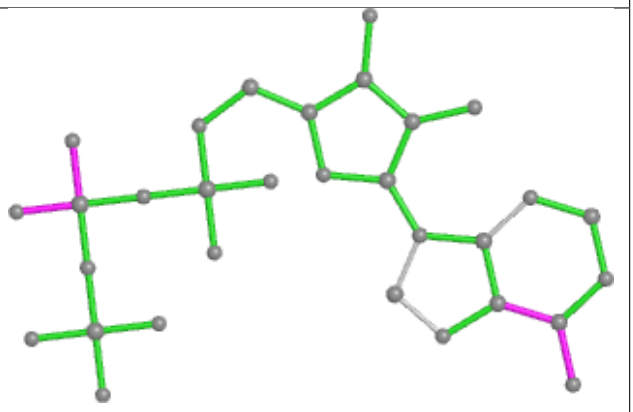

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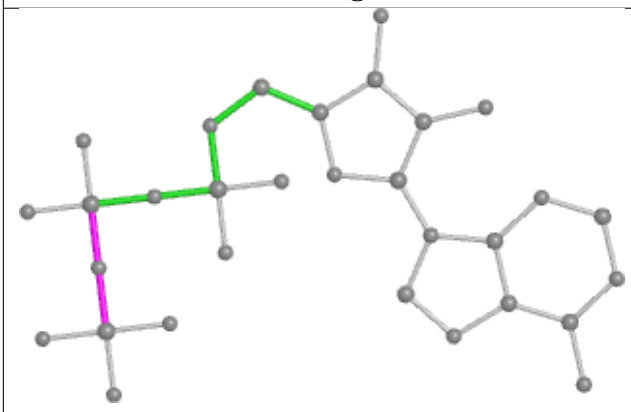

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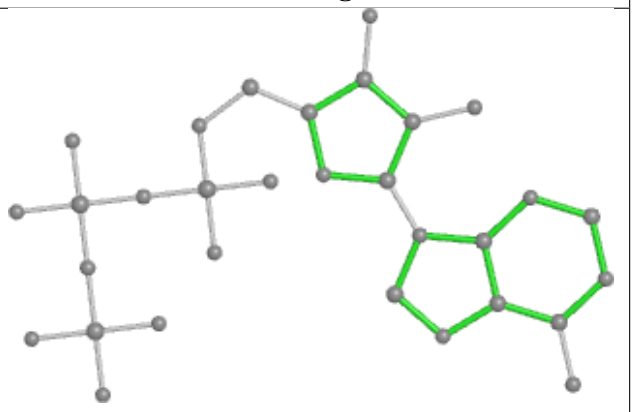
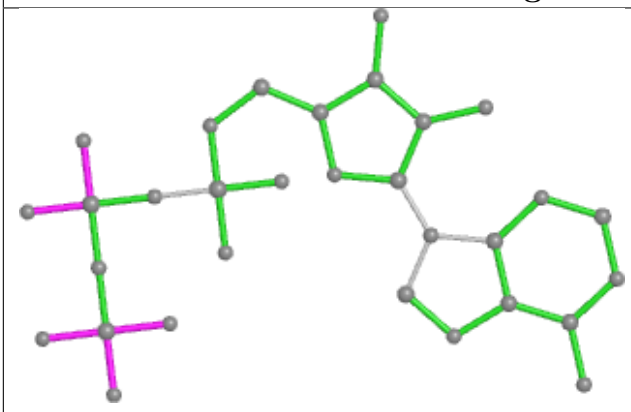


Rings

Ligand ANP L 601



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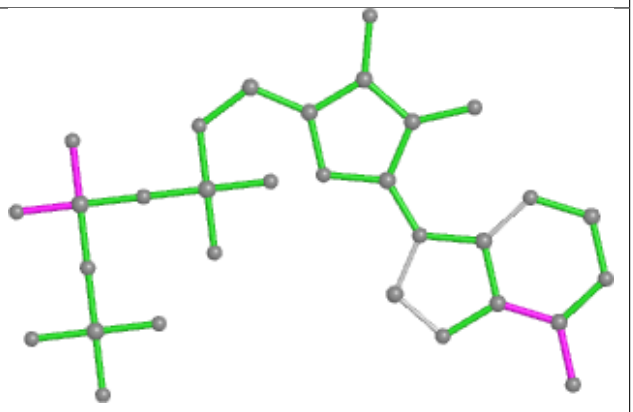

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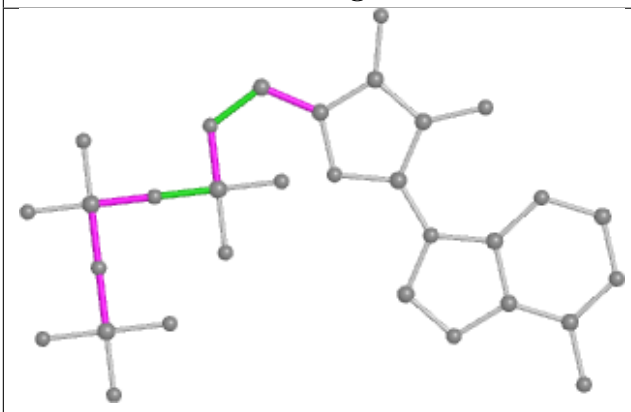

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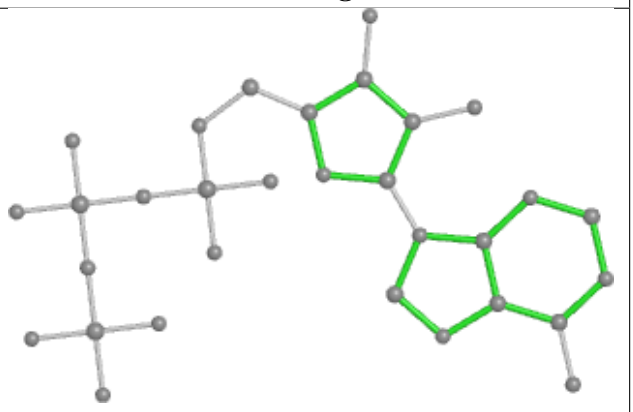
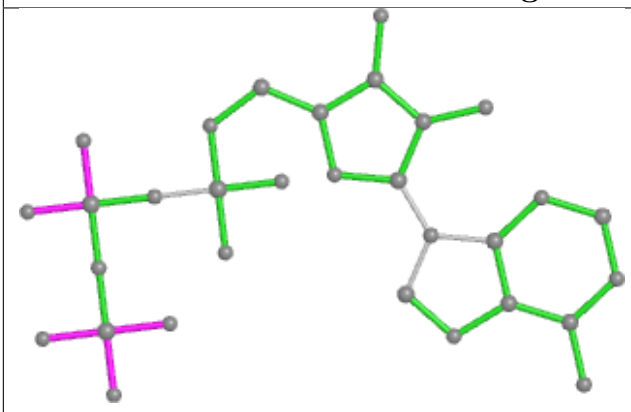


Rings

Ligand ANP A 601



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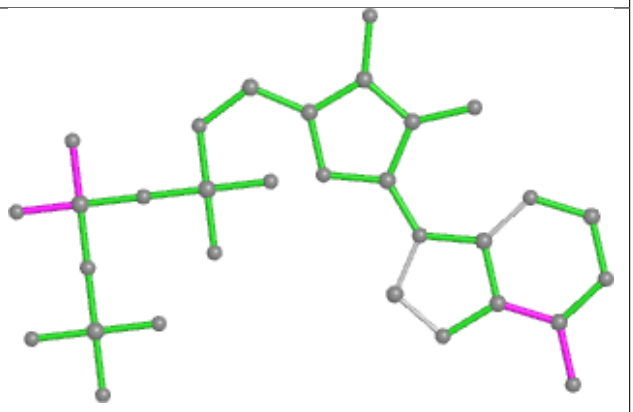

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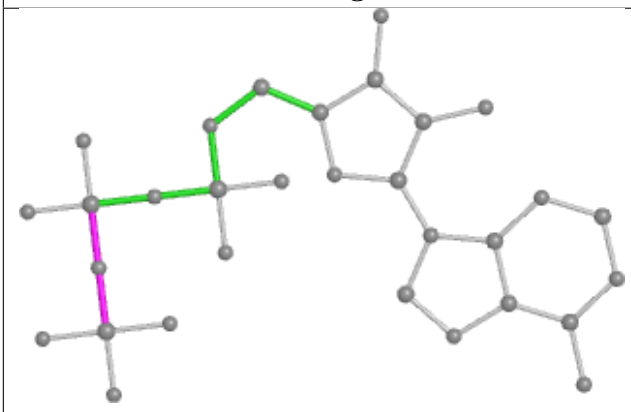
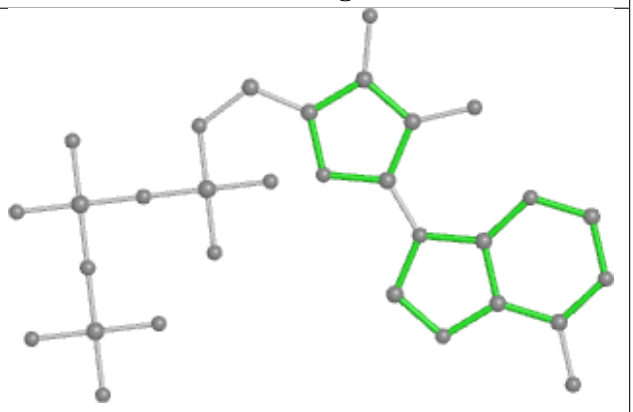
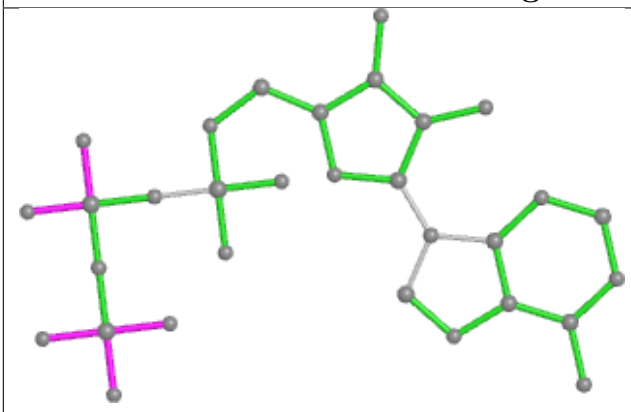


Torsions

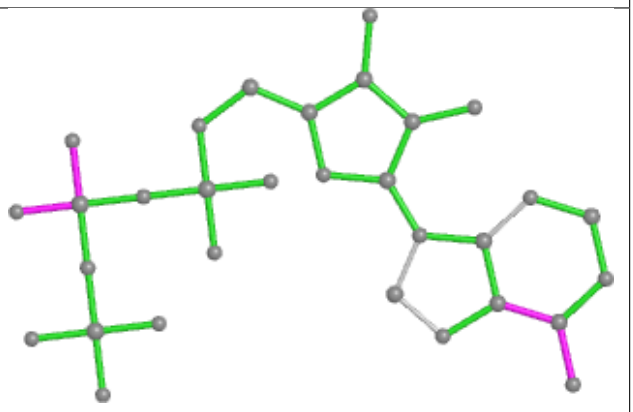


Rings

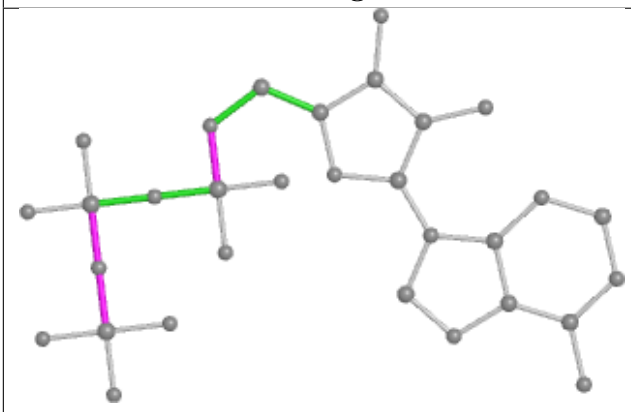
Ligand ANP B 602



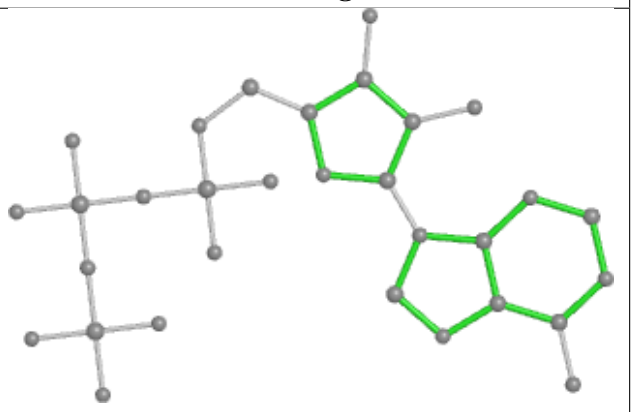
Bond lengths



Bond angles

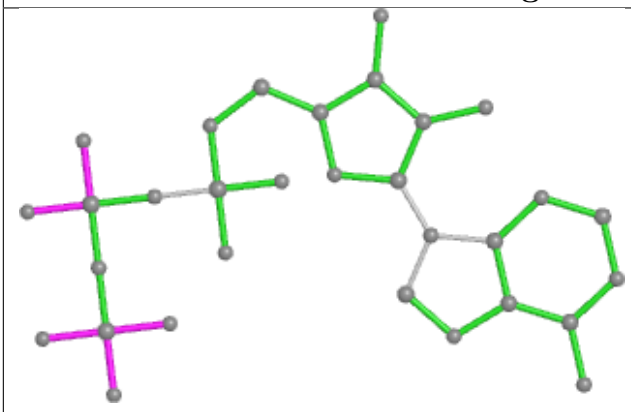


Torsions

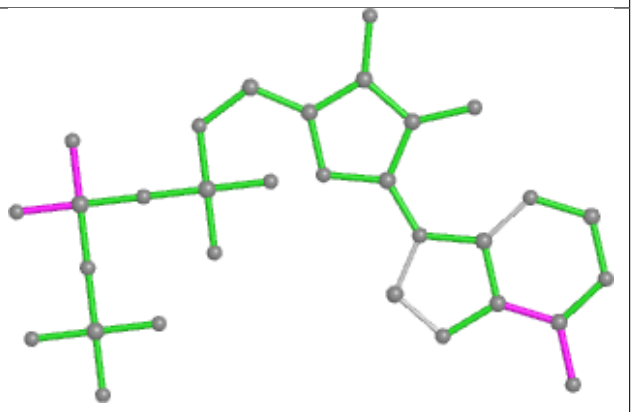


Rings

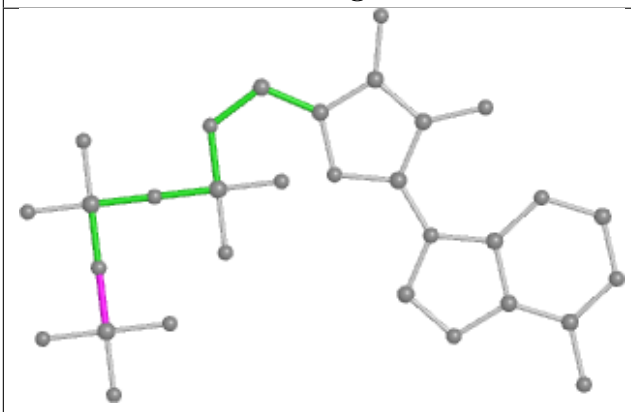
Ligand ANP C 602



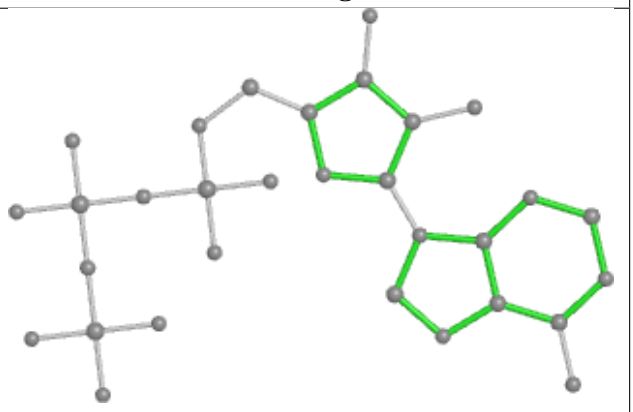
Bond lengths



Bond angles

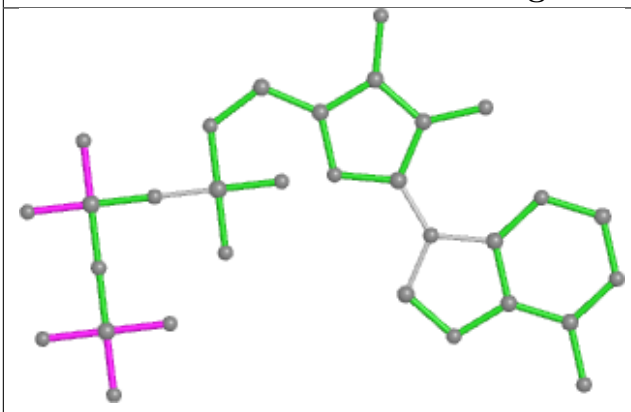


Torsions

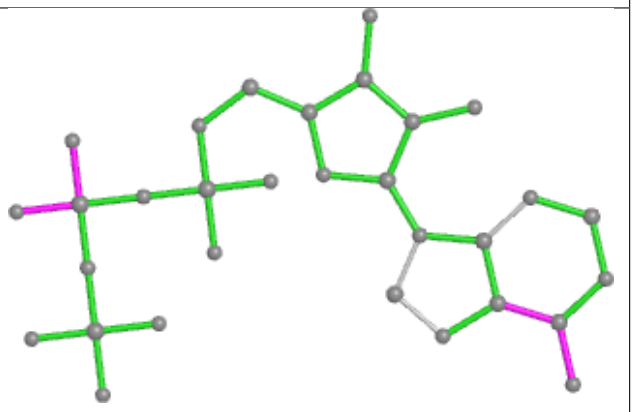


Rings

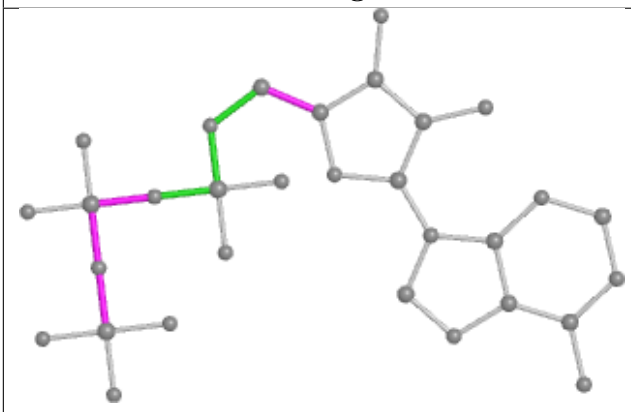
Ligand ANP I 601



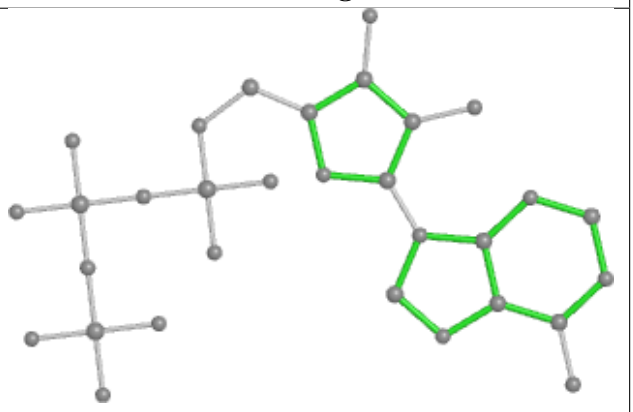
Bond lengths



Bond angles

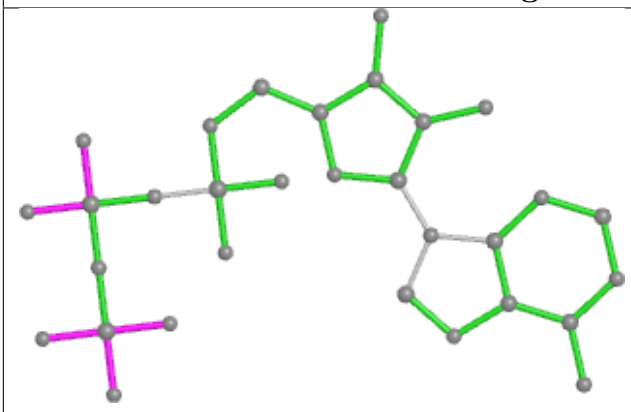


Torsions

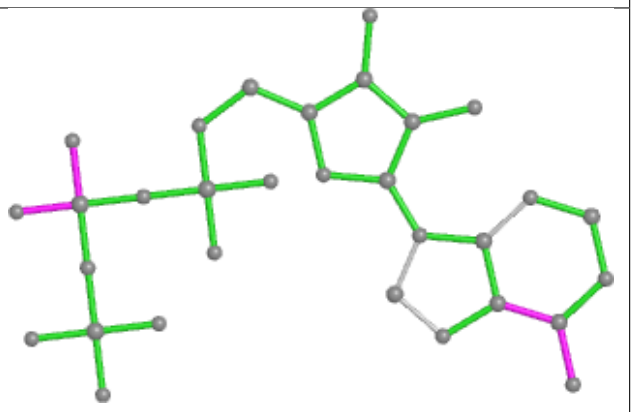


Rings

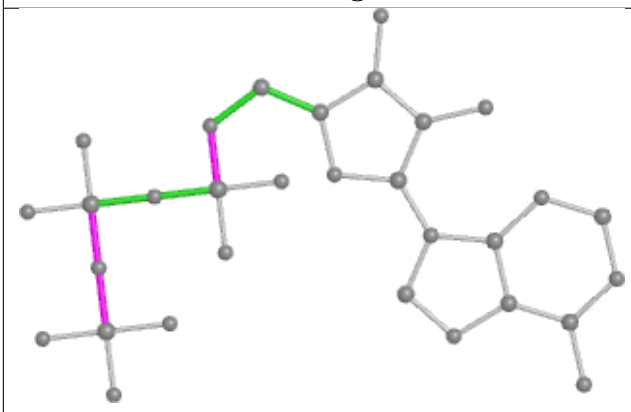
Ligand ANP D 602



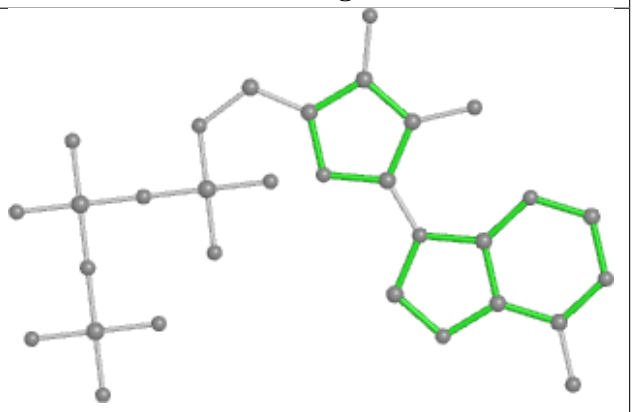
Bond lengths



Bond angles

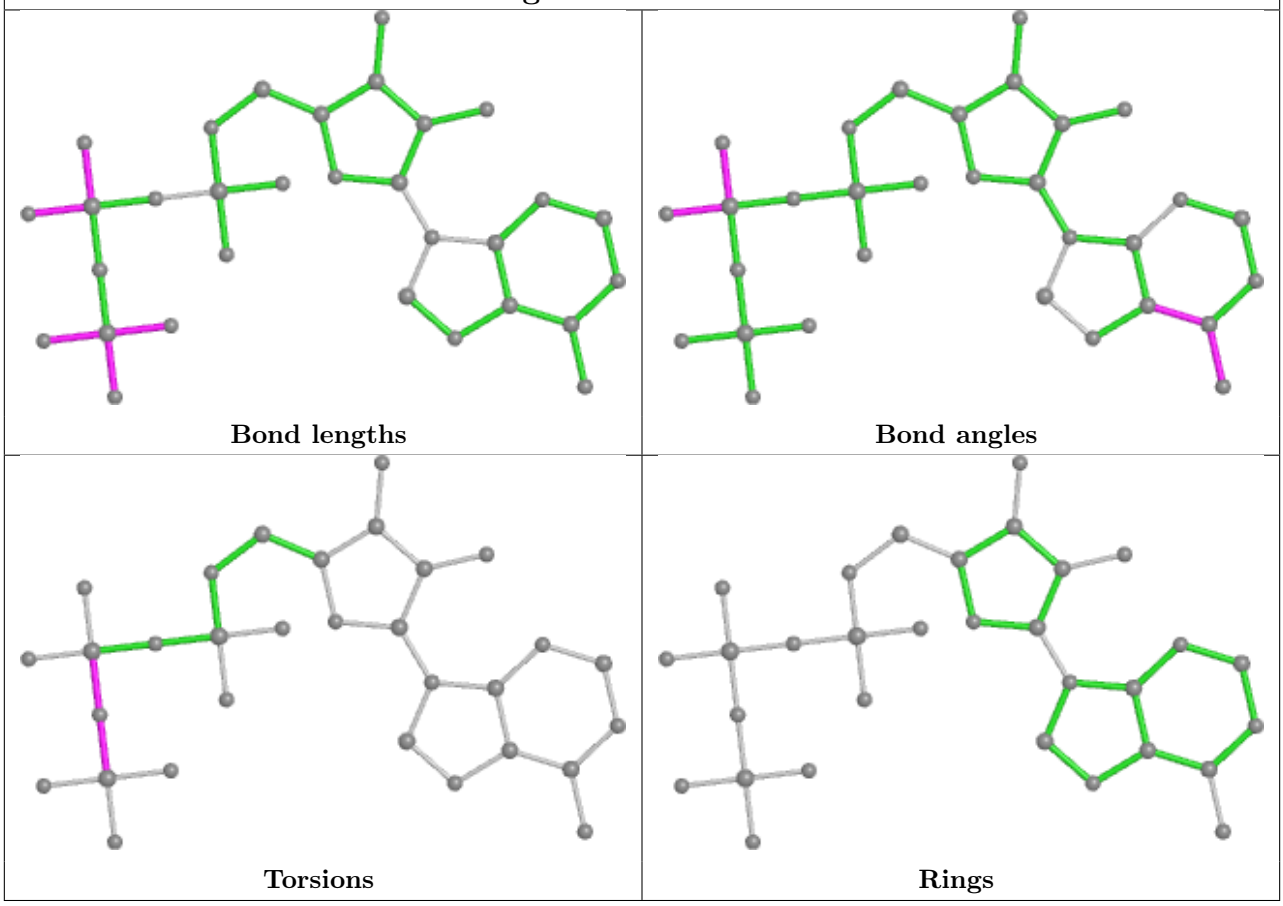


Torsions



Rings

Ligand ANP C 601



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	474/515 (92%)	0.31	12 (2%)	58	55	51, 74, 104, 127	0
1	F	468/515 (90%)	0.18	6 (1%)	74	72	52, 74, 108, 125	0
1	J	465/515 (90%)	0.26	9 (1%)	66	64	57, 77, 115, 140	0
1	K	459/515 (89%)	0.26	9 (1%)	64	62	52, 79, 107, 135	0
2	B	472/515 (91%)	0.21	5 (1%)	77	75	49, 74, 106, 144	0
2	C	471/515 (91%)	0.32	13 (2%)	55	51	57, 82, 111, 134	0
2	D	464/515 (90%)	0.28	8 (1%)	69	66	57, 81, 107, 135	0
2	E	476/515 (92%)	0.17	7 (1%)	71	69	51, 70, 102, 128	0
2	G	466/515 (90%)	0.20	10 (2%)	63	61	55, 76, 99, 124	0
2	H	473/515 (91%)	0.26	6 (1%)	74	72	55, 80, 104, 132	0
2	I	466/515 (90%)	0.29	7 (1%)	71	69	57, 78, 112, 132	0
2	L	471/515 (91%)	0.19	5 (1%)	77	75	55, 75, 100, 125	0
All	All	5625/6180 (91%)	0.24	97 (1%)	69	66	49, 77, 108, 144	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	423	ILE	3.9
2	D	153	ASP	3.8
1	A	154	ALA	3.5
2	C	148	VAL	3.3
2	I	255	ARG	3.3
2	E	125	ILE	3.2
1	F	420	SER	3.2
2	H	42	VAL	3.0
2	H	432	THR	3.0
1	J	54	SER	3.0
2	B	427	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	272	CYS	2.9
2	C	92	LEU	2.8
2	D	424	THR	2.8
1	A	427	HIS	2.8
2	B	428	ILE	2.8
2	C	154	ALA	2.8
2	C	331	ILE	2.8
2	E	54	SER	2.7
1	A	428	ILE	2.7
2	E	152	TYR	2.7
2	L	468	PHE	2.6
2	D	363	SER	2.6
2	I	154	ALA	2.6
1	J	417	PHE	2.6
2	C	397	VAL	2.6
2	E	427	HIS	2.5
1	K	247	LEU	2.5
2	D	157	VAL	2.5
2	D	110	PRO	2.5
2	L	419	GLY	2.5
1	K	140	VAL	2.5
2	C	423	ILE	2.5
2	H	253	THR	2.5
2	C	421	HIS	2.4
1	K	417	PHE	2.4
1	J	254	GLN	2.4
2	B	420	SER	2.4
2	C	420	SER	2.4
2	I	146	THR	2.4
2	G	426	SER	2.4
2	L	423	ILE	2.4
1	J	23	ILE	2.4
1	J	258	ASN	2.4
2	C	121	LEU	2.3
2	G	252	LEU	2.3
2	L	427	HIS	2.3
1	A	153	ASP	2.3
2	G	409	PHE	2.3
1	K	156	SER	2.3
2	G	26	PHE	2.3
2	H	468	PHE	2.3
2	I	432	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	419	GLY	2.2
2	C	149	PHE	2.2
2	I	145	VAL	2.2
1	J	468	PHE	2.2
2	B	109	ASP	2.2
1	K	42	VAL	2.2
2	E	495	ILE	2.2
2	G	43	SER	2.2
1	A	150	GLN	2.2
2	D	149	PHE	2.2
1	F	92	LEU	2.2
1	F	29	ILE	2.2
1	A	468	PHE	2.1
2	G	425	ASP	2.1
2	I	149	PHE	2.1
2	E	450	ALA	2.1
1	K	195	GLU	2.1
1	J	158	VAL	2.1
1	F	39	SER	2.1
2	G	420	SER	2.1
2	G	104	LEU	2.1
1	K	174	VAL	2.1
2	H	145	VAL	2.1
1	K	175	THR	2.1
1	A	254	GLN	2.1
1	K	39	SER	2.1
2	H	371	SER	2.1
2	I	155	ALA	2.1
2	G	124	LEU	2.0
1	J	279	ASP	2.0
2	C	416	GLN	2.0
1	F	155	ALA	2.0
2	D	196	GLU	2.0
2	E	423	ILE	2.0
1	J	418	MET	2.0
1	A	248	GLY	2.0
2	L	101	LEU	2.0
1	A	424	THR	2.0
2	C	236	THR	2.0
2	C	424	THR	2.0
1	A	479	ASP	2.0
1	A	351	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	255	ARG	2.0
1	A	421	HIS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	SEP	F	429	10/11	0.76	0.21	90,101,120,121	0
1	SEP	A	429	10/11	0.79	0.19	95,106,121,121	0
1	SEP	J	429	10/11	0.79	0.17	90,101,117,119	0
1	SEP	K	429	10/11	0.85	0.14	83,98,115,117	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
4	MG	E	604	1/1	0.62	0.15	90,90,90,90	0
4	MG	G	604	1/1	0.74	0.17	84,84,84,84	0
4	MG	K	604	1/1	0.74	0.09	82,82,82,82	0
4	MG	B	603	1/1	0.77	0.20	71,71,71,71	0
4	MG	A	604	1/1	0.85	0.14	69,69,69,69	0
4	MG	I	604	1/1	0.85	0.12	80,80,80,80	0
4	MG	L	604	1/1	0.87	0.10	73,73,73,73	0
4	MG	F	604	1/1	0.88	0.10	76,76,76,76	0
3	ANP	J	601	31/31	0.90	0.10	76,81,109,109	0
3	ANP	K	601	31/31	0.90	0.10	73,76,96,96	0
3	ANP	I	601	31/31	0.90	0.10	81,84,94,96	0
3	ANP	D	601	31/31	0.91	0.10	64,65,91,95	0

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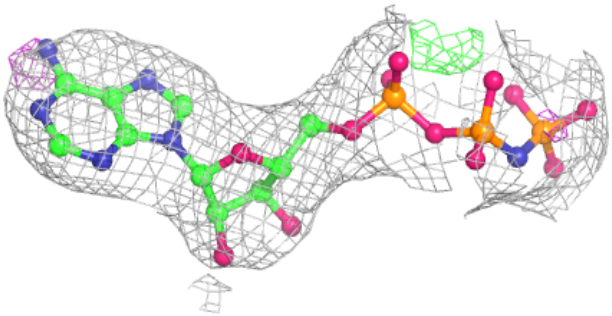
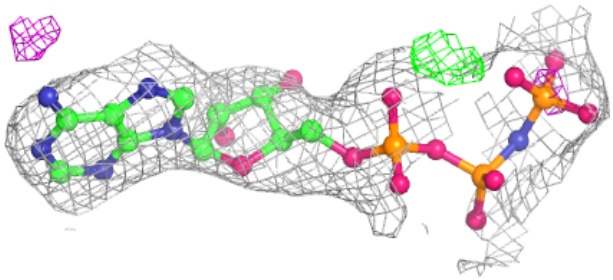
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	K	603	1/1	0.91	0.12	58,58,58,58	0
3	ANP	L	601	31/31	0.91	0.10	64,66,89,92	0
3	ANP	E	601	31/31	0.91	0.09	71,74,92,94	0
3	ANP	H	601	31/31	0.91	0.09	69,76,89,92	0
3	ANP	G	601	31/31	0.92	0.09	61,64,94,97	0
4	MG	H	604	1/1	0.92	0.06	74,74,74,74	0
3	ANP	F	601	31/31	0.92	0.09	71,72,91,95	0
3	ANP	A	602	31/31	0.92	0.10	62,66,84,86	0
3	ANP	B	601	31/31	0.92	0.09	68,71,92,94	0
3	ANP	C	601	31/31	0.92	0.09	71,77,90,91	0
3	ANP	G	602	31/31	0.93	0.08	67,76,81,82	0
3	ANP	I	602	31/31	0.94	0.07	61,63,74,75	0
3	ANP	F	602	31/31	0.94	0.08	58,61,66,68	0
3	ANP	K	602	31/31	0.94	0.07	62,66,70,71	0
3	ANP	C	602	31/31	0.95	0.07	65,69,78,79	0
3	ANP	H	602	31/31	0.95	0.07	70,73,77,78	0
3	ANP	B	602	31/31	0.95	0.07	55,58,60,61	0
3	ANP	D	602	31/31	0.95	0.07	65,66,74,76	0
3	ANP	J	602	31/31	0.95	0.07	63,67,72,73	0
3	ANP	L	602	31/31	0.96	0.06	56,58,64,65	0
3	ANP	E	602	31/31	0.96	0.07	63,67,70,71	0
3	ANP	A	601	31/31	0.96	0.06	54,61,62,64	0
4	MG	I	603	1/1	0.97	0.04	58,58,58,58	0
4	MG	D	603	1/1	0.97	0.06	57,57,57,57	0
4	MG	G	603	1/1	0.98	0.05	54,54,54,54	0
4	MG	H	603	1/1	0.99	0.03	76,76,76,76	0
4	MG	J	603	1/1	0.99	0.02	65,65,65,65	0
4	MG	L	603	1/1	1.00	0.03	55,55,55,55	0
4	MG	A	603	1/1	1.00	0.03	59,59,59,59	0
4	MG	C	603	1/1	1.00	0.03	71,71,71,71	0
4	MG	E	603	1/1	1.00	0.04	47,47,47,47	0
4	MG	F	603	1/1	1.00	0.01	49,49,49,49	0

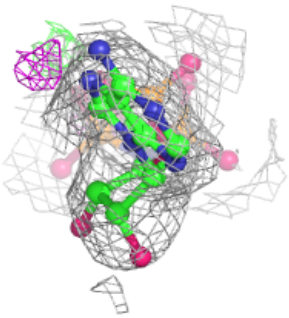
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP J 601:

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

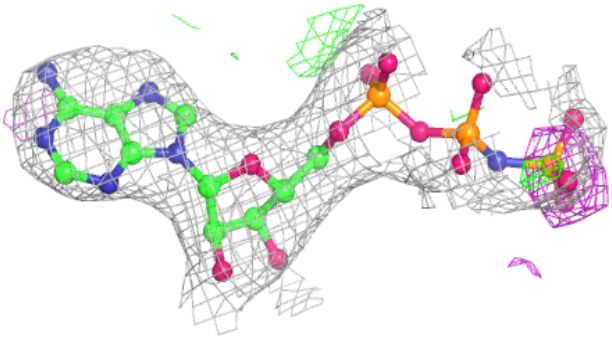


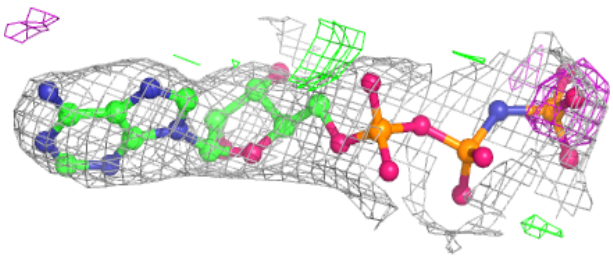


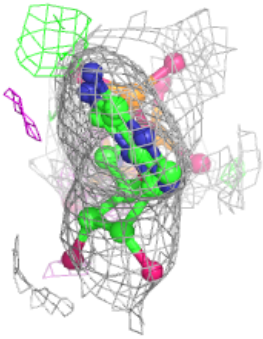


Electron density around ANP K 601:

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

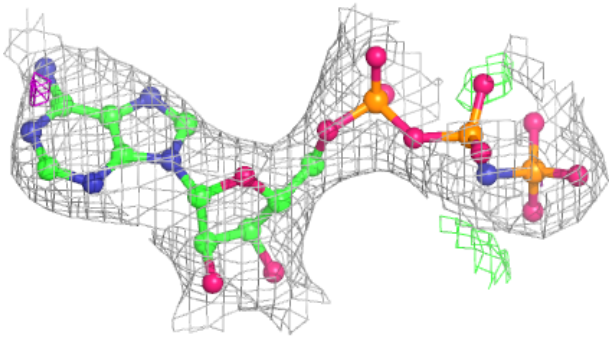


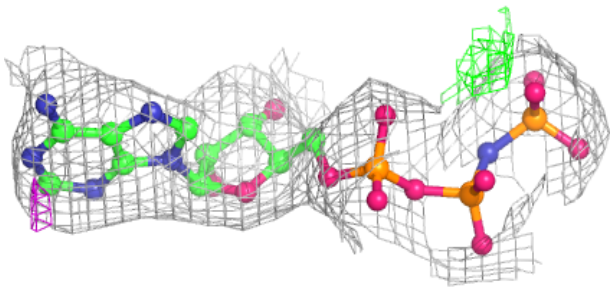


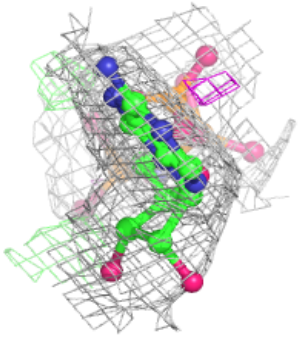


Electron density around ANP I 601:

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

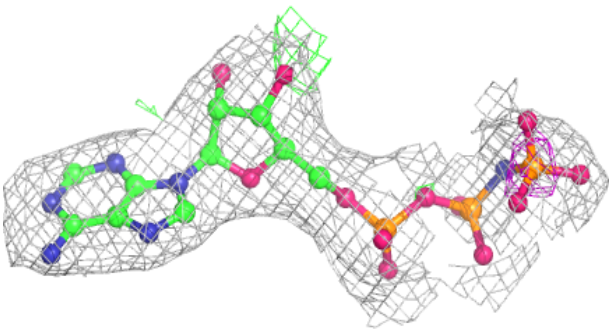


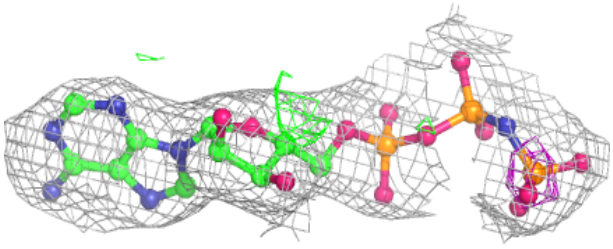


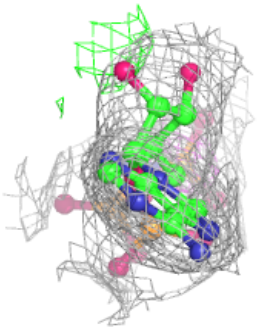


Electron density around ANP D 601:

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

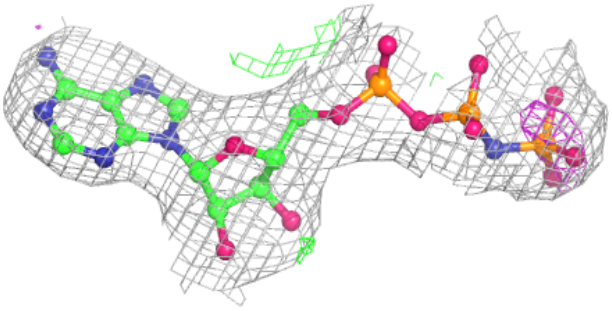


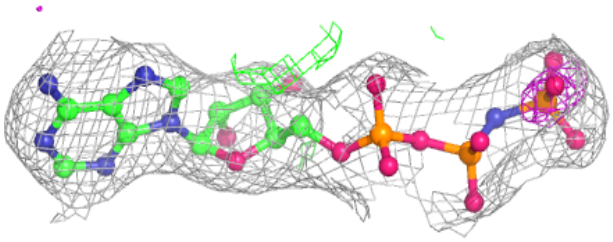


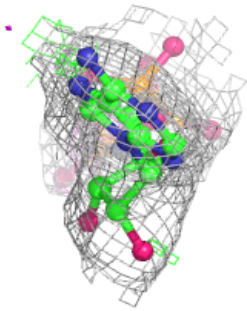


Electron density around ANP L 601:

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

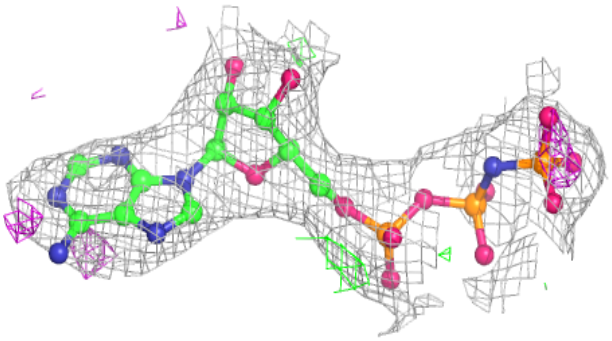


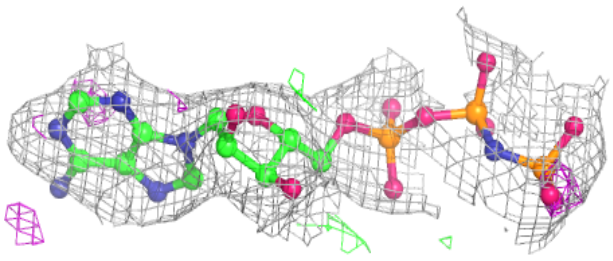


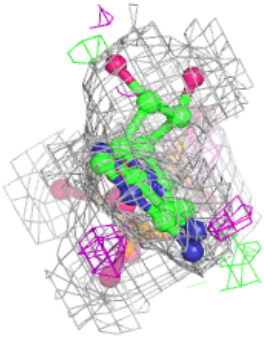


Electron density around ANP E 601:

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

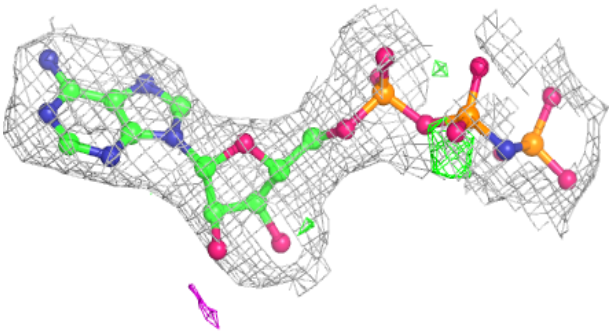


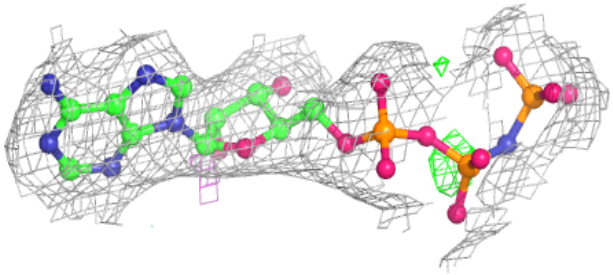


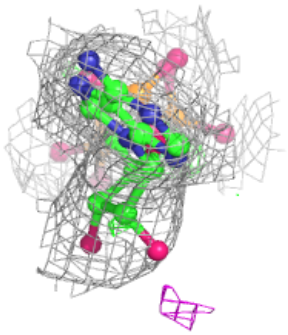


Electron density around ANP H 601:

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

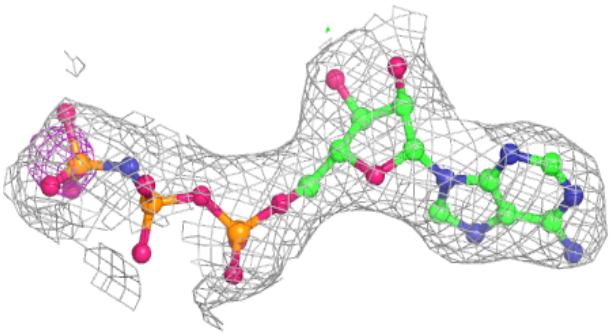


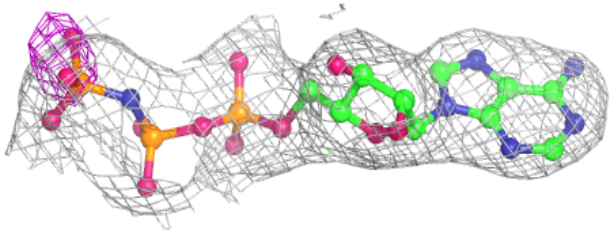


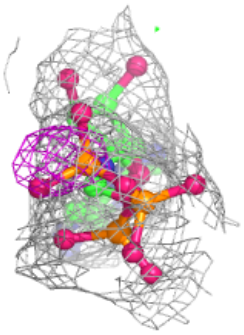


Electron density around ANP G 601:

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

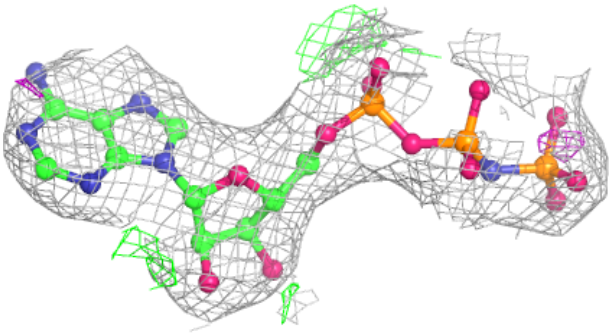


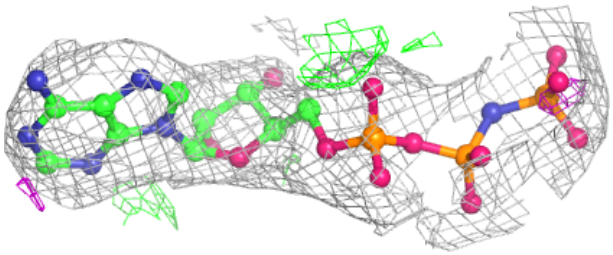


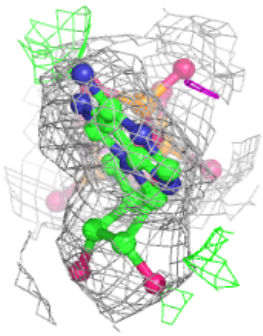


Electron density around ANP F 601:

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

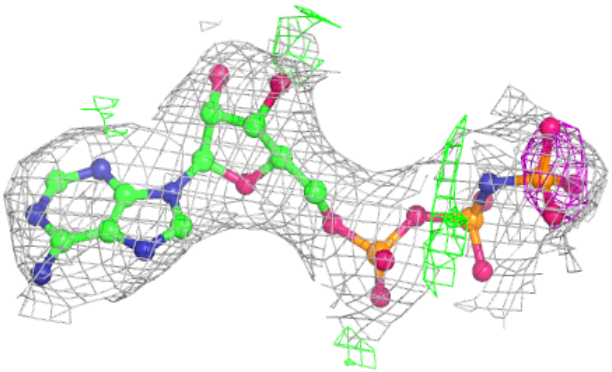


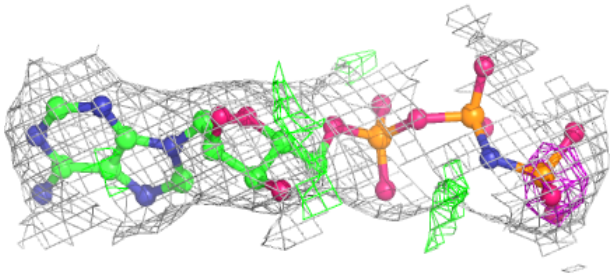


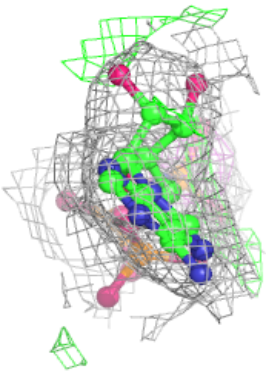


Electron density around ANP A 602:

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

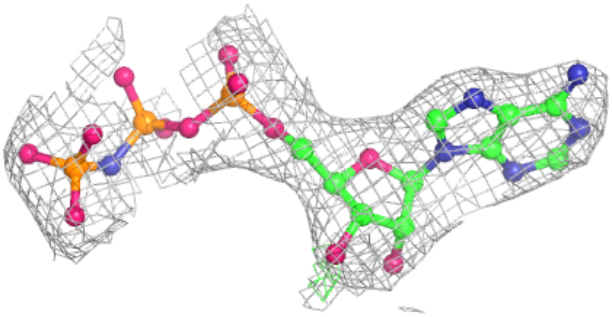


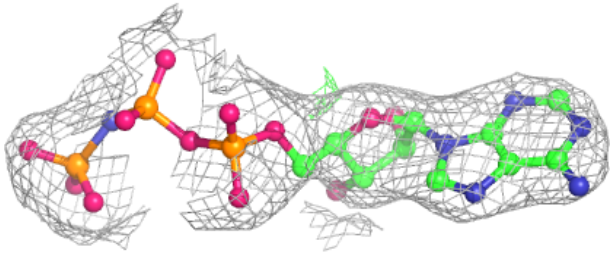


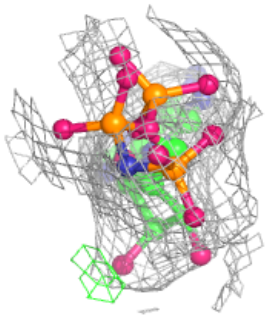


Electron density around ANP B 601:

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

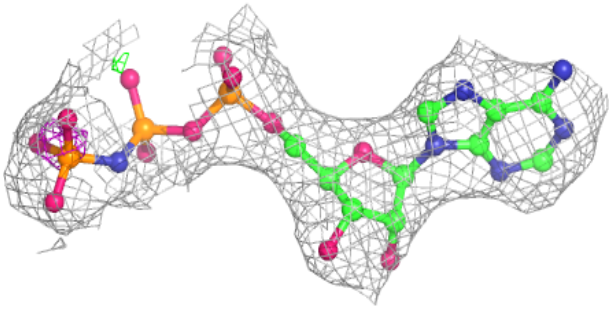


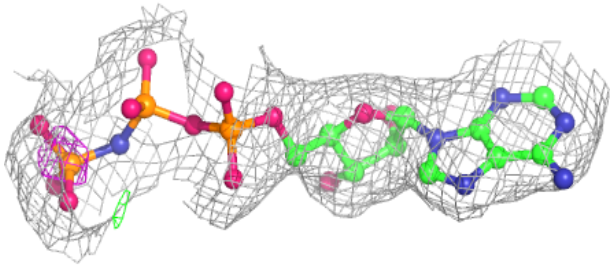


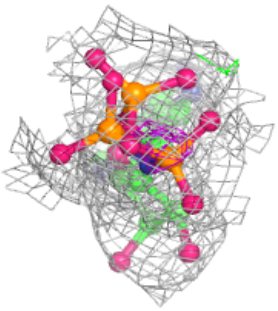


Electron density around ANP C 601:

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

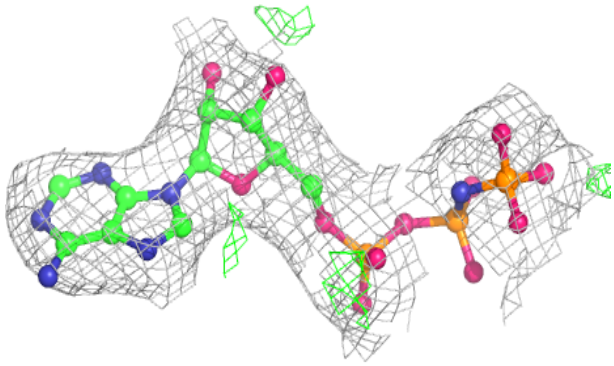


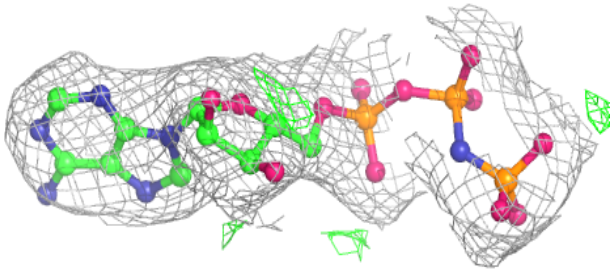


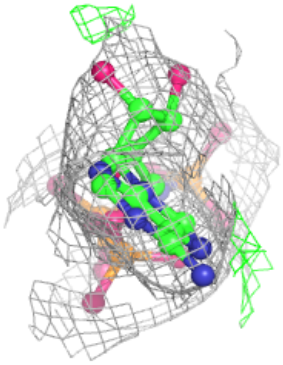


Electron density around ANP G 602:

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

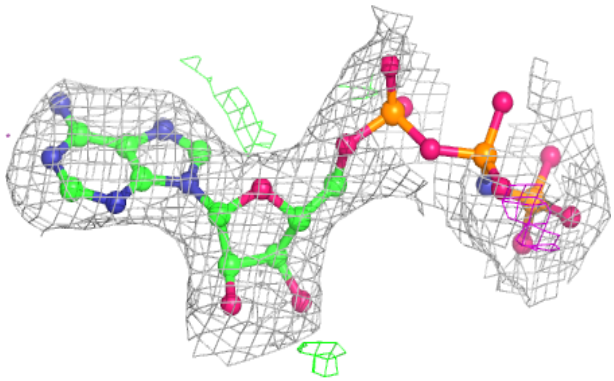


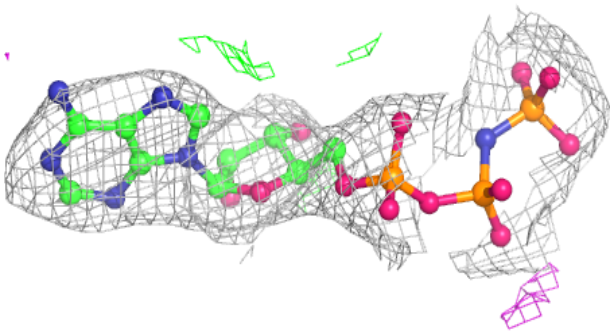


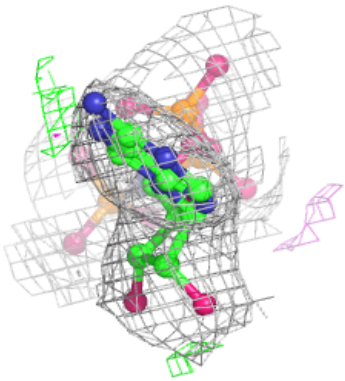


Electron density around ANP I 602:

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

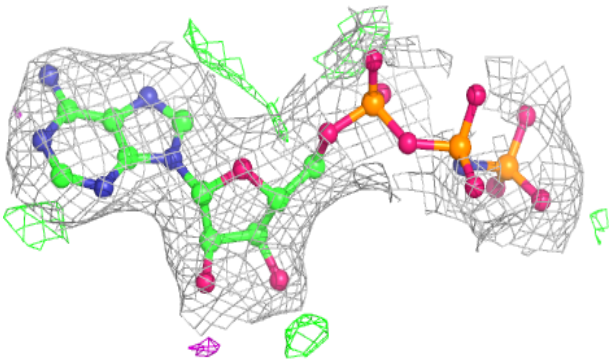


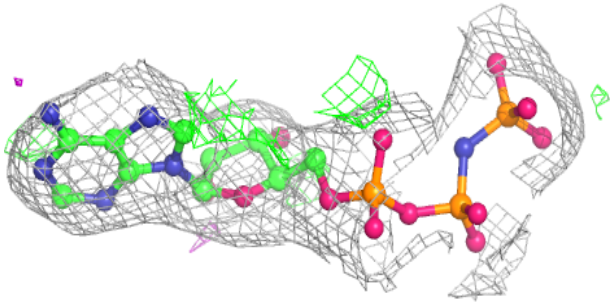


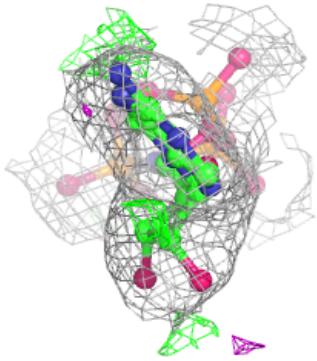


Electron density around ANP F 602:

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

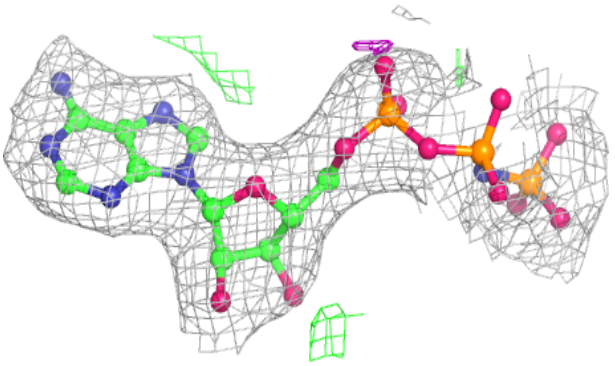


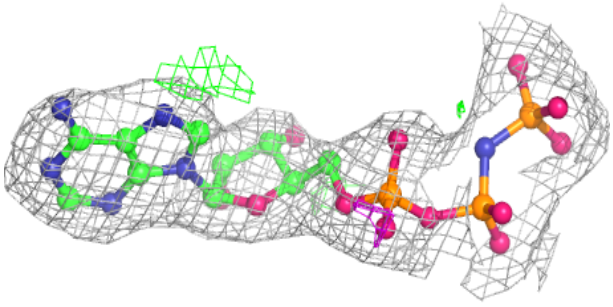


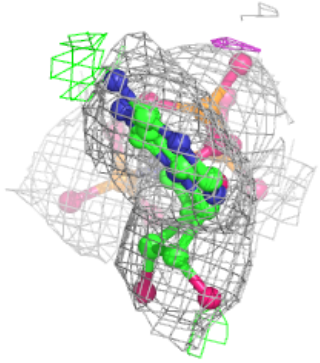


Electron density around ANP K 602:

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

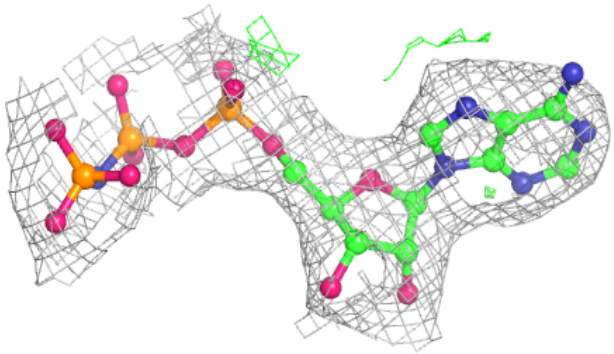


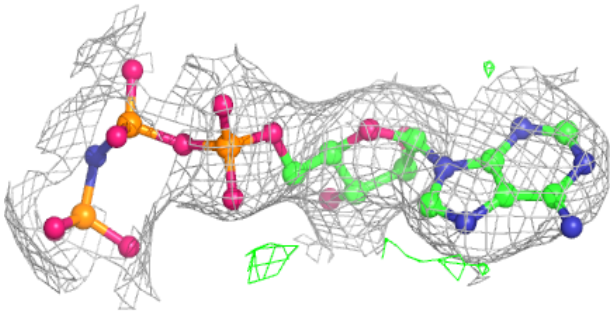


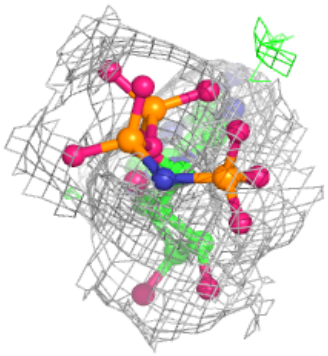


Electron density around ANP C 602:

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

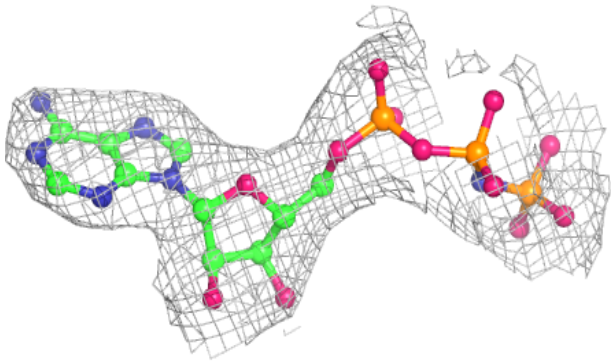


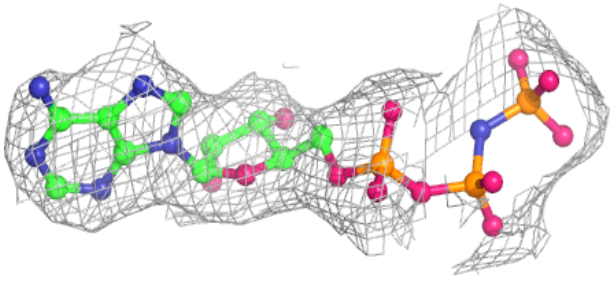


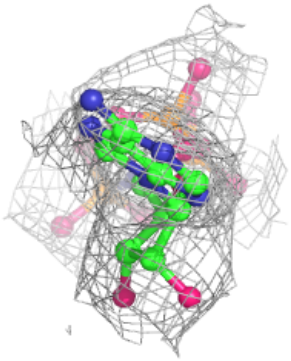


Electron density around ANP H 602:

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

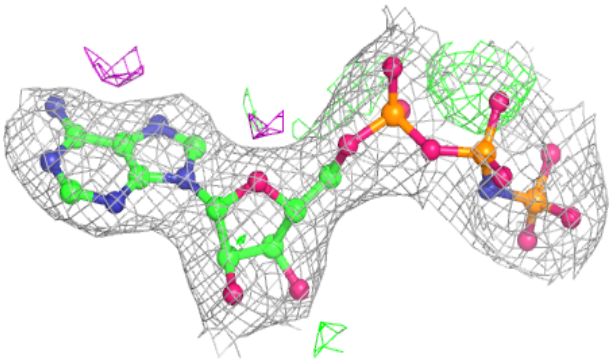


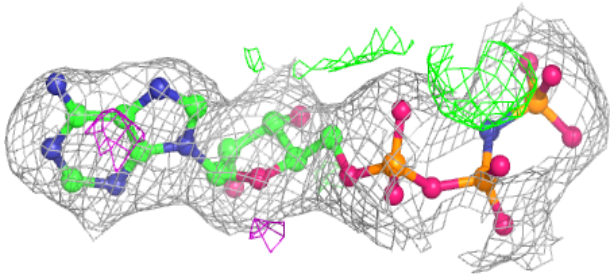


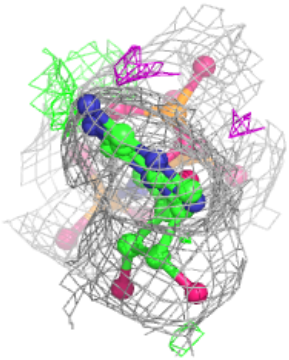


Electron density around ANP B 602:

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

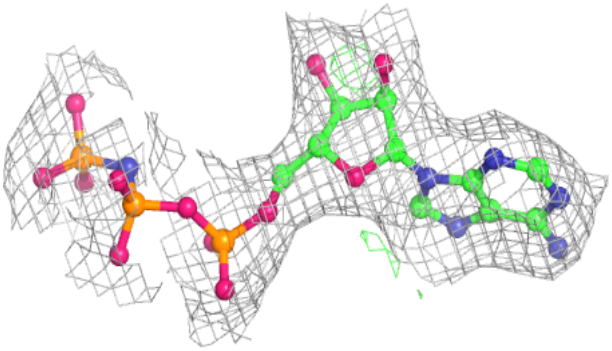


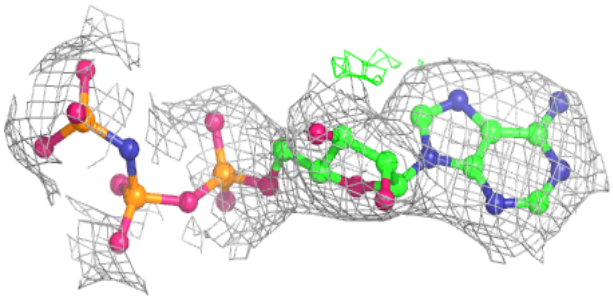


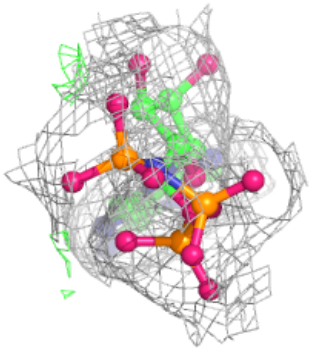


Electron density around ANP D 602:

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

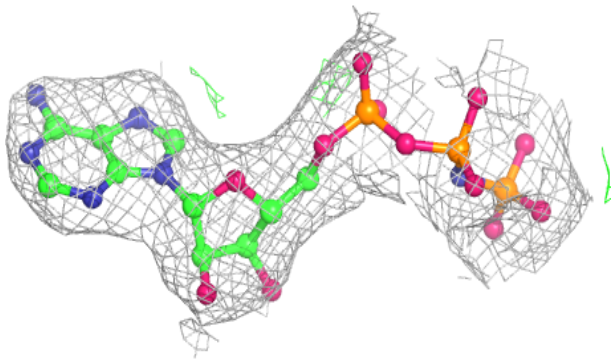


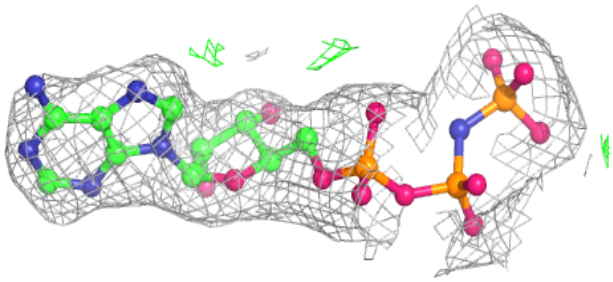


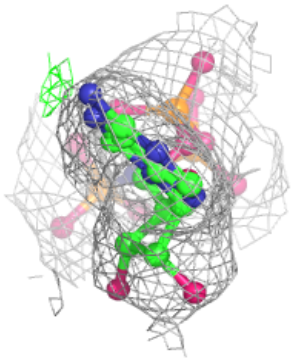


Electron density around ANP J 602:

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

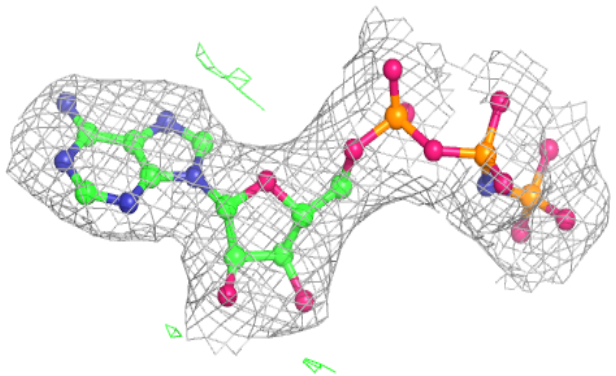


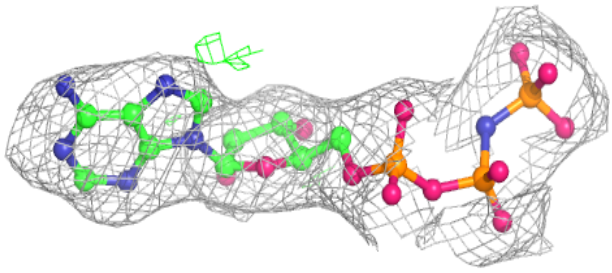


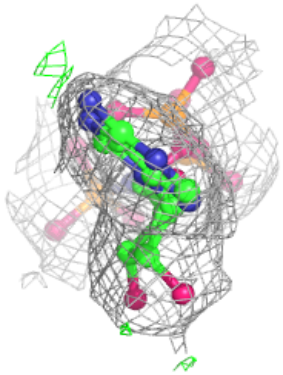


Electron density around ANP L 602:

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

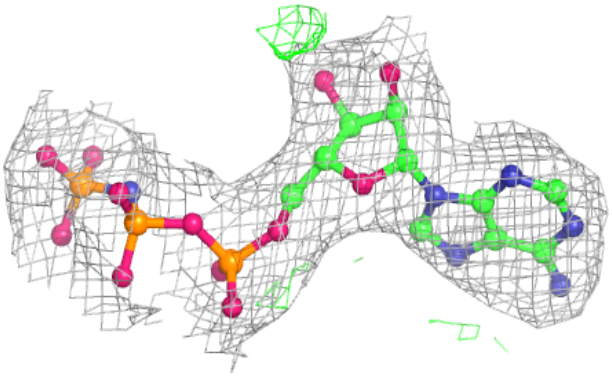


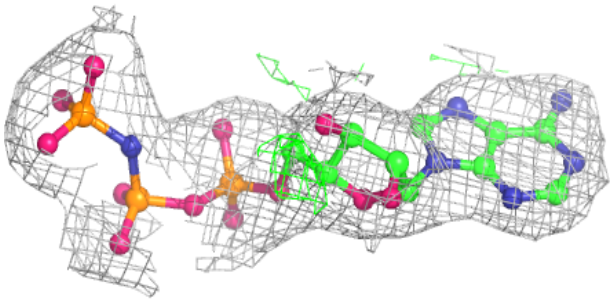


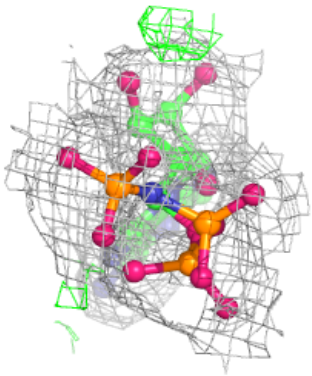


Electron density around ANP E 602:

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

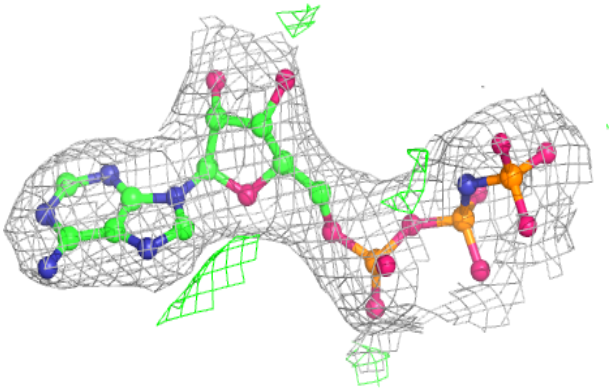


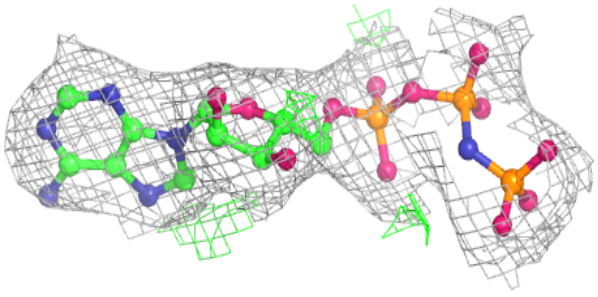


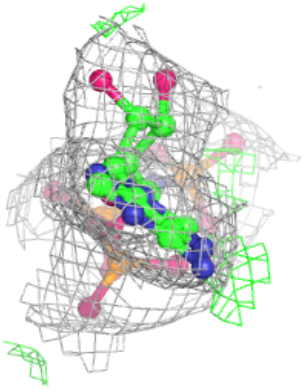


Electron density around ANP A 601:

$2mF_o$-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.