wwPDB X-ray Structure Validation Summary Report (i)

Sep 7, 2023 – 09:09 AM EDT

PDB ID	:	4GKH
Title	:	Crystal structure of the aminoglycoside phosphotransferase APH(3')-Ia, with substrate kanamycin and small molecule inhibitor 1-NA-PP1
Authors	:	Stogios, P.J.; Evdokimova, E.; Wawrzak, Z.; Minasov, G.; Egorova, O.; Di Leo, R.; Shakya, T.; Spanogiannopoulos, P.; Todorovic, N.; Capretta, A.; Wright, G.D.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2012-08-11
Resolution	:	1.86 Å(reported)

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

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

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

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

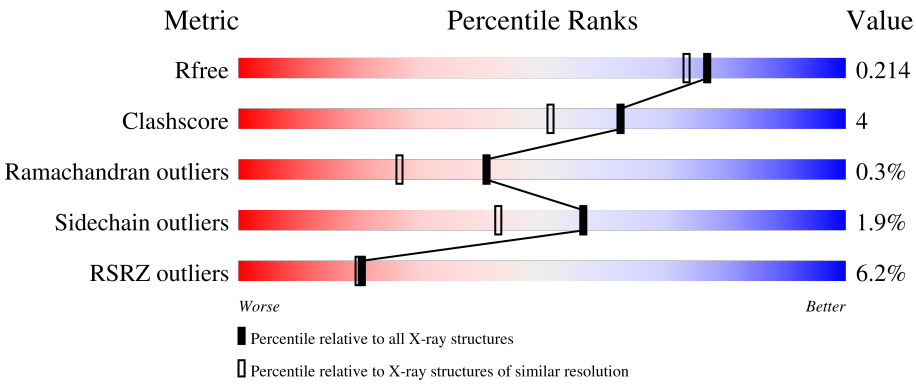
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 1.86 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	272	% 88% 6% 7%
1	B	272	4% 93% 6% •
1	C	272	6% 90% 6% • •

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

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Mol	Chain	Length	Quality of chain
1	D	272	11% 87% 10%
1	E	272	4% 90% 6%
1	F	272	6% 88% 10%
1	G	272	8% 88% 9%
1	H	272	3% 85% 8% 6%
1	I	272	4% 92% 5%
1	J	272	14% 86% 11%
1	K	272	9% 88% 9%
1	L	272	87% 6% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACT	L	304	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 29502 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 Aminoglycoside 3'-phosphotransferase AphA1-IAB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	254	2065	1325	350	380	4	6	0	5	0
1	B	268	2209	1404	385	408	5	7	0	7	0
1	C	267	2164	1377	374	402	5	6	0	3	0
1	D	265	2152	1371	374	396	5	6	0	2	0
1	E	261	2119	1354	364	391	4	6	0	4	0
1	F	271	2220	1412	385	411	5	7	0	7	0
1	G	267	2169	1382	374	401	5	7	0	4	0
1	H	255	2065	1322	350	383	4	6	0	4	0
1	I	266	2152	1369	374	398	5	6	0	2	0
1	J	267	2164	1379	374	399	5	7	0	2	0
1	K	269	2194	1398	379	405	5	7	0	5	0
1	L	254	2052	1314	349	379	4	6	0	2	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP B0VD92
B	0	GLY	-	expression tag	UNP B0VD92
C	0	GLY	-	expression tag	UNP B0VD92
D	0	GLY	-	expression tag	UNP B0VD92
E	0	GLY	-	expression tag	UNP B0VD92

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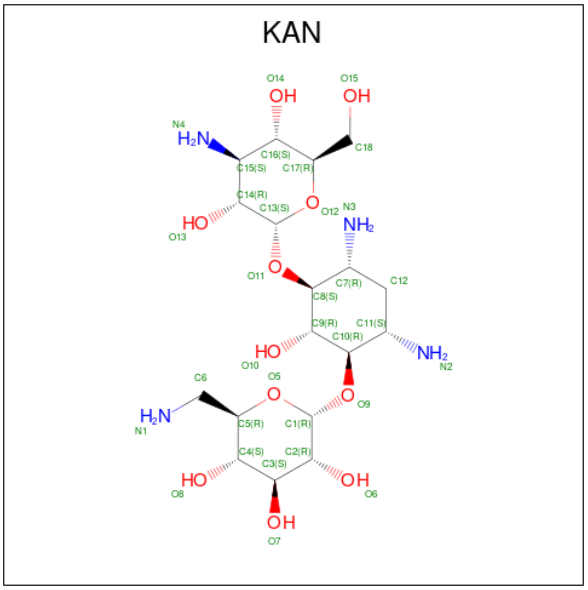
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	GLY	-	expression tag	UNP B0VD92
G	0	GLY	-	expression tag	UNP B0VD92
H	0	GLY	-	expression tag	UNP B0VD92
I	0	GLY	-	expression tag	UNP B0VD92
J	0	GLY	-	expression tag	UNP B0VD92
K	0	GLY	-	expression tag	UNP B0VD92
L	0	GLY	-	expression tag	UNP B0VD92

- Molecule 2 is KANAMYCIN A (three-letter code: KAN) (formula: $C_{18}H_{36}N_4O_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	33	18	4	11	0	0
2	B	1	33	18	4	11	0	0
2	C	1	33	18	4	11	0	0
2	D	1	33	18	4	11	0	0
2	E	1	33	18	4	11	0	0
2	F	1	33	18	4	11	0	0
2	G	1	33	18	4	11	0	0
2	H	1	33	18	4	11	0	0

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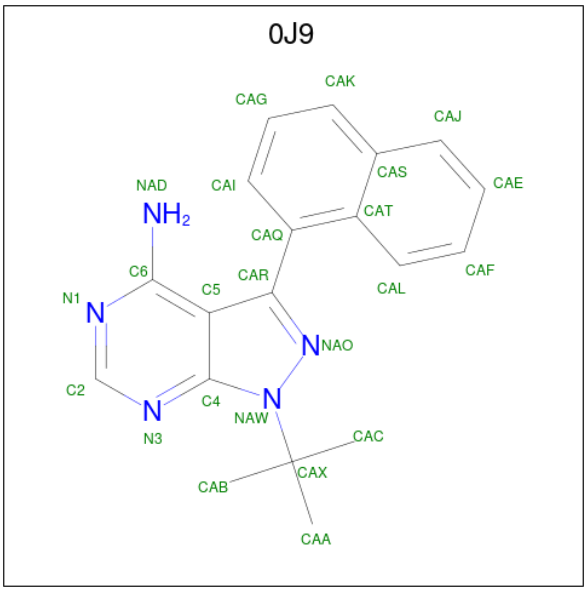
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	I	1	33	18	4	11	0	0
2	J	1	33	18	4	11	0	0
2	K	1	33	18	4	11	0	0
2	L	1	33	18	4	11	0	0

- Molecule 3 is 1-tert-butyl-3-(naphthalen-1-yl)-1H-pyrazolo[3,4-d]pyrimidin-4-amine (three-letter code: 0J9) (formula: $C_{19}H_{19}N_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
3	A	1	24	19	5	0	0
3	B	1	24	19	5	0	0
3	C	1	24	19	5	0	0
3	C	1	24	19	5	0	0
3	E	1	24	19	5	0	0
3	F	1	24	19	5	0	0
3	G	1	24	19	5	0	0

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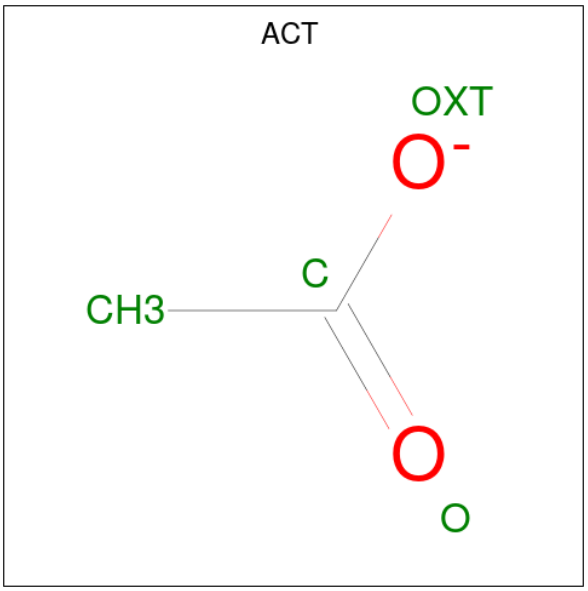
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
3	H	1	24	19	5	0	0
			Total	C	N		
3	I	1	24	19	5	0	0
			Total	C	N		
3	J	1	24	19	5	0	0
			Total	C	N		
3	K	1	24	19	5	0	0
			Total	C	N		
3	L	1	24	19	5	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	A	1	1	1	0	0
			Total	Na		
4	B	2	2	2	0	0
			Total	Na		
4	C	1	1	1	0	0
			Total	Na		
4	E	1	1	1	0	0
			Total	Na		
4	F	2	2	2	0	0
			Total	Na		
4	G	2	2	2	0	0
			Total	Na		
4	H	1	1	1	0	0
			Total	Na		
4	I	1	1	1	0	0
			Total	Na		
4	K	2	2	2	0	0
			Total	Na		
4	L	1	1	1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
5	A	1	4	2	2		0	0
			Total	C	O			
5	A	1	4	2	2		0	0
			Total	C	O			
5	A	1	4	2	2		0	0
			Total	C	O			
5	B	1	4	2	2		0	0
			Total	C	O			
5	B	1	4	2	2		0	0
			Total	C	O			
5	C	1	4	2	2		0	0
			Total	C	O			
5	C	1	4	2	2		0	0
			Total	C	O			
5	C	1	4	2	2		0	0
			Total	C	O			
5	D	1	4	2	2		0	0
			Total	C	O			
5	D	1	4	2	2		0	0
			Total	C	O			
5	D	1	4	2	2		0	0
			Total	C	O			
5	D	1	4	2	2		0	0
			Total	C	O			
5	E	1	4	2	2		0	0
			Total	C	O			
5	E	1	4	2	2		0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	E	1	4	2	2	0	0
5	F	1	4	2	2	0	0
5	F	1	4	2	2	0	0
5	F	1	4	2	2	0	0
5	F	1	4	2	2	0	0
5	G	1	4	2	2	0	0
5	G	1	4	2	2	0	0
5	G	1	4	2	2	0	0
5	H	1	4	2	2	0	0
5	H	1	4	2	2	0	0
5	I	1	4	2	2	0	0
5	I	1	4	2	2	0	0
5	I	1	4	2	2	0	0
5	J	1	4	2	2	0	0
5	K	1	4	2	2	0	0
5	K	1	4	2	2	0	0
5	K	1	4	2	2	0	0
5	L	1	4	2	2	0	0
5	L	1	4	2	2	0	0
5	L	1	4	2	2	0	0
5	L	1	4	2	2	0	0

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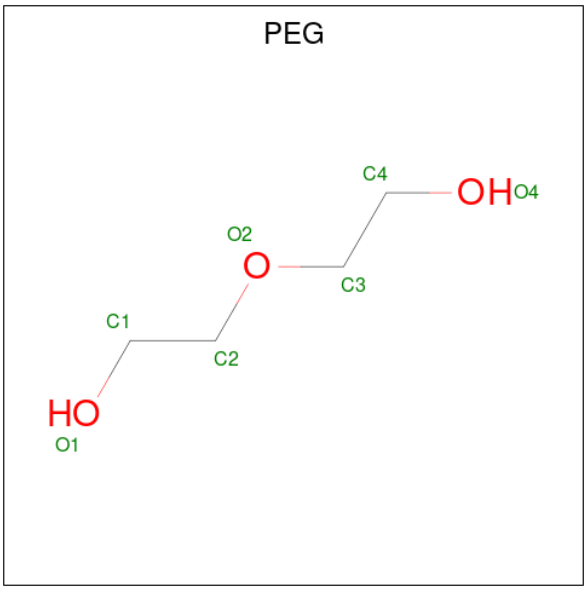
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	L	1	4	2	2	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
6	C	1	1	1	0	0
			Total	Cl		
6	I	1	1	1	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	D	1	7	4	3	0	0
			Total	C	O		
7	D	1	7	4	3	0	0
			Total	C	O		
7	H	1	7	4	3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	261	263	263	0	2

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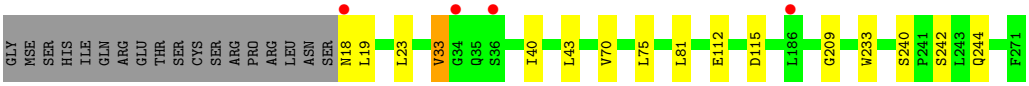
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	B	252	255	255	0	4
			Total	O		
8	C	245	247	247	0	2
			Total	O		
8	D	183	185	185	0	3
			Total	O		
8	E	256	265	265	0	9
			Total	O		
8	F	245	247	247	0	4
			Total	O		
8	G	254	258	258	0	4
			Total	O		
8	H	226	230	230	0	4
			Total	O		
8	I	274	276	276	0	2
			Total	O		
8	J	153	156	156	0	3
			Total	O		
8	K	259	263	263	0	4
			Total	O		
8	L	262	267	267	0	5

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.

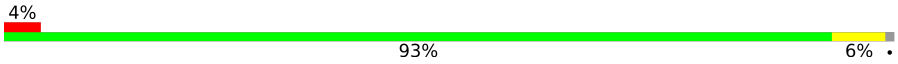
• Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

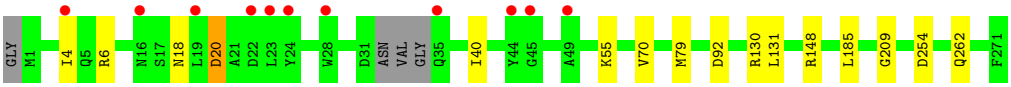
Chain A:



• Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

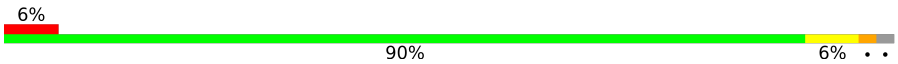
Chain B:

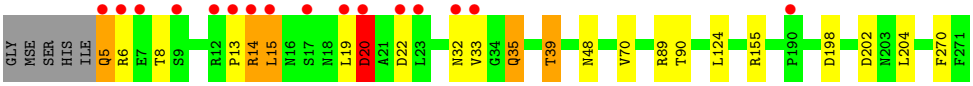




• Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

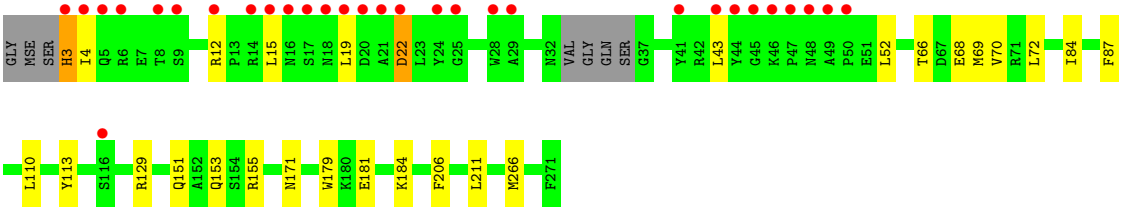
Chain C:





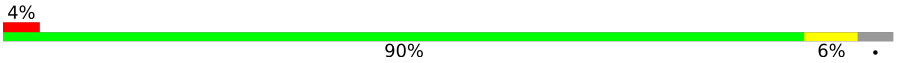
• Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

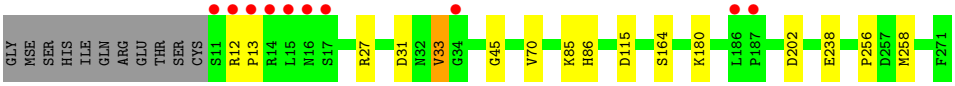
Chain D:



• Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

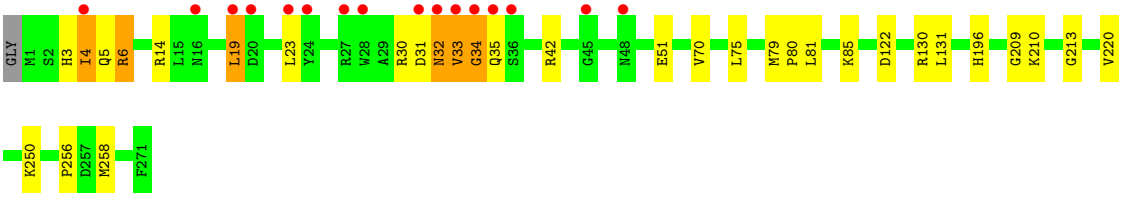
Chain E:





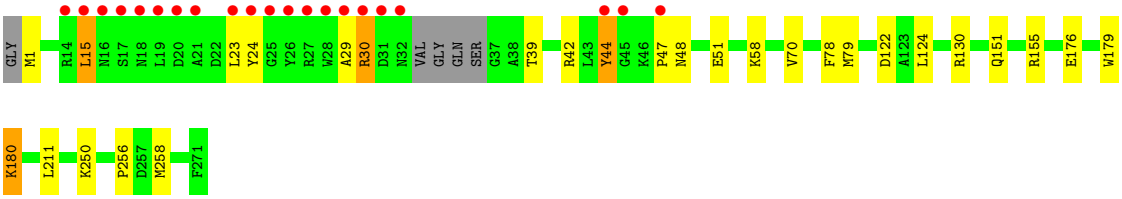
• Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

Chain F:



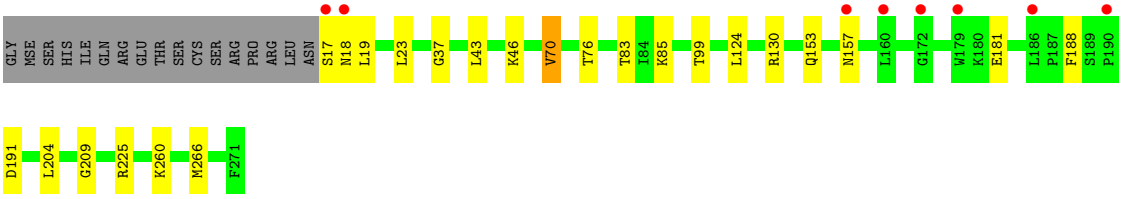
• Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

Chain G:



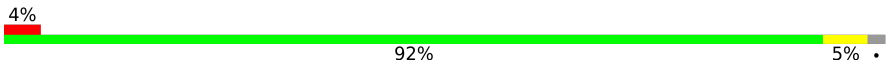
• Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

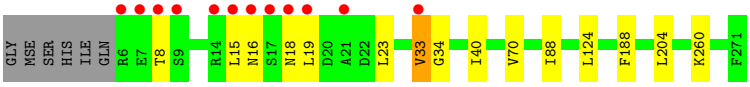
Chain H:



• Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

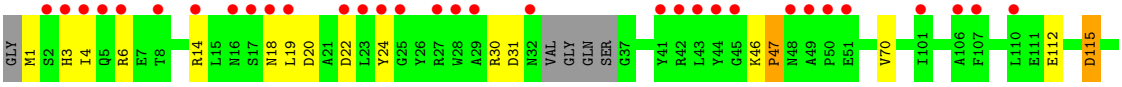
Chain I:

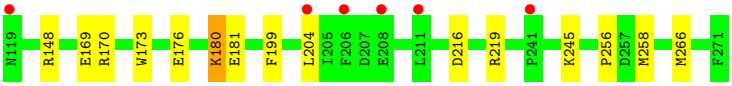




• Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

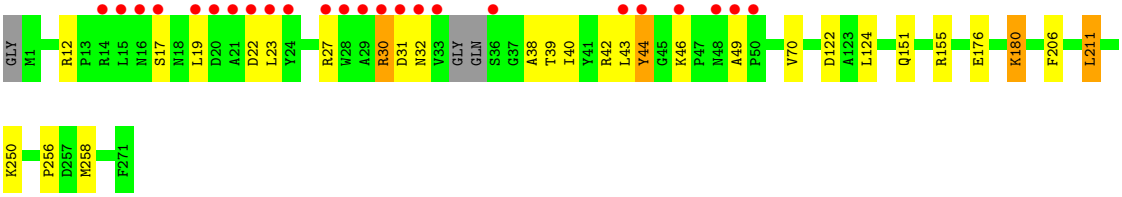
Chain J:





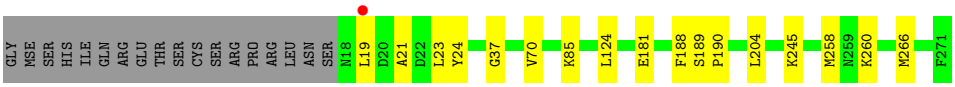
• Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

Chain K:



• Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	97.19Å 97.30Å 112.74Å 102.97° 106.21° 112.66°	Depositor
Resolution (Å)	54.78 – 1.86 80.87 – 1.86	Depositor EDS
% Data completeness (in resolution range)	94.6 (54.78-1.86) 88.4 (80.87-1.86)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 1.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.164 , 0.216 0.163 , 0.214	Depositor DCC
R_{free} test set	13573 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	20.6	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 59.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-h-k-l 0.011 for -k,-h,-l 0.000 for -h,-k,h+k+l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	29502	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 82.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0414e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, 0J9, CL, ACT, NA, KAN

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	0.39	0/2125	0.54	0/2876
1	B	0.36	0/2270	0.51	0/3066
1	C	0.38	0/2219	0.56	0/3001
1	D	0.33	0/2204	0.50	0/2981
1	E	0.39	0/2177	0.54	0/2946
1	F	0.38	0/2287	0.52	0/3091
1	G	0.36	0/2230	0.52	0/3014
1	H	0.37	0/2125	0.53	0/2876
1	I	0.39	0/2207	0.54	0/2984
1	J	0.30	0/2219	0.48	0/2999
1	K	0.38	0/2255	0.51	0/3047
1	L	0.39	0/2106	0.53	0/2850
All	All	0.37	0/26424	0.52	0/35731

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2065	0	2016	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2209	0	2150	10	0
1	C	2164	0	2100	20	0
1	D	2152	0	2089	22	0
1	E	2119	0	2064	12	0
1	F	2220	0	2166	23	0
1	G	2169	0	2113	16	0
1	H	2065	0	2007	15	0
1	I	2152	0	2090	15	0
1	J	2164	0	2106	19	0
1	K	2194	0	2142	19	0
1	L	2052	0	1990	12	0
2	A	33	0	36	0	0
2	B	33	0	36	0	0
2	C	33	0	36	0	0
2	D	33	0	36	0	0
2	E	33	0	36	0	0
2	F	33	0	36	0	0
2	G	33	0	36	0	0
2	H	33	0	36	0	0
2	I	33	0	36	0	0
2	J	33	0	36	0	0
2	K	33	0	36	1	0
2	L	33	0	36	0	0
3	A	24	0	19	5	0
3	B	24	0	19	4	0
3	C	48	0	38	8	0
3	E	24	0	19	5	0
3	F	24	0	19	5	0
3	G	24	0	19	4	0
3	H	24	0	19	4	0
3	I	24	0	19	5	0
3	J	24	0	19	5	0
3	K	24	0	19	4	0
3	L	24	0	19	4	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	2	0	0	0	0
4	L	1	0	0	0	0
5	A	12	0	9	1	0
5	B	8	0	6	1	0
5	C	12	0	9	0	0
5	D	16	0	12	0	0
5	E	12	0	9	1	0
5	F	16	0	12	1	0
5	G	12	0	9	0	0
5	H	8	0	6	1	0
5	I	12	0	9	0	0
5	J	4	0	3	0	0
5	K	12	0	9	1	0
5	L	20	0	15	3	0
6	C	1	0	0	0	0
6	I	1	0	0	0	0
7	D	14	0	16	2	0
7	H	7	0	8	1	0
8	A	263	0	0	2	0
8	B	255	0	0	1	0
8	C	247	0	0	2	0
8	D	185	0	0	2	0
8	E	265	0	0	2	0
8	F	247	0	0	1	0
8	G	258	0	0	0	0
8	H	230	0	0	2	0
8	I	276	0	0	1	0
8	J	156	0	0	1	0
8	K	263	0	0	2	0
8	L	267	0	0	1	0
All	All	29502	0	25825	225	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 4.

The worst 5 of 225 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)
3:G:302:0J9:H12	3:G:302:0J9:H15	1.06	1.07
3:K:302:0J9:H12	3:K:302:0J9:H15	1.16	1.06
3:F:302:0J9:H12	3:F:302:0J9:H15	1.25	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:VAL:HG11	1:D:70[B]:VAL:HG21	1.42	1.01
3:B:302:0J9:H12	3:B:302:0J9:H15	1.26	1.00

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	257/272 (94%)	252 (98%)	4 (2%)	1 (0%)	34	19
1	B	271/272 (100%)	262 (97%)	9 (3%)	0	100	100
1	C	268/272 (98%)	258 (96%)	8 (3%)	2 (1%)	22	9
1	D	263/272 (97%)	252 (96%)	11 (4%)	0	100	100
1	E	263/272 (97%)	257 (98%)	6 (2%)	0	100	100
1	F	276/272 (102%)	269 (98%)	5 (2%)	2 (1%)	22	9
1	G	267/272 (98%)	260 (97%)	6 (2%)	1 (0%)	34	19
1	H	257/272 (94%)	252 (98%)	4 (2%)	1 (0%)	34	19
1	I	266/272 (98%)	260 (98%)	6 (2%)	0	100	100
1	J	265/272 (97%)	255 (96%)	9 (3%)	1 (0%)	34	19
1	K	270/272 (99%)	264 (98%)	6 (2%)	0	100	100
1	L	254/272 (93%)	249 (98%)	4 (2%)	1 (0%)	34	19
All	All	3177/3264 (97%)	3090 (97%)	78 (2%)	9 (0%)	41	26

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	33	VAL
1	G	47	PRO
1	C	20	ASP

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Mol	Chain	Res	Type
1	J	47	PRO
1	F	33	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	226/231 (98%)	225 (100%)	1 (0%)	91	89
1	B	243/231 (105%)	239 (98%)	4 (2%)	62	49
1	C	237/231 (103%)	229 (97%)	8 (3%)	37	19
1	D	235/231 (102%)	231 (98%)	4 (2%)	60	47
1	E	232/231 (100%)	228 (98%)	4 (2%)	60	47
1	F	245/231 (106%)	239 (98%)	6 (2%)	49	33
1	G	239/231 (104%)	231 (97%)	8 (3%)	38	21
1	H	226/231 (98%)	223 (99%)	3 (1%)	69	58
1	I	235/231 (102%)	233 (99%)	2 (1%)	78	72
1	J	237/231 (103%)	228 (96%)	9 (4%)	33	16
1	K	242/231 (105%)	235 (97%)	7 (3%)	42	26
1	L	223/231 (96%)	223 (100%)	0	100	100
All	All	2820/2772 (102%)	2764 (98%)	56 (2%)	57	40

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	15	LEU
1	K	211	LEU
1	H	70[A]	VAL
1	K	180	LYS
1	K	17	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	16	ASN
1	I	18	ASN
1	D	16	ASN
1	E	73	ASN
1	F	3	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 79 ligands modelled in this entry, 16 are monoatomic - leaving 63 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	$\#\|Z\| > 2$
5	ACT	B	305	-	3,3,3	0.69	0	3,3,3	1.47	0
7	PEG	D	307	-	6,6,6	1.09	0	5,5,5	1.58	1 (20%)
5	ACT	D	304	-	3,3,3	0.76	0	3,3,3	1.32	0
5	ACT	E	306	-	3,3,3	0.82	0	3,3,3	1.11	0
5	ACT	C	306	-	3,3,3	0.75	0	3,3,3	1.40	0
5	ACT	K	305	-	3,3,3	0.79	0	3,3,3	1.24	0
5	ACT	F	305	-	3,3,3	0.73	0	3,3,3	1.37	0
3	0J9	J	302	-	22,27,27	1.50	3 (13%)	27,41,41	1.88	5 (18%)
3	0J9	I	302	-	22,27,27	1.60	4 (18%)	27,41,41	1.93	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	0J9	F	302	-	22,27,27	1.54	3 (13%)	27,41,41	1.90	4 (14%)
2	KAN	C	301	-	35,35,35	0.75	0	46,52,52	1.37	6 (13%)
5	ACT	A	304	-	3,3,3	0.77	0	3,3,3	1.17	0
3	0J9	E	302	-	22,27,27	1.59	3 (13%)	27,41,41	1.92	5 (18%)
3	0J9	C	302	-	22,27,27	1.47	3 (13%)	27,41,41	1.88	4 (14%)
3	0J9	H	302	-	22,27,27	1.66	4 (18%)	27,41,41	1.86	3 (11%)
5	ACT	F	308	-	3,3,3	0.89	0	3,3,3	1.43	0
5	ACT	G	306	4	3,3,3	0.78	0	3,3,3	1.34	0
3	0J9	C	303	-	22,27,27	1.57	3 (13%)	27,41,41	1.85	4 (14%)
2	KAN	L	301	-	35,35,35	0.81	2 (5%)	46,52,52	1.46	4 (8%)
7	PEG	H	306	-	6,6,6	0.94	0	5,5,5	3.11	3 (60%)
2	KAN	J	301	-	35,35,35	0.76	1 (2%)	46,52,52	1.28	4 (8%)
5	ACT	A	306	-	3,3,3	0.71	0	3,3,3	1.55	0
2	KAN	G	301	-	35,35,35	0.85	1 (2%)	46,52,52	1.37	5 (10%)
5	ACT	G	307	-	3,3,3	0.82	0	3,3,3	1.32	0
2	KAN	A	301	-	35,35,35	0.81	1 (2%)	46,52,52	1.38	5 (10%)
5	ACT	C	308	-	3,3,3	0.76	0	3,3,3	1.33	0
5	ACT	D	305	-	3,3,3	0.77	0	3,3,3	1.36	0
5	ACT	F	307	-	3,3,3	0.82	0	3,3,3	1.39	0
5	ACT	K	307	-	3,3,3	0.73	0	3,3,3	1.53	0
5	ACT	G	305	-	3,3,3	0.76	0	3,3,3	1.37	0
3	0J9	L	302	-	22,27,27	1.60	4 (18%)	27,41,41	1.89	4 (14%)
5	ACT	L	305	4	3,3,3	0.74	0	3,3,3	1.47	0
3	0J9	G	302	-	22,27,27	1.52	3 (13%)	27,41,41	1.92	4 (14%)
5	ACT	D	303	-	3,3,3	0.72	0	3,3,3	1.48	0
2	KAN	E	301	-	35,35,35	0.69	0	46,52,52	1.31	6 (13%)
5	ACT	E	305	-	3,3,3	0.80	0	3,3,3	1.44	0
5	ACT	B	306	-	3,3,3	0.87	0	3,3,3	1.31	0
5	ACT	I	307	-	3,3,3	0.78	0	3,3,3	1.26	0
2	KAN	H	301	-	35,35,35	0.81	0	46,52,52	1.33	7 (15%)
5	ACT	H	305	4	3,3,3	0.74	0	3,3,3	1.33	0
2	KAN	D	301	-	35,35,35	0.77	0	46,52,52	1.35	4 (8%)
5	ACT	D	302	-	3,3,3	0.76	0	3,3,3	1.33	0
3	0J9	A	302	-	22,27,27	1.57	4 (18%)	27,41,41	1.82	3 (11%)
3	0J9	K	302	-	22,27,27	1.53	3 (13%)	27,41,41	1.92	4 (14%)
5	ACT	A	305	-	3,3,3	0.84	0	3,3,3	1.23	0
5	ACT	H	304	-	3,3,3	0.76	0	3,3,3	1.22	0
5	ACT	I	305	4	3,3,3	0.78	0	3,3,3	1.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	PEG	D	306	-	6,6,6	1.01	0	5,5,5	2.28	3 (60%)
5	ACT	I	306	-	3,3,3	0.74	0	3,3,3	1.28	0
2	KAN	B	301	-	35,35,35	0.89	1 (2%)	46,52,52	1.48	7 (15%)
5	ACT	F	306	-	3,3,3	0.76	0	3,3,3	1.30	0
5	ACT	E	304	-	3,3,3	0.68	0	3,3,3	1.48	0
5	ACT	K	306	-	3,3,3	0.77	0	3,3,3	1.27	0
5	ACT	J	303	-	3,3,3	0.80	0	3,3,3	1.28	0
5	ACT	L	308	-	3,3,3	0.74	0	3,3,3	1.35	0
5	ACT	L	306	-	3,3,3	0.75	0	3,3,3	1.44	0
2	KAN	K	301	-	35,35,35	0.84	1 (2%)	46,52,52	1.38	8 (17%)
3	0J9	B	302	-	22,27,27	1.50	3 (13%)	27,41,41	1.94	5 (18%)
2	KAN	I	301	-	35,35,35	0.86	1 (2%)	46,52,52	1.18	5 (10%)
5	ACT	L	307	-	3,3,3	0.76	0	3,3,3	1.29	0
5	ACT	C	307	4	3,3,3	0.80	0	3,3,3	1.22	0
2	KAN	F	301	-	35,35,35	0.93	2 (5%)	46,52,52	1.41	4 (8%)
5	ACT	L	304	-	3,3,3	0.73	0	3,3,3	1.56	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
7	PEG	D	307	-	-	1/4/4/4	-
3	0J9	J	302	-	-	2/10/10/10	0/4/4/4
3	0J9	I	302	-	-	1/10/10/10	0/4/4/4
3	0J9	F	302	-	-	2/10/10/10	0/4/4/4
2	KAN	C	301	-	-	2/12/72/72	0/3/3/3
3	0J9	E	302	-	-	1/10/10/10	0/4/4/4
3	0J9	C	302	-	-	1/10/10/10	0/4/4/4
3	0J9	H	302	-	-	1/10/10/10	0/4/4/4
3	0J9	C	303	-	-	1/10/10/10	0/4/4/4
2	KAN	L	301	-	-	2/12/72/72	0/3/3/3
7	PEG	H	306	-	-	2/4/4/4	-
2	KAN	J	301	-	-	2/12/72/72	0/3/3/3
2	KAN	G	301	-	-	2/12/72/72	0/3/3/3
2	KAN	A	301	-	-	2/12/72/72	0/3/3/3
3	0J9	L	302	-	-	1/10/10/10	0/4/4/4
3	0J9	G	302	-	-	2/10/10/10	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KAN	E	301	-	-	1/12/72/72	0/3/3/3
2	KAN	H	301	-	-	2/12/72/72	0/3/3/3
2	KAN	D	301	-	-	2/12/72/72	0/3/3/3
7	PEG	D	306	-	-	0/4/4/4	-
3	0J9	A	302	-	-	1/10/10/10	0/4/4/4
3	0J9	K	302	-	-	3/10/10/10	0/4/4/4
2	KAN	B	301	-	-	1/12/72/72	0/3/3/3
2	KAN	K	301	-	-	2/12/72/72	0/3/3/3
3	0J9	B	302	-	-	2/10/10/10	0/4/4/4
2	KAN	I	301	-	-	2/12/72/72	0/3/3/3
2	KAN	F	301	-	-	2/12/72/72	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	302	0J9	C2-N3	5.15	1.40	1.32
3	H	302	0J9	C2-N3	4.56	1.39	1.32
3	F	302	0J9	C2-N3	4.55	1.39	1.32
3	C	303	0J9	C2-N3	4.47	1.39	1.32
3	A	302	0J9	C2-N3	4.45	1.39	1.32

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	302	0J9	N3-C2-N1	-7.76	116.56	128.68
3	I	302	0J9	N3-C2-N1	-7.75	116.56	128.68
3	B	302	0J9	N3-C2-N1	-7.70	116.64	128.68
3	A	302	0J9	N3-C2-N1	-7.65	116.72	128.68
3	L	302	0J9	N3-C2-N1	-7.65	116.73	128.68

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	0J9	CAI-CAQ-CAR-NAO
3	B	302	0J9	CAT-CAQ-CAR-C5
3	C	302	0J9	CAI-CAQ-CAR-NAO
3	C	303	0J9	CAI-CAQ-CAR-NAO
3	E	302	0J9	CAI-CAQ-CAR-NAO

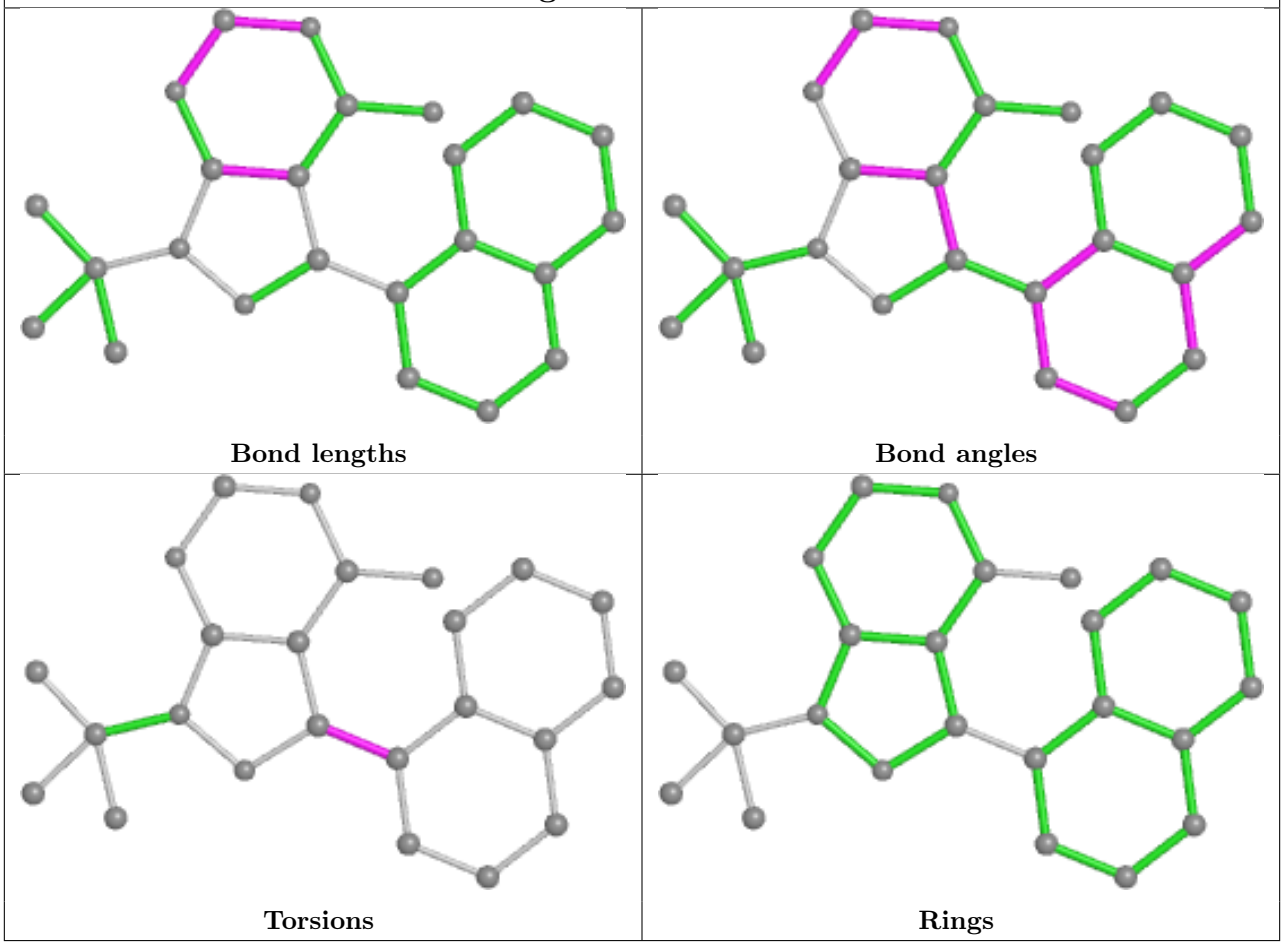
There are no ring outliers.

24 monomers are involved in 65 short contacts:

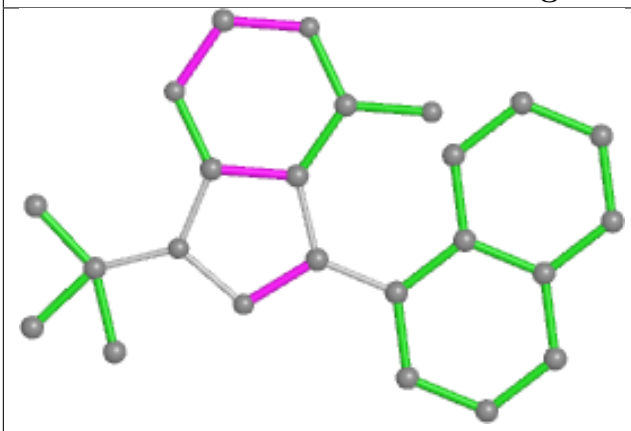
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	305	ACT	1	0
7	D	307	PEG	1	0
5	E	306	ACT	1	0
5	F	305	ACT	1	0
3	J	302	0J9	5	0
3	I	302	0J9	5	0
3	F	302	0J9	5	0
5	A	304	ACT	1	0
3	E	302	0J9	5	0
3	C	302	0J9	4	0
3	H	302	0J9	4	0
3	C	303	0J9	4	0
7	H	306	PEG	1	0
5	K	307	ACT	1	0
3	L	302	0J9	4	0
3	G	302	0J9	4	0
5	H	305	ACT	1	0
3	A	302	0J9	5	0
3	K	302	0J9	4	0
7	D	306	PEG	1	0
2	K	301	KAN	1	0
3	B	302	0J9	4	0
5	L	307	ACT	1	0
5	L	304	ACT	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.

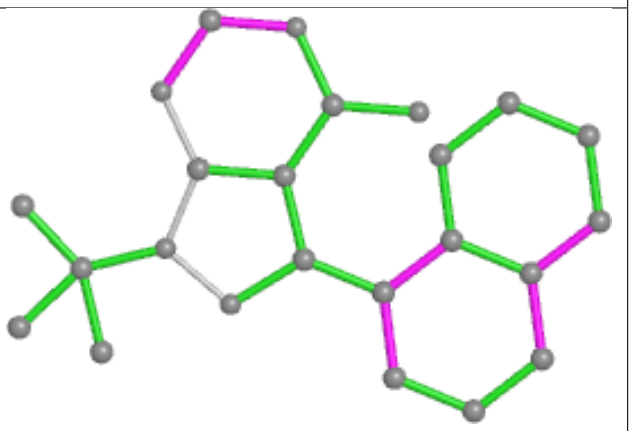
Ligand 0J9 J 302



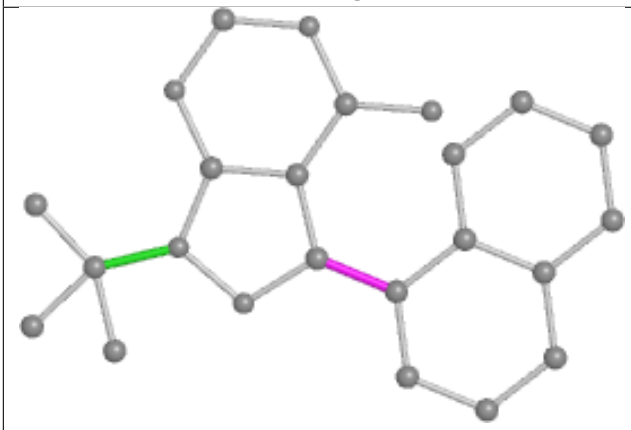
Ligand 0J9 I 302



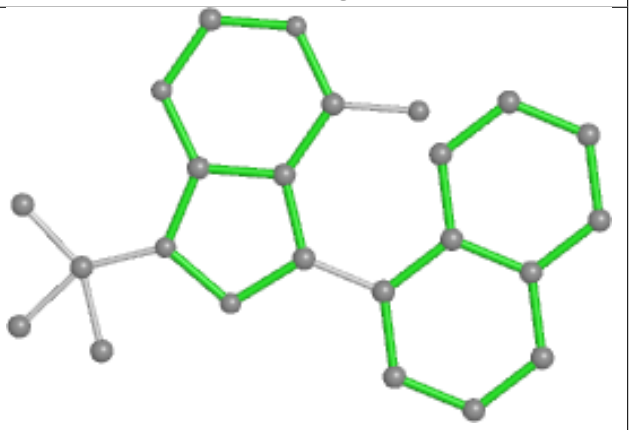
Bond lengths



Bond angles

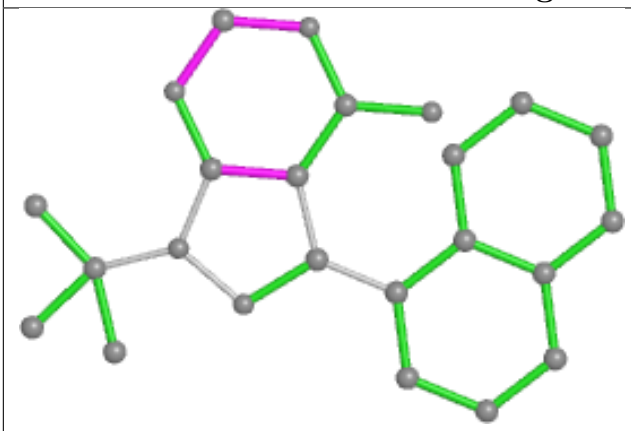


Torsions

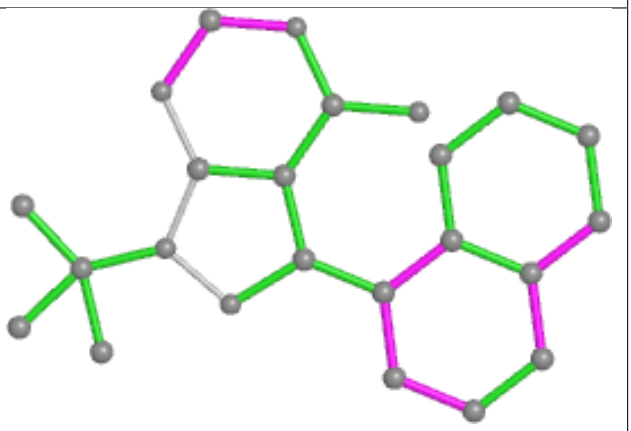


Rings

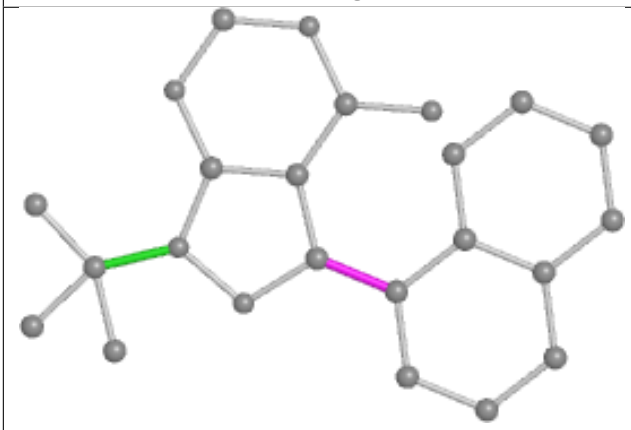
Ligand 0J9 F 302



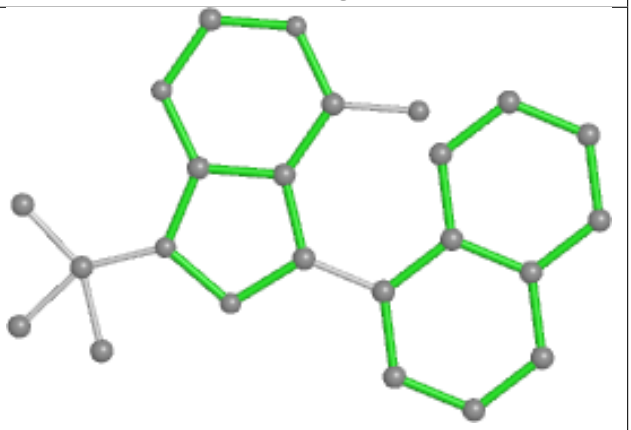
Bond lengths



Bond angles

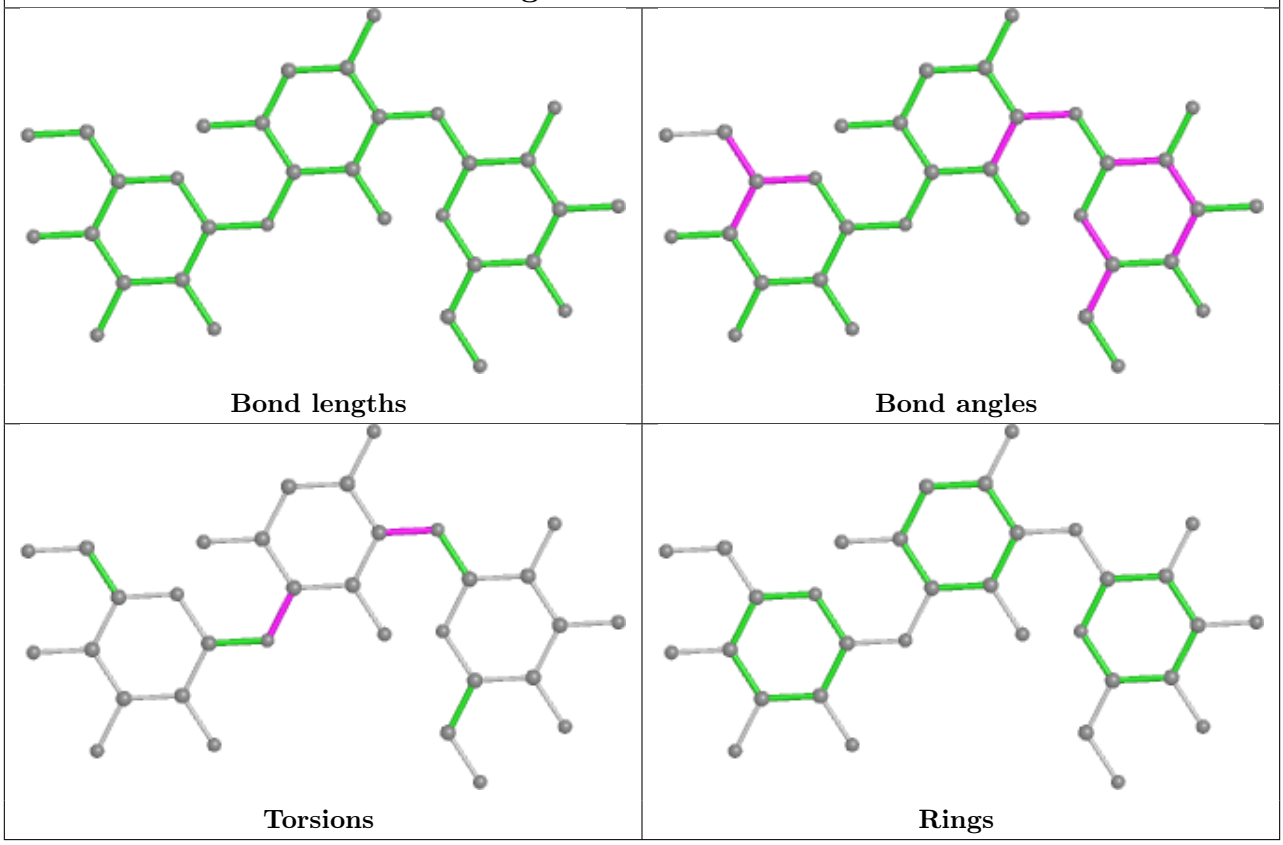


Torsions

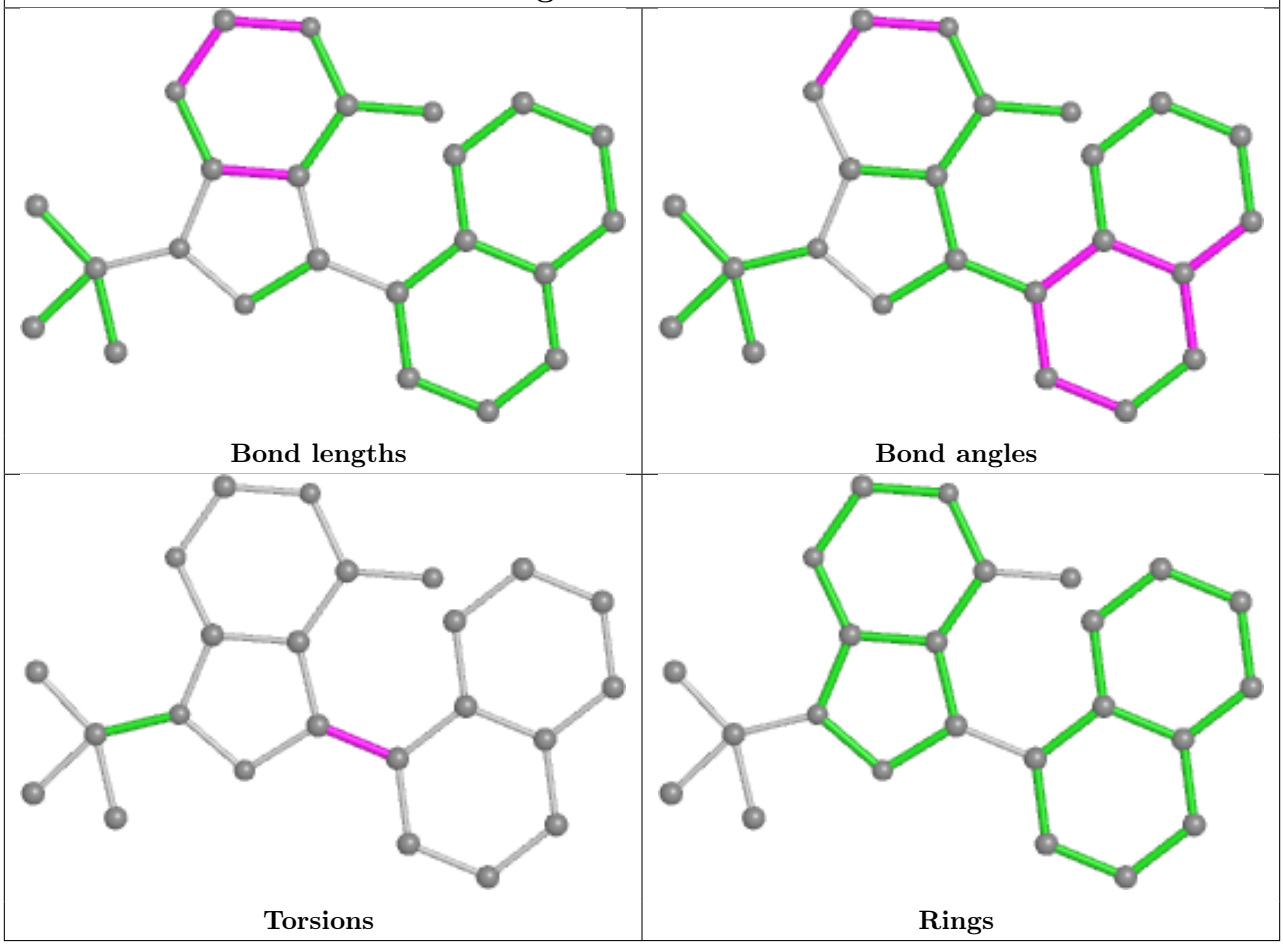


Rings

Ligand KAN C 301



Ligand 0J9 E 302



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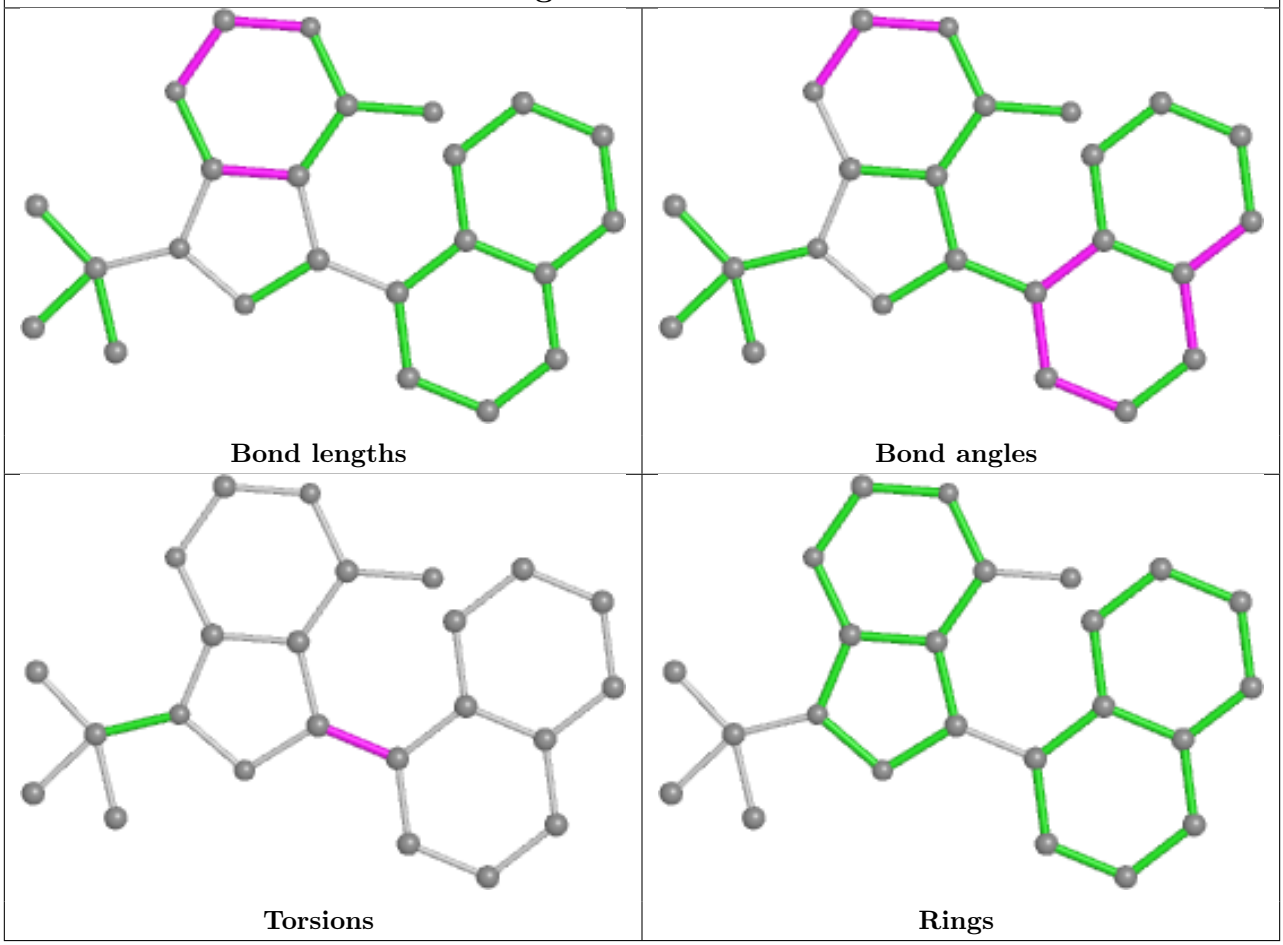
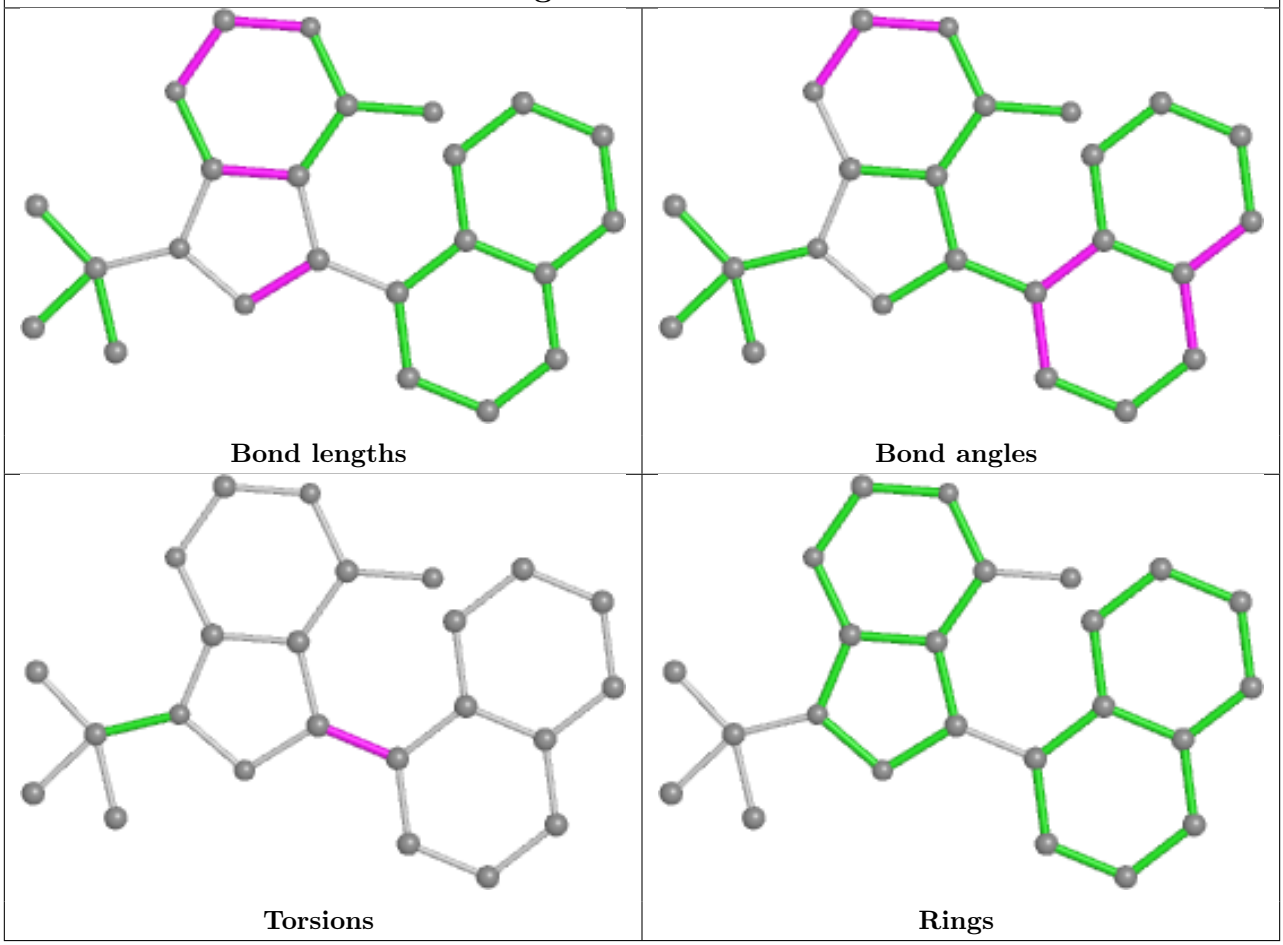


Ligand 0J9 H 302



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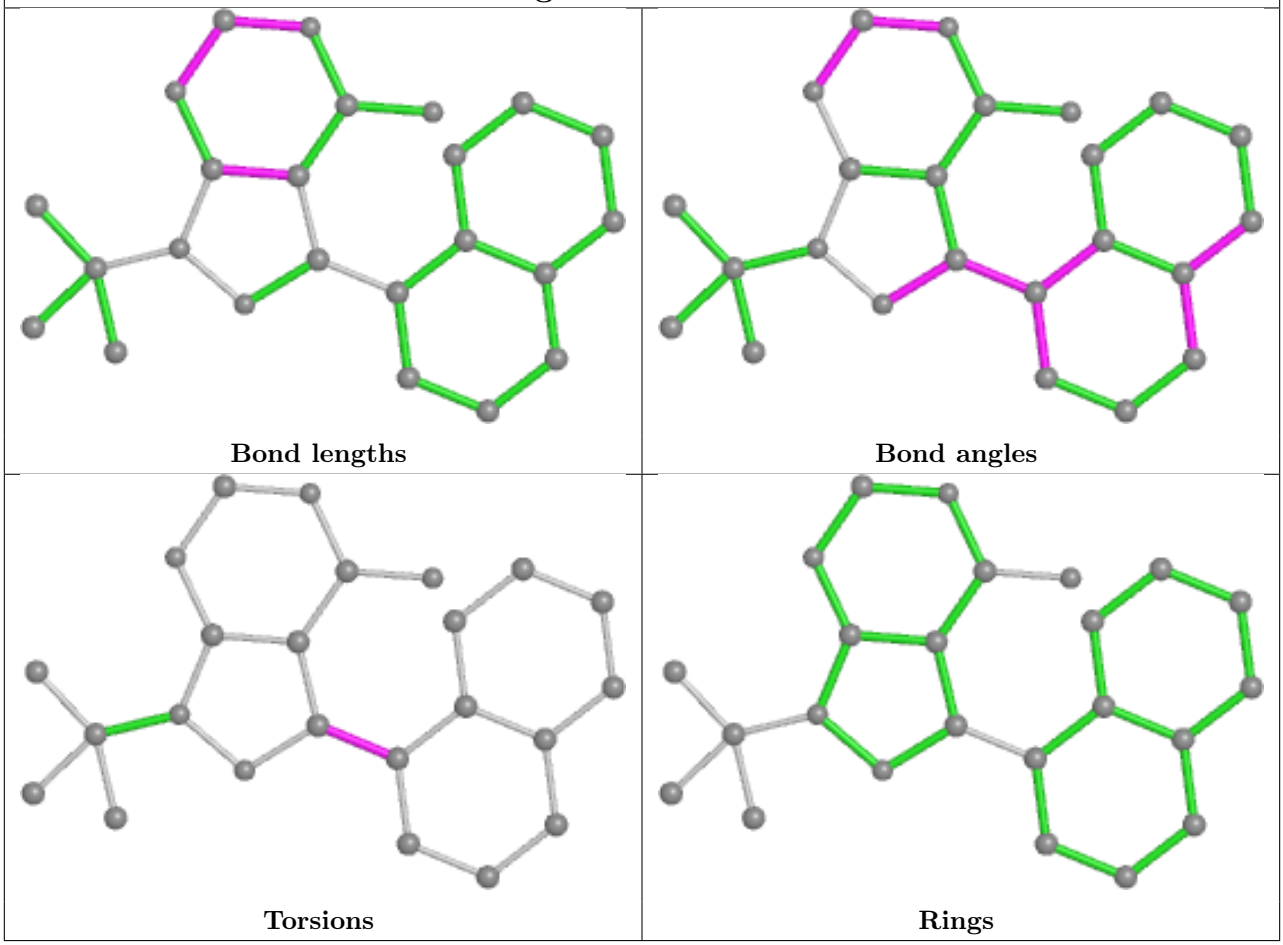

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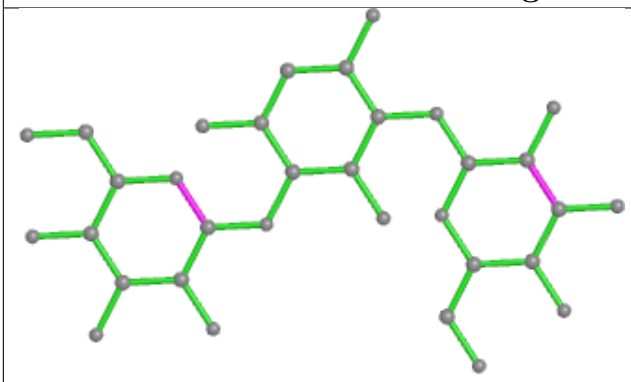
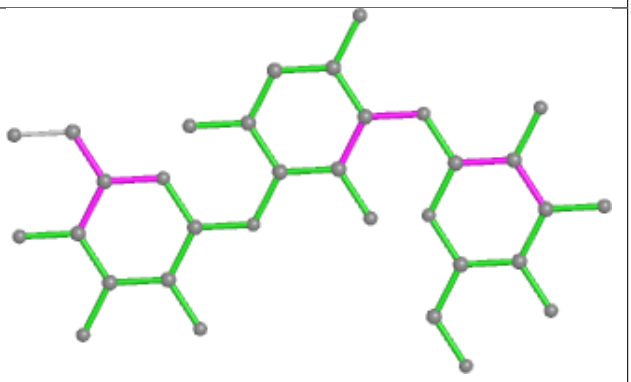


Bond lengths



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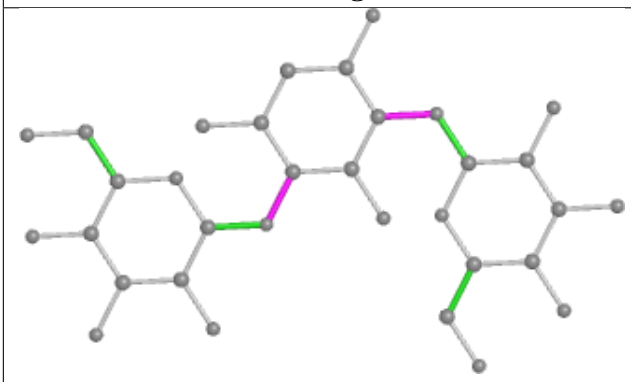
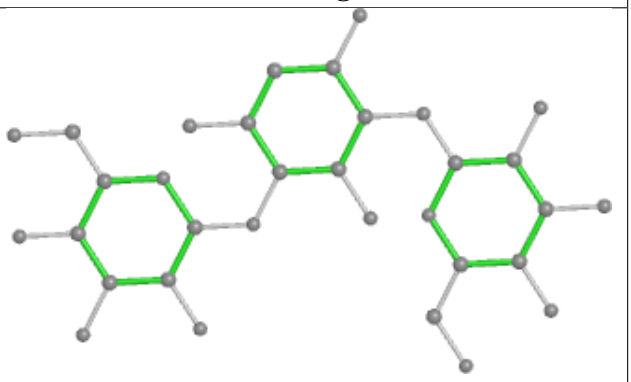
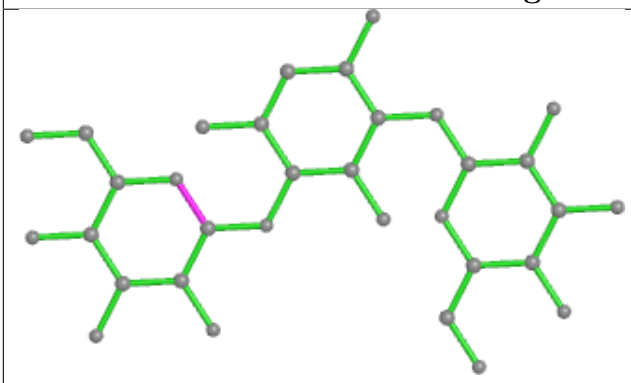


Torsions



Rings

Ligand KAN J 301



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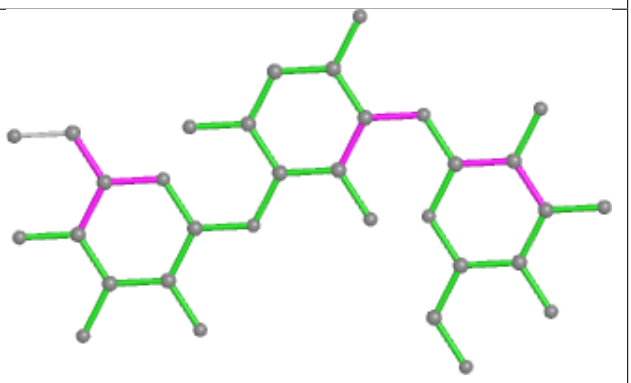

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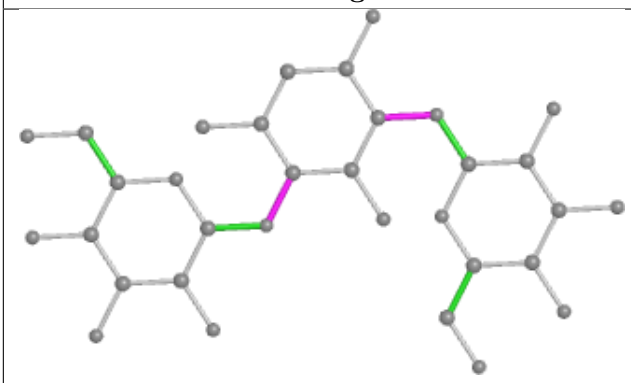

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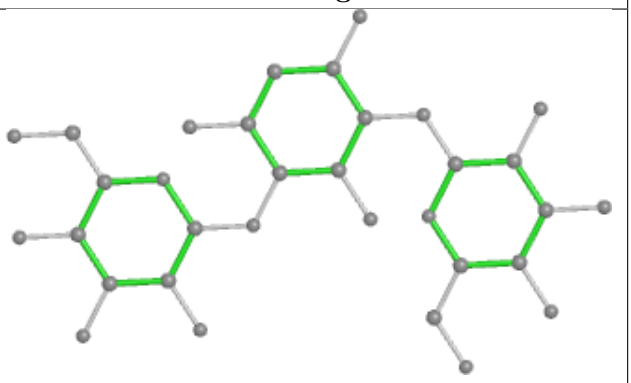

Rings

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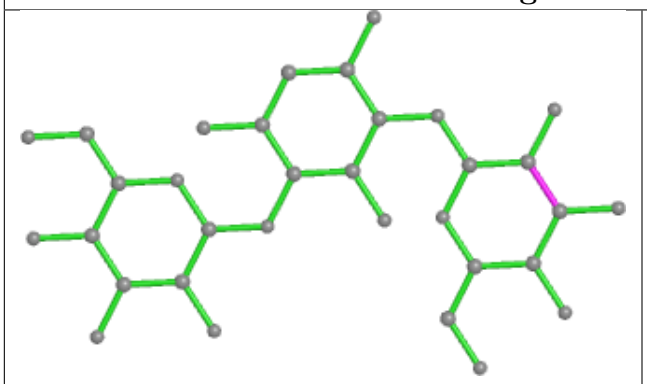

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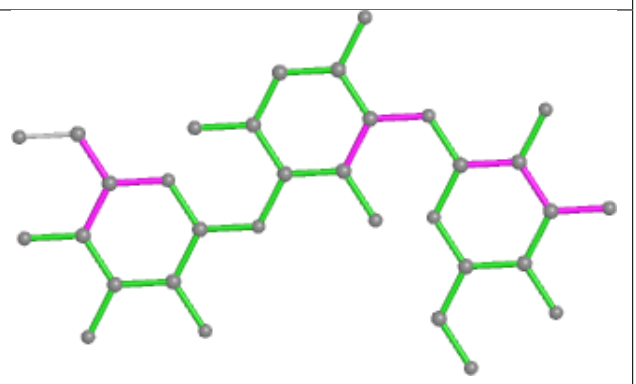

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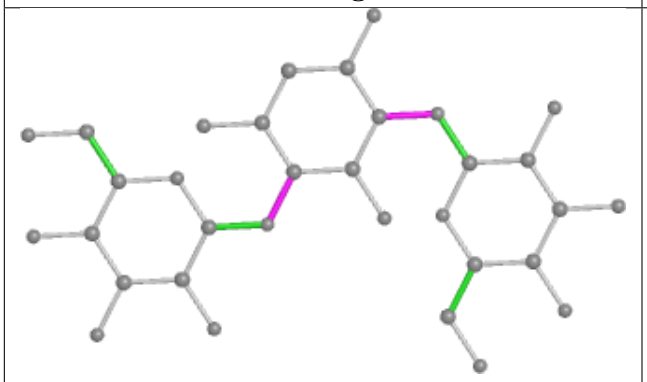

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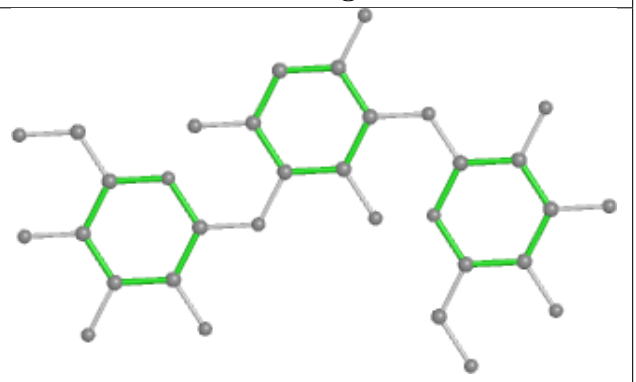

Rings

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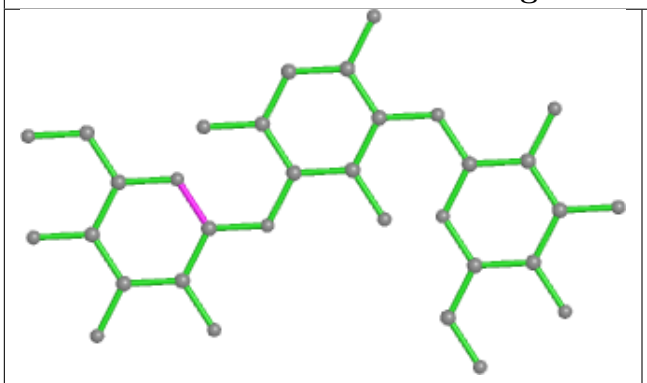

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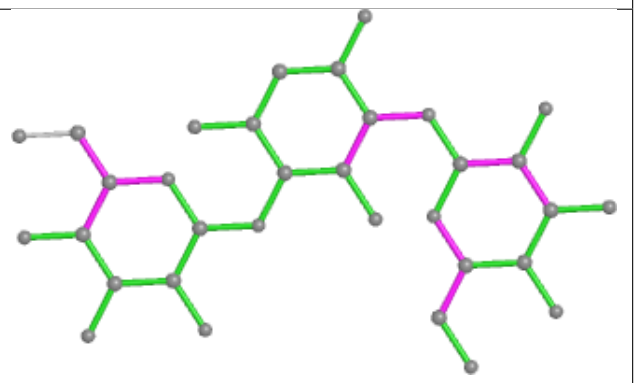

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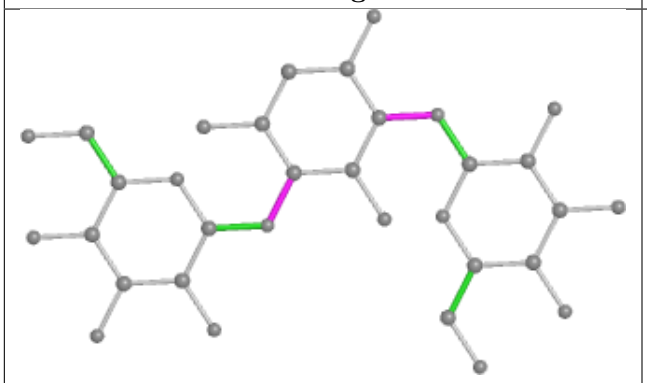

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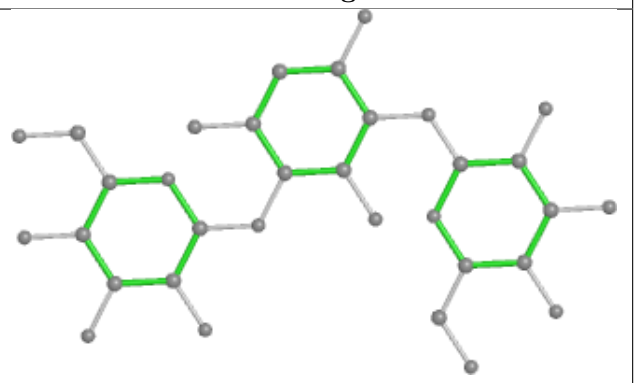
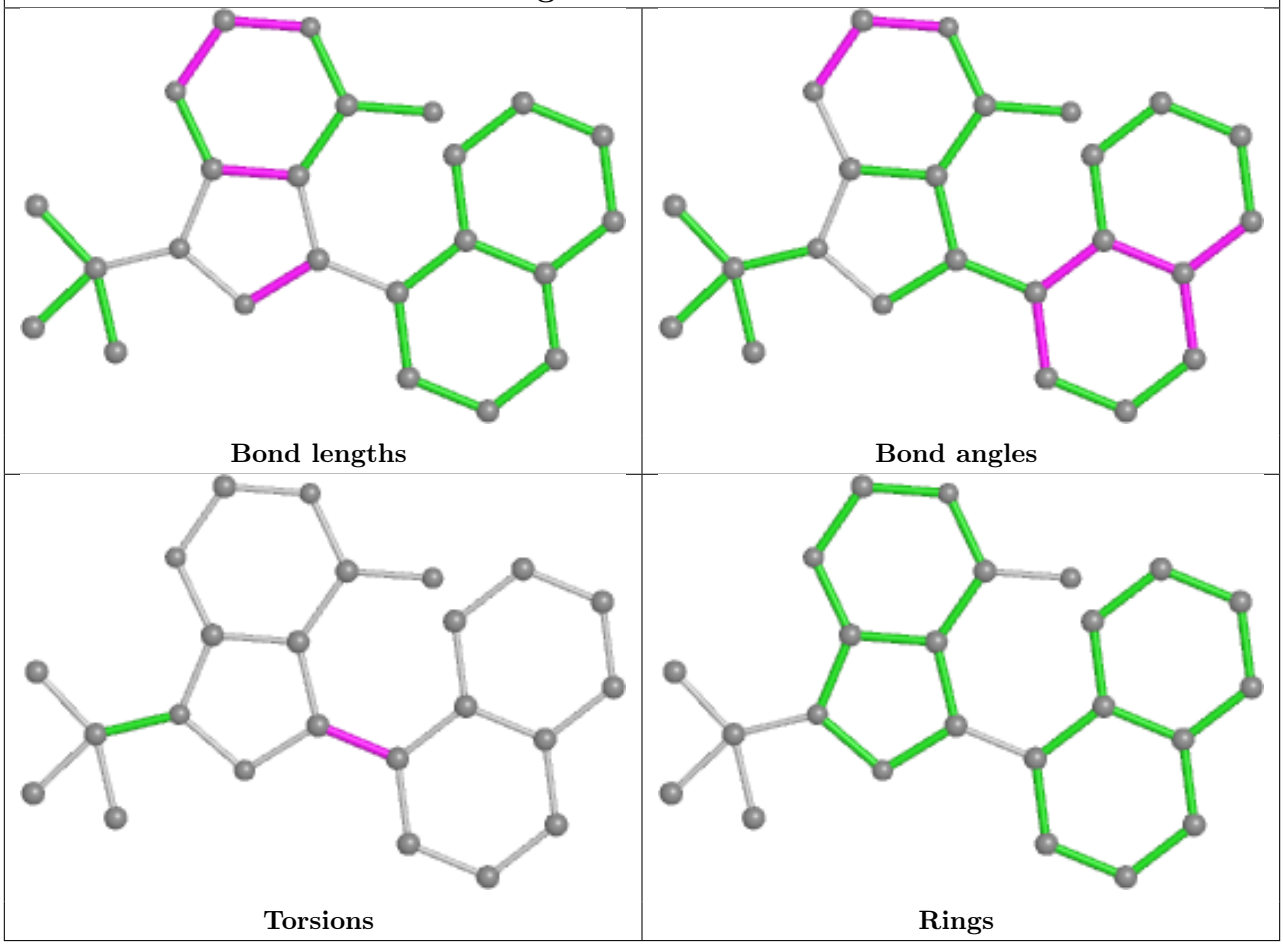
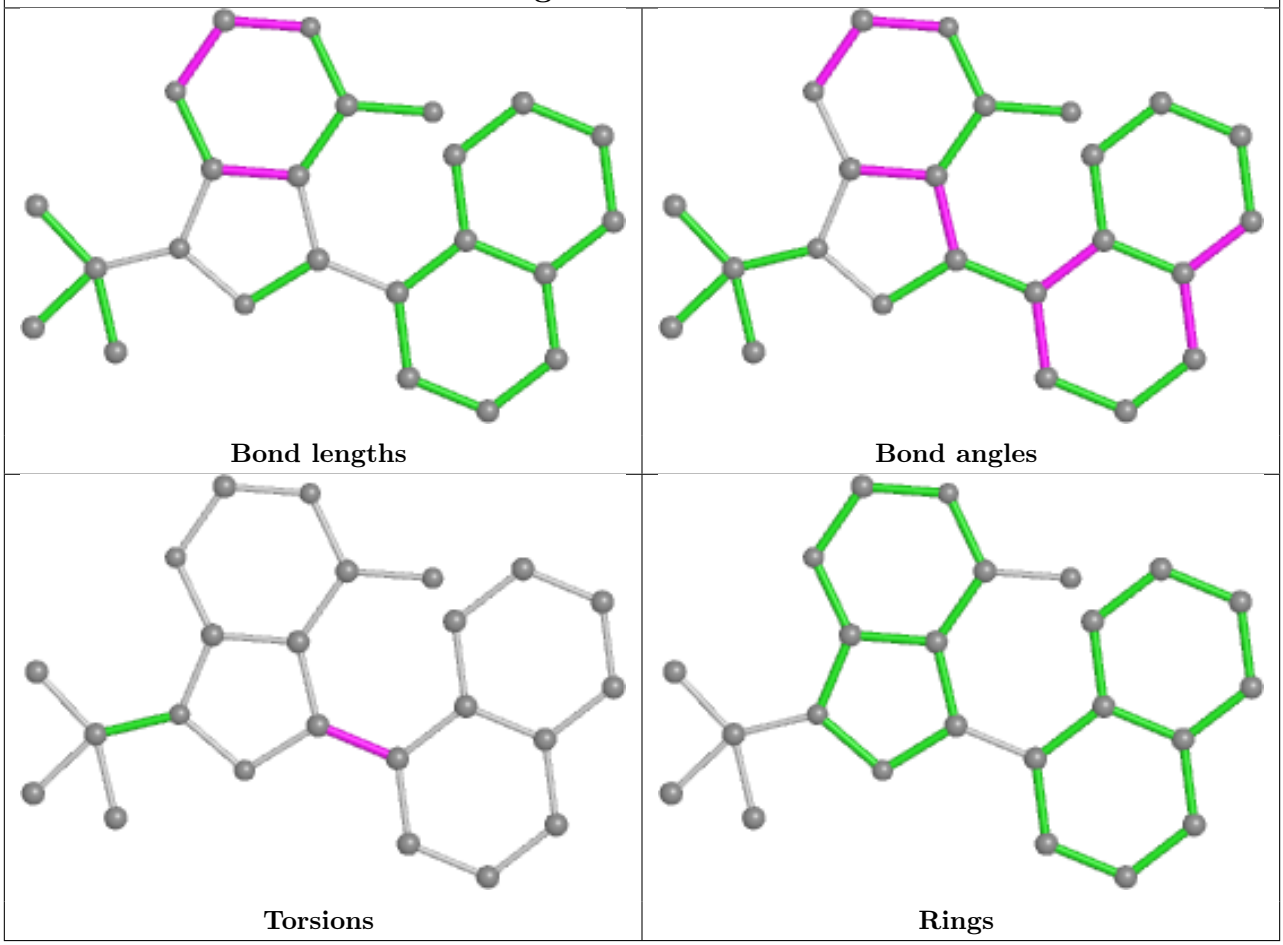


Rings

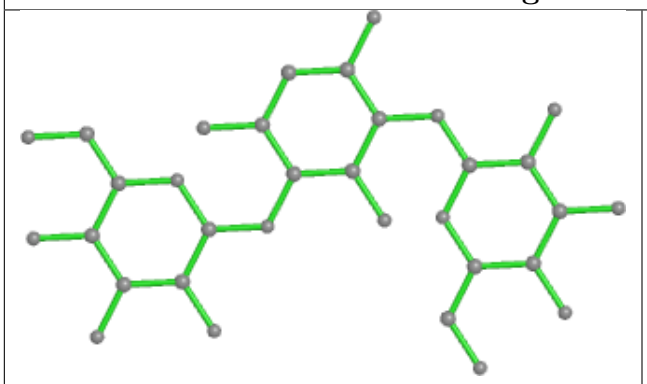
Ligand 0J9 L 302



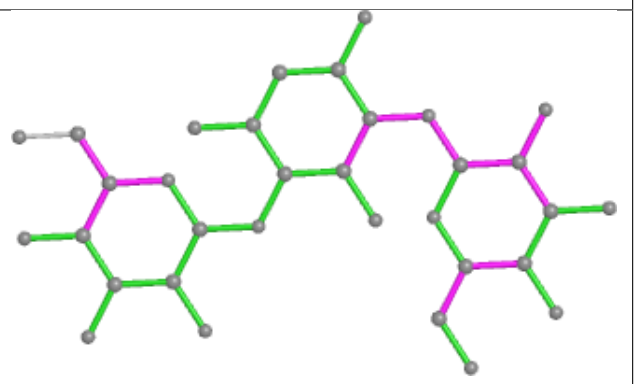
Ligand 0J9 G 302



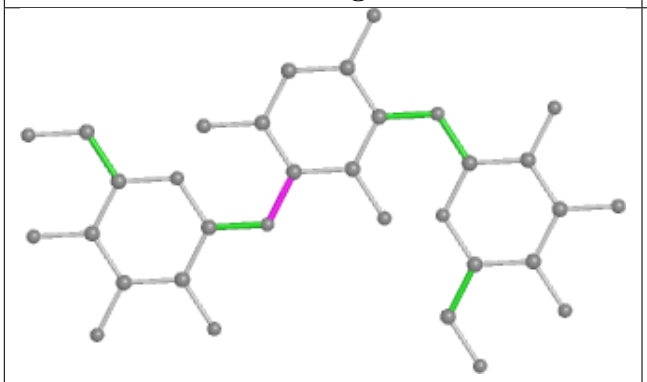
Ligand KAN E 301



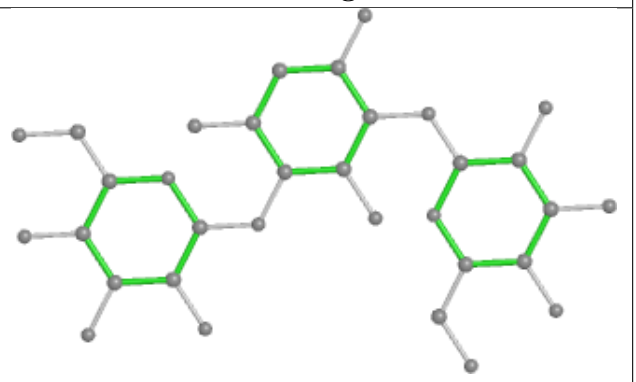
Bond lengths



Bond angles

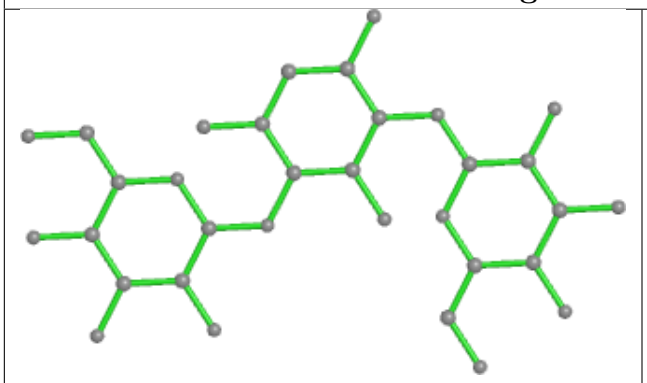


Torsions



Rings

Ligand KAN H 301



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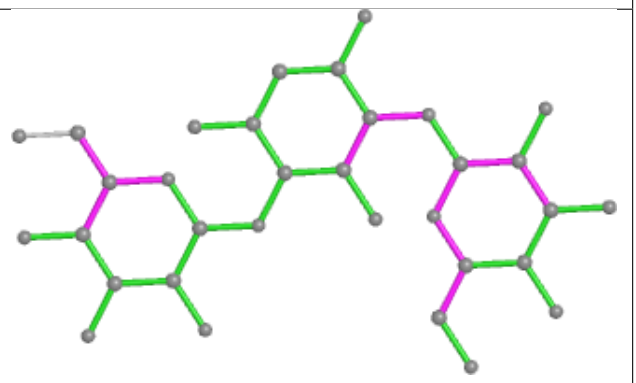

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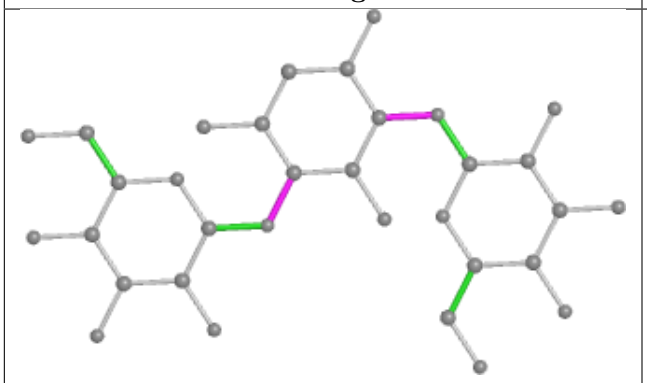

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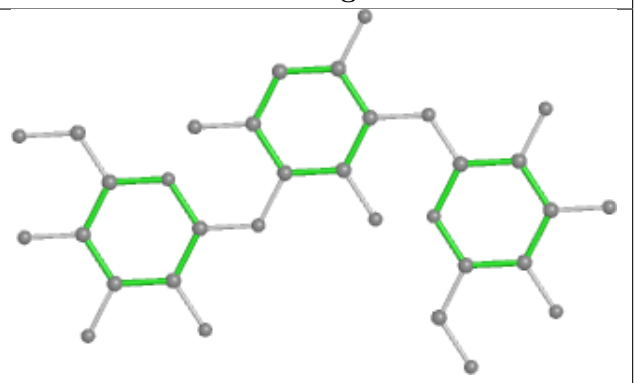
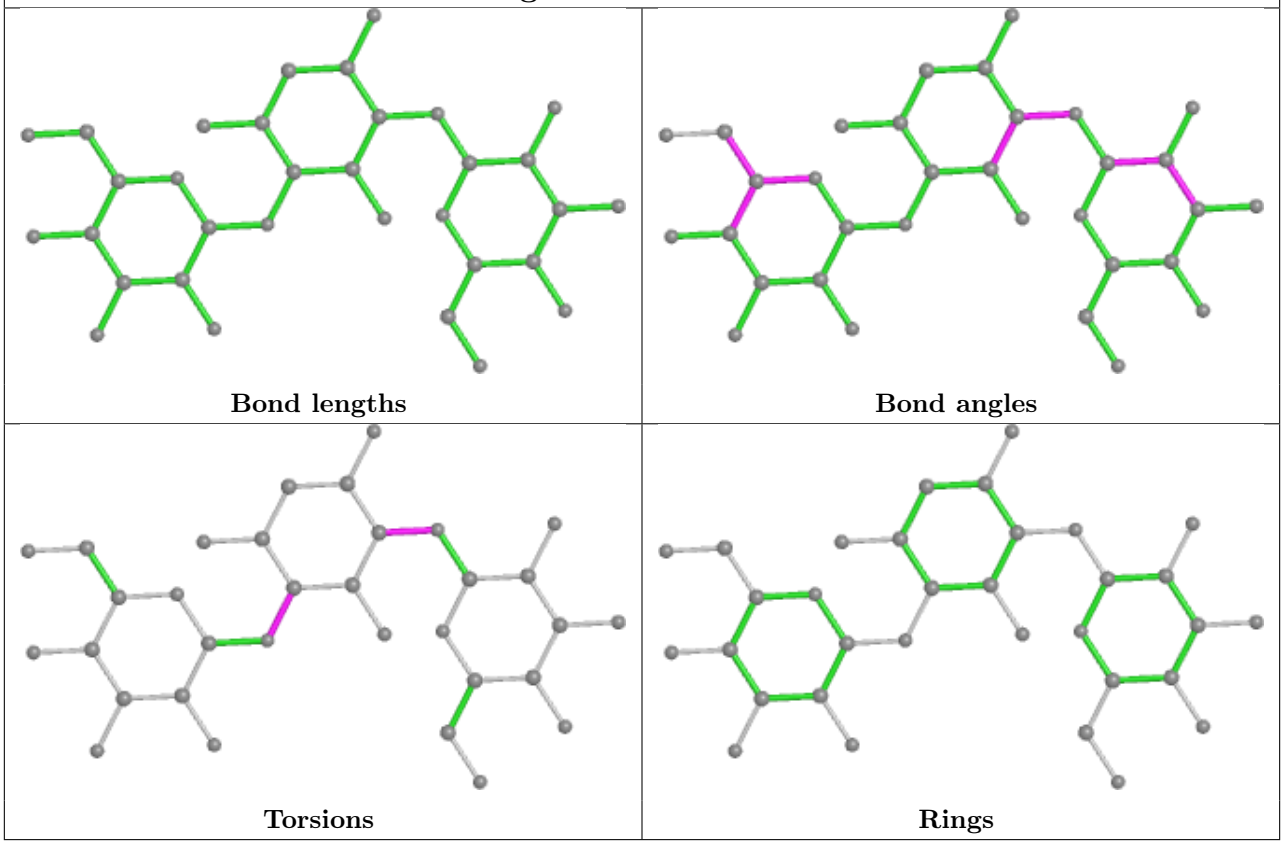
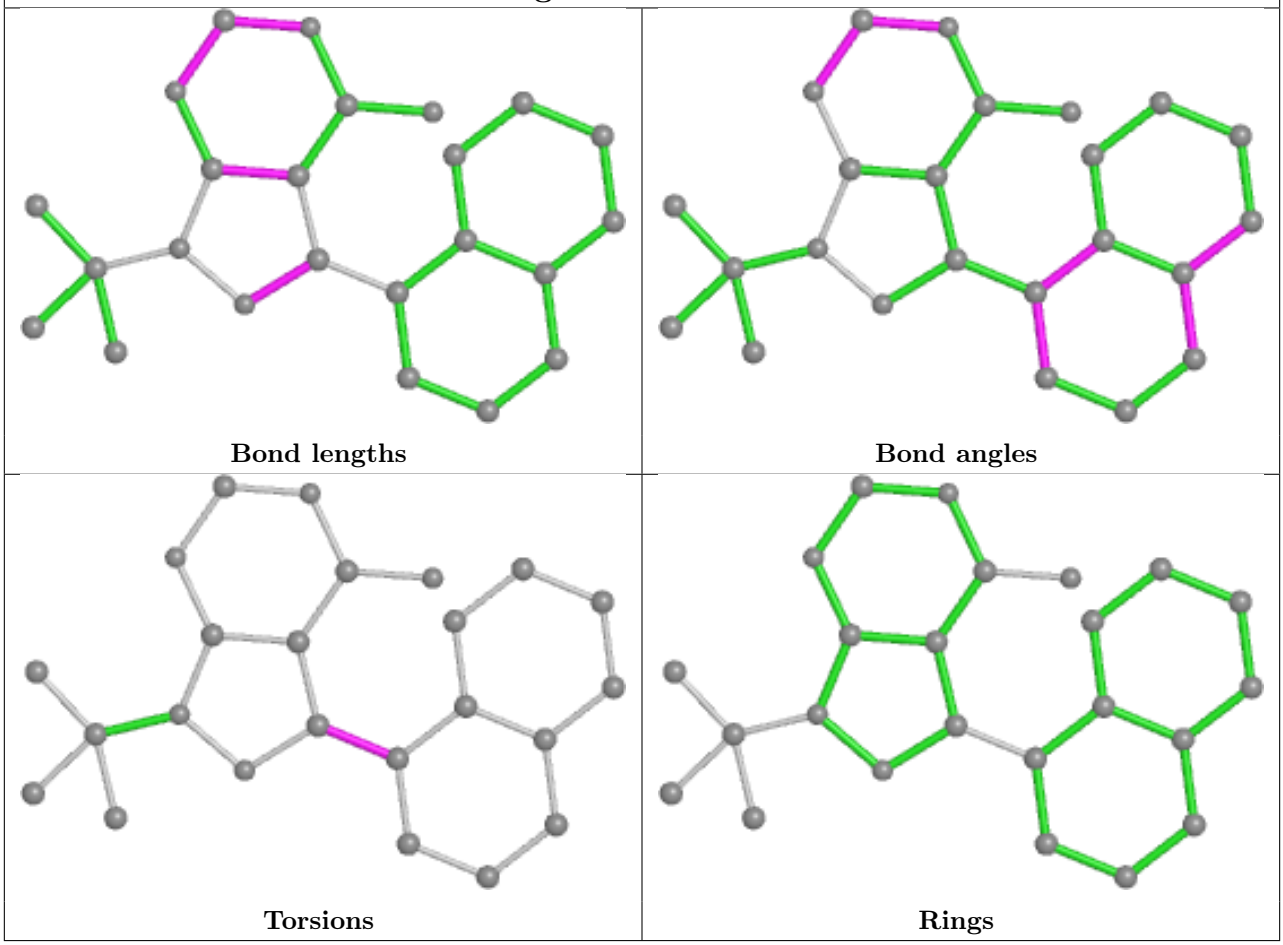


Rings

Ligand KAN D 301



Ligand 0J9 A 302



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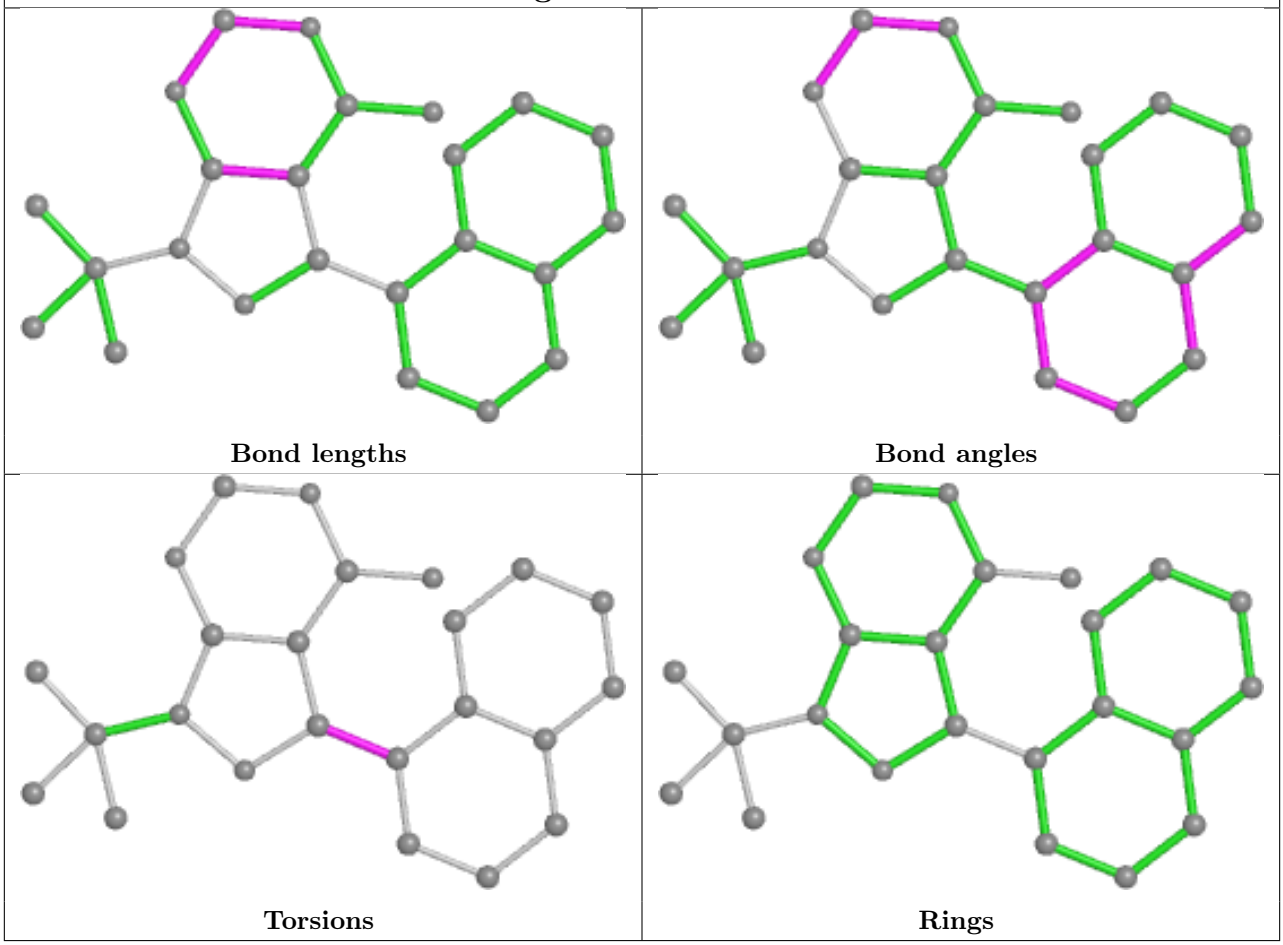
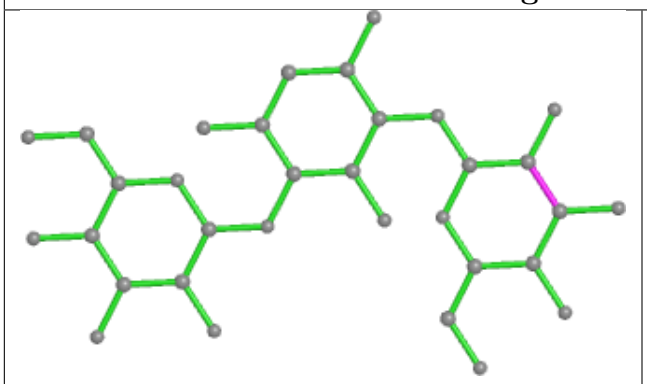
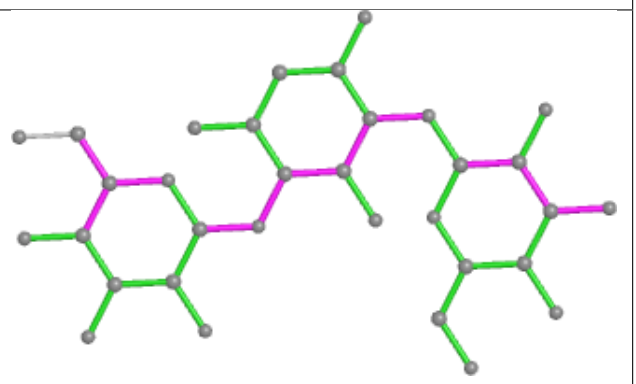


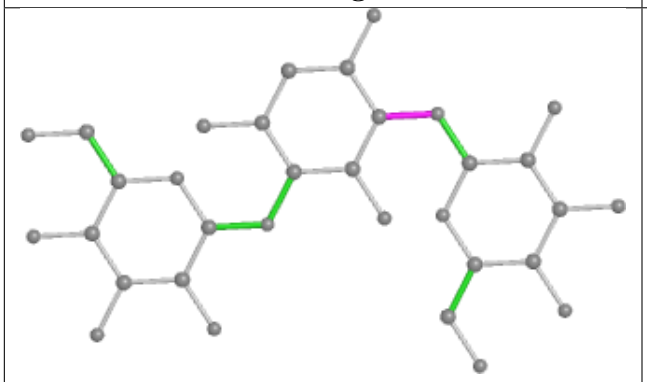
Ligand KAN B 301



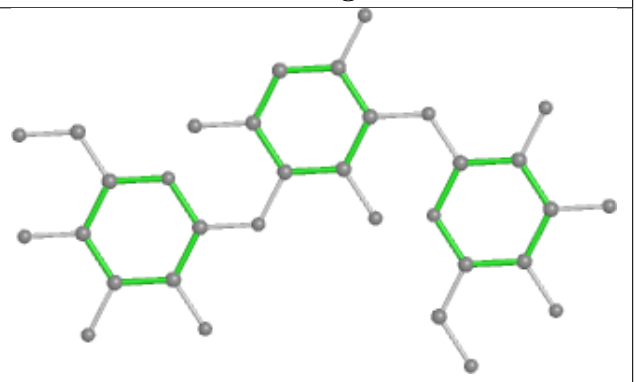
Bond lengths



Bond angles

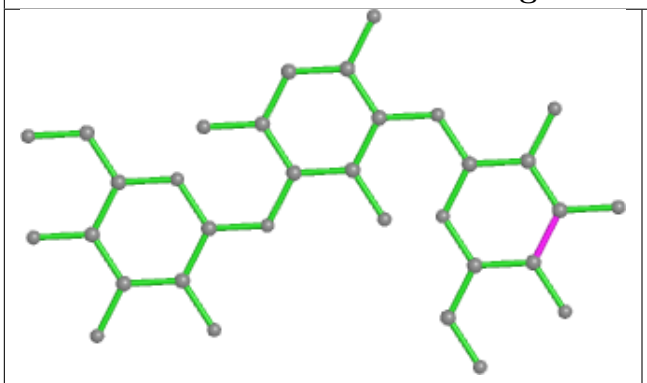


Torsions

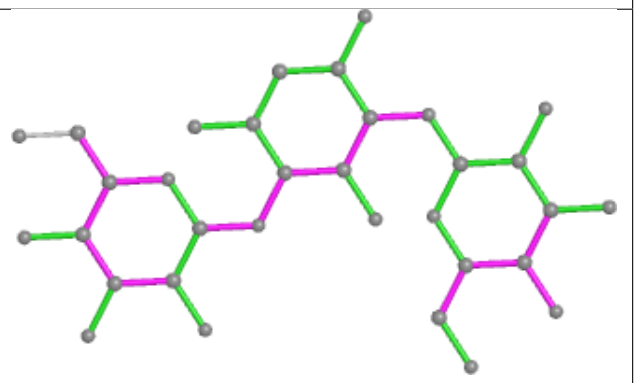


Rings

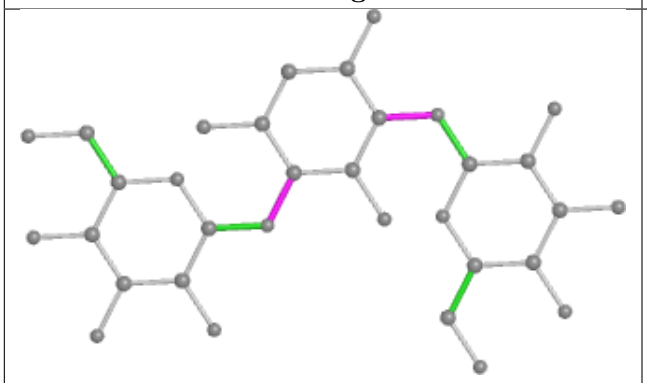
Ligand KAN K 301



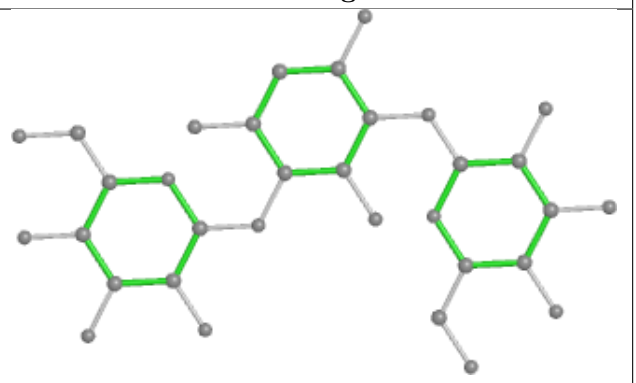
Bond lengths



Bond angles

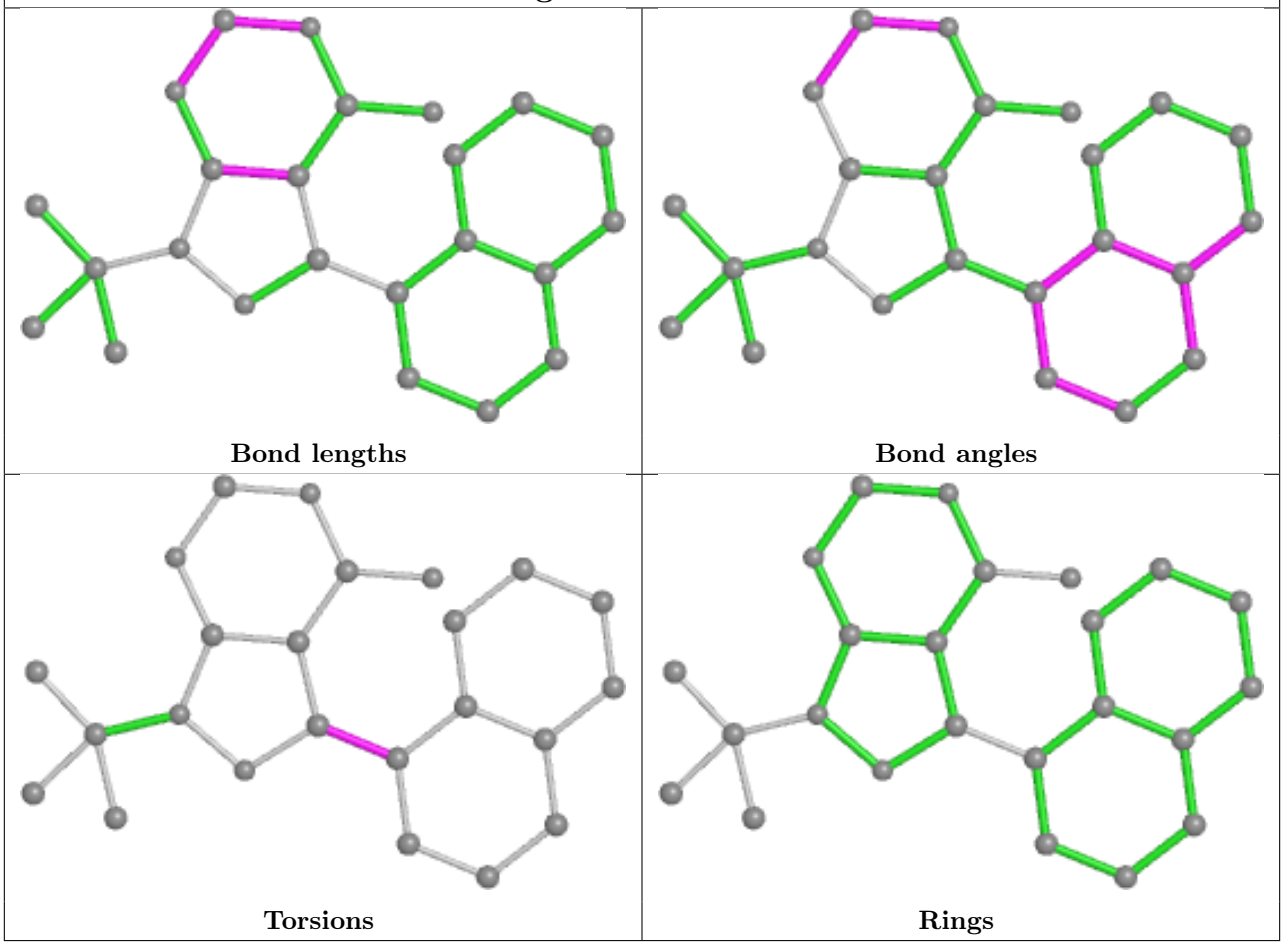


Torsions

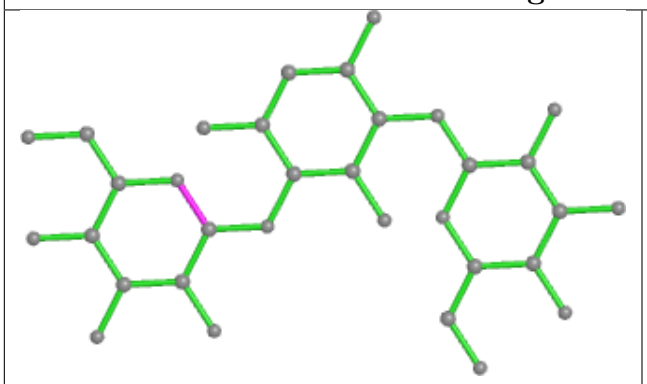


Rings

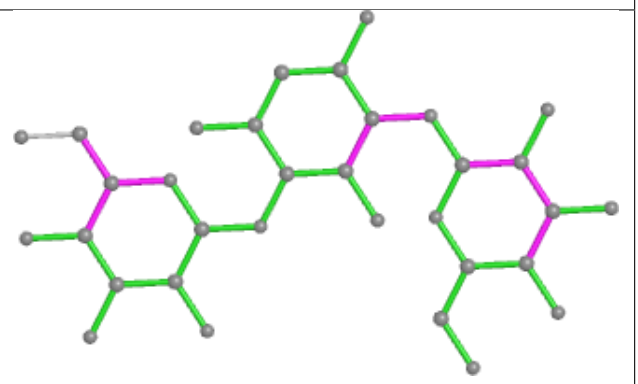
Ligand 0J9 B 302



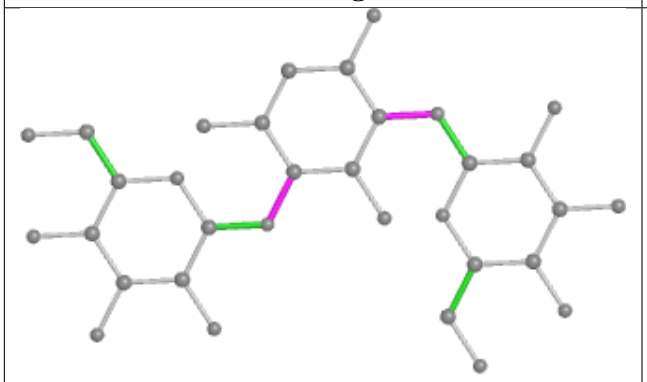
Ligand KAN I 301



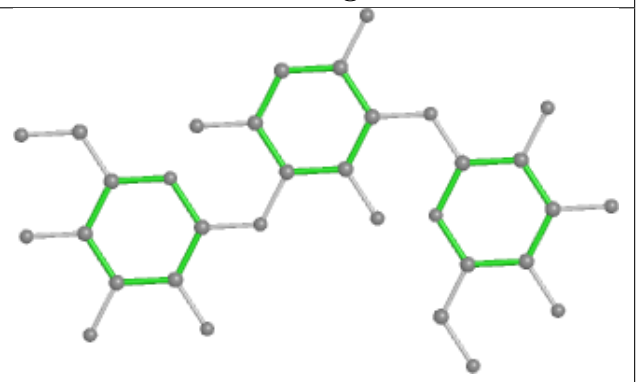
Bond lengths



Bond angles

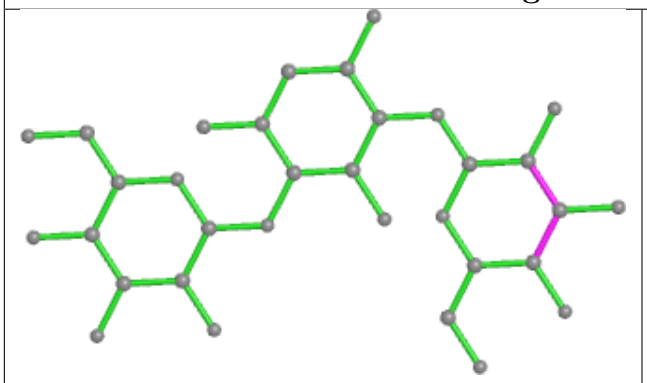


Torsions

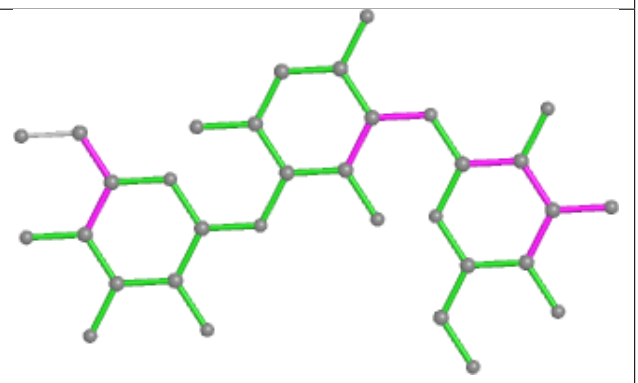


Rings

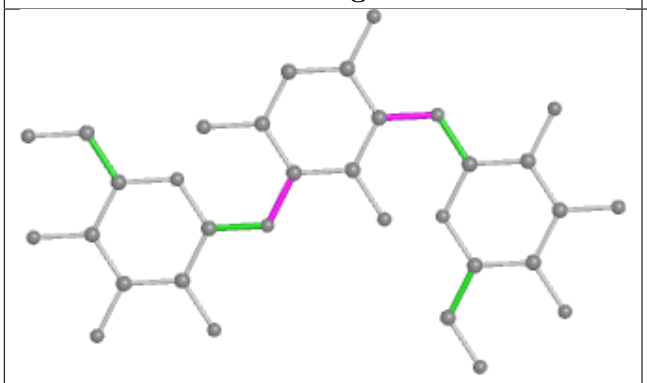
Ligand KAN F 301



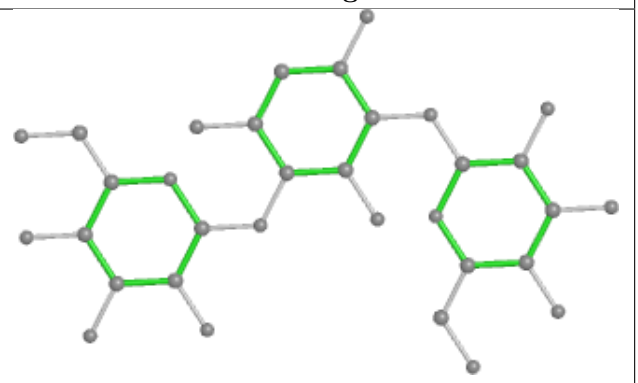
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	248/272 (91%)	-0.07	4 (1%)	72	72	29, 38, 62, 106	0
1	B	261/272 (95%)	0.11	11 (4%)	36	34	30, 42, 94, 114	0
1	C	261/272 (95%)	0.12	16 (6%)	21	20	29, 39, 100, 143	0
1	D	259/272 (95%)	0.54	30 (11%)	4	4	32, 50, 106, 140	0
1	E	255/272 (93%)	0.07	10 (3%)	39	38	27, 37, 68, 130	0
1	F	264/272 (97%)	0.13	16 (6%)	21	20	29, 42, 94, 122	0
1	G	260/272 (95%)	0.13	21 (8%)	12	12	30, 44, 107, 141	0
1	H	249/272 (91%)	0.01	8 (3%)	47	45	30, 40, 69, 98	0
1	I	260/272 (95%)	0.07	12 (4%)	32	31	29, 39, 93, 141	0
1	J	260/272 (95%)	0.69	38 (14%)	2	2	33, 57, 106, 148	0
1	K	262/272 (96%)	0.22	24 (9%)	9	8	28, 43, 106, 147	0
1	L	248/272 (91%)	-0.04	1 (0%)	92	92	28, 39, 64, 97	0
All	All	3087/3264 (94%)	0.17	191 (6%)	20	20	27, 42, 95, 148	0

The worst 5 of 191 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4	ILE	17.1
1	J	22	ASP	15.4
1	J	4	ILE	13.3
1	K	33	VAL	10.2
1	G	17	SER	9.5

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

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

6.3 Carbohydrates (i)

There are no 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ACT	G	306	4/4	0.51	0.27	61,77,85,118	0
5	ACT	D	305	4/4	0.66	0.28	64,85,93,106	0
5	ACT	H	305	4/4	0.69	0.19	48,71,71,129	0
5	ACT	L	304	4/4	0.75	0.14	53,64,69,95	0
5	ACT	L	305	4/4	0.76	0.15	53,63,78,126	0
5	ACT	C	307	4/4	0.78	0.22	46,63,66,128	0
3	0J9	G	302	24/24	0.78	0.36	38,76,106,128	24
5	ACT	D	303	4/4	0.78	0.29	71,71,80,84	0
5	ACT	D	304	4/4	0.78	0.20	55,81,91,119	0
7	PEG	D	306	7/7	0.78	0.18	51,76,102,118	0
3	0J9	K	302	24/24	0.81	0.30	36,60,79,117	24
3	0J9	B	302	24/24	0.81	0.23	36,54,92,106	24
5	ACT	I	306	4/4	0.83	0.16	63,74,91,92	0
5	ACT	F	307	4/4	0.83	0.14	47,70,78,94	0
5	ACT	K	306	4/4	0.85	0.19	40,57,69,100	0
3	0J9	F	302	24/24	0.85	0.24	33,46,88,114	24
3	0J9	J	302	24/24	0.86	0.20	43,59,79,105	24
5	ACT	L	306	4/4	0.86	0.17	52,70,83,83	0
5	ACT	A	304	4/4	0.86	0.19	74,75,88,89	0
5	ACT	E	306	4/4	0.87	0.19	54,71,73,84	0
7	PEG	D	307	7/7	0.87	0.26	60,72,103,118	0
5	ACT	H	304	4/4	0.87	0.18	44,44,75,117	0
7	PEG	H	306	7/7	0.87	0.17	57,86,114,138	0
5	ACT	G	305	4/4	0.88	0.17	43,48,79,88	0
5	ACT	C	306	4/4	0.88	0.21	59,71,79,111	0
5	ACT	C	308	4/4	0.89	0.13	49,77,89,106	0
5	ACT	K	307	4/4	0.89	0.26	45,61,75,109	0
5	ACT	L	307	4/4	0.89	0.21	55,63,72,85	0
3	0J9	C	302	24/24	0.90	0.12	34,45,64,85	0
4	NA	G	303	1/1	0.90	0.12	49,49,49,49	0
6	CL	I	304	1/1	0.90	0.10	65,65,65,65	0
5	ACT	E	304	4/4	0.91	0.16	36,37,38,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	0J9	C	303	24/24	0.91	0.15	37,53,74,123	24
3	0J9	I	302	24/24	0.91	0.14	32,43,70,93	0
5	ACT	B	306	4/4	0.91	0.13	39,49,61,85	0
5	ACT	I	307	4/4	0.91	0.15	51,84,91,99	0
4	NA	F	303	1/1	0.92	0.07	33,33,33,33	1
5	ACT	I	305	4/4	0.92	0.09	58,65,67,123	0
3	0J9	E	302	24/24	0.93	0.12	30,34,50,70	0
5	ACT	J	303	4/4	0.93	0.10	45,57,57,71	0
5	ACT	L	308	4/4	0.93	0.14	50,52,57,93	0
5	ACT	E	305	4/4	0.93	0.14	56,61,82,84	0
4	NA	A	303	1/1	0.93	0.09	57,57,57,57	0
4	NA	K	303	1/1	0.93	0.08	41,41,41,41	1
4	NA	L	303	1/1	0.93	0.13	37,37,37,37	1
3	0J9	L	302	24/24	0.94	0.11	29,35,41,57	0
3	0J9	H	302	24/24	0.94	0.10	30,36,45,48	0
2	KAN	C	301	33/33	0.94	0.13	30,37,52,57	0
6	CL	C	305	1/1	0.94	0.10	66,66,66,66	0
5	ACT	F	306	4/4	0.95	0.13	51,69,72,78	0
5	ACT	K	305	4/4	0.95	0.11	44,45,54,63	0
2	KAN	J	301	33/33	0.95	0.11	37,46,53,57	0
5	ACT	F	308	4/4	0.95	0.11	47,49,51,90	0
2	KAN	K	301	33/33	0.95	0.10	29,34,42,49	0
2	KAN	L	301	33/33	0.95	0.10	32,42,47,48	0
5	ACT	G	307	4/4	0.95	0.10	31,45,46,108	0
4	NA	H	303	1/1	0.95	0.08	40,40,40,40	1
2	KAN	A	301	33/33	0.95	0.09	26,37,48,55	0
2	KAN	D	301	33/33	0.95	0.10	32,40,45,50	0
2	KAN	E	301	33/33	0.95	0.10	28,36,48,58	0
5	ACT	A	306	4/4	0.95	0.14	36,40,47,86	0
2	KAN	I	301	33/33	0.95	0.10	30,38,44,55	0
2	KAN	H	301	33/33	0.96	0.08	36,40,45,46	0
5	ACT	A	305	4/4	0.96	0.14	48,51,53,91	0
5	ACT	B	305	4/4	0.96	0.09	45,58,72,73	0
3	0J9	A	302	24/24	0.96	0.10	29,34,53,59	0
4	NA	B	303	1/1	0.96	0.12	39,39,39,39	1
4	NA	E	303	1/1	0.96	0.07	53,53,53,53	0
5	ACT	F	305	4/4	0.96	0.16	53,57,62,68	0
2	KAN	G	301	33/33	0.96	0.11	28,33,39,42	0
2	KAN	F	301	33/33	0.97	0.09	25,32,37,41	0
4	NA	G	304	1/1	0.97	0.19	47,47,47,47	0
4	NA	C	304	1/1	0.97	0.19	43,43,43,43	1
5	ACT	D	302	4/4	0.97	0.10	43,59,84,90	0

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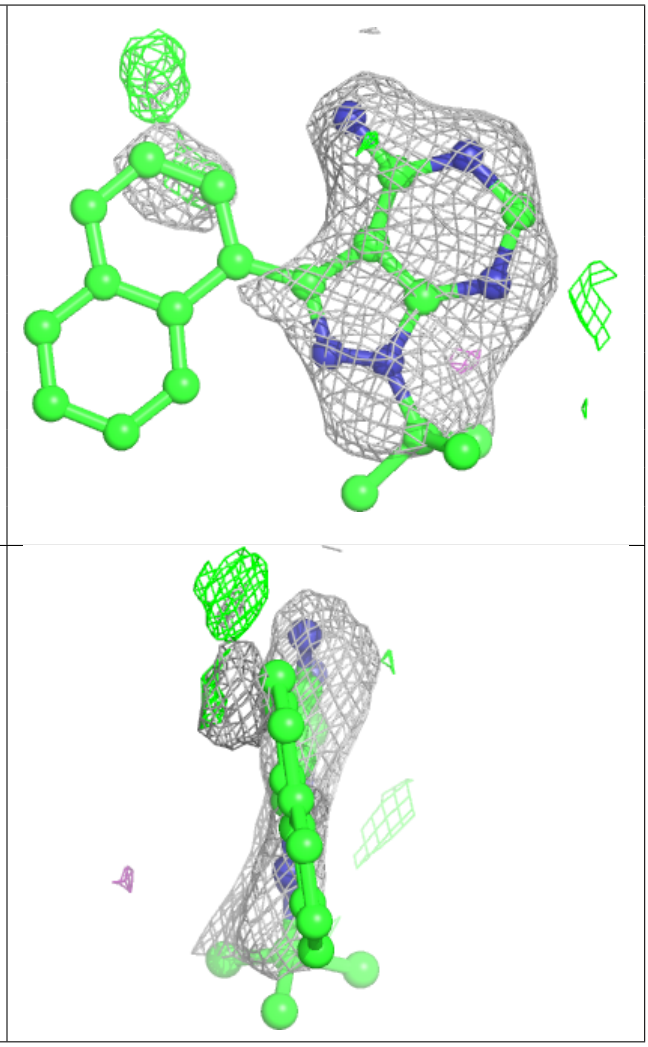
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NA	I	303	1/1	0.97	0.16	35,35,35,35	1
4	NA	F	304	1/1	0.98	0.20	41,41,41,41	0
4	NA	B	304	1/1	0.98	0.09	51,51,51,51	0
2	KAN	B	301	33/33	0.98	0.09	29,34,40,46	0
4	NA	K	304	1/1	0.99	0.18	43,43,43,43	0

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

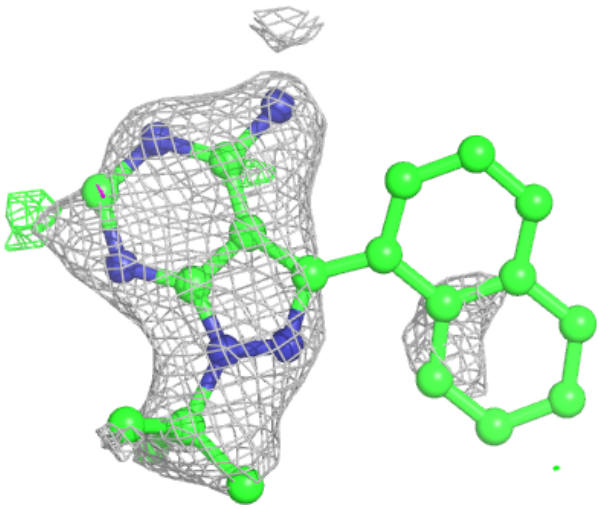
Electron density around 0J9 G 302:

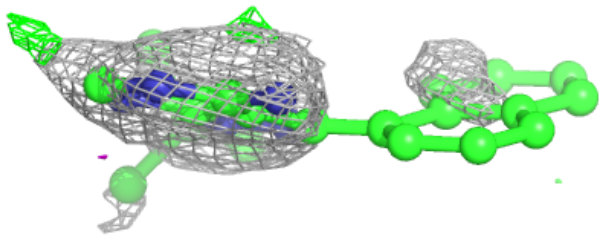
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

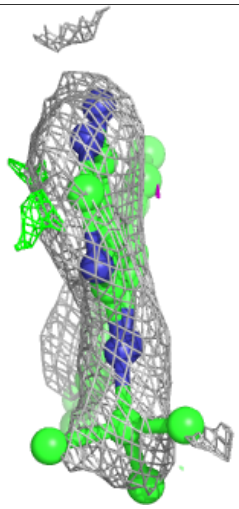


Electron density around 0J9 K 302:

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

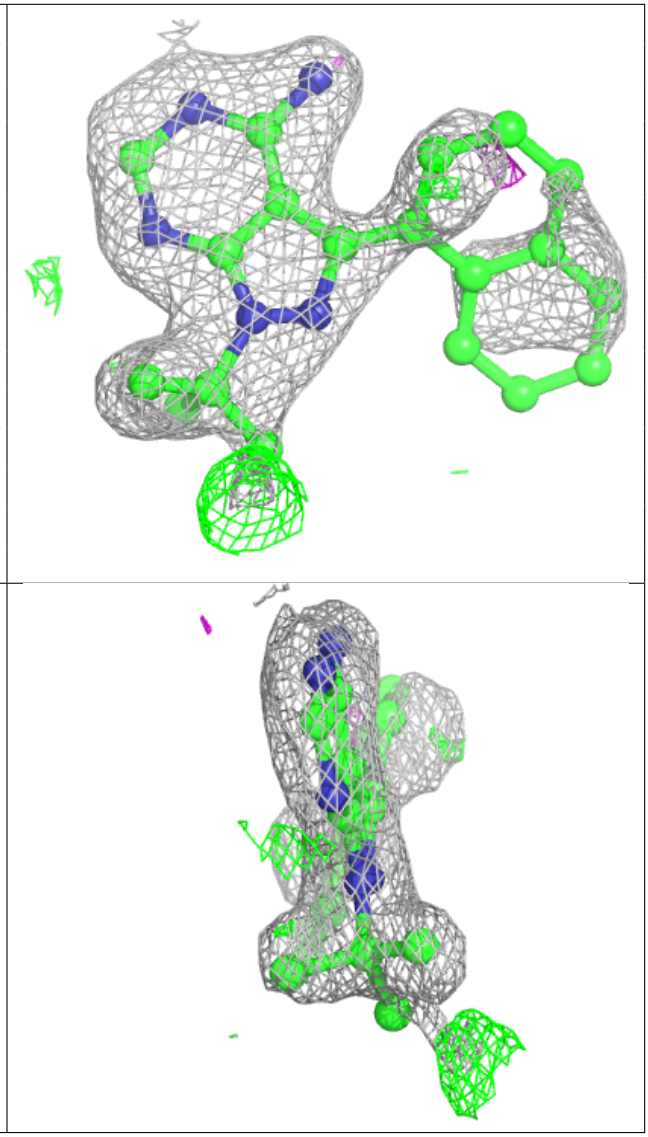






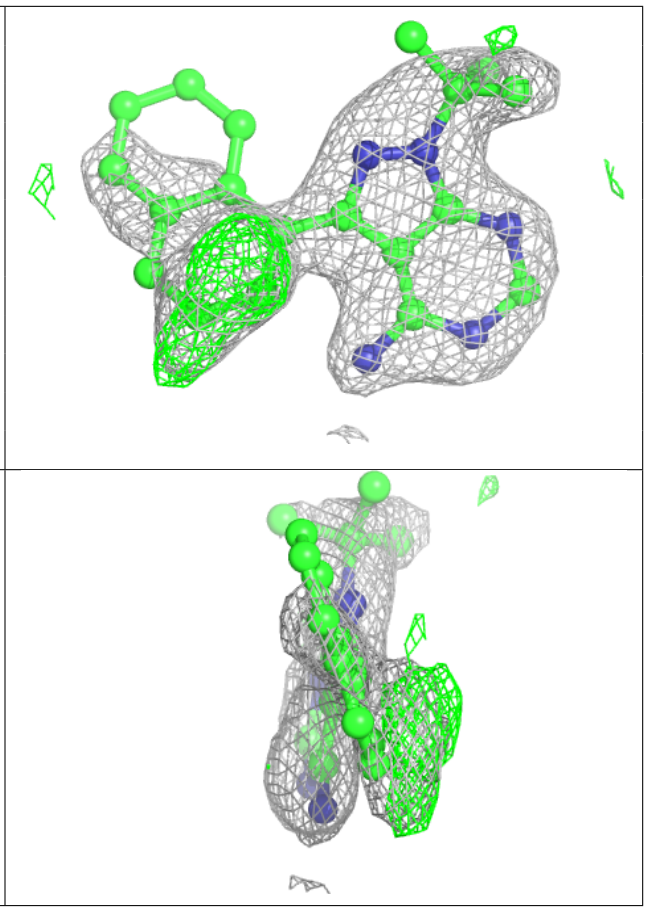
Electron density around 0J9 B 302:

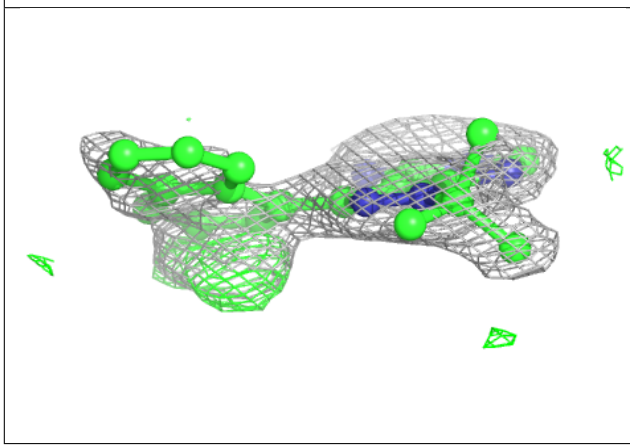
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 0J9 F 302:

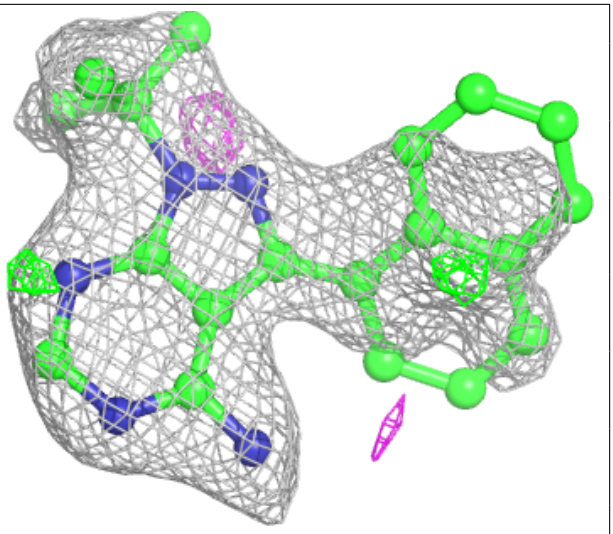
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

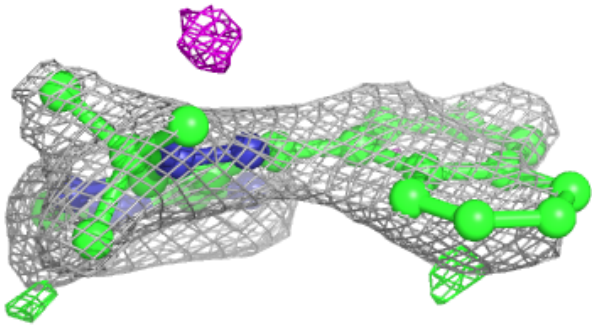


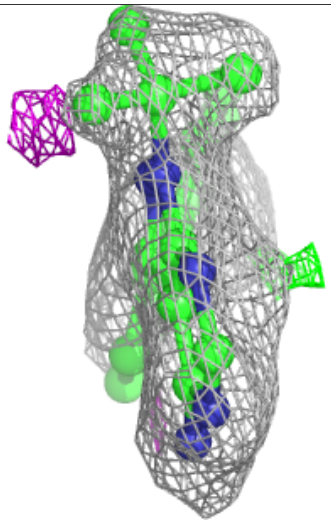


Electron density around 0J9 J 302:

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

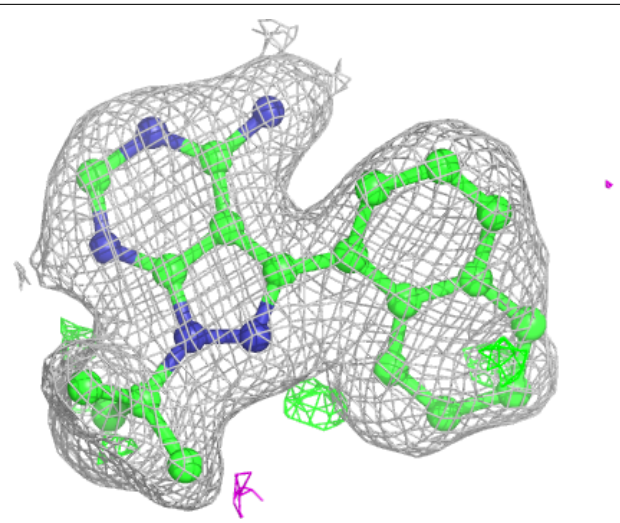


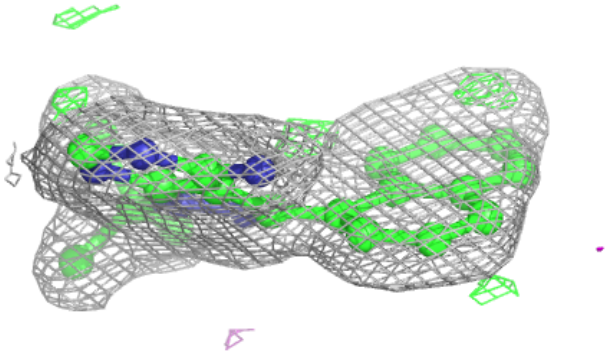


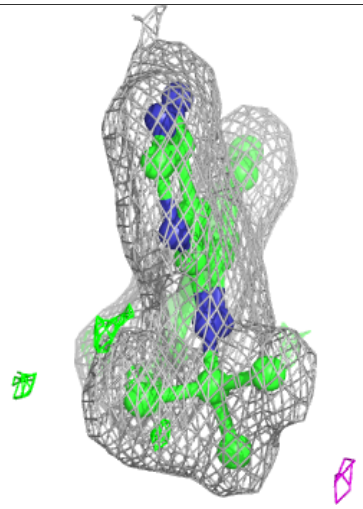


Electron density around 0J9 C 302:

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

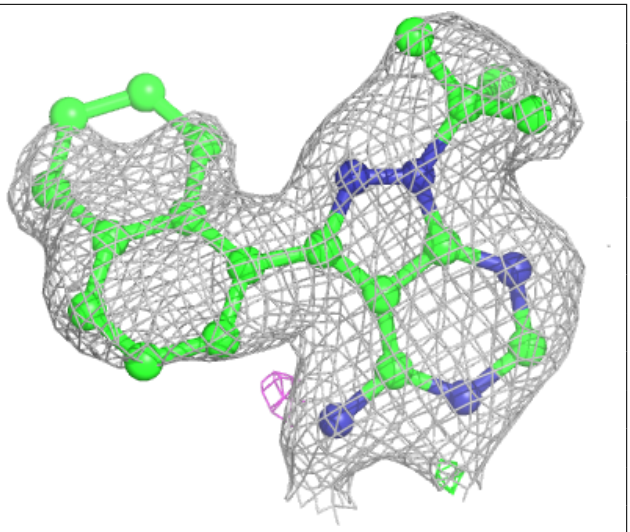


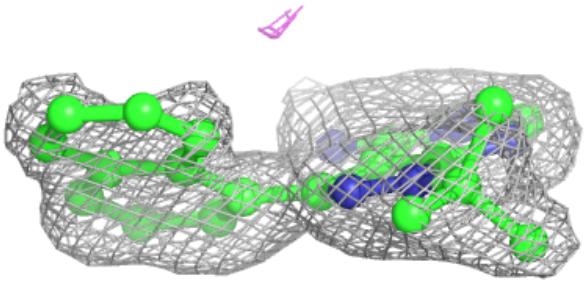


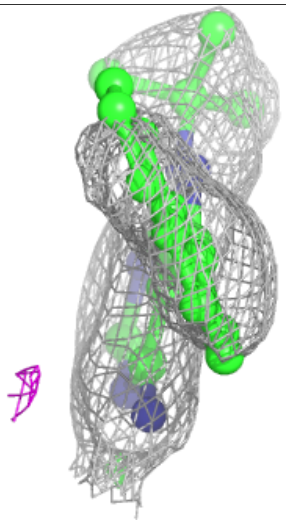


Electron density around 0J9 C 303:

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

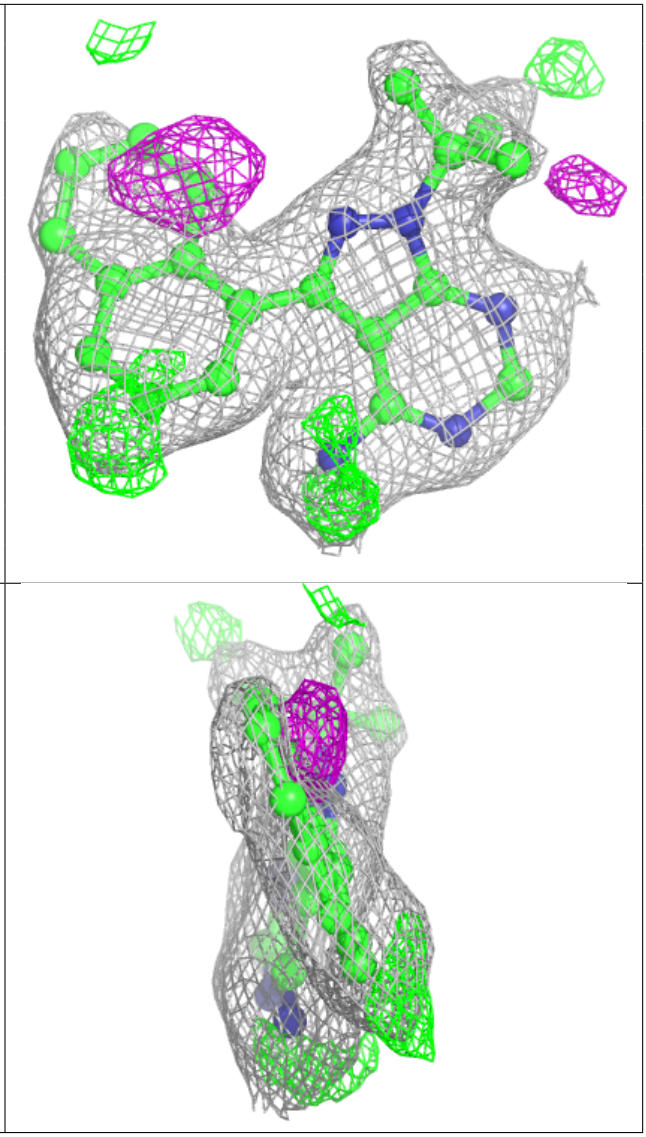


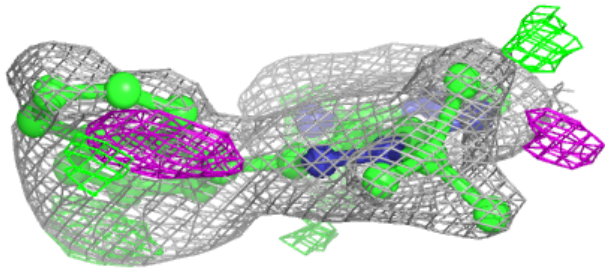




Electron density around 0J9 I 302:

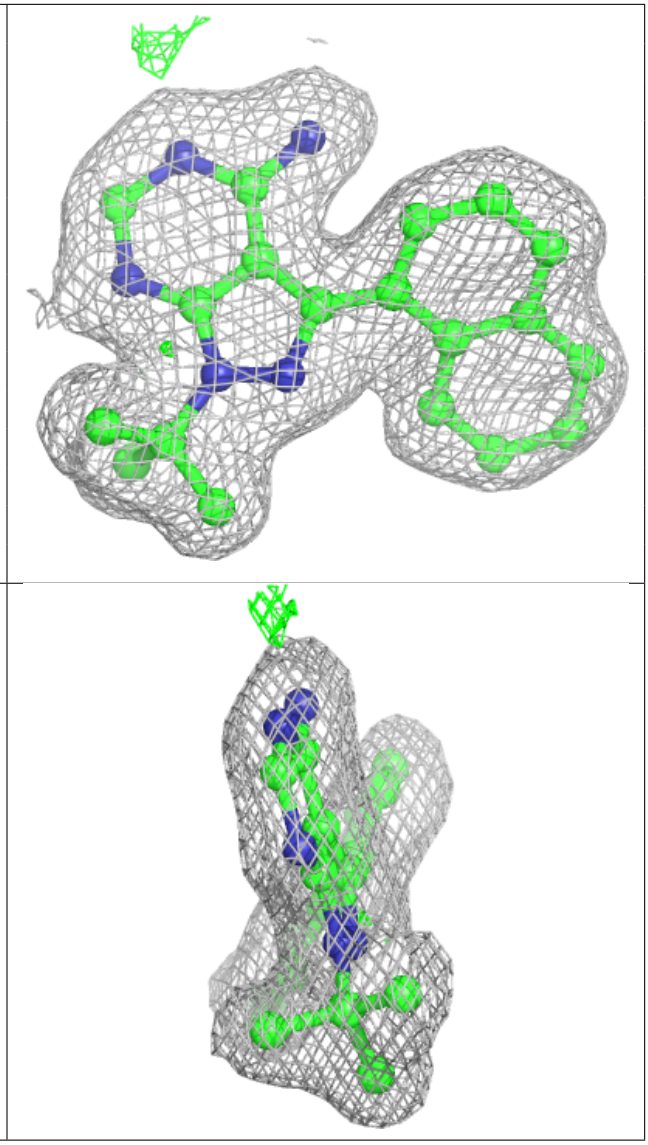
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





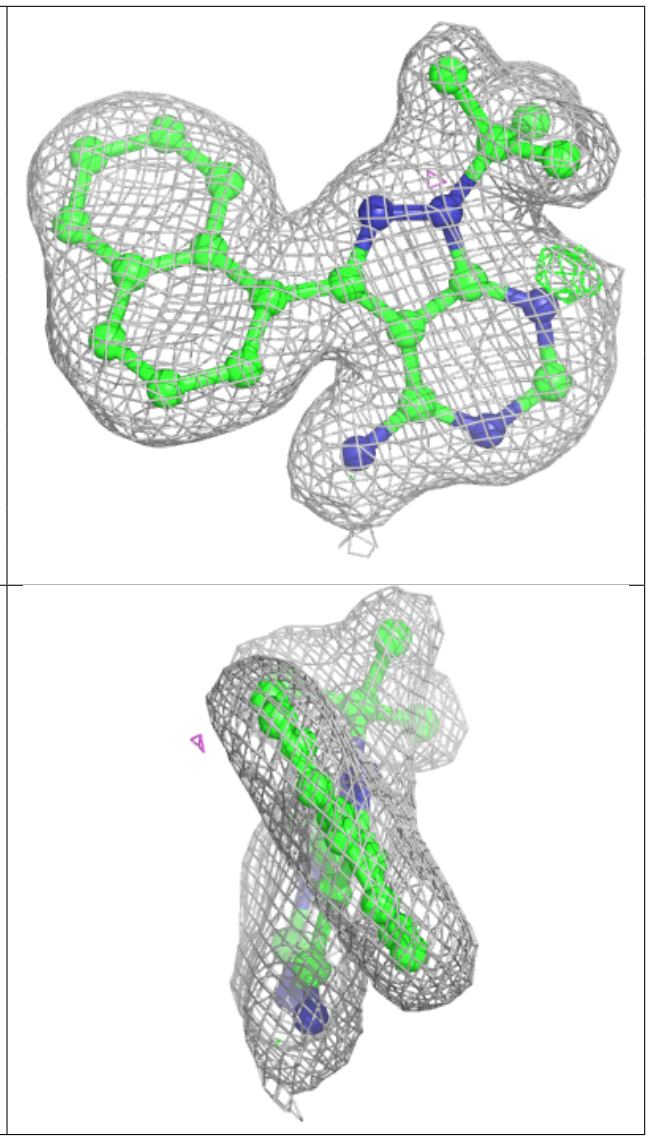
Electron density around 0J9 E 302:

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



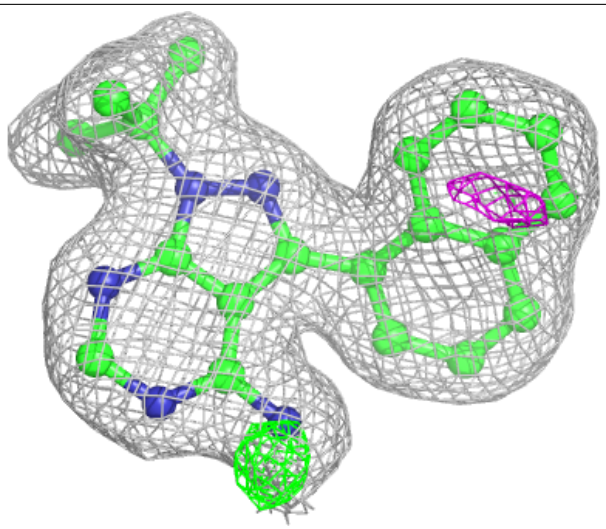
Electron density around 0J9 L 302:

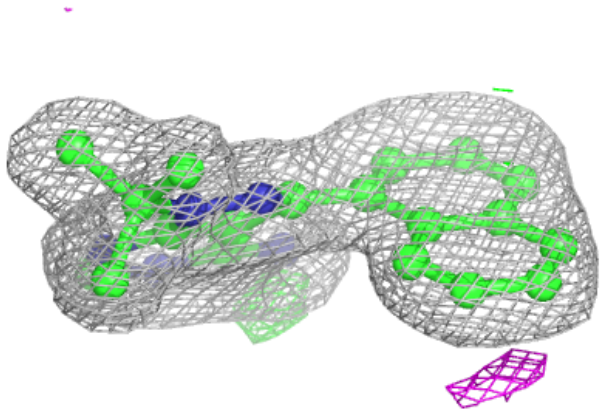
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

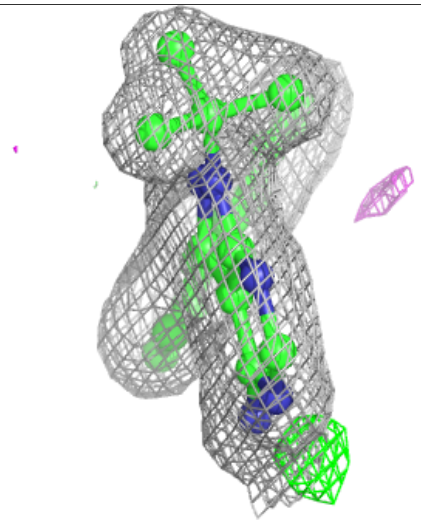


Electron density around 0J9 H 302:

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

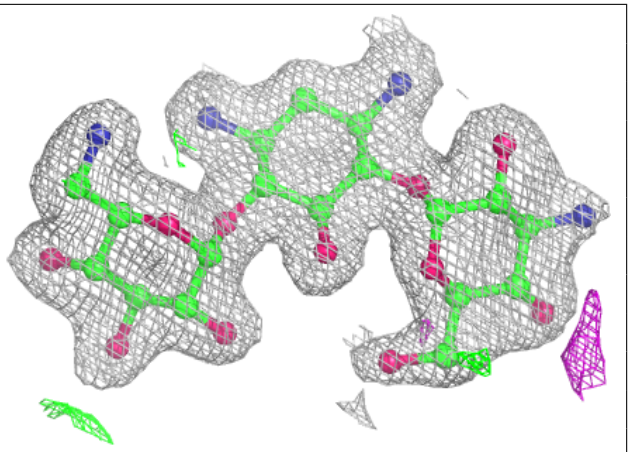


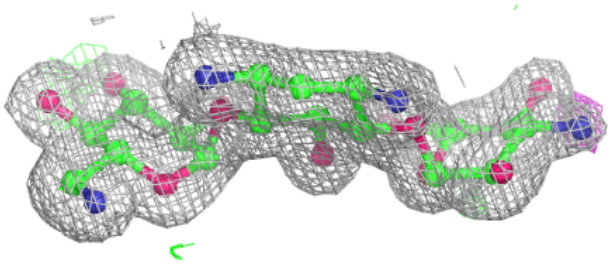


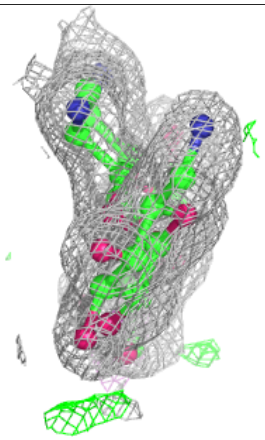


Electron density around KAN C 301:

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

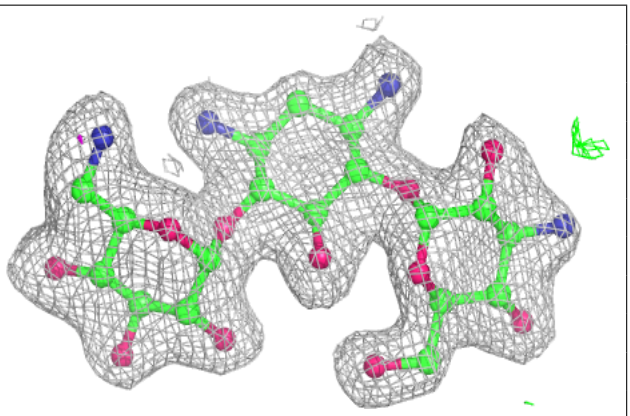


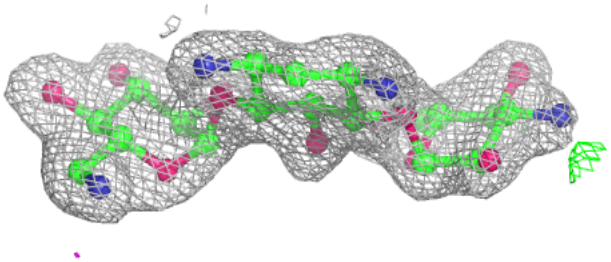


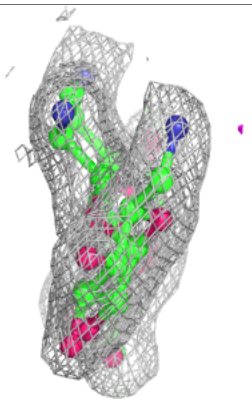


Electron density around KAN J 301:

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

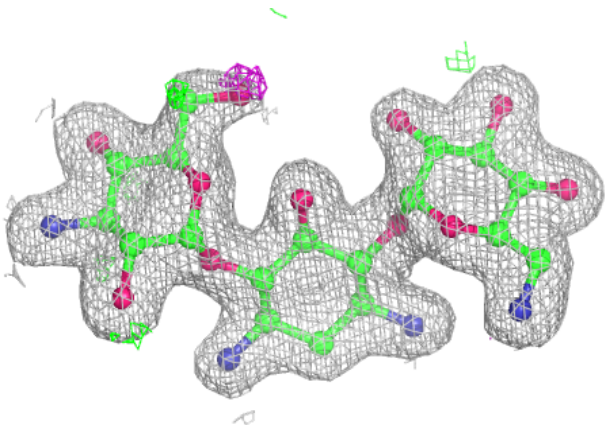


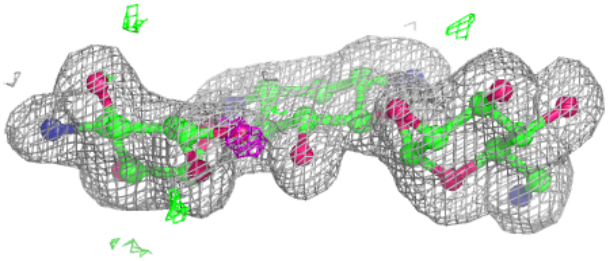


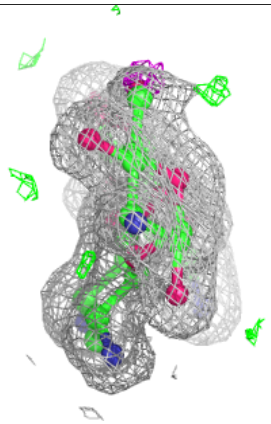


Electron density around KAN K 301:

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

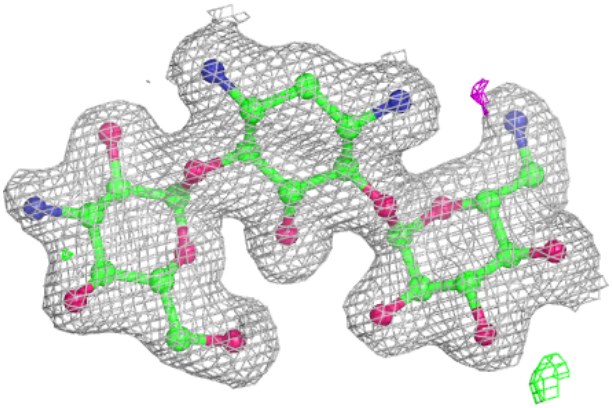


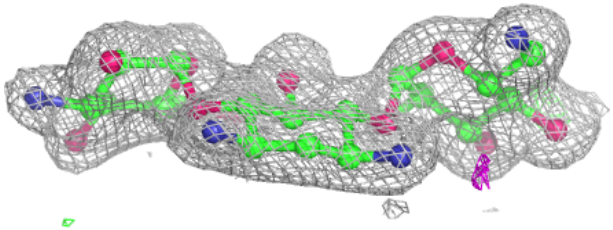


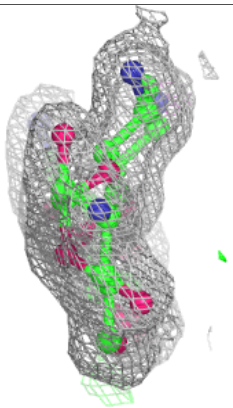


Electron density around KAN L 301:

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

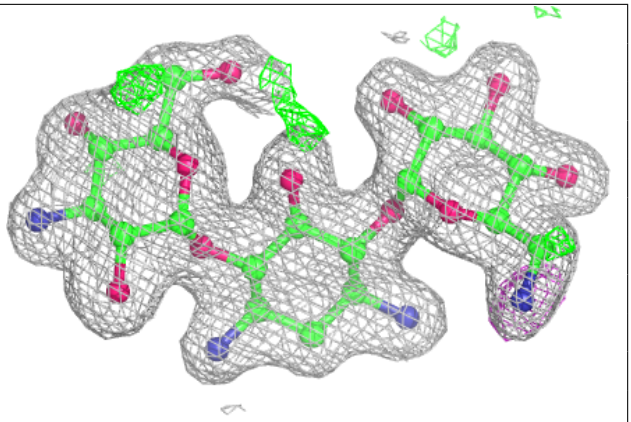


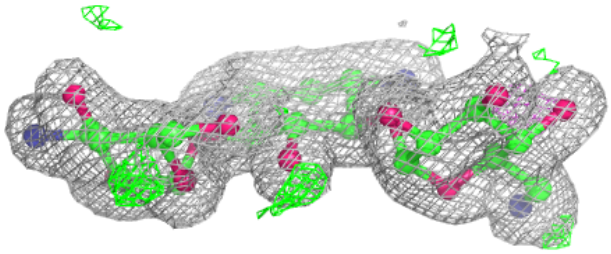


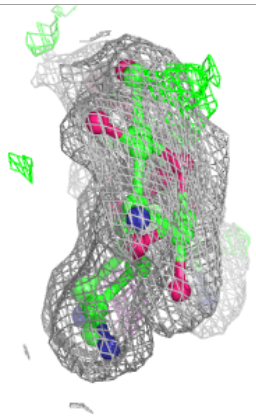


Electron density around KAN A 301:

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

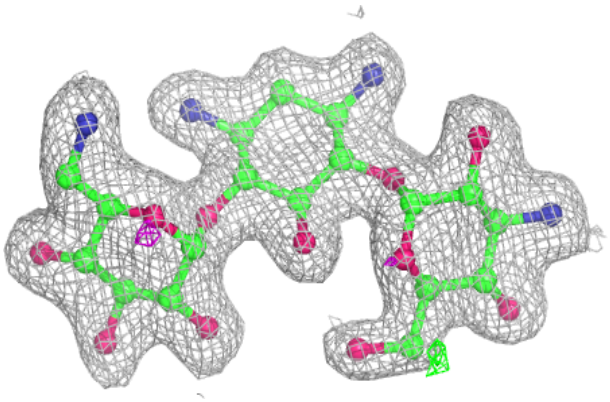


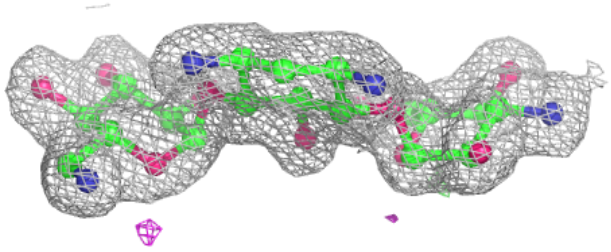


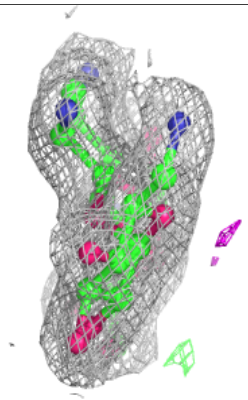


Electron density around KAN D 301:

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

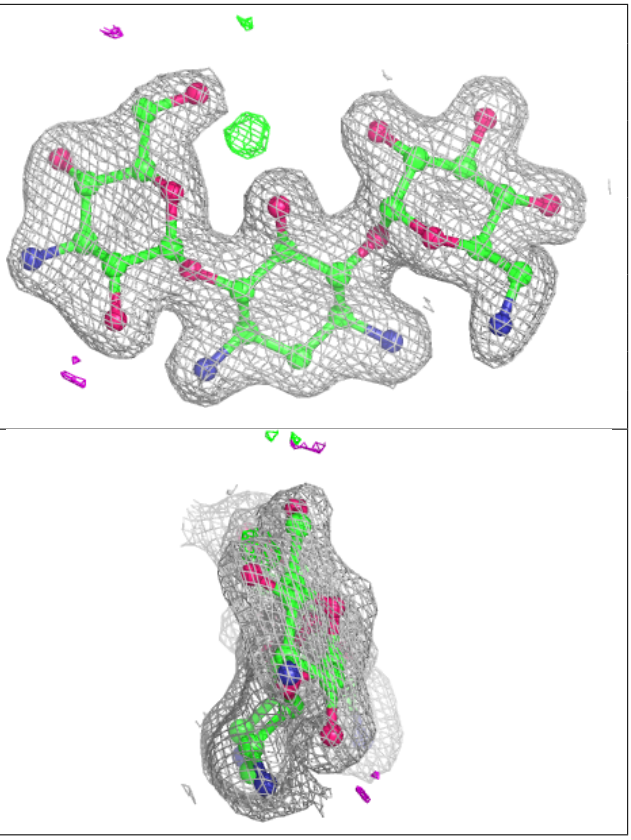






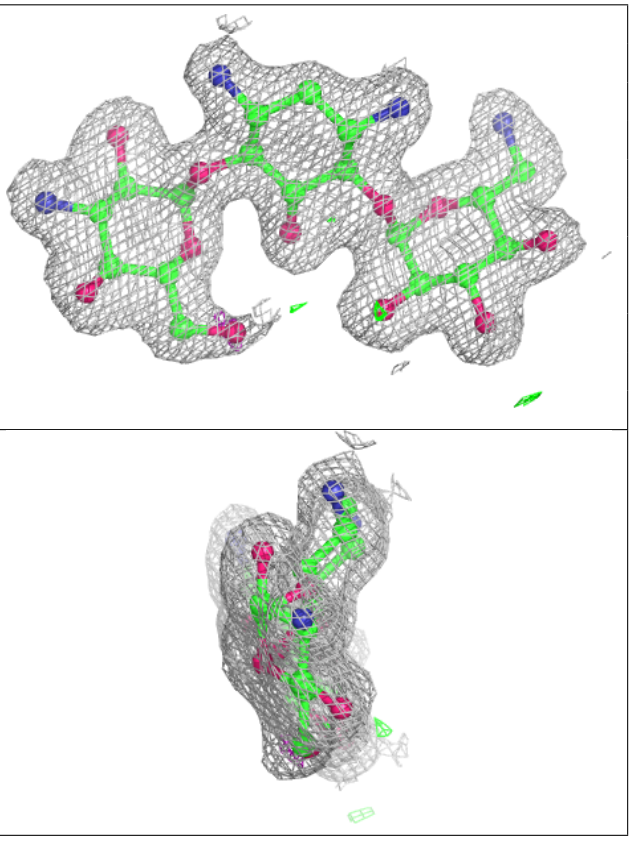
Electron density around KAN E 301:

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



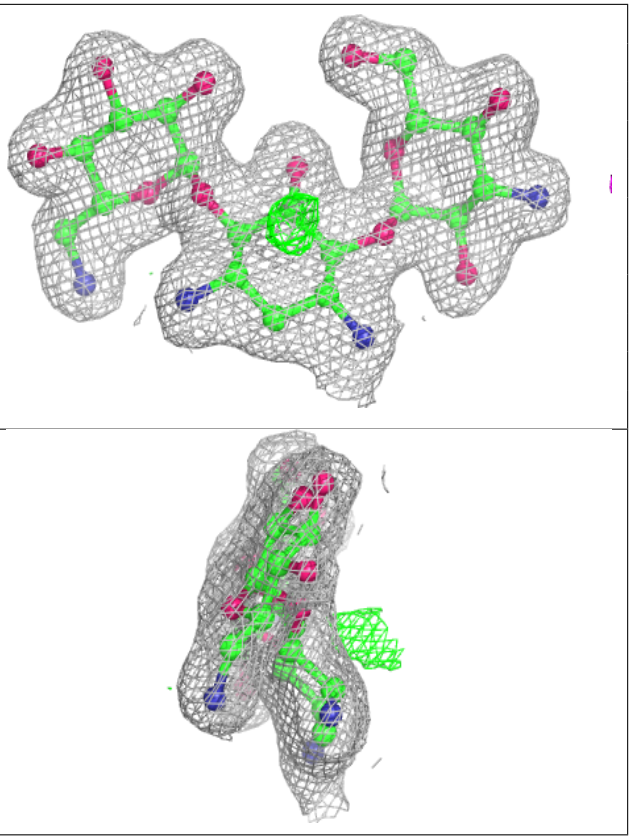
Electron density around KAN I 301:

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



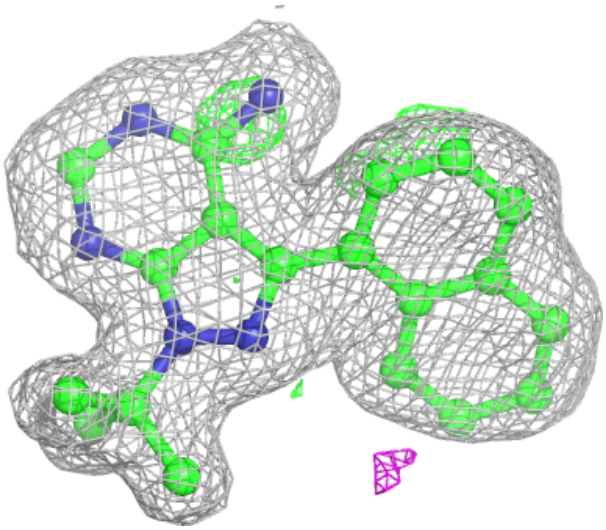
Electron density around KAN H 301:

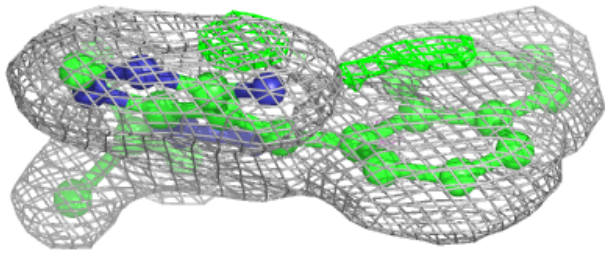
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

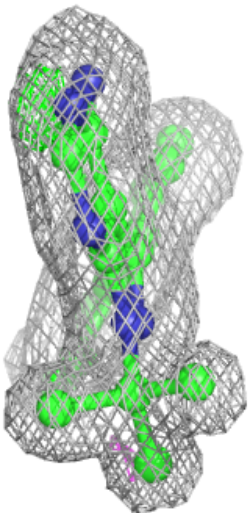


Electron density around 0J9 A 302:

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

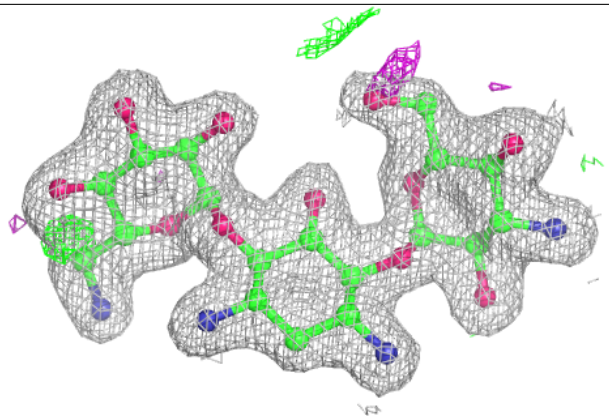


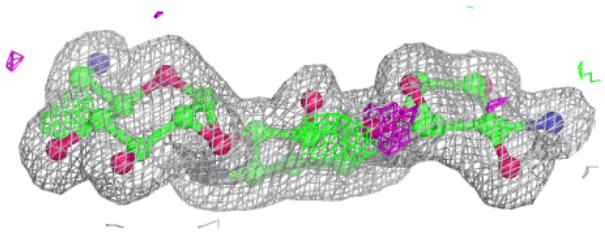


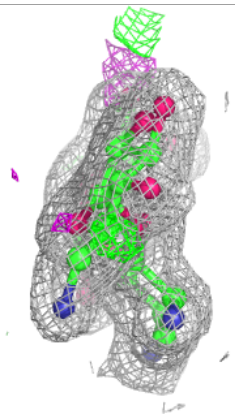


Electron density around KAN G 301:

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

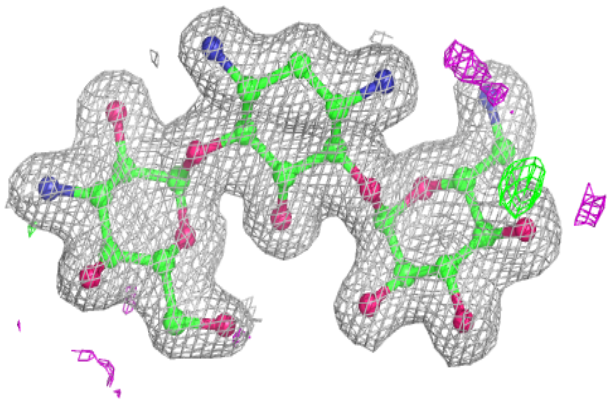


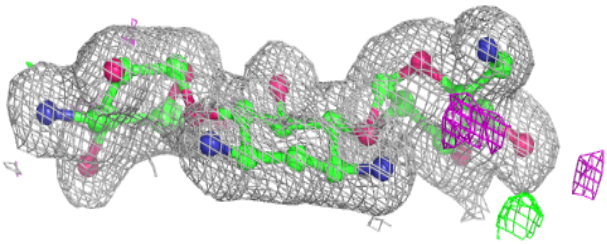


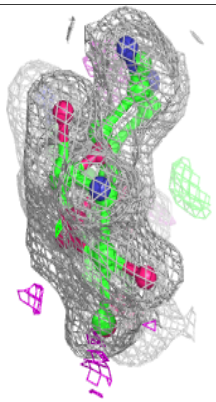


Electron density around KAN F 301:

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

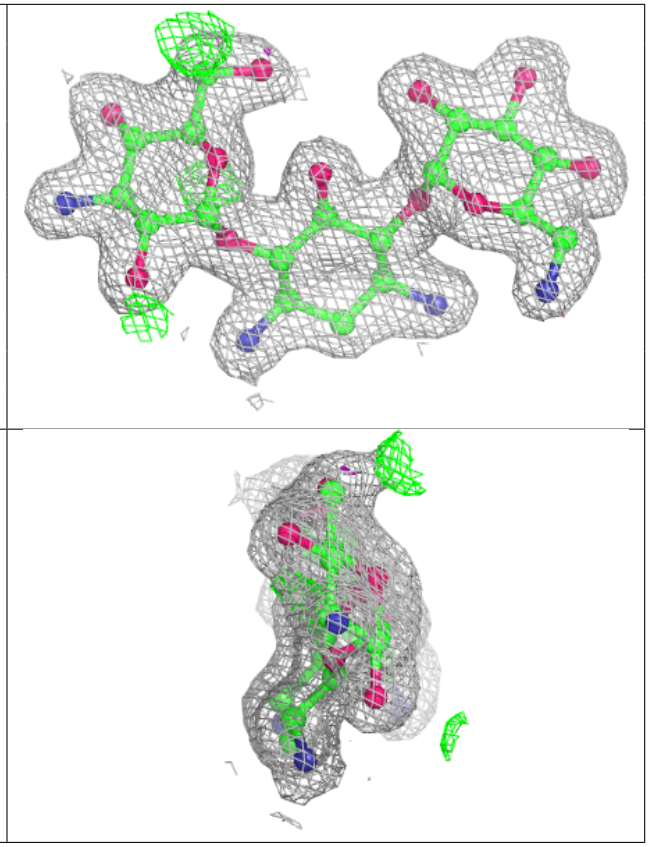






Electron density around KAN B 301:

$2mF_o$-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.