



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 02:09 AM BST

PDB ID : 4GKI
Title : Crystal structure of the aminoglycoside phosphotransferase APH(3')-Ia, with substrate kanamycin and small molecule inhibitor 1-NM-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 : 1.88 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 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)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

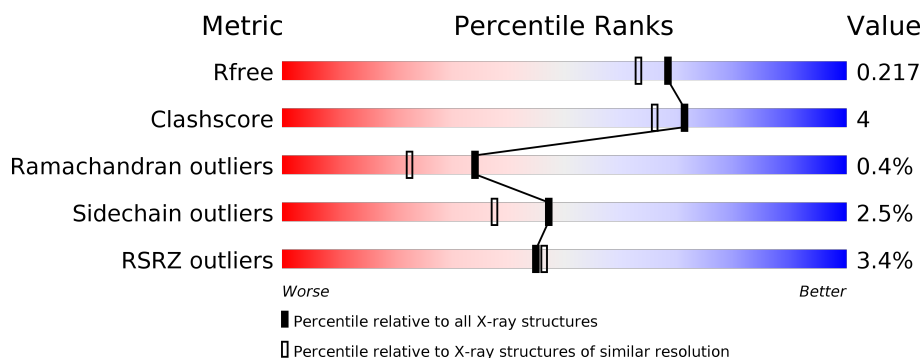
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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.





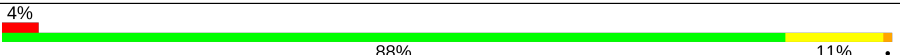
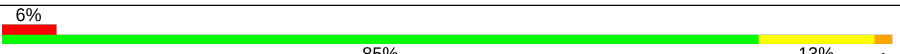
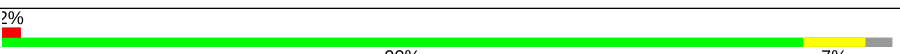
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 on 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 $\leq 5\%$. 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	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>.</div> </div> </div>
1	B	272	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>6%</div> </div> </div>
1	C	272	<div> <div>6%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div> </div>
1	D	272	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>5%</div> <div>7%</div> </div> </div>
1	E	272	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div>.</div> </div> </div>
1	F	272	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	272	
1	H	272	
1	I	272	
1	J	272	
1	K	272	
1	L	272	

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
3	0JN	C	302	-	-	-	X
3	0JN	G	302	-	-	-	X
6	ACT	H	305	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 30104 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
1	A	272	Total	C	N	O	S	Se	0	8	0
			2236	1423	391	410	5	7			
1	B	257	Total	C	N	O	S	Se	0	9	0
			2117	1356	362	389	4	6			
1	C	272	Total	C	N	O	S	Se	0	6	0
			2224	1413	388	411	5	7			
1	D	254	Total	C	N	O	S	Se	0	4	0
			2069	1323	354	382	4	6			
1	E	266	Total	C	N	O	S	Se	0	4	0
			2166	1378	375	402	5	6			
1	F	261	Total	C	N	O	S	Se	0	2	0
			2125	1356	370	388	5	6			
1	G	272	Total	C	N	O	S	Se	0	5	0
			2222	1411	391	408	5	7			
1	H	255	Total	C	N	O	S	Se	0	7	0
			2101	1344	361	386	4	6			
1	I	254	Total	C	N	O	S	Se	0	4	0
			2062	1321	350	381	4	6			
1	J	272	Total	C	N	O	S	Se	0	7	0
			2223	1415	385	411	5	7			
1	K	271	Total	C	N	O	S	Se	0	3	0
			2195	1397	382	404	5	7			
1	L	265	Total	C	N	O	S	Se	0	2	0
			2136	1360	367	398	5	6			

There are 12 discrepancies between the modelled and reference sequences:

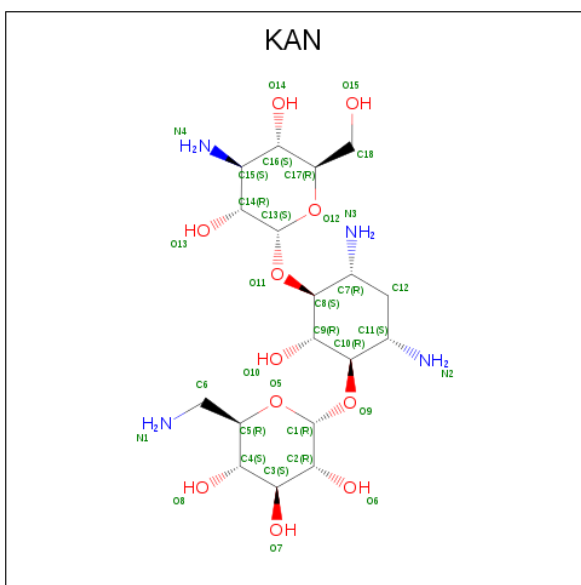
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP B0VD92
B	0	GLY	-	EXPRESSION TAG	UNP B0VD92
C	0	GLY	-	EXPRESSION TAG	UNP B0VD92
D	0	GLY	-	EXPRESSION TAG	UNP B0VD92
E	0	GLY	-	EXPRESSION TAG	UNP B0VD92

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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: $C_{18}H_{36}N_4O_{11}$).



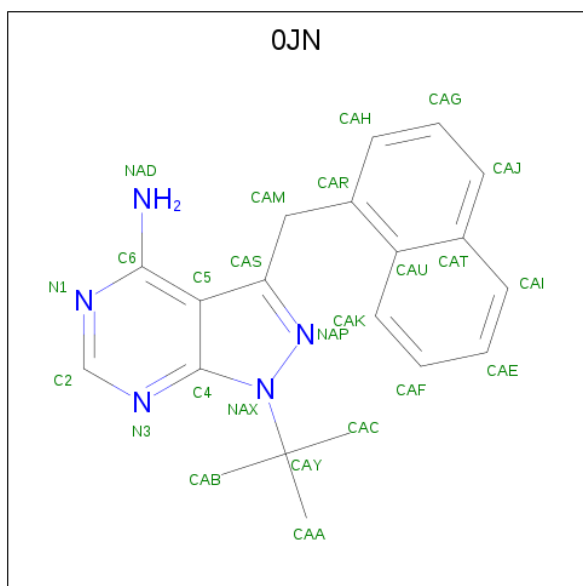
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	18	4	11		
2	B	1	Total	C	N	O	0	0
			33	18	4	11		
2	C	1	Total	C	N	O	0	0
			33	18	4	11		
2	D	1	Total	C	N	O	0	0
			33	18	4	11		
2	E	1	Total	C	N	O	0	0
			33	18	4	11		
2	F	1	Total	C	N	O	0	0
			33	18	4	11		
2	G	1	Total	C	N	O	0	0
			33	18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

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

- Molecule 3 is 1-tert-butyl-3-(naphthalen-1-ylmethyl)-1H-pyrazolo[3,4-d]pyrimidin-4-amine (three-letter code: OJN) (formula: C₂₀H₂₁N₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N		0	0
			25	20	5			
3	B	1	Total	C	N		0	0
			25	20	5			
3	C	1	Total	C	N		0	0
			25	20	5			
3	D	1	Total	C	N		0	0
			25	20	5			
3	E	1	Total	C	N		0	0
			25	20	5			
3	F	1	Total	C	N		0	0
			25	20	5			
3	G	1	Total	C	N		0	0
			25	20	5			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	N	0	0
			25	20	5		
3	I	1	Total	C	N	0	0
			25	20	5		
3	J	1	Total	C	N	0	0
			25	20	5		
3	K	1	Total	C	N	0	0
			25	20	5		
3	L	1	Total	C	N	0	0
			25	20	5		

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

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



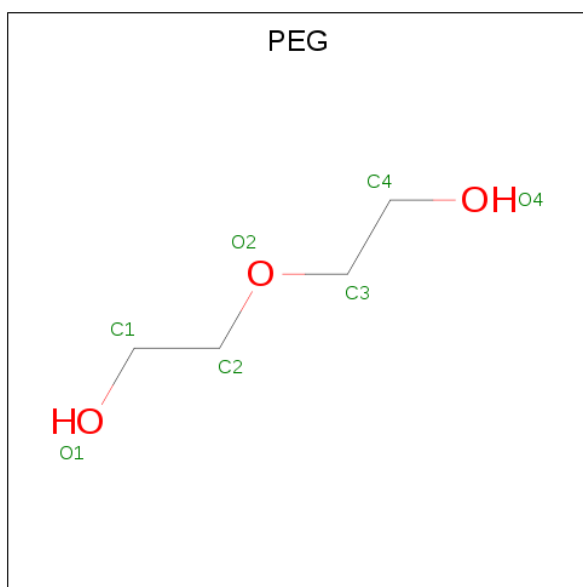
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total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

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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		
7	I	1	Total	C	O	0	0
			7	4	3		
7	J	1	Total	C	O	0	0
			7	4	3		
7	J	1	Total	C	O	0	0
			7	4	3		
7	J	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	274	Total	O	0	4
			277	277		
8	B	284	Total	O	0	8
			289	289		
8	C	272	Total	O	0	6
			278	278		
8	D	272	Total	O	0	2
			274	274		
8	E	307	Total	O	0	6
			313	313		
8	F	241	Total	O	0	6
			246	246		

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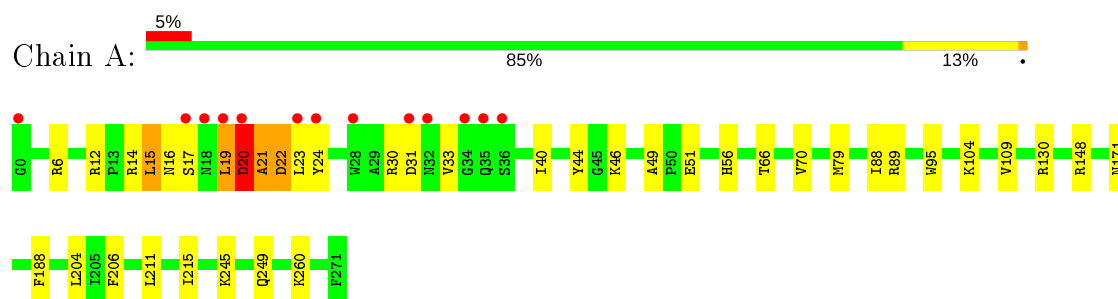
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	309	Total 317	O 317	0	8
8	H	267	Total 270	O 270	0	4
8	I	291	Total 297	O 297	0	7
8	J	284	Total 287	O 287	0	4
8	K	198	Total 202	O 202	0	5
8	L	309	Total 313	O 313	0	4

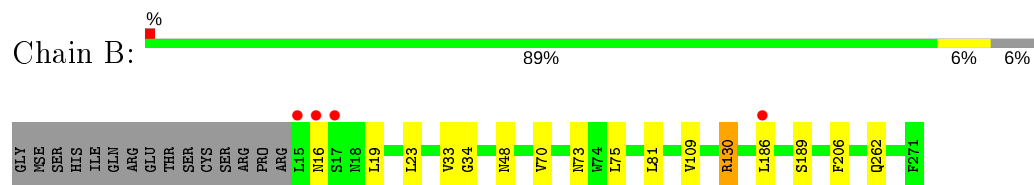
3 Residue-property plots

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.

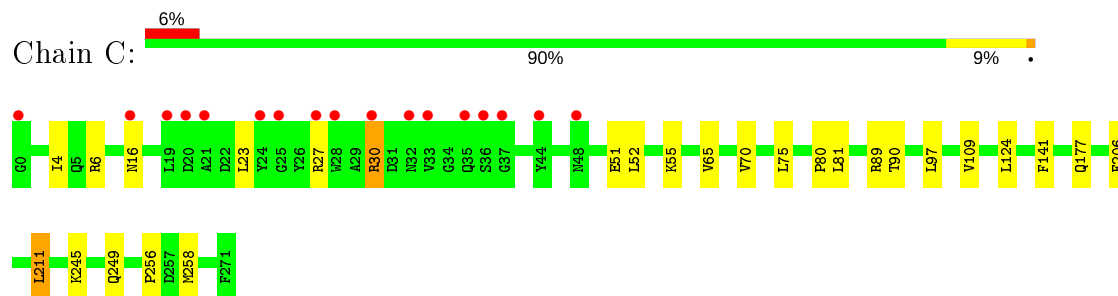
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



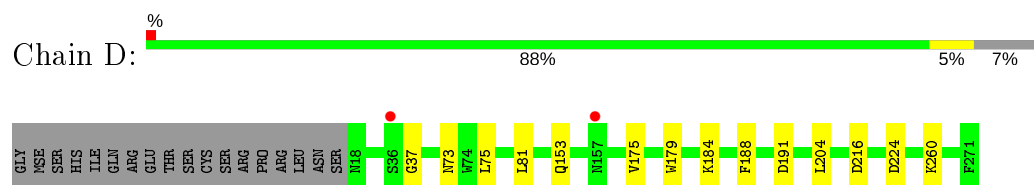
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



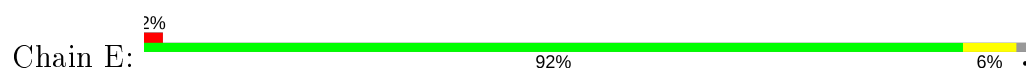
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



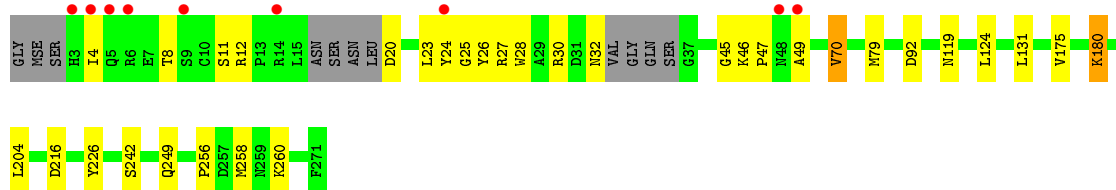
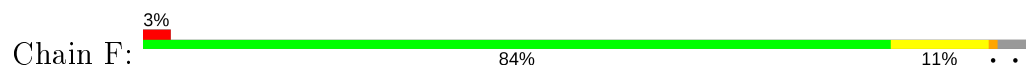
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



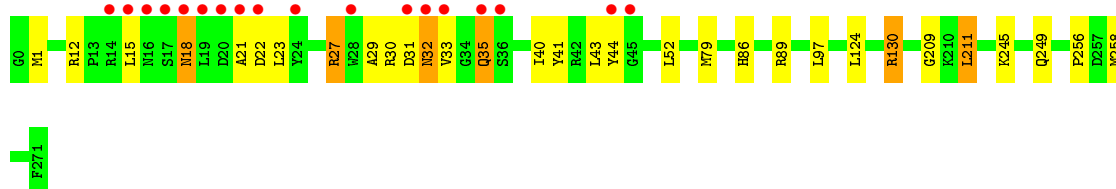
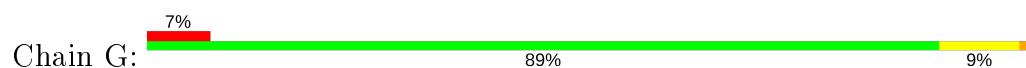
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



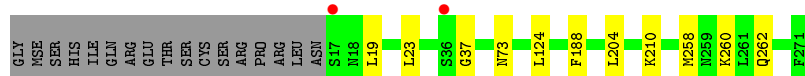
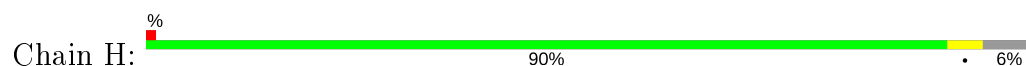
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



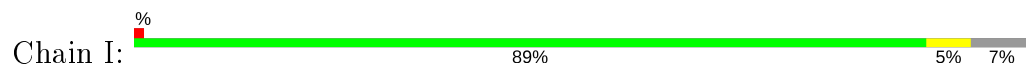
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



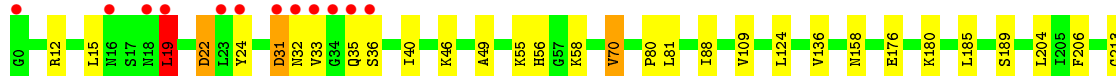
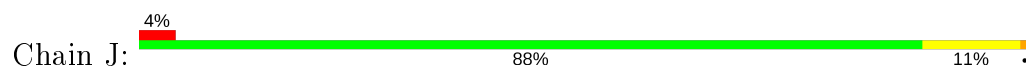
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

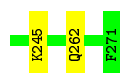


- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

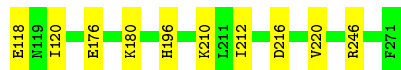
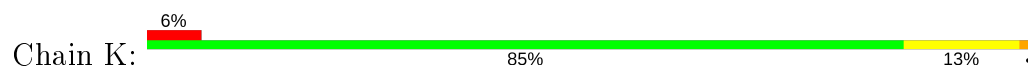


- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

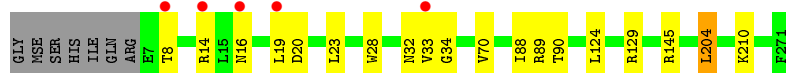
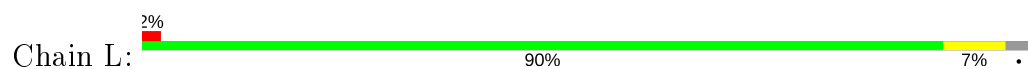




- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	96.84Å 97.10Å 112.13Å 103.24° 106.18° 112.66°	Depositor
Resolution (Å)	54.38 – 1.88 82.90 – 1.88	Depositor EDS
% Data completeness (in resolution range)	94.4 (54.38-1.88) 87.0 (82.90-1.88)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 1.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.166 , 0.216 0.167 , 0.217	Depositor DCC
R_{free} test set	13002 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-h-k-l 0.015 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	30104	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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 86.99 % 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 7.9096e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 0JN, CL, NA, KAN, ACT, PEG

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	0.37	0/2305	0.52	0/3111
1	B	0.40	0/2189	0.55	0/2960
1	C	0.38	0/2285	0.52	0/3086
1	D	0.36	0/2126	0.53	1/2876 (0.0%)
1	E	0.38	0/2221	0.53	0/3002
1	F	0.34	0/2176	0.51	0/2939
1	G	0.38	0/2283	0.54	0/3082
1	H	0.38	0/2158	0.54	0/2918
1	I	0.39	0/2119	0.54	1/2868 (0.0%)
1	J	0.38	0/2290	0.55	0/3094
1	K	0.34	0/2254	0.50	0/3047
1	L	0.38	0/2191	0.54	1/2964 (0.0%)
All	All	0.37	0/26597	0.53	3/35947 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	204	LEU	CA-CB-CG	-5.33	103.05	115.30
1	L	204	LEU	CA-CB-CG	-5.30	103.11	115.30
1	I	204	LEU	CA-CB-CG	-5.10	103.56	115.30

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	2236	0	2193	30	0
1	B	2117	0	2077	13	0
1	C	2224	0	2167	15	0
1	D	2069	0	2008	8	0
1	E	2166	0	2103	10	0
1	F	2125	0	2066	18	0
1	G	2222	0	2169	25	0
1	H	2101	0	2048	8	0
1	I	2062	0	2004	10	0
1	J	2223	0	2172	23	0
1	K	2195	0	2143	26	0
1	L	2136	0	2069	13	0
2	A	33	0	36	0	0
2	B	33	0	36	0	0
2	C	33	0	36	1	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	0	0
2	L	33	0	36	0	0
3	A	25	0	21	3	0
3	B	25	0	21	0	0
3	C	25	0	21	2	0
3	D	25	0	21	0	0
3	E	25	0	21	1	0
3	F	25	0	21	1	0
3	G	25	0	21	6	0
3	H	25	0	21	0	0
3	I	25	0	21	0	0
3	J	25	0	21	2	0
3	K	25	0	21	1	0
3	L	25	0	21	1	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	2	0	0	0	0
4	H	1	0	0	0	0
4	J	2	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	A	1	0	0	0	0
6	A	12	0	9	0	0
6	B	4	0	3	0	0
6	C	16	0	12	1	0
6	D	8	0	6	0	0
6	E	20	0	15	0	0
6	F	4	0	3	0	0
6	G	8	0	6	1	0
6	H	12	0	9	2	0
6	I	4	0	3	0	0
6	J	8	0	6	0	0
6	K	4	0	3	0	0
6	L	12	0	9	0	0
7	A	7	0	8	0	0
7	B	7	0	9	0	0
7	I	7	0	8	0	0
7	J	21	0	24	5	0
8	A	277	0	0	8	0
8	B	289	0	0	2	0
8	C	278	0	0	1	0
8	D	274	0	0	2	0
8	E	313	0	0	1	0
8	F	246	0	0	4	0
8	G	317	0	0	2	0
8	H	270	0	0	1	0
8	I	297	0	0	2	0
8	J	287	0	0	0	0
8	K	202	0	0	4	0
8	L	313	0	0	1	0
All	All	30104	0	26036	187	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.

All (187) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:CYS:HB3	1:F:28:TRP:HB2	1.59	0.83
3:C:302:0JN:H18	3:C:302:0JN:CAH	2.02	0.72
1:F:12:ARG:NH2	8:F:631:HOH:O	2.25	0.70
1:J:158:ASN:HB3	7:J:309:PEG:H32	1.74	0.69
1:J:12:ARG:HH21	1:J:15:LEU:HD12	1.56	0.69
1:F:46:LYS:HD3	1:F:47:PRO:HD2	1.74	0.68
1:C:256:PRO:HB2	1:C:258:MSE:HE2	1.74	0.68
1:H:258:MSE:HE3	6:H:305:ACT:H1	1.76	0.67
1:F:256:PRO:HB2	1:F:258:MSE:HE2	1.76	0.66
1:A:16:ASN:ND2	1:A:17:SER:O	2.30	0.65
3:K:302:0JN:H18	3:K:302:0JN:CAH	2.11	0.64
1:A:79:MSE:SE	1:A:130:ARG:HG2	2.49	0.63
1:C:89[A]:ARG:HH21	1:D:73:ASN:HD21	1.46	0.63
1:A:6[B]:ARG:NH2	8:A:584:HOH:O	2.22	0.62
1:A:70[A]:VAL:HG11	1:B:70[A]:VAL:HG11	1.81	0.62
1:G:89[B]:ARG:HH21	1:H:73:ASN:HD21	1.47	0.62
1:I:130:ARG:NH1	8:I:611:HOH:O	2.21	0.60
1:D:153:GLN:NE2	1:K:111:GLU:O	2.30	0.59
1:I:75:LEU:HB3	1:I:81:LEU:HD11	1.84	0.59
1:I:23:LEU:HD12	1:J:15:LEU:HD11	1.85	0.58
1:G:18:ASN:HA	1:G:86:HIS:HE1	1.69	0.58
1:H:210[A]:LYS:NZ	8:H:623:HOH:O	2.35	0.58
3:J:302:0JN:H18	3:J:302:0JN:CAH	2.17	0.58
3:G:302:0JN:H18	3:G:302:0JN:CAH	2.17	0.57
1:F:46:LYS:HG3	1:F:49:ALA:HB3	1.87	0.57
3:C:302:0JN:H18	3:C:302:0JN:CAR	2.16	0.57
1:I:19:LEU:HD22	1:I:88:ILE:HD12	1.87	0.57
1:L:124:LEU:HD22	1:L:204:LEU:HD13	1.87	0.57
1:L:19:LEU:HB2	1:L:88:ILE:HD11	1.87	0.57
1:H:262:GLN:HB2	6:H:305:ACT:H3	1.87	0.56
1:L:32:ASN:OD1	1:L:33:VAL:HB	2.06	0.56
1:H:124:LEU:HD22	1:H:204:LEU:HD13	1.88	0.55
1:A:20:ASP:N	1:A:20:ASP:OD1	2.36	0.55
1:J:176:GLU:HG3	1:J:180:LYS:HE2	1.88	0.55
1:A:19:LEU:O	1:A:21:ALA:N	2.38	0.55
1:K:20:ASP:OD1	1:K:21:ALA:N	2.40	0.55
1:C:124:LEU:HD23	1:C:211:LEU:HD21	1.90	0.54
1:G:18:ASN:HA	1:G:86:HIS:CE1	2.42	0.54
1:G:12:ARG:HE	1:G:15:LEU:HD21	1.73	0.54
1:I:89:ARG:NH1	1:I:90:THR:O	2.41	0.54
1:K:104:LYS:NZ	1:K:112:GLU:OE1	2.34	0.54
1:A:14:ARG:NH2	8:A:661:HOH:O	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:ILE:HG23	1:C:6[A]:ARG:HG3	1.88	0.53
1:H:19:LEU:O	1:H:23:LEU:HG	2.09	0.53
3:F:302:0JN:CAH	3:F:302:0JN:H18	2.21	0.53
1:B:186:LEU:H	1:B:186:LEU:HD23	1.72	0.53
1:F:175:VAL:HG23	8:F:559:HOH:O	2.09	0.53
1:G:124:LEU:HD23	1:G:211:LEU:HD21	1.91	0.53
1:K:118:GLU:OE2	1:K:246:ARG:NH1	2.42	0.53
1:A:109:VAL:HG21	1:A:206:PHE:HB2	1.90	0.52
1:F:27:ARG:HG3	1:F:45:GLY:HA3	1.92	0.52
1:J:19:LEU:HG	1:J:88[B]:ILE:HD12	1.92	0.52
1:D:175:VAL:HG23	8:D:648:HOH:O	2.08	0.52
1:A:46:LYS:HB3	1:A:49:ALA:HB3	1.90	0.52
1:G:31:ASP:CG	3:G:302:0JN:H9	2.30	0.52
1:J:40:ILE:HG12	1:J:55:LYS:HG3	1.91	0.51
1:D:184:LYS:NZ	8:D:562:HOH:O	2.37	0.51
1:G:31:ASP:OD2	3:G:302:0JN:H9	2.10	0.51
1:J:46:LYS:HB3	1:J:49:ALA:HB3	1.92	0.50
1:C:245:LYS:O	1:C:249:GLN:HG3	2.11	0.50
1:K:42:ARG:NH2	1:K:51:GLU:OE2	2.45	0.50
1:A:66:THR:OG1	1:A:89[B]:ARG:NH1	2.43	0.50
1:L:145:ARG:NH2	8:L:664:HOH:O	2.38	0.50
1:K:27:ARG:NH2	8:K:562:HOH:O	2.41	0.49
1:J:22:ASP:OD1	1:J:22:ASP:N	2.43	0.49
1:B:73:ASN:ND2	8:B:631:HOH:O	2.45	0.49
1:D:153:GLN:HB2	1:D:179:TRP:CH2	2.48	0.49
3:J:302:0JN:H18	3:J:302:0JN:CAR	2.25	0.49
1:K:15:LEU:CD2	1:L:19:LEU:HD23	2.43	0.48
1:D:188:PHE:CD1	1:D:260:LYS:HE2	2.48	0.48
1:J:58:LYS:HB3	7:J:307:PEG:H32	1.96	0.48
1:K:70[A]:VAL:HG11	1:L:70:VAL:HG11	1.95	0.48
1:G:245:LYS:HE2	1:G:249[A]:GLN:NE2	2.29	0.48
1:K:16:ASN:ND2	1:L:90:THR:HG21	2.28	0.48
1:E:12:ARG:NH2	1:F:23:LEU:O	2.45	0.47
1:K:40:ILE:HG12	1:K:55:LYS:HG2	1.96	0.47
1:A:30:ARG:HD2	1:A:33:VAL:HG12	1.96	0.47
1:B:130[B]:ARG:NH2	8:B:641:HOH:O	2.25	0.47
1:F:226:TYR:CD1	1:F:260:LYS:HE2	2.49	0.47
1:K:32:ASN:OD1	1:K:32:ASN:N	2.46	0.47
1:G:32:ASN:O	1:G:35:GLN:HB2	2.16	0.46
1:A:245:LYS:O	1:A:249:GLN:HG3	2.15	0.46
1:G:23:LEU:HD12	1:G:23:LEU:HA	1.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:110:LEU:HD13	1:K:120:ILE:HG21	1.97	0.46
1:J:58:LYS:O	7:J:307:PEG:H41	2.16	0.46
1:A:22:ASP:OD1	1:A:22:ASP:N	2.49	0.46
1:C:177:GLN:OE1	8:C:524:HOH:O	2.21	0.46
1:K:87:PHE:HB3	1:L:89:ARG:HB3	1.96	0.46
8:A:593:HOH:O	1:B:33:VAL:HA	2.14	0.46
1:A:130:ARG:HD2	8:A:619:HOH:O	2.15	0.46
1:A:31:ASP:HB3	3:A:302:OJN:H8	1.97	0.46
1:B:75:LEU:HB3	1:B:81:LEU:HD11	1.98	0.45
1:J:12:ARG:NH2	1:J:15:LEU:HD12	2.26	0.45
1:E:210:LYS:HD3	1:E:212:ILE:HG22	1.98	0.45
1:E:14:ARG:HH12	1:F:20:ASP:HA	1.81	0.45
1:K:110:LEU:HD12	1:K:110:LEU:HA	1.83	0.45
1:A:56:HIS:HB2	1:A:95:TRP:CZ3	2.52	0.45
1:F:124:LEU:HD22	1:F:204:LEU:HD13	1.97	0.45
1:A:70[A]:VAL:HG11	1:B:70[A]:VAL:CG1	2.47	0.45
1:G:43:LEU:HB2	1:G:52:LEU:HB2	1.99	0.45
1:J:80:PRO:HG2	1:J:213:GLY:HA2	1.99	0.45
1:K:27:ARG:NH1	8:K:498:HOH:O	2.42	0.45
1:K:176:GLU:O	1:K:180:LYS:HD3	2.18	0.44
1:A:14:ARG:NH1	8:A:526:HOH:O	2.50	0.44
1:J:15:LEU:HD23	1:J:15:LEU:HA	1.72	0.44
1:C:80:PRO:HD3	6:C:308:ACT:H3	2.00	0.44
1:J:109:VAL:HG21	1:J:206:PHE:HB2	1.99	0.44
1:G:256:PRO:HB2	1:G:258:MSE:HE2	1.99	0.44
1:I:70[B]:VAL:HG21	1:J:70:VAL:HG11	2.00	0.44
1:J:35:GLN:HG2	1:J:36:SER:H	1.82	0.44
1:C:109:VAL:HG21	1:C:206:PHE:HB2	1.99	0.44
1:C:55:LYS:HD3	1:C:65:VAL:HG22	1.99	0.44
1:G:23:LEU:HD13	1:G:97:LEU:HD21	1.98	0.44
1:J:19:LEU:HG	1:J:88[B]:ILE:CD1	2.48	0.44
1:K:70[A]:VAL:CG1	1:L:70:VAL:HG11	2.48	0.44
1:B:19:LEU:O	1:B:23:LEU:HG	2.18	0.44
1:A:15:LEU:HD21	1:B:23:LEU:HD12	2.00	0.44
1:E:70:VAL:HG11	1:F:70[A]:VAL:HG11	1.98	0.44
1:G:209:GLY:HA2	6:G:306:ACT:H1	1.98	0.43
1:J:185:LEU:HD11	1:J:262[A]:GLN:HG2	1.98	0.43
1:F:25:GLY:O	1:F:46:LYS:HE3	2.18	0.43
1:A:44:TYR:HB3	1:A:51:GLU:HG3	2.00	0.43
1:C:23:LEU:HD21	1:C:97:LEU:HD21	2.00	0.43
1:H:188:PHE:CD1	1:H:260:LYS:HE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:80:PRO:O	1:I:81:LEU:HD23	2.18	0.43
3:A:302:OJN:H18	3:A:302:OJN:H11	1.82	0.43
1:E:238:GLU:HG3	8:E:609:HOH:O	2.18	0.43
1:G:27:ARG:HB3	1:G:44:TYR:CZ	2.53	0.43
1:J:158:ASN:O	7:J:309:PEG:H12	2.18	0.43
1:K:5:GLN:HA	8:K:593:HOH:O	2.18	0.43
1:A:104:LYS:NZ	8:A:662:HOH:O	2.46	0.43
1:E:210:LYS:NZ	1:G:33:VAL:HG11	2.33	0.43
1:G:30:ARG:HG2	1:G:31:ASP:O	2.18	0.43
1:A:188:PHE:CD1	1:A:260:LYS:HD3	2.54	0.43
1:A:89[A]:ARG:HH21	1:B:73:ASN:HD21	1.66	0.43
1:I:146[A]:VAL:HG23	8:I:595:HOH:O	2.17	0.43
1:K:5:GLN:HG2	1:K:5:GLN:H	1.61	0.43
1:L:33:VAL:HG22	1:L:34:GLY:H	1.83	0.43
1:K:210:LYS:O	1:K:212:ILE:HG23	2.19	0.42
1:A:204:LEU:HB3	1:A:211:LEU:HD11	2.01	0.42
1:D:75:LEU:HB3	1:D:81:LEU:HD11	2.01	0.42
1:A:30:ARG:HA	1:A:40:ILE:O	2.19	0.42
1:F:119:ASN:ND2	8:F:625:HOH:O	2.41	0.42
1:F:180:LYS:HD2	8:F:607:HOH:O	2.19	0.42
1:E:75:LEU:HB3	1:E:81:LEU:HD11	1.99	0.42
1:F:20:ASP:N	1:F:23:LEU:HD13	2.34	0.42
3:G:302:OJN:H11	8:G:622:HOH:O	2.18	0.42
1:I:70[B]:VAL:HG12	1:I:141:PHE:HZ	1.84	0.42
1:A:148[B]:ARG:HD2	8:A:434:HOH:O	2.19	0.42
3:L:302:OJN:H18	3:L:302:OJN:CAH	2.32	0.42
1:D:191:ASP:HB3	1:D:224:ASP:OD2	2.20	0.42
1:E:12:ARG:HG3	1:E:12:ARG:O	2.19	0.42
1:K:35:GLN:HB3	8:K:512:HOH:O	2.19	0.42
1:J:124:LEU:HD22	1:J:204:LEU:HD13	2.02	0.42
1:K:196:HIS:HA	1:K:220:VAL:HG22	2.01	0.42
1:G:31:ASP:OD1	3:G:302:OJN:H9	2.20	0.42
1:L:19:LEU:O	1:L:23:LEU:HG	2.20	0.42
1:K:16:ASN:CG	1:L:90:THR:HG21	2.41	0.42
1:G:35:GLN:NE2	8:G:569:HOH:O	2.53	0.41
1:I:70[B]:VAL:HG21	1:J:70:VAL:CG1	2.50	0.41
1:K:69:MSE:HG3	1:K:87:PHE:CG	2.55	0.41
3:G:302:OJN:H18	3:G:302:OJN:H11	1.85	0.41
1:A:19:LEU:HB2	1:A:88:ILE:HD11	2.02	0.41
1:A:70[A]:VAL:CG1	1:B:70[A]:VAL:HG11	2.49	0.41
2:C:301:KAN:O10	2:C:301:KAN:H1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:VAL:HG22	1:B:34:GLY:H	1.86	0.41
3:E:302:OJN:H18	3:E:302:OJN:CAH	2.33	0.41
1:F:79:MSE:HE2	1:F:131:LEU:HB2	2.02	0.41
1:J:80:PRO:O	1:J:81:LEU:HD23	2.21	0.41
1:G:29:ALA:O	1:G:41:TYR:HA	2.21	0.41
1:J:56:HIS:O	7:J:307:PEG:H21	2.20	0.41
1:C:89[A]:ARG:NH1	1:C:90:THR:O	2.54	0.41
1:G:79:MSE:SE	1:G:130[B]:ARG:HG2	2.71	0.41
1:G:27:ARG:HD2	1:G:44:TYR:OH	2.21	0.41
1:B:109[A]:VAL:HG21	1:B:206:PHE:HB2	2.03	0.41
1:G:30:ARG:HA	1:G:40:ILE:O	2.21	0.41
1:G:89[B]:ARG:NH2	1:H:73:ASN:HD21	2.15	0.41
1:E:70:VAL:HG11	1:F:70[A]:VAL:CG1	2.51	0.41
1:A:215:ILE:HD12	3:A:302:OJN:H14	2.04	0.40
1:C:51:GLU:O	1:C:52:LEU:HD23	2.21	0.40
1:K:12:ARG:HB3	1:L:28:TRP:CE2	2.57	0.40
1:A:171:ASN:ND2	8:A:588:HOH:O	2.47	0.40
1:C:70[B]:VAL:HG12	1:C:141:PHE:HZ	1.86	0.40
1:C:30:ARG:HD3	1:C:30:ARG:H	1.86	0.40
1:C:75:LEU:HB3	1:C:81:LEU:HD11	2.04	0.40
1:G:21:ALA:C	1:G:23:LEU:H	2.25	0.40
1:K:53:PHE:O	1:K:97:LEU:HD12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	278/272 (102%)	270 (97%)	6 (2%)	2 (1%)	22	11
1	B	264/272 (97%)	260 (98%)	4 (2%)	0	100	100
1	C	276/272 (102%)	268 (97%)	7 (2%)	1 (0%)	34	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	256/272 (94%)	252 (98%)	3 (1%)	1 (0%)	34	22
1	E	268/272 (98%)	259 (97%)	7 (3%)	2 (1%)	22	11
1	F	257/272 (94%)	247 (96%)	9 (4%)	1 (0%)	34	22
1	G	275/272 (101%)	261 (95%)	13 (5%)	1 (0%)	34	22
1	H	260/272 (96%)	255 (98%)	4 (2%)	1 (0%)	34	22
1	I	256/272 (94%)	251 (98%)	5 (2%)	0	100	100
1	J	277/272 (102%)	266 (96%)	9 (3%)	2 (1%)	22	11
1	K	272/272 (100%)	260 (96%)	9 (3%)	3 (1%)	14	5
1	L	265/272 (97%)	259 (98%)	6 (2%)	0	100	100
All	All	3204/3264 (98%)	3108 (97%)	82 (3%)	14 (0%)	34	22

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	11	SER
1	F	24	TYR
1	G	32	ASN
1	A	20	ASP
1	K	36	SER
1	C	16	ASN
1	D	37	GLY
1	K	23	LEU
1	A	21	ALA
1	J	31	ASP
1	H	37	GLY
1	J	19	LEU
1	K	47	PRO
1	E	33	VAL

5.3.2 Protein sidechains ⓘ

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	246/231 (106%)	239 (97%)	7 (3%)	43	33
1	B	233/231 (101%)	226 (97%)	7 (3%)	41	30
1	C	244/231 (106%)	241 (99%)	3 (1%)	71	67
1	D	225/231 (97%)	224 (100%)	1 (0%)	91	90
1	E	237/231 (103%)	230 (97%)	7 (3%)	41	30
1	F	231/231 (100%)	218 (94%)	13 (6%)	21	10
1	G	243/231 (105%)	235 (97%)	8 (3%)	38	26
1	H	229/231 (99%)	229 (100%)	0	100	100
1	I	225/231 (97%)	225 (100%)	0	100	100
1	J	245/231 (106%)	234 (96%)	11 (4%)	27	16
1	K	241/231 (104%)	230 (95%)	11 (5%)	27	15
1	L	234/231 (101%)	228 (97%)	6 (3%)	46	36
All	All	2833/2772 (102%)	2759 (97%)	74 (3%)	47	36

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	15	LEU
1	A	19	LEU
1	A	20	ASP
1	A	22	ASP
1	A	23	LEU
1	A	24	TYR
1	B	16	ASN
1	B	48	ASN
1	B	130[A]	ARG
1	B	130[B]	ARG
1	B	189	SER
1	B	262[A]	GLN
1	B	262[B]	GLN
1	C	27	ARG
1	C	30	ARG
1	C	211	LEU
1	D	216	ASP
1	E	8	THR
1	E	9	SER
1	E	10	CYS
1	E	20	ASP

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Mol	Chain	Res	Type
1	E	23	LEU
1	E	32	ASN
1	E	216	ASP
1	F	4	ILE
1	F	8	THR
1	F	11	SER
1	F	26	TYR
1	F	30	ARG
1	F	32	ASN
1	F	70[A]	VAL
1	F	70[B]	VAL
1	F	92	ASP
1	F	180	LYS
1	F	216	ASP
1	F	242	SER
1	F	249	GLN
1	G	1	MSE
1	G	18	ASN
1	G	22	ASP
1	G	27	ARG
1	G	35	GLN
1	G	130[A]	ARG
1	G	130[B]	ARG
1	G	211	LEU
1	J	19	LEU
1	J	22	ASP
1	J	24	TYR
1	J	31	ASP
1	J	32	ASN
1	J	33	VAL
1	J	70	VAL
1	J	136[A]	VAL
1	J	136[B]	VAL
1	J	189	SER
1	J	245	LYS
1	K	1	MSE
1	K	4	ILE
1	K	5	GLN
1	K	32	ASN
1	K	36	SER
1	K	70[A]	VAL
1	K	70[B]	VAL

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Mol	Chain	Res	Type
1	K	92	ASP
1	K	110	LEU
1	K	115	ASP
1	K	216	ASP
1	L	8	THR
1	L	14	ARG
1	L	16	ASN
1	L	20	ASP
1	L	129	ARG
1	L	210	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	73	ASN
1	C	158	ASN
1	D	73	ASN
1	G	73	ASN
1	G	86	HIS
1	H	73	ASN
1	J	73	ASN
1	K	16	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 73 ligands modelled in this entry, 15 are monoatomic - leaving 58 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$
6	ACT	E	306	-	1,3,3	1.25	0	0,3,3	0.00	-
2	KAN	I	301	-	35,35,35	0.90	2 (5%)	46,52,52	1.42	7 (15%)
3	0JN	F	302	-	24,28,28	2.14	5 (20%)	28,42,42	1.61	3 (10%)
6	ACT	J	306	4	1,3,3	1.37	0	0,3,3	0.00	-
6	ACT	D	304	4	1,3,3	1.17	0	0,3,3	0.00	-
3	0JN	A	302	-	24,28,28	2.00	5 (20%)	28,42,42	1.60	2 (7%)
6	ACT	L	305	-	1,3,3	1.27	0	0,3,3	0.00	-
2	KAN	J	301	-	35,35,35	0.91	2 (5%)	46,52,52	1.38	4 (8%)
6	ACT	G	305	-	1,3,3	1.12	0	0,3,3	0.00	-
2	KAN	H	301	-	35,35,35	0.86	1 (2%)	46,52,52	1.39	4 (8%)
2	KAN	A	301	-	35,35,35	0.95	2 (5%)	46,52,52	1.24	4 (8%)
7	PEG	I	304	-	6,6,6	1.06	0	5,5,5	2.04	2 (40%)
2	KAN	C	301	-	35,35,35	0.99	2 (5%)	46,52,52	1.34	7 (15%)
7	PEG	J	309	-	6,6,6	1.03	0	5,5,5	1.79	2 (40%)
7	PEG	J	308	-	6,6,6	1.06	0	5,5,5	1.96	2 (40%)
6	ACT	L	304	4	1,3,3	1.15	0	0,3,3	0.00	-
7	PEG	J	307	-	6,6,6	1.07	0	5,5,5	1.85	2 (40%)
6	ACT	L	306	-	1,3,3	1.42	0	0,3,3	0.00	-
3	0JN	B	302	-	24,28,28	1.96	5 (20%)	28,42,42	1.76	3 (10%)
3	0JN	K	302	-	24,28,28	2.03	5 (20%)	28,42,42	1.65	2 (7%)
6	ACT	A	307	4	1,3,3	1.52	0	0,3,3	0.00	-
3	0JN	I	302	-	24,28,28	2.11	5 (20%)	28,42,42	1.74	2 (7%)
6	ACT	H	305	-	1,3,3	1.39	0	0,3,3	0.00	-
3	0JN	G	302	-	24,28,28	2.02	5 (20%)	28,42,42	1.76	3 (10%)
7	PEG	A	309	-	6,6,6	1.03	0	5,5,5	1.80	2 (40%)
2	KAN	F	301	-	35,35,35	0.67	1 (2%)	46,52,52	1.30	5 (10%)
6	ACT	F	304	-	1,3,3	1.42	0	0,3,3	0.00	-
6	ACT	G	306	-	1,3,3	1.11	0	0,3,3	0.00	-
3	0JN	L	302	-	24,28,28	2.07	5 (20%)	28,42,42	1.64	3 (10%)
6	ACT	E	305	-	1,3,3	0.86	0	0,3,3	0.00	-
3	0JN	J	302	-	24,28,28	2.12	5 (20%)	28,42,42	1.82	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	KAN	K	301	-	35,35,35	0.74	1 (2%)	46,52,52	1.29	5 (10%)
7	PEG	B	304	-	6,6,6	1.05	0	5,5,5	1.74	2 (40%)
6	ACT	K	304	-	1,3,3	1.72	0	0,3,3	0.00	-
2	KAN	D	301	-	35,35,35	0.83	1 (2%)	46,52,52	1.38	6 (13%)
6	ACT	D	305	-	1,3,3	1.52	0	0,3,3	0.00	-
6	ACT	H	304	4	1,3,3	1.49	0	0,3,3	0.00	-
6	ACT	E	308	-	1,3,3	1.72	0	0,3,3	0.00	-
6	ACT	C	305	-	1,3,3	1.02	0	0,3,3	0.00	-
3	0JN	D	302	-	24,28,28	2.02	5 (20%)	28,42,42	1.89	4 (14%)
6	ACT	C	306	-	1,3,3	1.40	0	0,3,3	0.00	-
6	ACT	A	306	-	1,3,3	1.53	0	0,3,3	0.00	-
2	KAN	G	301	-	35,35,35	0.95	1 (2%)	46,52,52	1.28	5 (10%)
6	ACT	B	303	-	1,3,3	1.47	0	0,3,3	0.00	-
6	ACT	E	307	4	1,3,3	1.13	0	0,3,3	0.00	-
6	ACT	E	304	-	1,3,3	1.39	0	0,3,3	0.00	-
6	ACT	C	307	-	1,3,3	1.35	0	0,3,3	0.00	-
6	ACT	H	306	-	1,3,3	1.44	0	0,3,3	0.00	-
2	KAN	B	301	-	35,35,35	0.75	0	46,52,52	1.20	4 (8%)
3	0JN	E	302	-	24,28,28	1.93	5 (20%)	28,42,42	1.78	3 (10%)
3	0JN	C	302	-	24,28,28	2.08	5 (20%)	28,42,42	1.67	2 (7%)
6	ACT	A	308	-	1,3,3	1.50	0	0,3,3	0.00	-
6	ACT	I	303	-	1,3,3	1.61	0	0,3,3	0.00	-
6	ACT	C	308	4	1,3,3	1.22	0	0,3,3	0.00	-
6	ACT	J	305	-	1,3,3	1.16	0	0,3,3	0.00	-
3	0JN	H	302	-	24,28,28	2.14	5 (20%)	28,42,42	1.79	3 (10%)
2	KAN	L	301	-	35,35,35	0.82	1 (2%)	46,52,52	1.22	4 (8%)
2	KAN	E	301	-	35,35,35	0.80	1 (2%)	46,52,52	1.44	7 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KAN	I	301	-	-	1/12/72/72	0/3/3/3
3	0JN	F	302	-	-	0/10/10/10	0/4/4/4
3	0JN	A	302	-	-	0/10/10/10	0/4/4/4
2	KAN	J	301	-	-	1/12/72/72	0/3/3/3
2	KAN	H	301	-	-	2/12/72/72	0/3/3/3
2	KAN	A	301	-	-	1/12/72/72	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PEG	I	304	-	-	0/4/4/4	-
2	KAN	C	301	-	-	2/12/72/72	0/3/3/3
7	PEG	J	308	-	-	0/4/4/4	-
7	PEG	J	307	-	-	1/4/4/4	-
3	0JN	B	302	-	-	0/10/10/10	0/4/4/4
3	0JN	K	302	-	-	1/10/10/10	0/4/4/4
3	0JN	I	302	-	-	0/10/10/10	0/4/4/4
3	0JN	G	302	-	-	0/10/10/10	0/4/4/4
7	PEG	A	309	-	-	1/4/4/4	-
2	KAN	F	301	-	-	1/12/72/72	0/3/3/3
3	0JN	L	302	-	-	0/10/10/10	0/4/4/4
3	0JN	J	302	-	-	1/10/10/10	0/4/4/4
2	KAN	K	301	-	-	1/12/72/72	0/3/3/3
7	PEG	B	304	-	-	2/4/4/4	-
2	KAN	D	301	-	-	2/12/72/72	0/3/3/3
3	0JN	D	302	-	-	0/10/10/10	0/4/4/4
2	KAN	G	301	-	-	0/12/72/72	0/3/3/3
2	KAN	B	301	-	-	2/12/72/72	0/3/3/3
3	0JN	E	302	-	-	0/10/10/10	0/4/4/4
3	0JN	C	302	-	-	2/10/10/10	0/4/4/4
7	PEG	J	309	-	-	1/4/4/4	-
3	0JN	H	302	-	-	0/10/10/10	0/4/4/4
2	KAN	L	301	-	-	2/12/72/72	0/3/3/3
2	KAN	E	301	-	-	1/12/72/72	0/3/3/3

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	302	0JN	CAM-CAS	6.27	1.56	1.51
3	J	302	0JN	CAM-CAS	6.10	1.56	1.51
3	F	302	0JN	CAM-CAS	6.01	1.56	1.51
3	C	302	0JN	CAM-CAS	5.97	1.56	1.51
3	L	302	0JN	CAM-CAS	5.88	1.56	1.51
3	I	302	0JN	CAM-CAS	5.82	1.56	1.51
3	G	302	0JN	CAM-CAS	5.77	1.56	1.51
3	D	302	0JN	CAM-CAS	5.60	1.55	1.51
3	B	302	0JN	C2-N3	5.19	1.40	1.32
3	A	302	0JN	CAM-CAS	5.05	1.55	1.51
3	K	302	0JN	CAM-CAS	5.01	1.55	1.51
3	J	302	0JN	C2-N3	4.97	1.40	1.32
3	F	302	0JN	C2-N3	4.96	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	OJN	C2-N3	4.91	1.40	1.32
3	I	302	OJN	C2-N3	4.86	1.39	1.32
3	G	302	OJN	C2-N3	4.81	1.39	1.32
3	D	302	OJN	C2-N3	4.76	1.39	1.32
3	K	302	OJN	C2-N3	4.73	1.39	1.32
3	L	302	OJN	C2-N3	4.73	1.39	1.32
3	H	302	OJN	C2-N3	4.69	1.39	1.32
3	E	302	OJN	C2-N3	4.65	1.39	1.32
3	C	302	OJN	C2-N3	4.65	1.39	1.32
3	E	302	OJN	CAM-CAS	4.63	1.55	1.51
3	B	302	OJN	CAM-CAS	4.36	1.55	1.51
3	B	302	OJN	C2-N1	3.44	1.40	1.33
3	K	302	OJN	CAM-CAR	-3.41	1.39	1.52
3	C	302	OJN	CAM-CAR	-3.39	1.39	1.52
3	F	302	OJN	C2-N1	3.38	1.40	1.33
3	H	302	OJN	C2-N1	3.37	1.40	1.33
3	I	302	OJN	C2-N1	3.34	1.40	1.33
3	D	302	OJN	C2-N1	3.30	1.40	1.33
3	E	302	OJN	CAM-CAR	-3.26	1.40	1.52
3	J	302	OJN	CAM-CAR	-3.26	1.40	1.52
3	A	302	OJN	C5-C4	-3.24	1.34	1.43
3	L	302	OJN	CAM-CAR	-3.24	1.40	1.52
3	K	302	OJN	C2-N1	3.20	1.39	1.33
3	F	302	OJN	C5-C4	-3.19	1.34	1.43
3	C	302	OJN	C5-C4	-3.18	1.34	1.43
3	A	302	OJN	CAM-CAR	-3.18	1.40	1.52
3	F	302	OJN	CAM-CAR	-3.16	1.40	1.52
3	A	302	OJN	C2-N1	3.14	1.39	1.33
3	J	302	OJN	C2-N1	3.13	1.39	1.33
3	H	302	OJN	CAM-CAR	-3.12	1.40	1.52
3	B	302	OJN	CAM-CAR	-3.12	1.40	1.52
3	E	302	OJN	C2-N1	3.12	1.39	1.33
3	I	302	OJN	C5-C4	-3.07	1.34	1.43
3	G	302	OJN	C5-C4	-3.07	1.34	1.43
3	K	302	OJN	C5-C4	-3.05	1.34	1.43
3	G	302	OJN	C2-N1	3.05	1.39	1.33
3	L	302	OJN	C5-C4	-3.04	1.34	1.43
3	L	302	OJN	C2-N1	3.04	1.39	1.33
3	J	302	OJN	C5-C4	-3.02	1.35	1.43
3	I	302	OJN	CAM-CAR	-2.97	1.41	1.52
3	B	302	OJN	C5-C4	-2.91	1.35	1.43
3	H	302	OJN	C5-C4	-2.90	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	302	OJN	CAM-CAR	-2.85	1.41	1.52
3	D	302	OJN	C5-C4	-2.81	1.35	1.43
3	C	302	OJN	C2-N1	2.80	1.39	1.33
3	E	302	OJN	C5-C4	-2.73	1.35	1.43
3	D	302	OJN	CAM-CAR	-2.72	1.42	1.52
2	H	301	KAN	O5-C1	2.71	1.48	1.41
2	G	301	KAN	C14-C15	-2.63	1.50	1.53
2	A	301	KAN	O5-C1	2.56	1.48	1.41
2	C	301	KAN	C6-C5	2.55	1.55	1.52
2	I	301	KAN	O5-C1	2.52	1.48	1.41
2	A	301	KAN	C6-C5	2.50	1.55	1.52
2	E	301	KAN	O5-C1	2.32	1.47	1.41
2	L	301	KAN	O5-C1	2.25	1.47	1.41
2	F	301	KAN	O5-C1	2.23	1.47	1.41
2	J	301	KAN	C14-C15	-2.20	1.50	1.53
2	I	301	KAN	C6-C5	2.18	1.55	1.52
2	K	301	KAN	O5-C1	2.17	1.47	1.41
2	C	301	KAN	C14-C15	-2.16	1.50	1.53
2	J	301	KAN	C16-C15	-2.09	1.50	1.53
2	D	301	KAN	O5-C1	2.04	1.47	1.41

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	OJN	N3-C2-N1	-7.45	117.03	128.68
3	I	302	OJN	N3-C2-N1	-7.43	117.07	128.68
3	D	302	OJN	N3-C2-N1	-7.38	117.14	128.68
3	G	302	OJN	N3-C2-N1	-7.32	117.23	128.68
3	E	302	OJN	N3-C2-N1	-7.29	117.28	128.68
3	J	302	OJN	N3-C2-N1	-7.10	117.58	128.68
3	A	302	OJN	N3-C2-N1	-7.08	117.61	128.68
3	B	302	OJN	N3-C2-N1	-7.00	117.73	128.68
3	H	302	OJN	N3-C2-N1	-6.96	117.80	128.68
3	F	302	OJN	N3-C2-N1	-6.91	117.88	128.68
3	L	302	OJN	N3-C2-N1	-6.75	118.13	128.68
3	K	302	OJN	N3-C2-N1	-6.72	118.18	128.68
2	I	301	KAN	C6-C5-C4	-4.55	104.16	113.10
2	J	301	KAN	C6-C5-C4	-4.43	104.38	113.10
3	J	302	OJN	CAR-CAM-CAS	4.33	122.04	114.50
3	H	302	OJN	CAR-CAM-CAS	4.03	121.53	114.50
2	L	301	KAN	C6-C5-C4	-3.95	105.32	113.10
3	D	302	OJN	CAR-CAM-CAS	3.89	121.29	114.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	302	0JN	CAR-CAM-CAS	3.74	121.02	114.50
2	K	301	KAN	C6-C5-C4	-3.71	105.79	113.10
2	E	301	KAN	C6-C5-C4	-3.57	106.08	113.10
2	D	301	KAN	C13-C14-C15	3.44	115.02	110.40
2	F	301	KAN	C6-C5-C4	-3.43	106.36	113.10
2	A	301	KAN	C6-C5-C4	-3.38	106.45	113.10
3	K	302	0JN	CAR-CAM-CAS	3.37	120.37	114.50
2	J	301	KAN	O5-C5-C6	3.36	112.27	106.01
2	D	301	KAN	C6-C5-C4	-3.31	106.59	113.10
2	E	301	KAN	C13-C14-C15	3.31	114.84	110.40
2	H	301	KAN	O11-C8-C9	3.30	116.06	107.28
2	J	301	KAN	O11-C8-C9	3.30	116.05	107.28
2	H	301	KAN	C13-C14-C15	3.25	114.76	110.40
2	C	301	KAN	O11-C8-C9	3.23	115.87	107.28
2	E	301	KAN	O11-C8-C9	3.23	115.86	107.28
3	I	302	0JN	CAR-CAM-CAS	3.21	120.09	114.50
2	G	301	KAN	C6-C5-C4	-3.18	106.85	113.10
2	G	301	KAN	O11-C8-C9	3.16	115.69	107.28
3	B	302	0JN	CAR-CAM-CAS	3.15	119.99	114.50
2	L	301	KAN	O11-C8-C9	3.12	115.57	107.28
2	D	301	KAN	O11-C8-C9	3.11	115.54	107.28
3	L	302	0JN	CAR-CAM-CAS	3.10	119.90	114.50
2	F	301	KAN	C13-C14-C15	3.08	114.54	110.40
2	H	301	KAN	C6-C5-C4	-3.05	107.10	113.10
2	K	301	KAN	O11-C8-C9	3.05	115.39	107.28
2	B	301	KAN	O11-C8-C9	3.00	115.26	107.28
2	C	301	KAN	O5-C5-C6	3.00	111.59	106.01
2	A	301	KAN	O11-C8-C9	2.97	115.17	107.28
2	F	301	KAN	O11-C8-C9	2.90	114.98	107.28
3	D	302	0JN	CAM-CAR-CAH	-2.88	117.07	121.28
2	I	301	KAN	O11-C8-C9	2.83	114.81	107.28
3	B	302	0JN	CAM-CAR-CAH	-2.83	117.15	121.28
2	B	301	KAN	C6-C5-C4	-2.81	107.58	113.10
2	H	301	KAN	O5-C5-C6	2.80	111.21	106.01
2	C	301	KAN	C13-C14-C15	2.69	114.01	110.40
7	I	304	PEG	O2-C2-C1	2.68	121.83	110.07
7	A	309	PEG	O2-C2-C1	2.67	121.78	110.07
7	I	304	PEG	O2-C3-C4	2.66	121.77	110.07
3	E	302	0JN	CAM-CAR-CAH	-2.66	117.41	121.28
2	D	301	KAN	O12-C17-C18	2.65	113.01	106.44
7	J	308	PEG	O2-C2-C1	2.60	121.49	110.07
2	A	301	KAN	C18-C17-C16	-2.59	106.95	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	309	PEG	O2-C2-C1	2.57	121.38	110.07
2	G	301	KAN	C14-C15-N4	-2.54	105.85	111.05
3	A	302	0JN	C5-C6-NAD	-2.53	118.10	122.67
7	J	308	PEG	O2-C3-C4	2.52	121.12	110.07
2	F	301	KAN	C13-O12-C17	2.51	118.62	113.69
2	E	301	KAN	O12-C17-C18	2.51	112.67	106.44
3	F	302	0JN	C5-C6-NAD	-2.51	118.15	122.67
2	E	301	KAN	C1-O9-C10	-2.48	111.82	117.96
7	J	307	PEG	O2-C3-C4	2.47	120.94	110.07
2	C	301	KAN	C6-C5-C4	-2.47	108.24	113.10
2	G	301	KAN	O5-C5-C6	2.47	110.60	106.01
2	D	301	KAN	O5-C5-C6	2.46	110.59	106.01
7	J	307	PEG	O2-C2-C1	2.42	120.69	110.07
3	G	302	0JN	C5-C6-NAD	-2.41	118.32	122.67
2	I	301	KAN	O12-C17-C18	2.38	112.36	106.44
2	I	301	KAN	C13-C14-C15	2.35	113.56	110.40
2	K	301	KAN	C13-C14-C15	2.31	113.50	110.40
3	C	302	0JN	CAR-CAM-CAS	2.31	118.52	114.50
3	J	302	0JN	C5-C6-NAD	-2.30	118.51	122.67
2	C	301	KAN	C1-O9-C10	-2.29	112.30	117.96
2	I	301	KAN	O5-C5-C6	2.26	110.22	106.01
7	B	304	PEG	O2-C3-C4	2.24	119.90	110.07
3	G	302	0JN	CAJ-CAT-CAI	-2.21	118.01	123.19
3	H	302	0JN	CAM-CAR-CAH	-2.21	118.06	121.28
7	B	304	PEG	O2-C2-C1	2.20	119.72	110.07
2	G	301	KAN	C1-O9-C10	-2.17	112.59	117.96
7	A	309	PEG	O2-C3-C4	2.16	119.58	110.07
2	A	301	KAN	C13-C14-C15	2.16	113.30	110.40
2	K	301	KAN	C1-O9-C10	-2.14	112.67	117.96
2	B	301	KAN	O13-C14-C15	2.13	114.05	110.22
2	B	301	KAN	C1-O9-C10	-2.12	112.71	117.96
2	L	301	KAN	C16-C15-C14	-2.12	106.46	111.06
3	F	302	0JN	CAR-CAM-CAS	2.10	118.16	114.50
2	E	301	KAN	O12-C13-C14	-2.09	105.92	110.35
7	J	309	PEG	O2-C3-C4	2.09	119.26	110.07
2	L	301	KAN	C13-C14-C15	2.08	113.20	110.40
2	I	301	KAN	C1-O9-C10	-2.08	112.82	117.96
2	K	301	KAN	C16-C15-C14	-2.07	106.56	111.06
2	D	301	KAN	O12-C13-C14	-2.07	105.96	110.35
2	J	301	KAN	C13-C14-C15	2.06	113.17	110.40
2	F	301	KAN	C1-O9-C10	-2.05	112.88	117.96
2	I	301	KAN	O14-C16-C15	-2.05	106.53	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	302	0JN	C5-C6-NAD	-2.05	118.98	122.67
2	C	301	KAN	O14-C16-C15	-2.04	106.56	110.22
3	D	302	0JN	CAJ-CAT-CAI	-2.02	118.48	123.19
2	C	301	KAN	C16-C15-N4	-2.01	106.93	111.05
2	E	301	KAN	C16-C15-C14	-2.01	106.69	111.06

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	J	307	PEG	C1-C2-O2-C3
7	J	309	PEG	C1-C2-O2-C3
7	A	309	PEG	C1-C2-O2-C3
7	B	304	PEG	O2-C3-C4-O4
7	B	304	PEG	O1-C1-C2-O2
2	A	301	KAN	C9-C8-O11-C13
2	H	301	KAN	C9-C8-O11-C13
3	K	302	0JN	CAR-CAM-CAS-NAP
3	J	302	0JN	CAR-CAM-CAS-NAP
3	C	302	0JN	CAR-CAM-CAS-NAP
2	J	301	KAN	C9-C8-O11-C13
2	E	301	KAN	C9-C8-O11-C13
2	K	301	KAN	C9-C8-O11-C13
2	D	301	KAN	C9-C10-O9-C1
2	L	301	KAN	C9-C8-O11-C13
2	F	301	KAN	C9-C8-O11-C13
3	C	302	0JN	CAR-CAM-CAS-C5
2	D	301	KAN	C9-C8-O11-C13
2	C	301	KAN	C9-C8-O11-C13
2	C	301	KAN	C9-C10-O9-C1
2	H	301	KAN	C9-C10-O9-C1
2	I	301	KAN	C9-C8-O11-C13
2	B	301	KAN	C9-C10-O9-C1
2	B	301	KAN	C9-C8-O11-C13
2	L	301	KAN	C9-C10-O9-C1

There are no ring outliers.

14 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	302	0JN	1	0

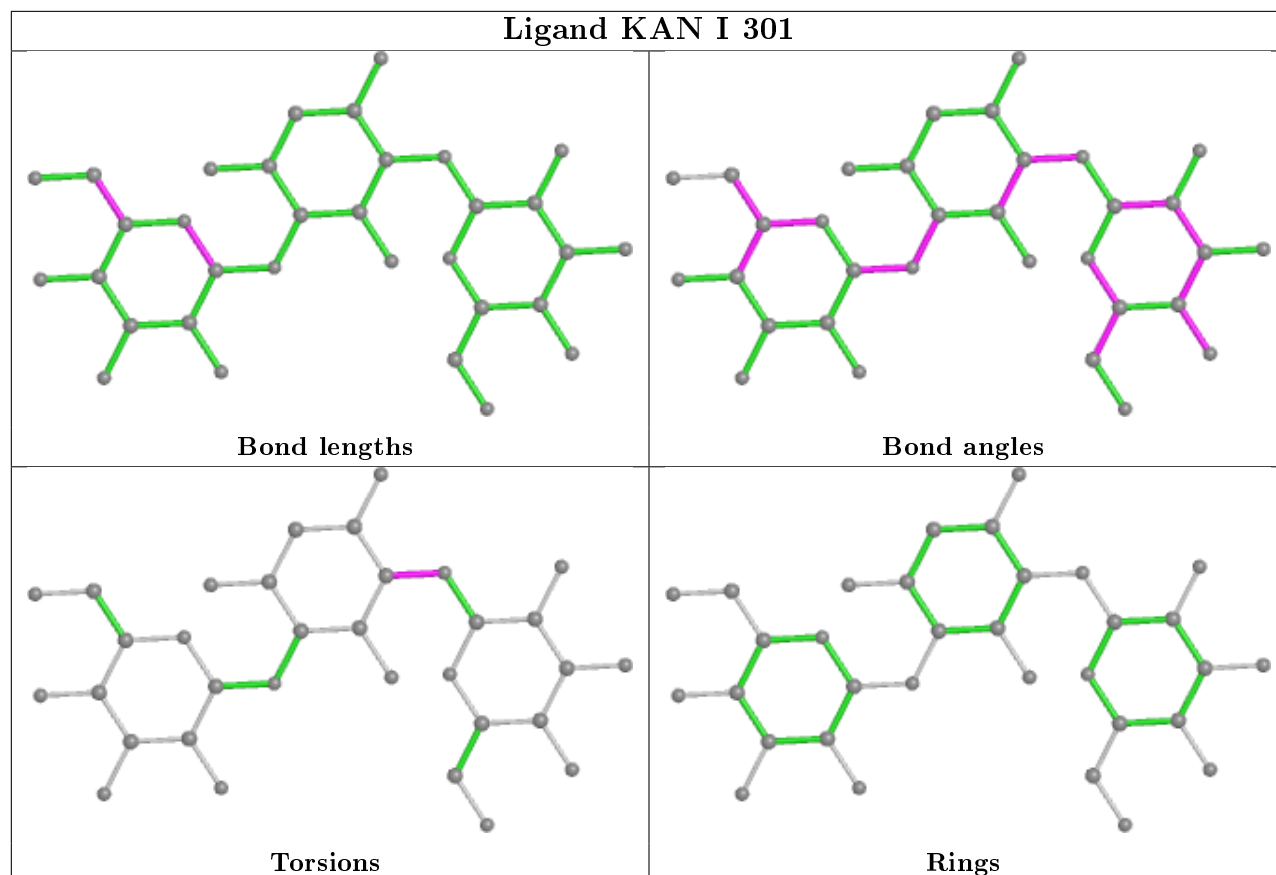
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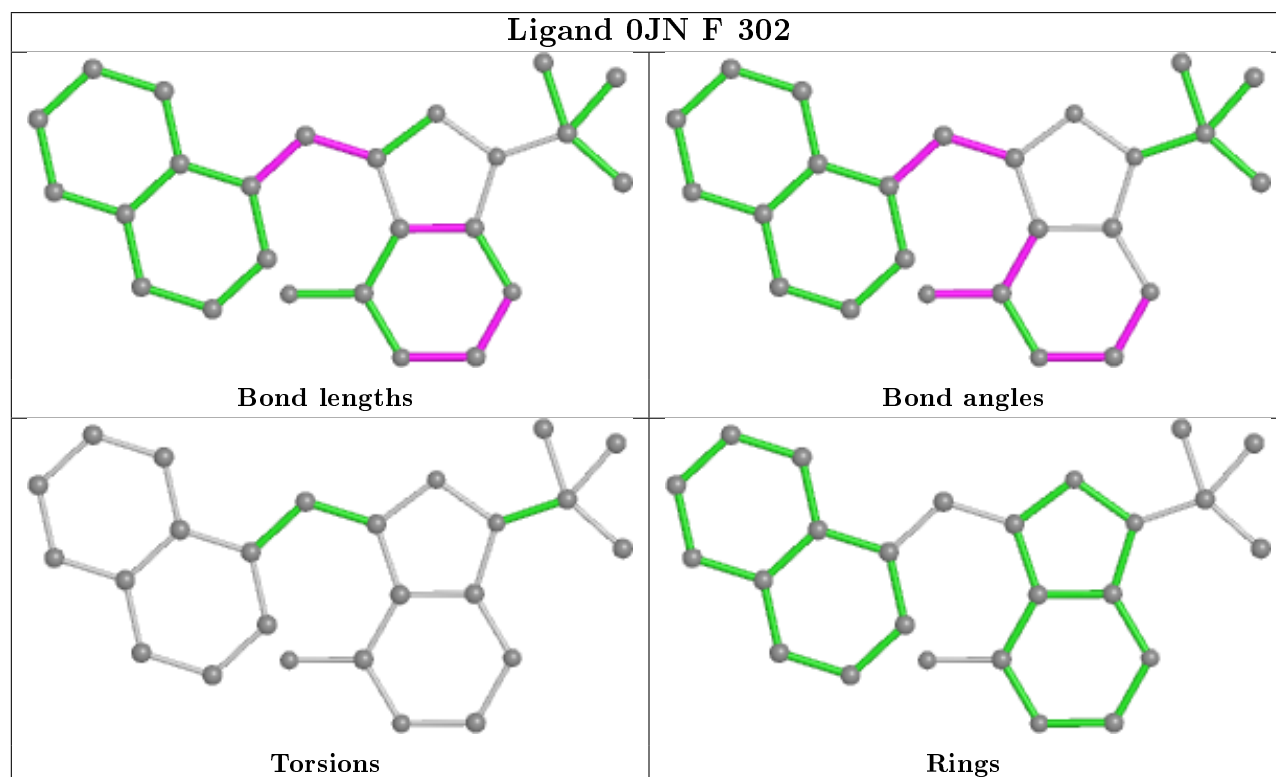
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	OJN	3	0
2	C	301	KAN	1	0
7	J	309	PEG	2	0
7	J	307	PEG	3	0
3	K	302	OJN	1	0
6	H	305	ACT	2	0
3	G	302	OJN	6	0
6	G	306	ACT	1	0
3	L	302	OJN	1	0
3	J	302	OJN	2	0
3	E	302	OJN	1	0
3	C	302	OJN	2	0
6	C	308	ACT	1	0

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 than 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.

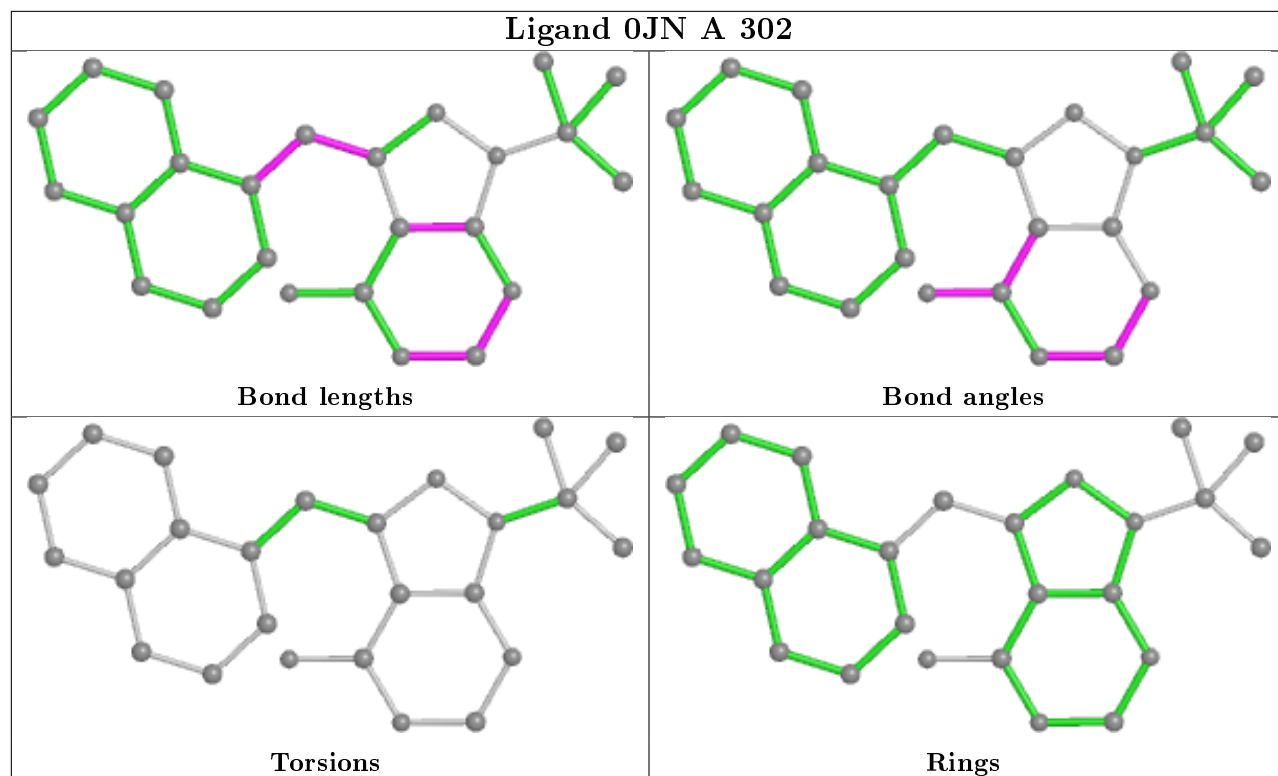
Ligand KAN I 301



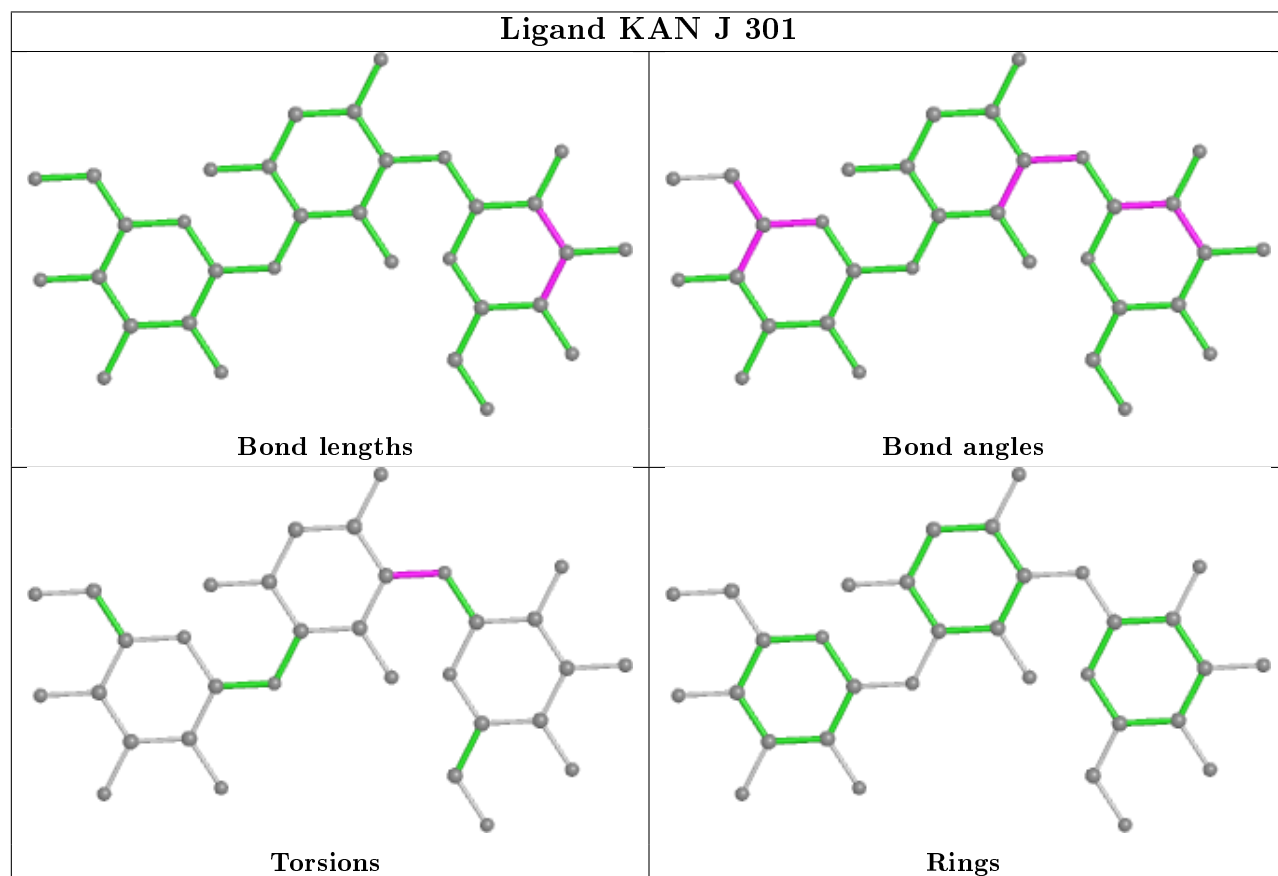
Ligand 0JN F 302

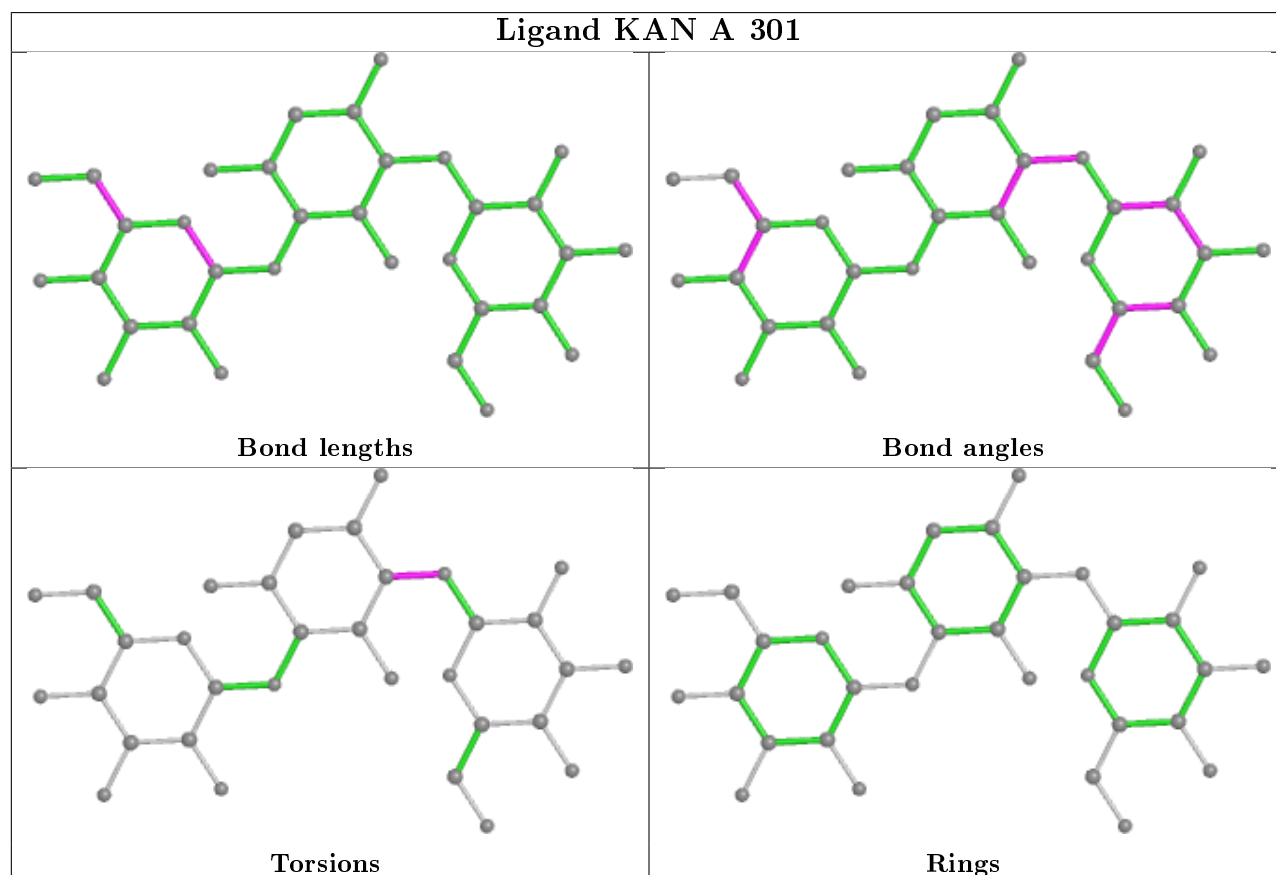
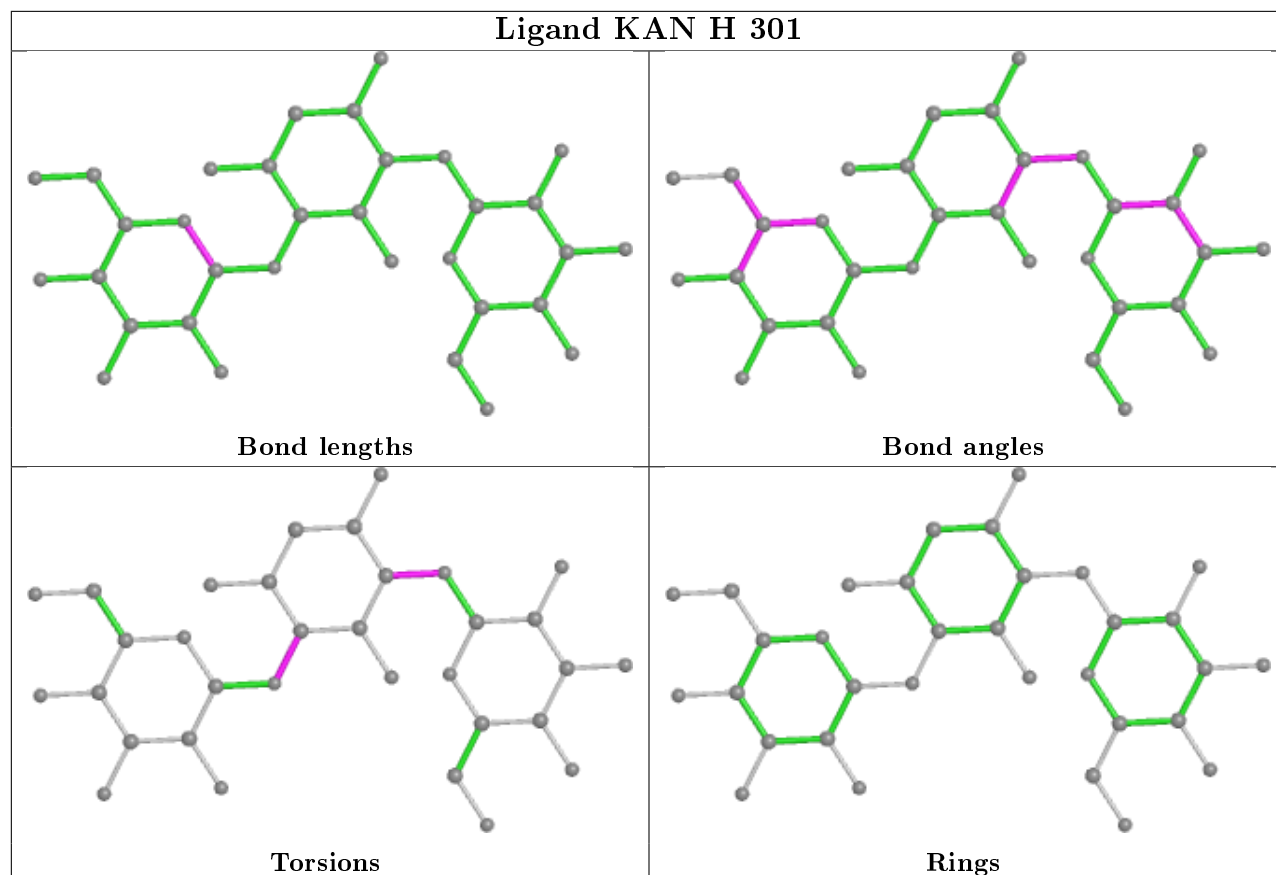


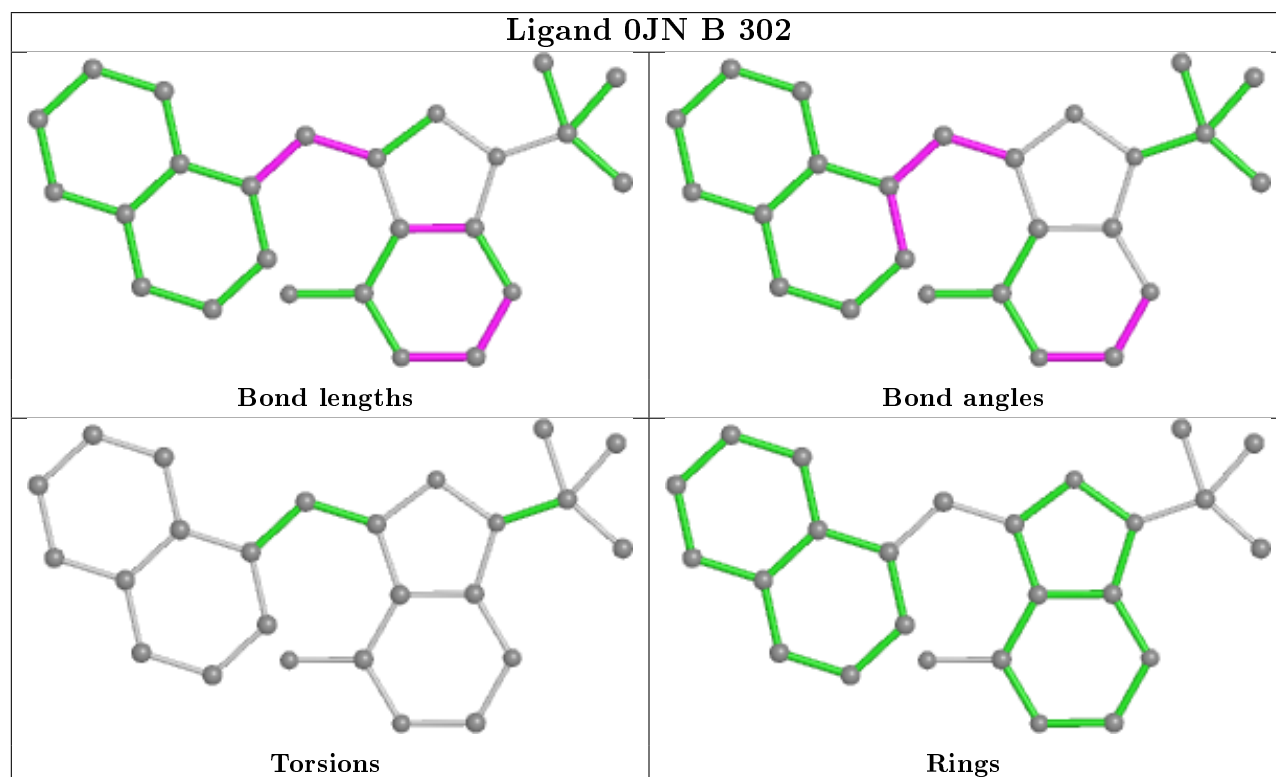
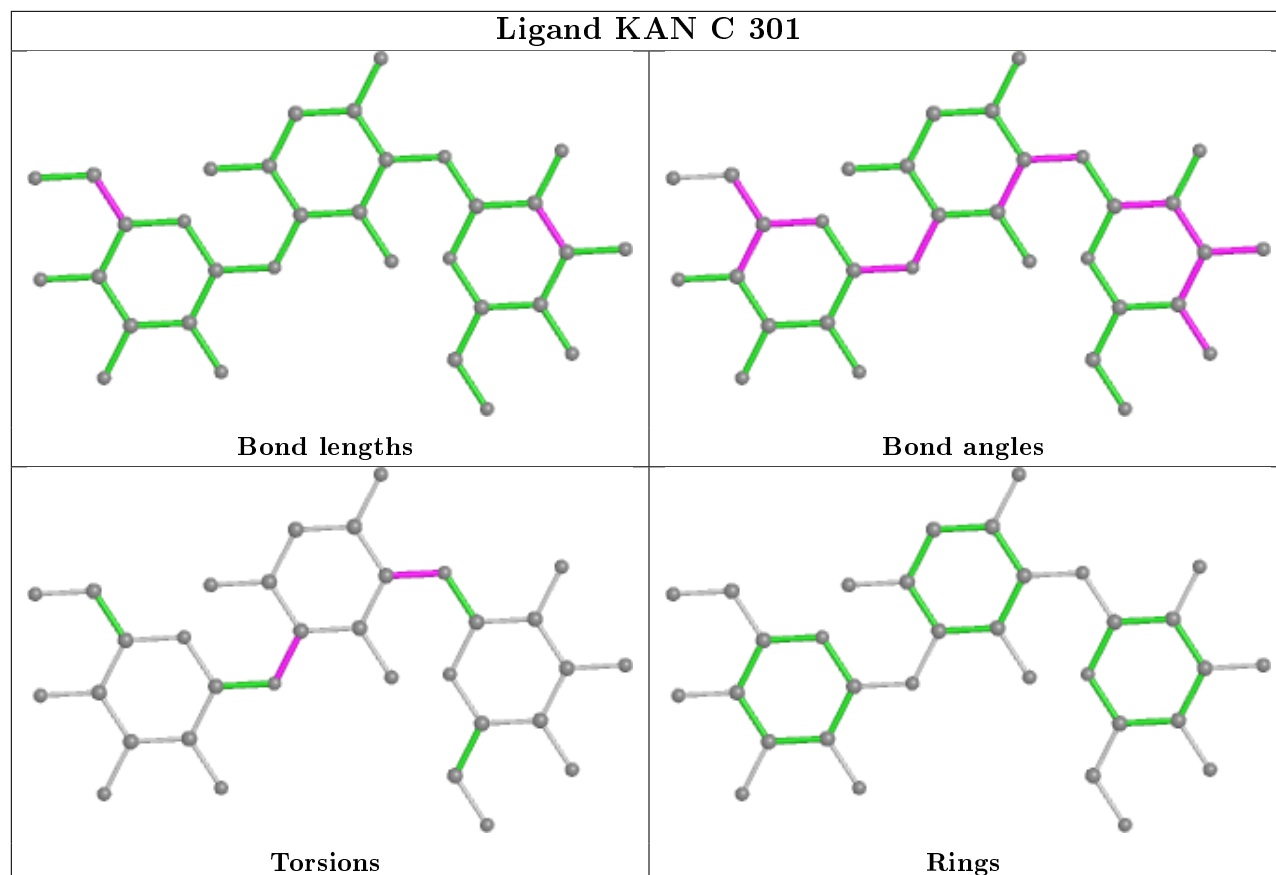
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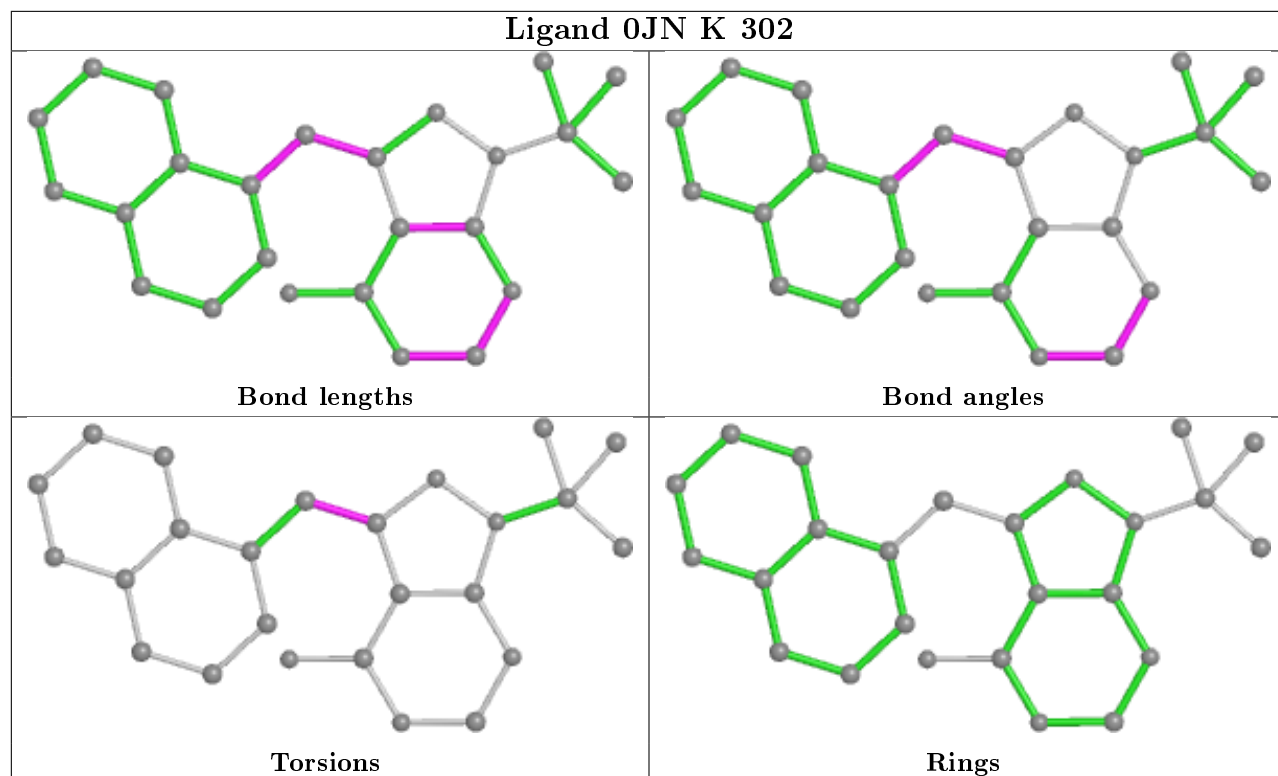
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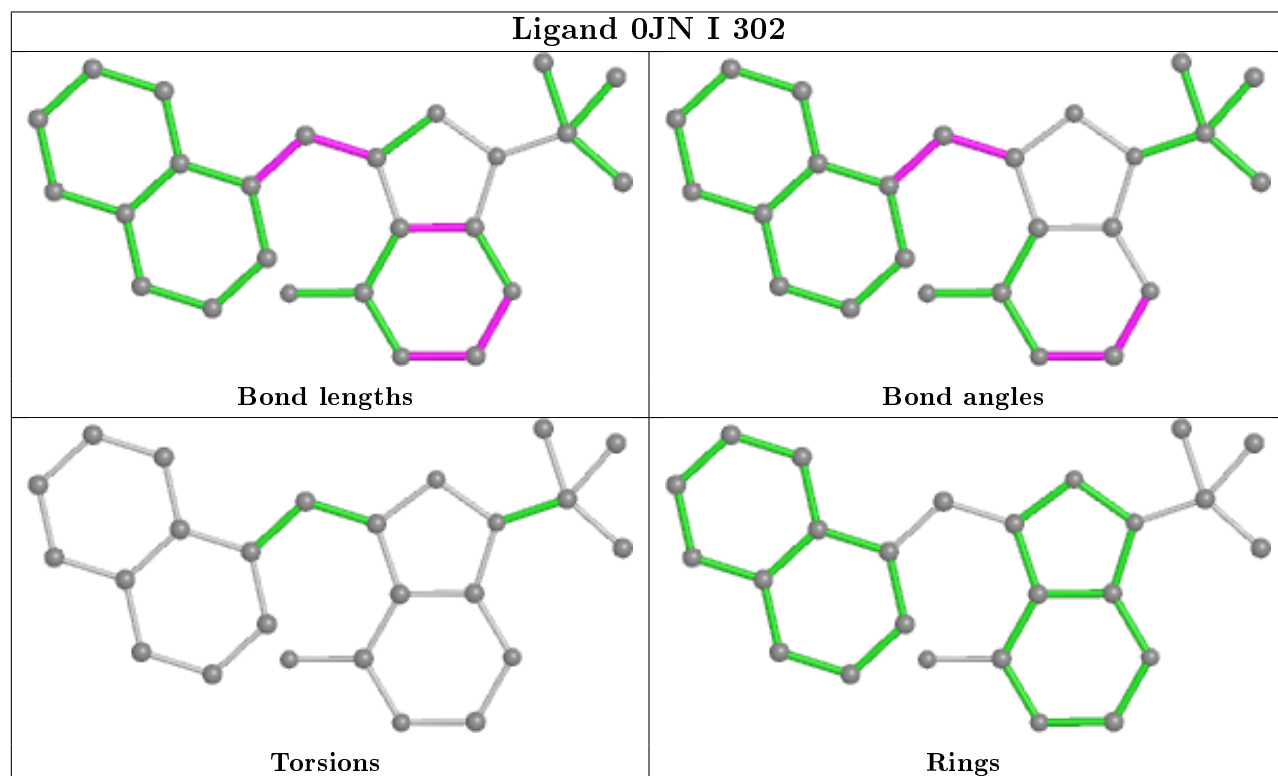




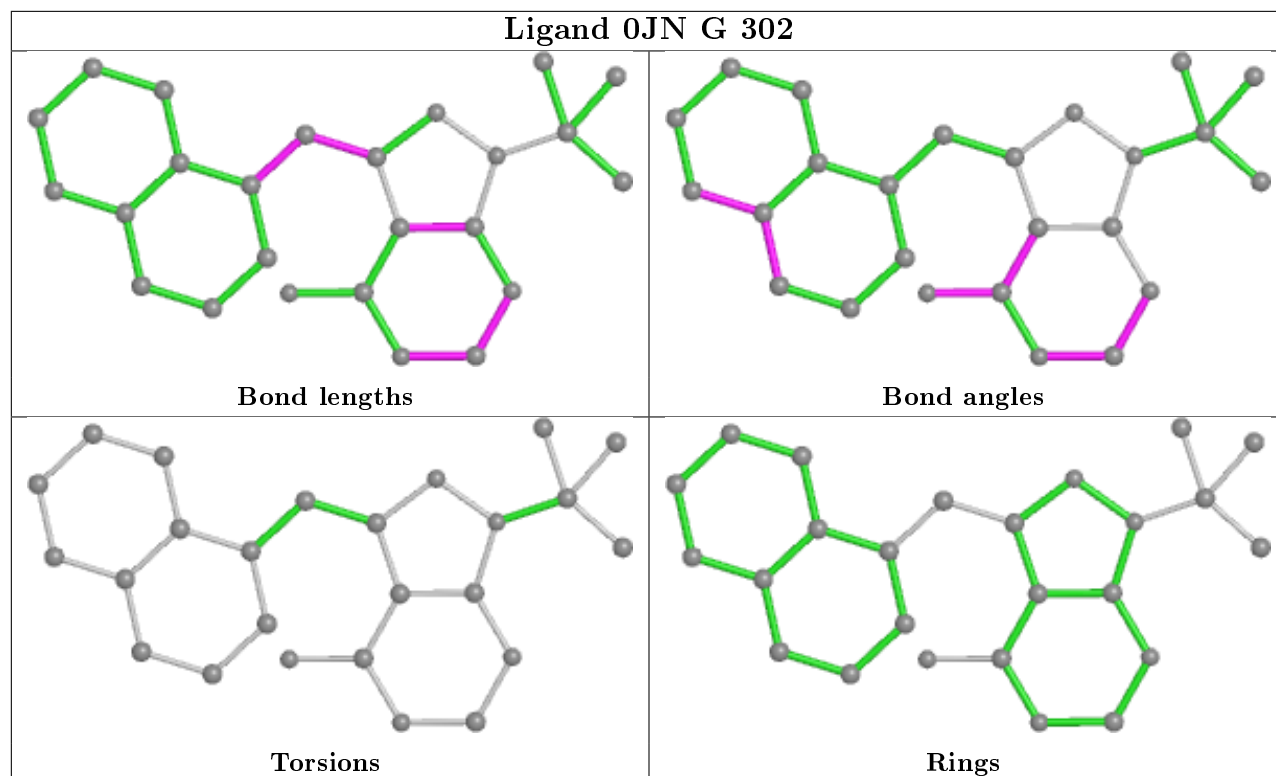
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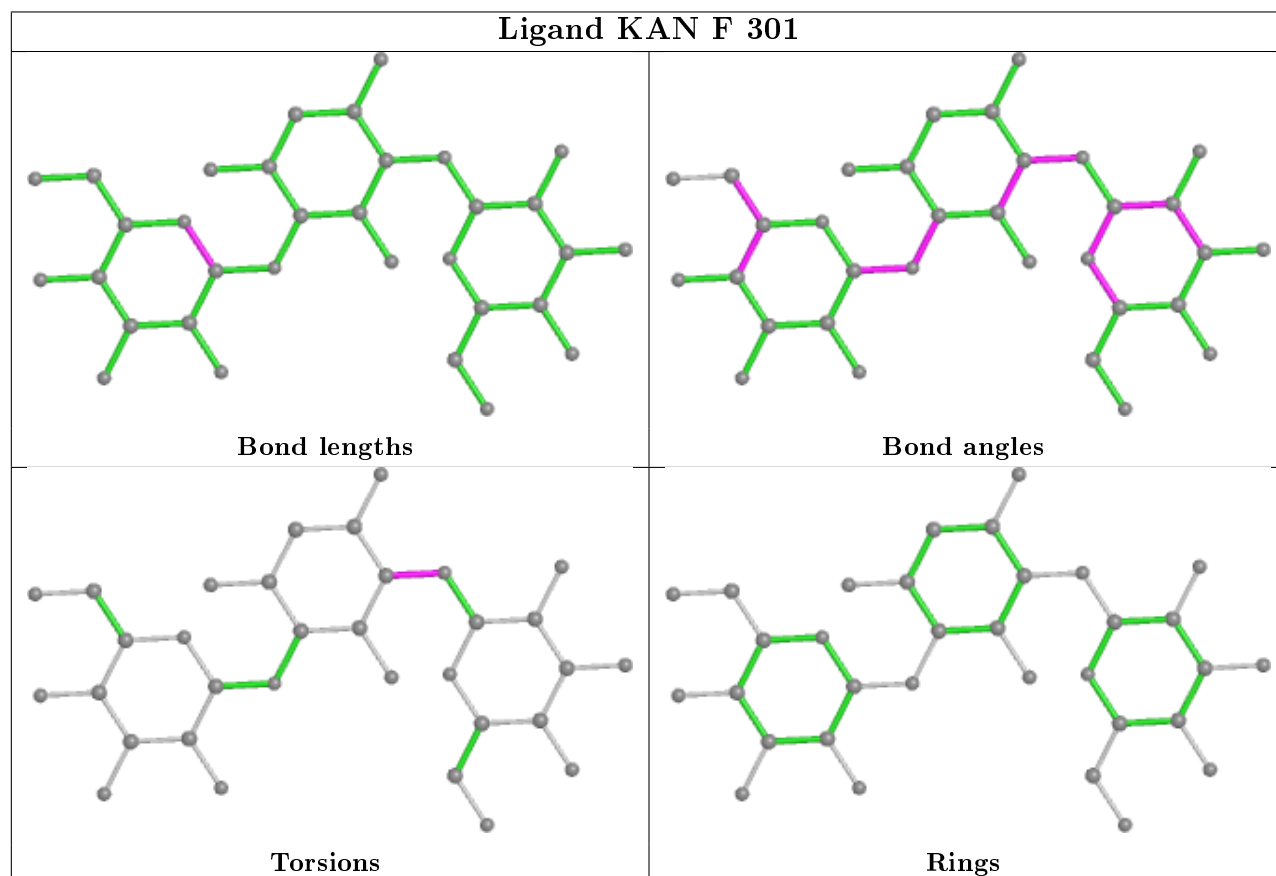
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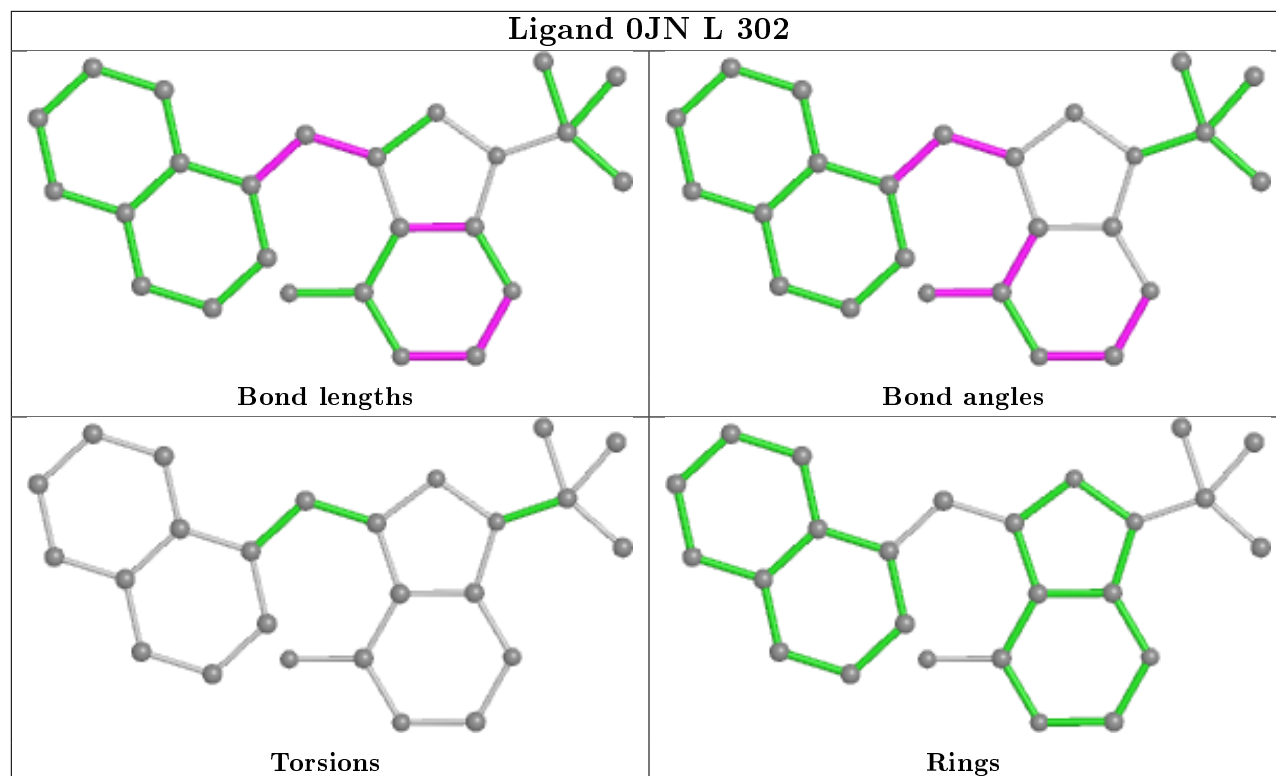
Ligand 0JN G 302



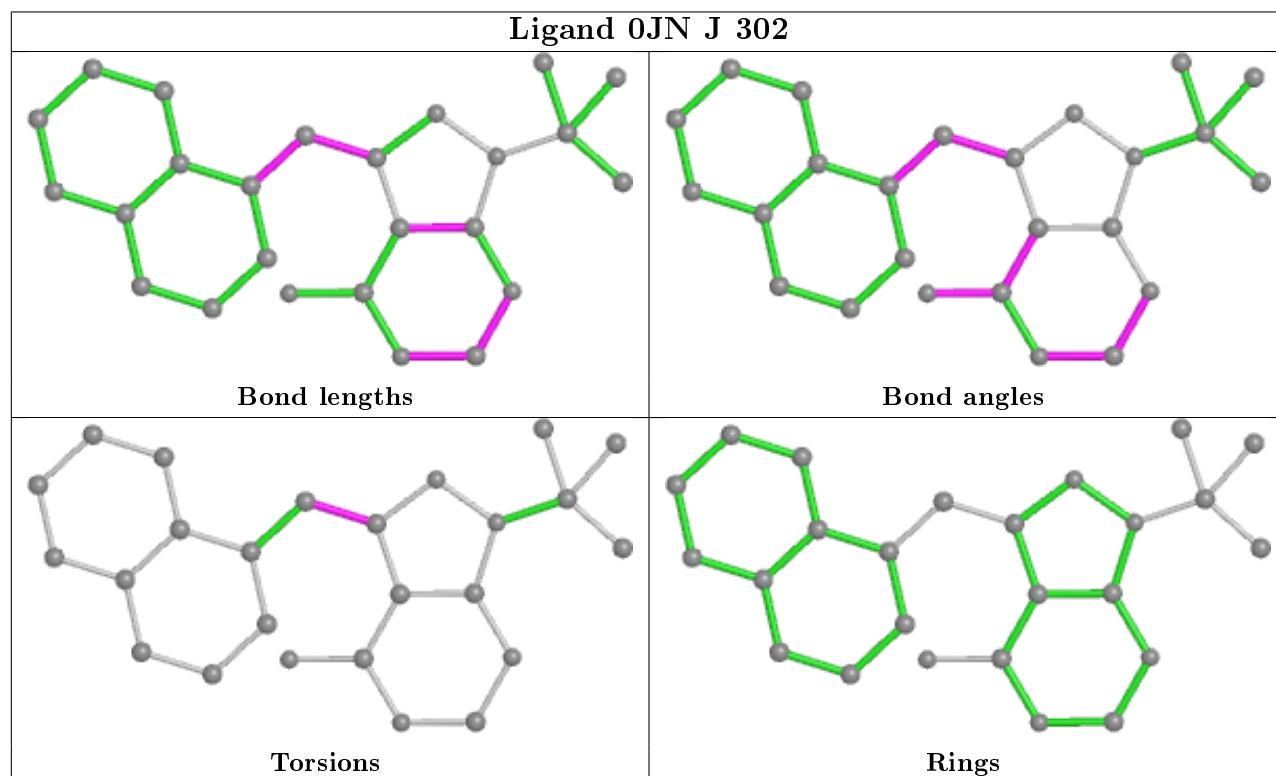
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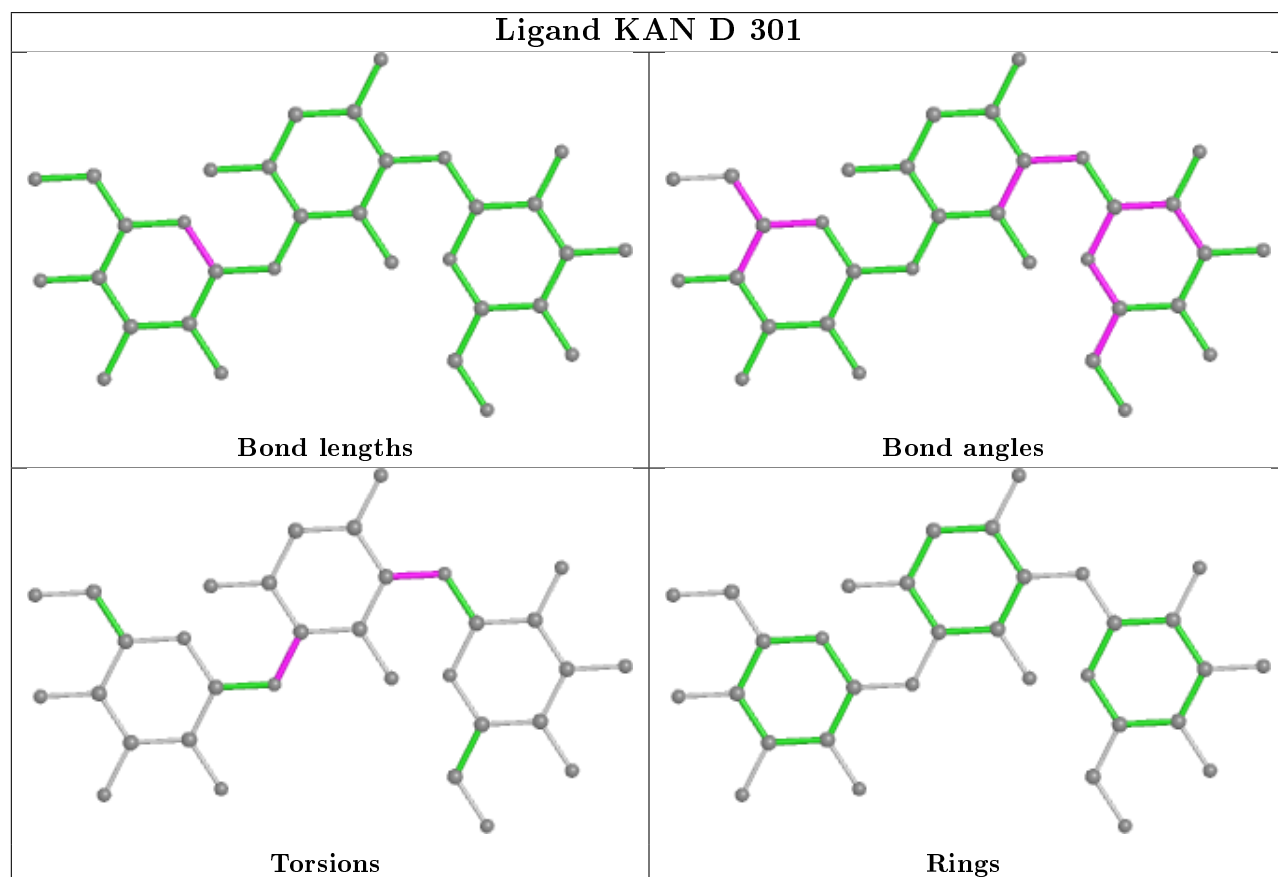
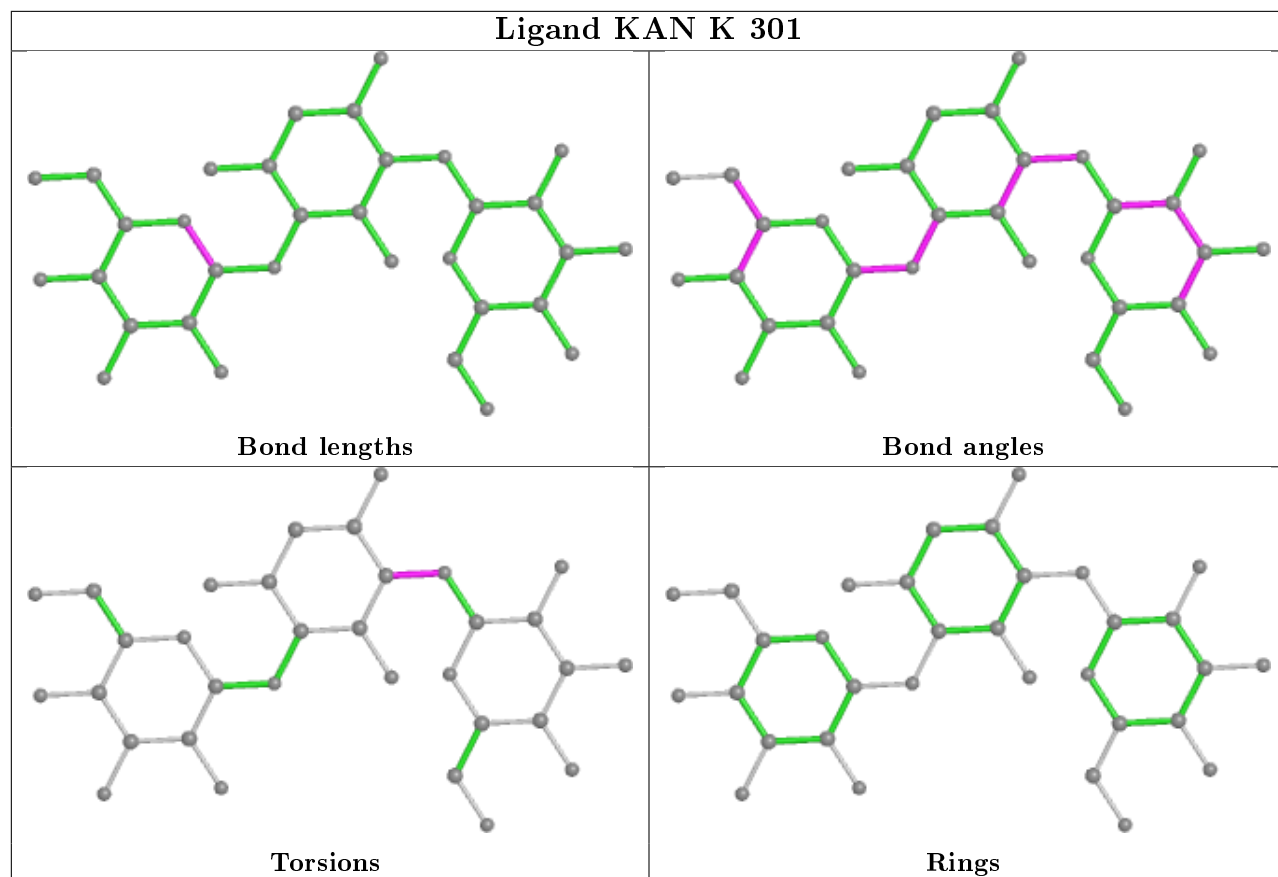


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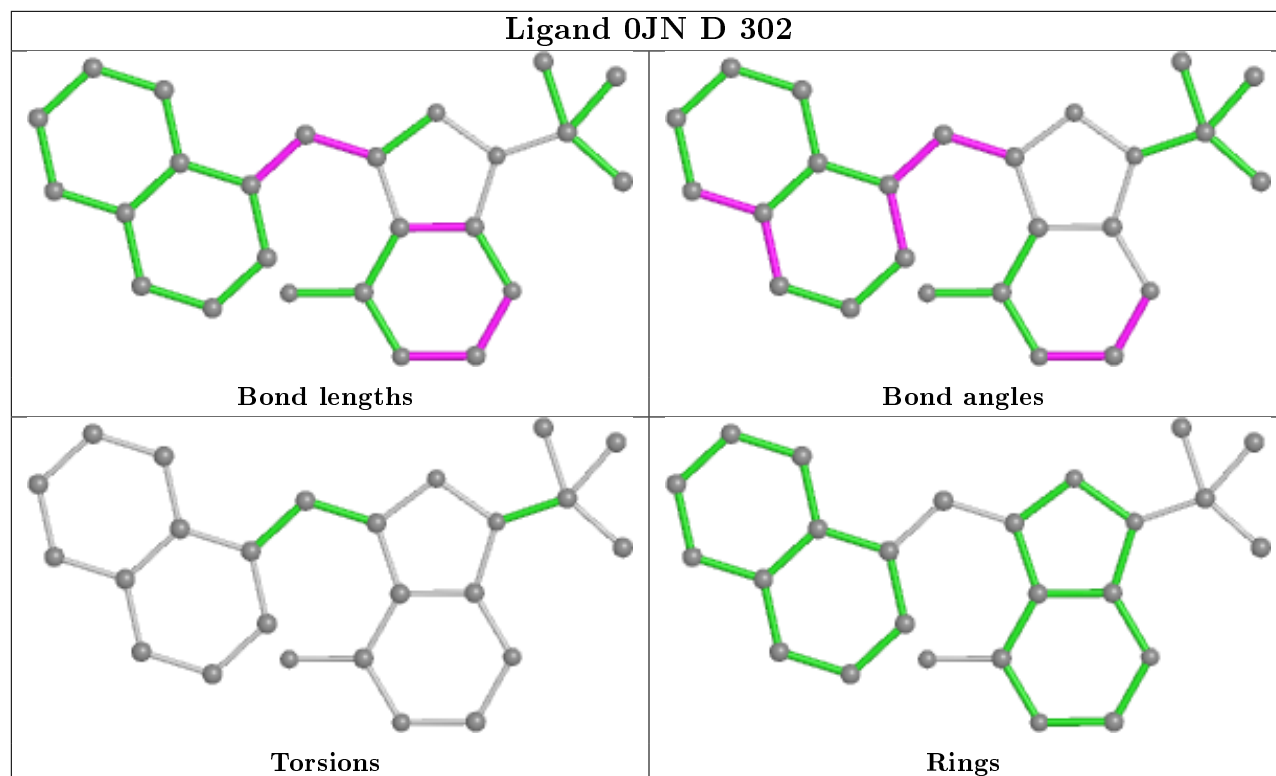


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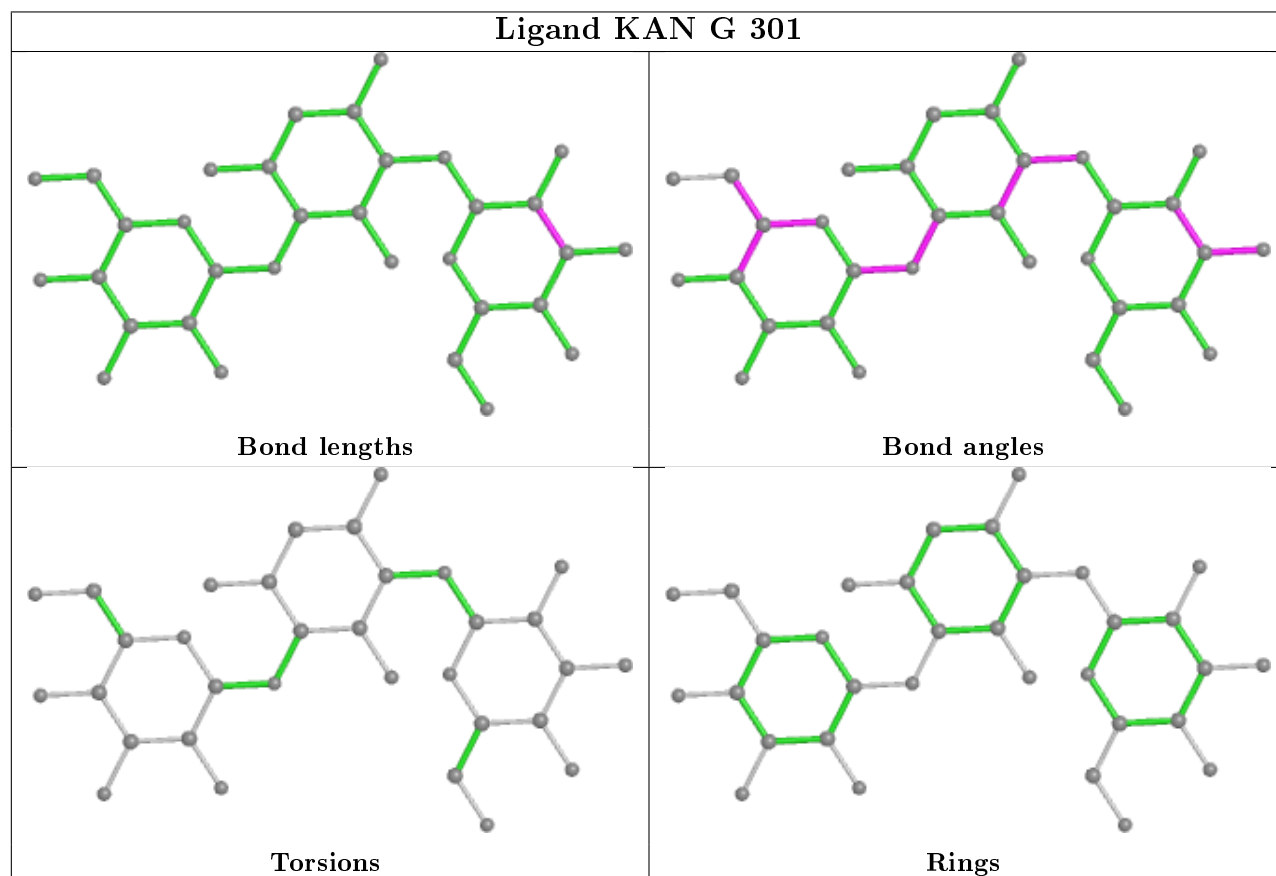


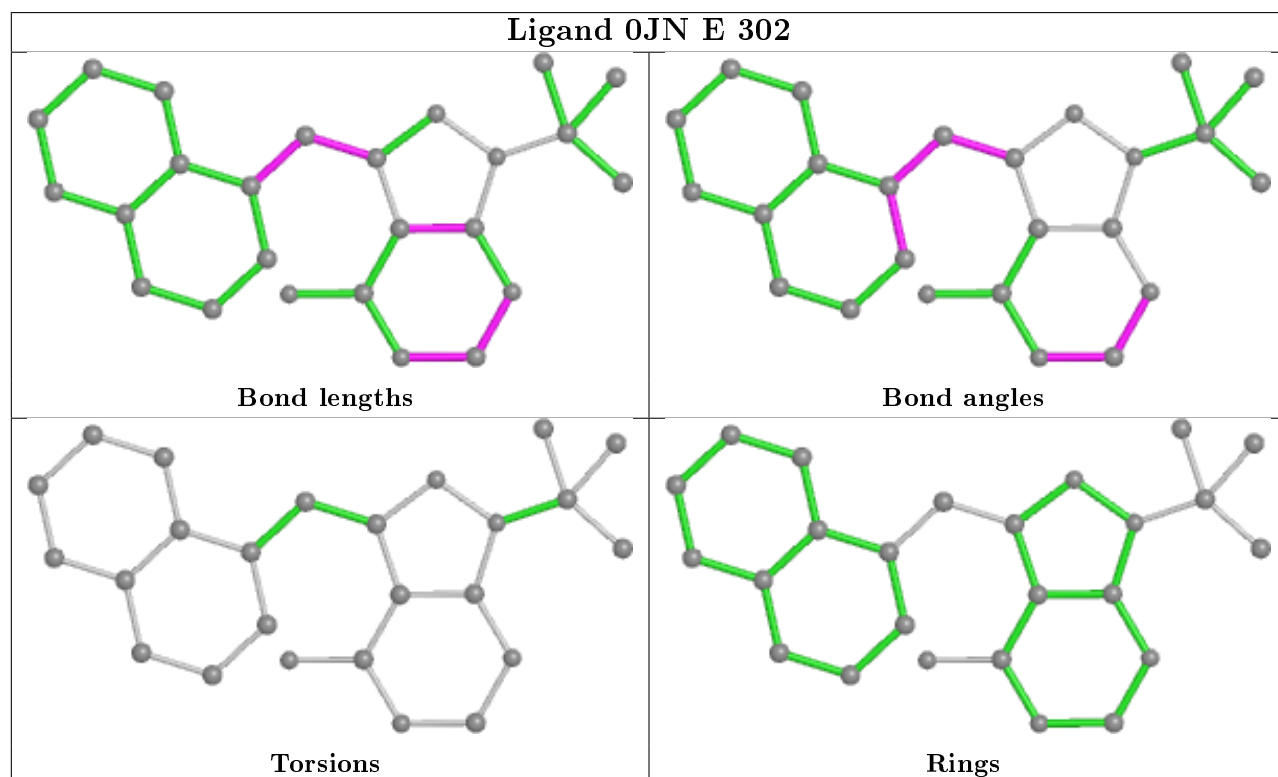
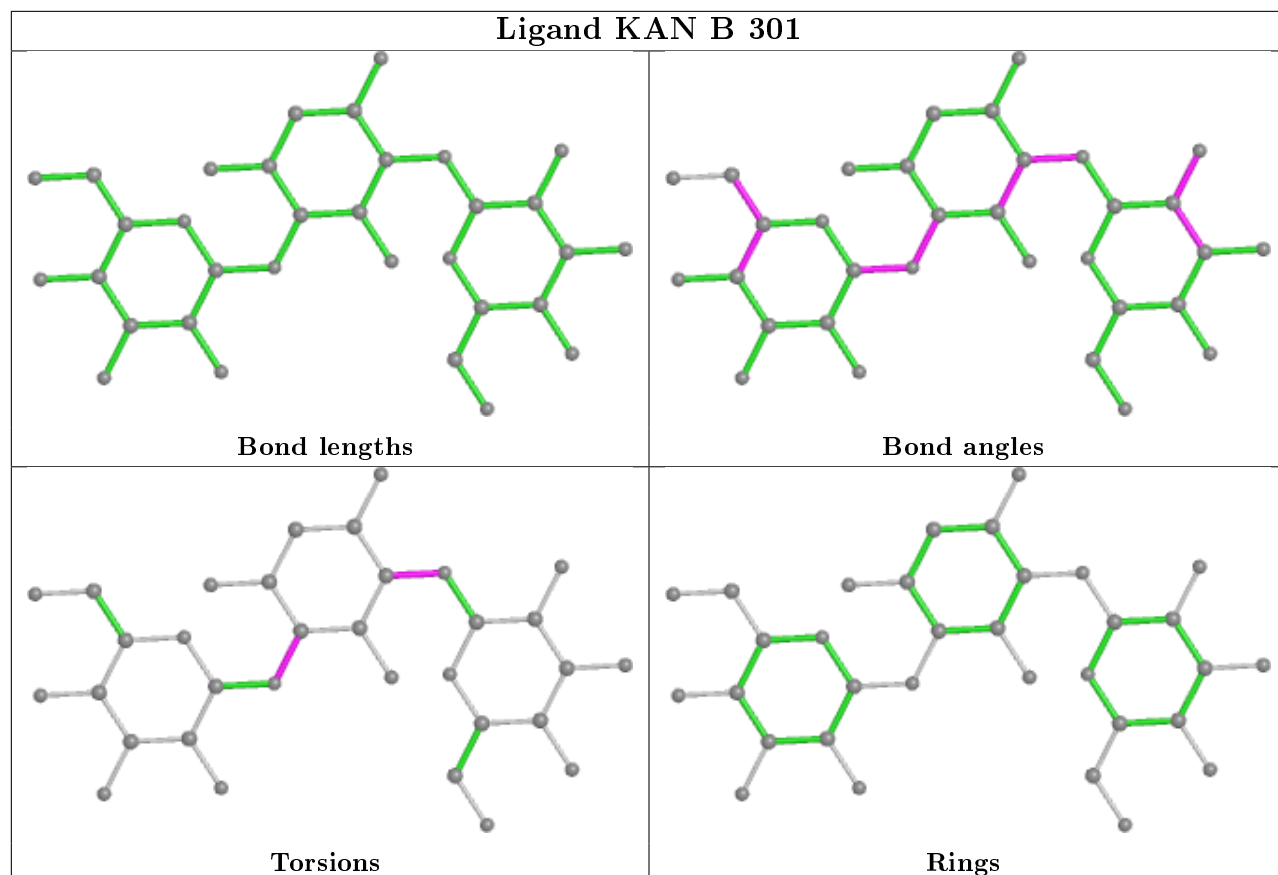


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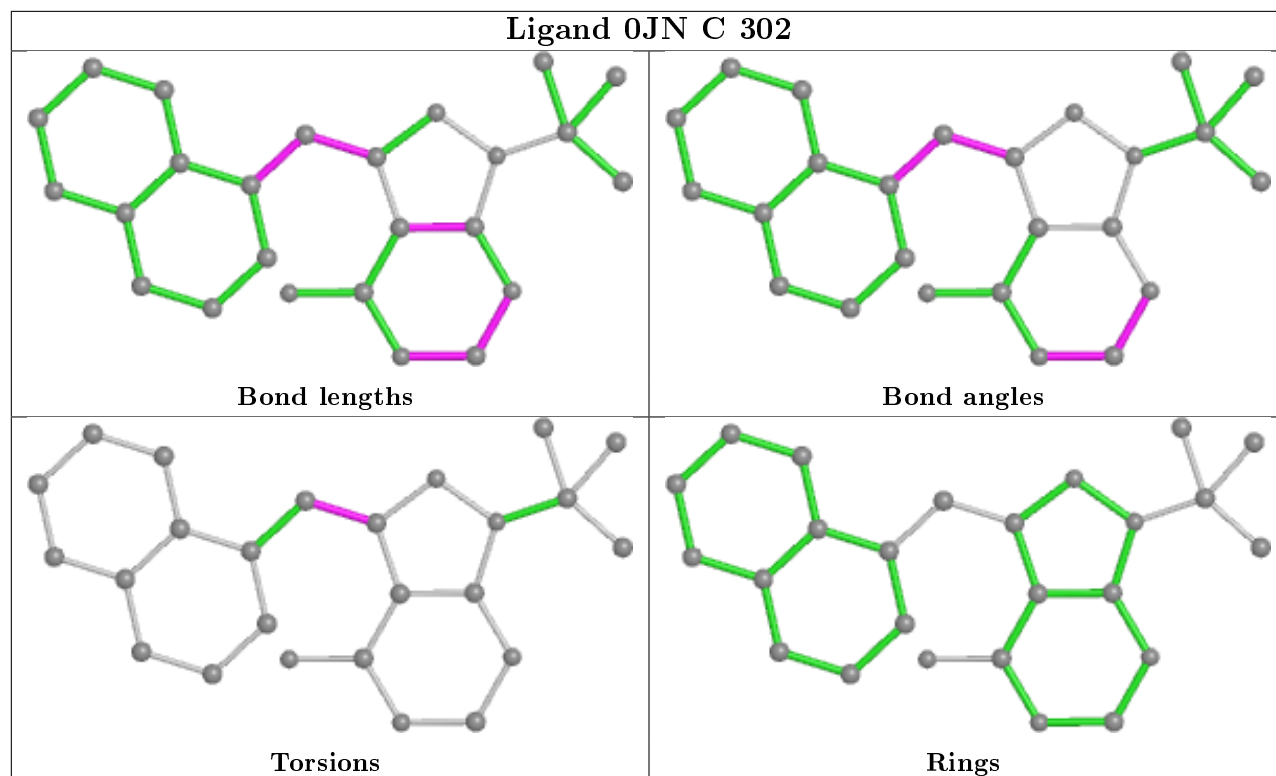


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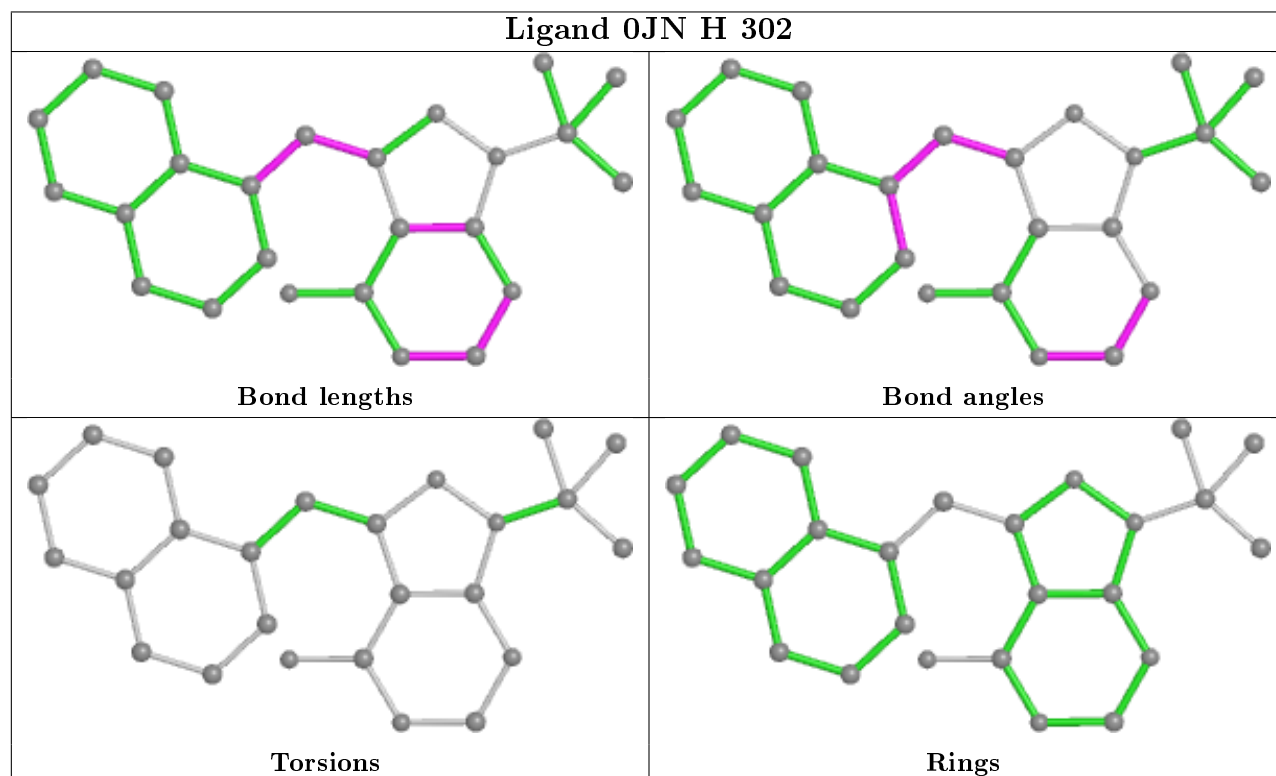


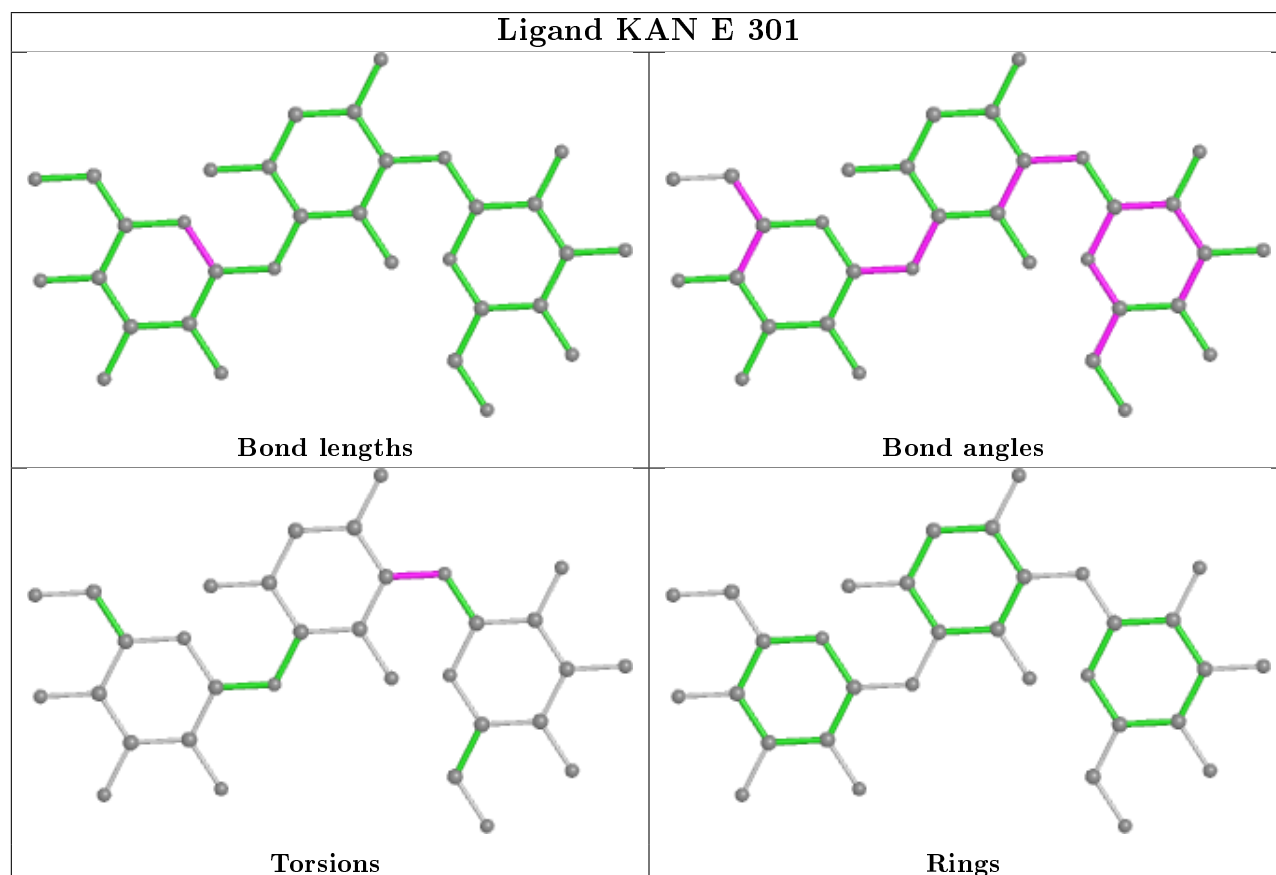
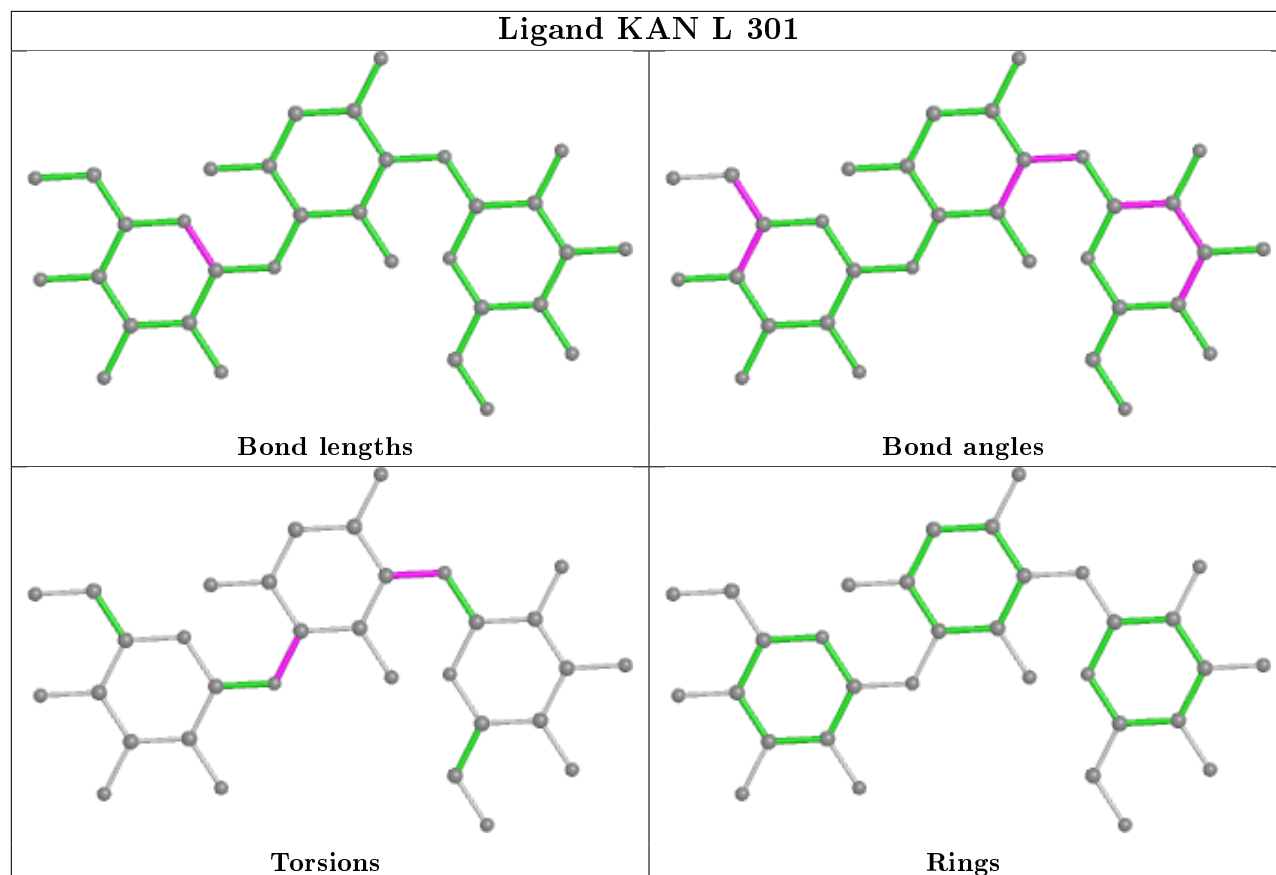


Ligand 0JN C 302



Ligand 0JN H 302





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	265/272 (97%)	-0.29	13 (4%) 29 31	19, 30, 86, 133	0
1	B	251/272 (92%)	-0.52	4 (1%) 72 74	18, 27, 55, 112	0
1	C	265/272 (97%)	-0.21	17 (6%) 19 20	19, 33, 95, 146	0
1	D	248/272 (91%)	-0.49	2 (0%) 86 87	19, 29, 55, 68	0
1	E	260/272 (95%)	-0.42	5 (1%) 66 68	17, 27, 79, 143	0
1	F	255/272 (93%)	-0.26	9 (3%) 44 45	22, 37, 83, 128	0
1	G	265/272 (97%)	-0.18	18 (6%) 17 18	17, 31, 90, 146	0
1	H	249/272 (91%)	-0.52	2 (0%) 86 87	17, 28, 56, 109	0
1	I	248/272 (91%)	-0.55	2 (0%) 86 87	17, 27, 53, 96	0
1	J	265/272 (97%)	-0.26	12 (4%) 33 34	20, 32, 92, 124	0
1	K	264/272 (97%)	-0.04	17 (6%) 19 20	22, 45, 94, 126	0
1	L	259/272 (95%)	-0.48	5 (1%) 66 68	17, 29, 70, 119	0
All	All	3094/3264 (94%)	-0.35	106 (3%) 45 46	17, 31, 80, 146	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	24	TYR	8.5
1	G	24	TYR	8.1
1	K	4	ILE	7.6
1	K	33	VAL	7.1
1	E	16	ASN	6.9
1	K	2	SER	6.8
1	C	24	TYR	6.4
1	G	22	ASP	5.9
1	C	19	LEU	5.9
1	C	35	GLN	5.8
1	G	35	GLN	5.8

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Mol	Chain	Res	Type	RSRZ
1	C	33	VAL	5.7
1	C	21	ALA	5.5
1	A	0	GLY	5.5
1	J	24	TYR	5.5
1	K	36	SER	5.2
1	A	24	TYR	5.2
1	G	45	GLY	5.1
1	A	32	ASN	5.0
1	J	19	LEU	4.9
1	J	0	GLY	4.9
1	J	33	VAL	4.7
1	G	17	SER	4.6
1	G	16	ASN	4.6
1	G	33	VAL	4.5
1	H	17	SER	4.5
1	J	36	SER	4.5
1	J	32	ASN	4.4
1	K	16	ASN	4.4
1	K	34	GLY	4.3
1	K	35	GLN	4.3
1	A	23	LEU	4.2
1	F	6	ARG	4.2
1	B	17	SER	4.2
1	C	44	TYR	4.1
1	G	19	LEU	4.1
1	F	14	ARG	4.0
1	C	16	ASN	4.0
1	K	17	SER	3.9
1	B	16	ASN	3.9
1	F	4	ILE	3.9
1	J	35	GLN	3.8
1	G	44	TYR	3.8
1	A	35	GLN	3.8
1	F	3	HIS	3.8
1	A	19	LEU	3.8
1	J	16	ASN	3.7
1	A	36	SER	3.7
1	C	36	SER	3.7
1	J	23	LEU	3.6
1	A	34	GLY	3.5
1	G	32	ASN	3.5
1	F	48	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	36	SER	3.4
1	K	3	HIS	3.2
1	B	15	LEU	3.1
1	G	36	SER	3.1
1	J	31	ASP	3.1
1	G	28	TRP	3.0
1	C	30	ARG	2.9
1	E	15	LEU	2.9
1	D	157	ASN	2.9
1	F	5	GLN	2.9
1	G	31	ASP	2.8
1	K	18	ASN	2.8
1	K	14	ARG	2.7
1	A	18	ASN	2.7
1	C	28	TRP	2.7
1	C	25	GLY	2.6
1	E	17	SER	2.6
1	F	9	SER	2.5
1	E	10	CYS	2.5
1	A	28	TRP	2.5
1	B	186	LEU	2.5
1	C	0	GLY	2.4
1	G	21	ALA	2.4
1	L	14	ARG	2.4
1	L	8	THR	2.4
1	C	48	ASN	2.4
1	C	32	ASN	2.4
1	D	36	SER	2.4
1	L	19	LEU	2.4
1	K	32	ASN	2.4
1	C	20	ASP	2.3
1	K	19	LEU	2.3
1	K	49	ALA	2.3
1	G	20	ASP	2.3
1	G	18	ASN	2.3
1	I	36	SER	2.3
1	A	20	ASP	2.2
1	F	49	ALA	2.2
1	L	33	VAL	2.2
1	C	27	ARG	2.2
1	A	17	SER	2.2
1	J	18	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	16	ASN	2.2
1	A	31	ASP	2.2
1	I	19	LEU	2.2
1	K	24	TYR	2.2
1	K	22	ASP	2.1
1	G	15	LEU	2.1
1	K	5	GLN	2.1
1	C	37	GLY	2.1
1	E	14	ARG	2.0
1	G	14	ARG	2.0
1	J	34	GLY	2.0

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
3	0JN	C	302	25/25	0.54	0.45	83,86,94,94	25
3	0JN	G	302	25/25	0.62	0.46	76,81,90,90	25
3	0JN	A	302	25/25	0.66	0.34	77,82,87,87	25
4	NA	K	303	1/1	0.68	0.20	56,56,56,56	1
6	ACT	I	303	4/4	0.71	0.20	36,58,82,117	0
7	PEG	J	309	7/7	0.72	0.23	45,61,173,174	0
6	ACT	A	307	4/4	0.73	0.15	41,61,64,139	0
3	0JN	J	302	25/25	0.76	0.29	49,56,65,66	25
6	ACT	L	304	4/4	0.78	0.11	36,52,52,112	0
6	ACT	D	304	4/4	0.82	0.13	41,60,62,83	0
4	NA	H	303	1/1	0.82	0.17	48,48,48,48	0
6	ACT	E	307	4/4	0.83	0.14	45,56,66,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	ACT	J	306	4/4	0.83	0.16	34,71,73,138	0
6	ACT	E	304	4/4	0.84	0.19	65,69,77,77	0
6	ACT	H	304	4/4	0.85	0.11	47,51,55,138	0
7	PEG	B	304	7/7	0.86	0.15	39,55,125,135	0
6	ACT	C	308	4/4	0.86	0.10	53,58,73,91	0
6	ACT	L	306	4/4	0.87	0.13	65,67,75,121	0
7	PEG	J	308	7/7	0.88	0.18	43,62,105,124	0
3	0JN	K	302	25/25	0.88	0.15	39,44,56,58	25
6	ACT	E	306	4/4	0.88	0.20	48,60,81,92	0
4	NA	F	303	1/1	0.89	0.17	53,53,53,53	0
6	ACT	B	303	4/4	0.89	0.15	45,54,60,76	0
6	ACT	H	306	4/4	0.90	0.13	54,57,60,80	0
7	PEG	A	309	7/7	0.91	0.11	41,64,81,109	0
6	ACT	E	308	4/4	0.92	0.13	41,49,65,73	0
4	NA	A	303	1/1	0.92	0.09	31,31,31,31	1
7	PEG	I	304	7/7	0.92	0.12	45,62,88,106	0
4	NA	D	303	1/1	0.92	0.24	43,43,43,43	0
3	0JN	F	302	25/25	0.93	0.12	34,39,46,48	25
6	ACT	E	305	4/4	0.93	0.18	55,68,106,115	0
6	ACT	D	305	4/4	0.93	0.14	38,53,67,97	0
3	0JN	E	302	25/25	0.94	0.10	22,28,39,42	0
6	ACT	C	305	4/4	0.94	0.11	38,47,57,72	0
6	ACT	A	308	4/4	0.94	0.11	36,44,61,80	0
6	ACT	C	307	4/4	0.94	0.12	52,66,66,82	0
6	ACT	K	304	4/4	0.94	0.14	33,38,60,65	0
7	PEG	J	307	7/7	0.95	0.15	33,36,129,146	0
3	0JN	L	302	25/25	0.95	0.10	31,35,45,45	0
6	ACT	L	305	4/4	0.95	0.10	53,54,58,101	0
6	ACT	A	306	4/4	0.95	0.09	34,45,48,57	0
2	KAN	H	301	33/33	0.96	0.09	24,31,37,38	0
4	NA	A	304	1/1	0.96	0.07	24,24,24,24	1
3	0JN	I	302	25/25	0.96	0.07	20,23,25,26	0
3	0JN	D	302	25/25	0.96	0.08	26,27,31,32	0
6	ACT	H	305	4/4	0.96	0.12	53,62,69,95	0
3	0JN	B	302	25/25	0.96	0.08	21,25,28,29	0
6	ACT	J	305	4/4	0.96	0.12	38,48,58,86	0
2	KAN	L	301	33/33	0.96	0.08	17,25,31,42	0
2	KAN	K	301	33/33	0.96	0.09	24,33,40,47	0
2	KAN	E	301	33/33	0.96	0.09	16,24,38,45	0
2	KAN	D	301	33/33	0.97	0.08	24,30,36,37	0
2	KAN	J	301	33/33	0.97	0.07	16,23,29,36	0
6	ACT	G	305	4/4	0.97	0.12	37,40,45,59	0

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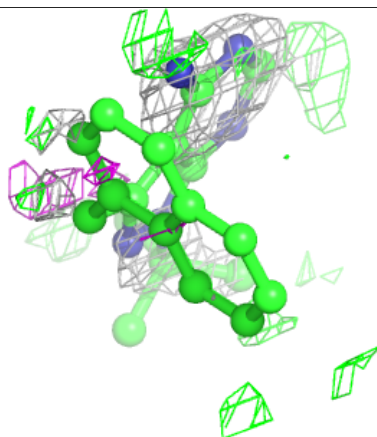
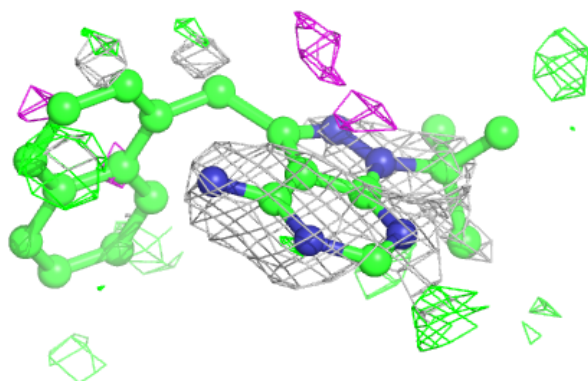
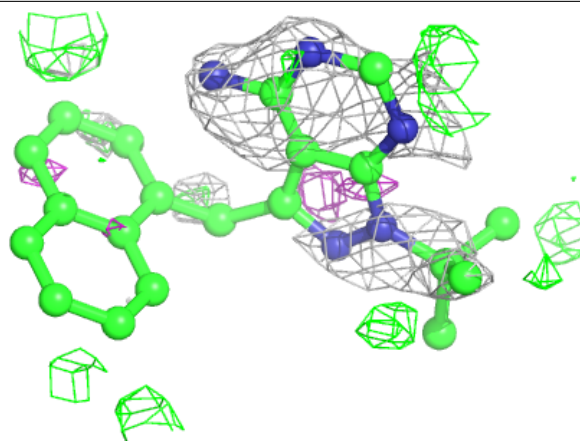
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NA	J	303	1/1	0.97	0.08	29,29,29,29	1
2	KAN	B	301	33/33	0.97	0.07	17,25,36,40	0
2	KAN	I	301	33/33	0.97	0.07	19,24,34,37	0
6	ACT	G	306	4/4	0.97	0.09	40,48,49,55	0
2	KAN	F	301	33/33	0.97	0.07	20,30,34,41	0
5	CL	A	305	1/1	0.97	0.08	62,62,62,62	0
6	ACT	F	304	4/4	0.97	0.09	38,42,54,82	0
2	KAN	C	301	33/33	0.97	0.08	16,21,27,32	0
3	0JN	H	302	25/25	0.97	0.07	24,26,30,32	0
6	ACT	C	306	4/4	0.97	0.09	23,35,39,62	0
4	NA	G	303	1/1	0.97	0.07	34,34,34,34	0
2	KAN	G	301	33/33	0.97	0.07	15,21,28,36	0
4	NA	C	303	1/1	0.98	0.08	39,39,39,39	0
4	NA	E	303	1/1	0.98	0.08	28,28,28,28	1
2	KAN	A	301	33/33	0.98	0.07	13,20,24,28	0
4	NA	J	304	1/1	0.98	0.08	25,25,25,25	1
4	NA	L	303	1/1	0.98	0.17	43,43,43,43	0
4	NA	G	304	1/1	0.99	0.10	32,32,32,32	0
4	NA	C	304	1/1	0.99	0.11	37,37,37,37	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.

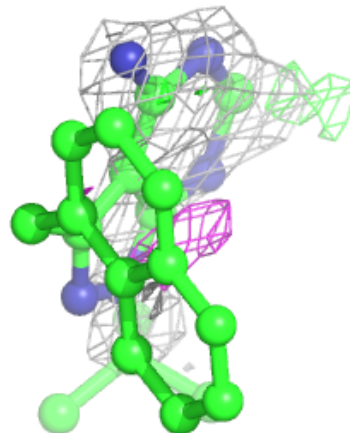
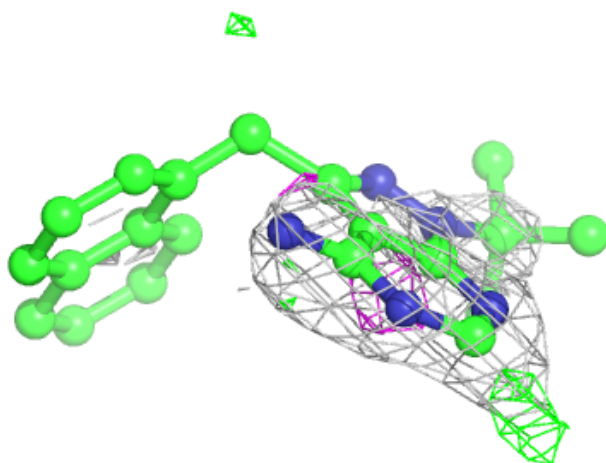
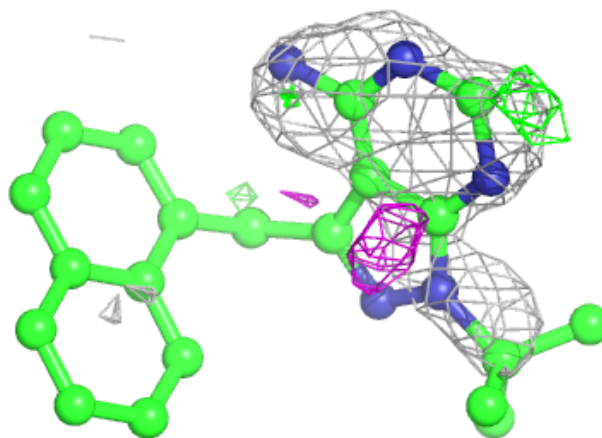
Electron density around 0JN C 302:

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



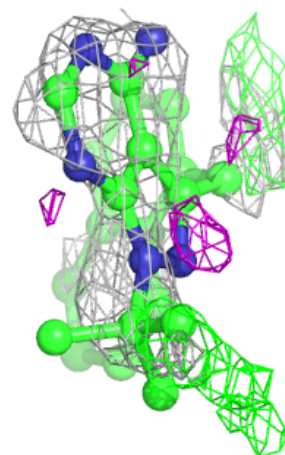
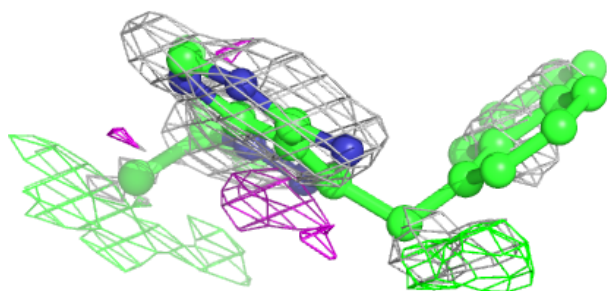
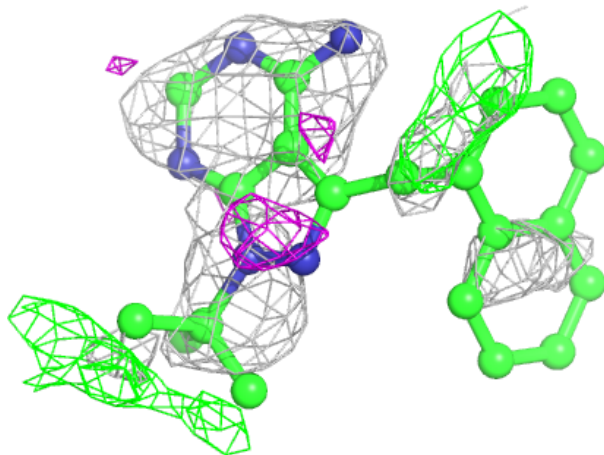
Electron density around 0JN G 302:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



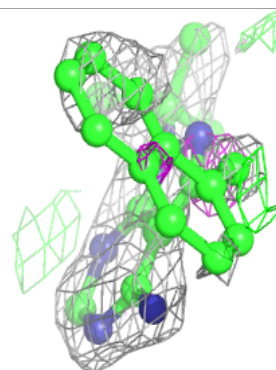
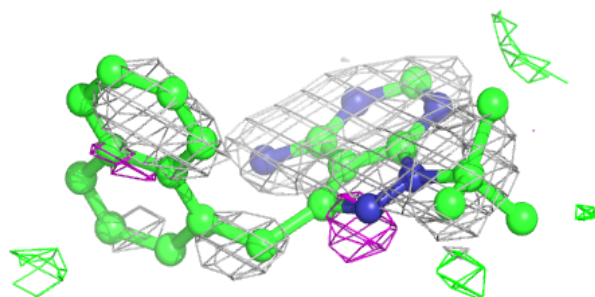
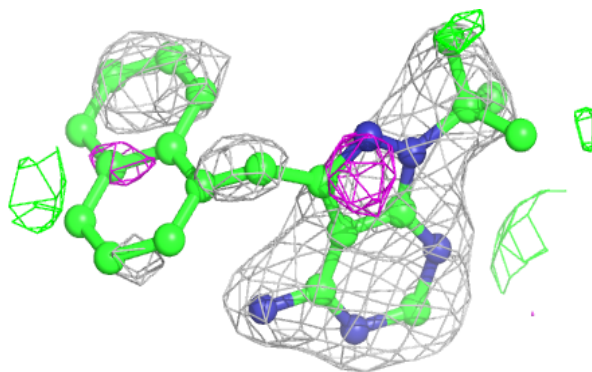
Electron density around 0JN A 302:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

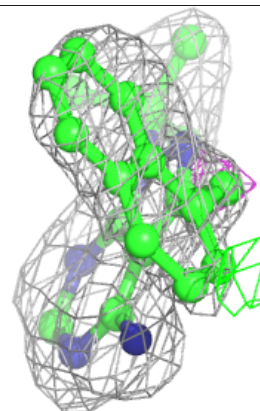
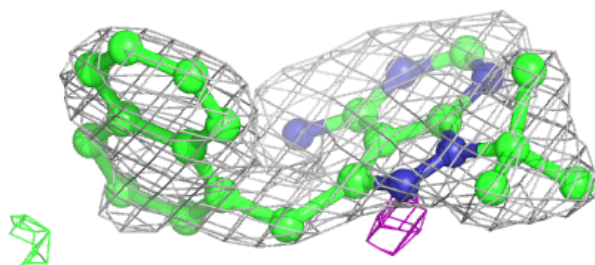
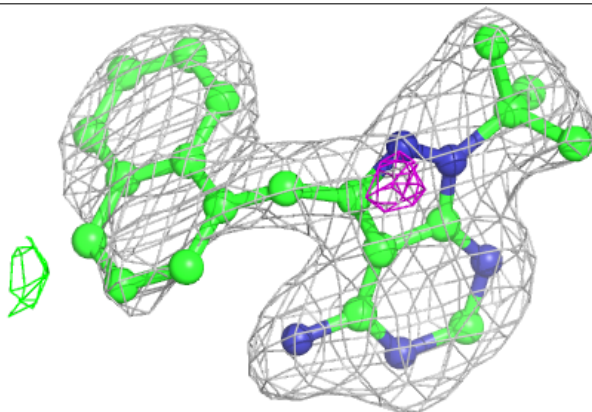


Electron density around 0JN J 302:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

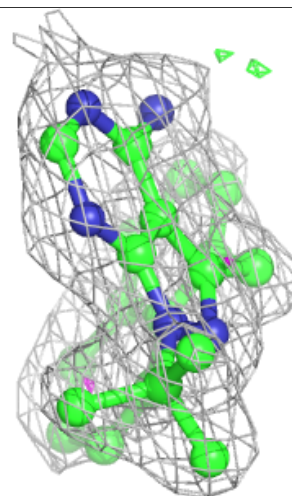
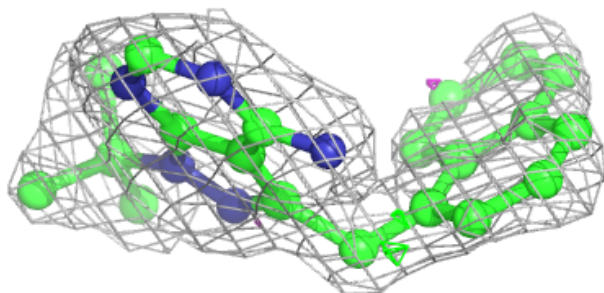
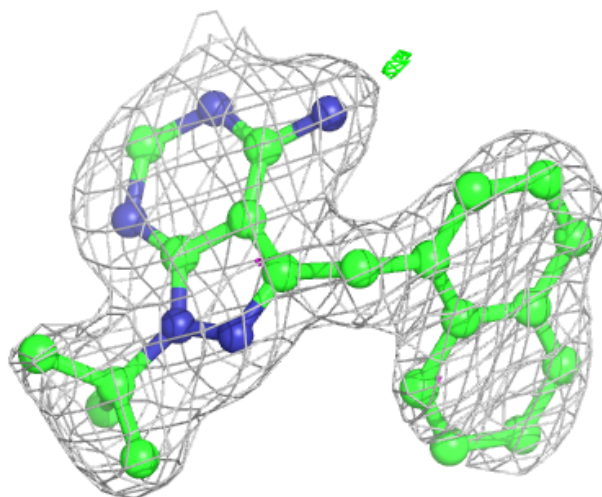
**Electron density around 0JN K 302:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



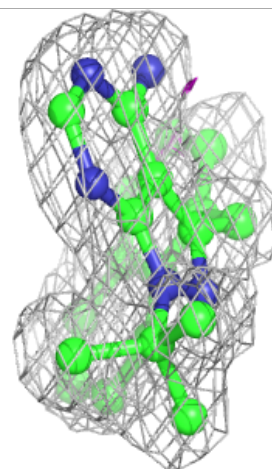
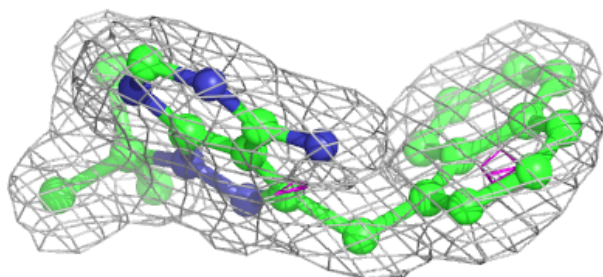
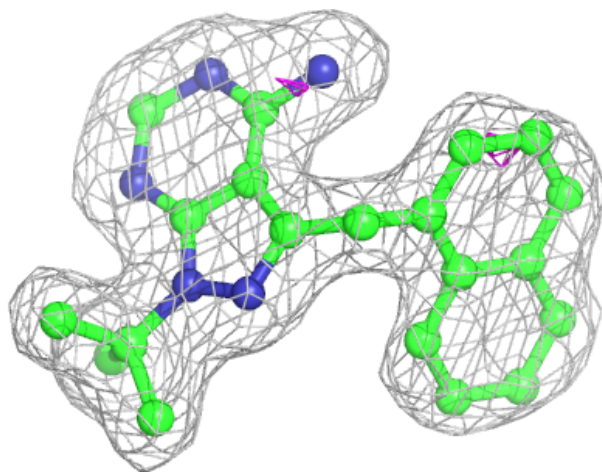
Electron density around 0JN F 302:

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



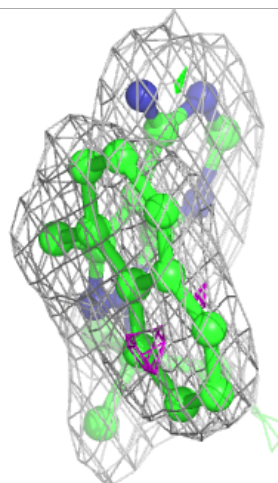
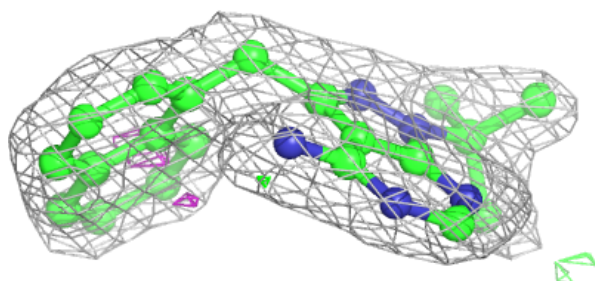
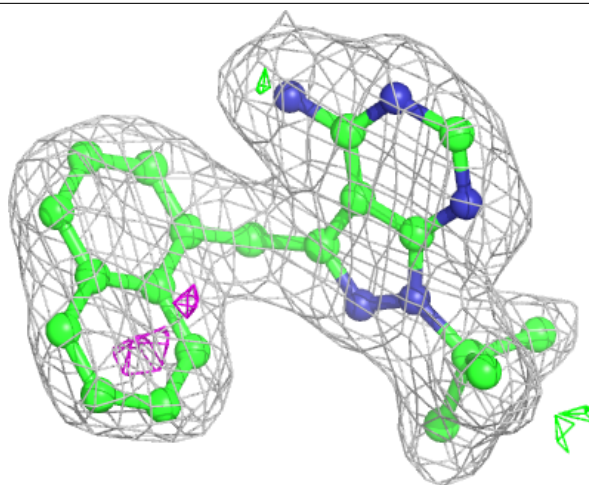
Electron density around 0JN E 302:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



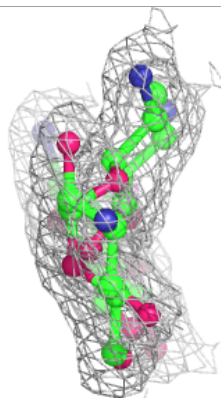
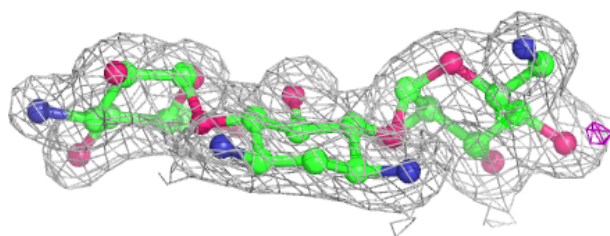
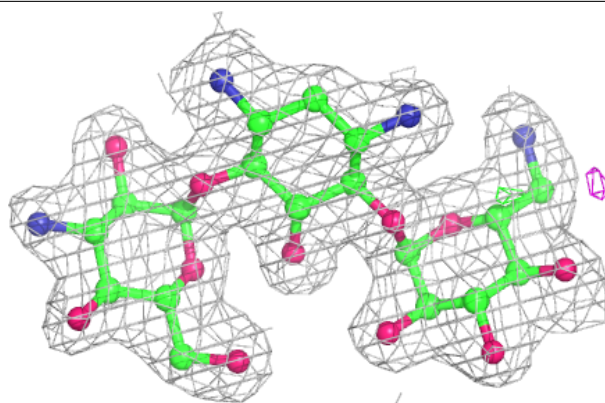
Electron density around 0JN L 302:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



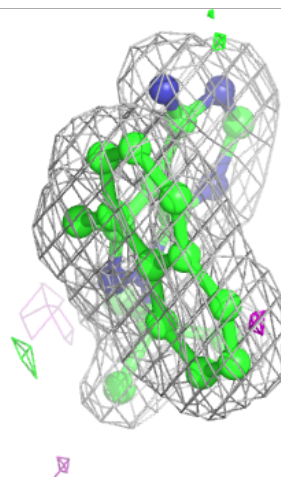
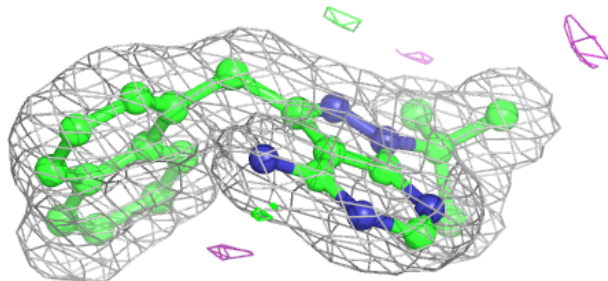
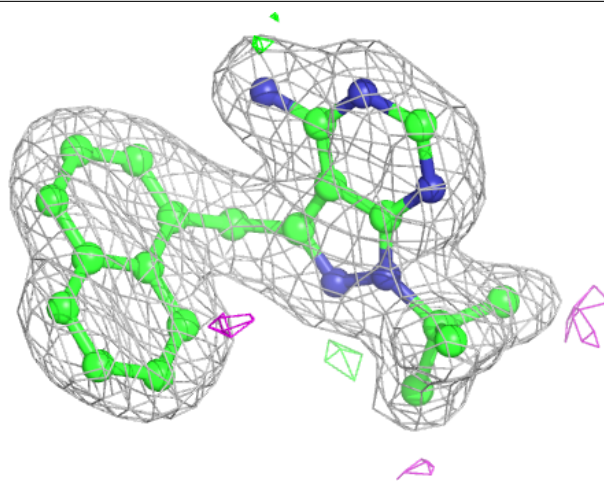
Electron density around KAN H 301:

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



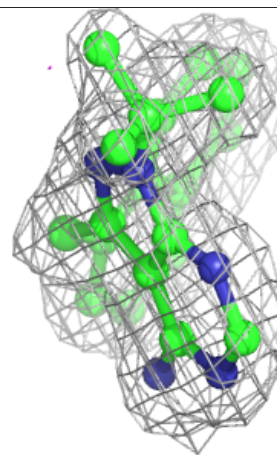
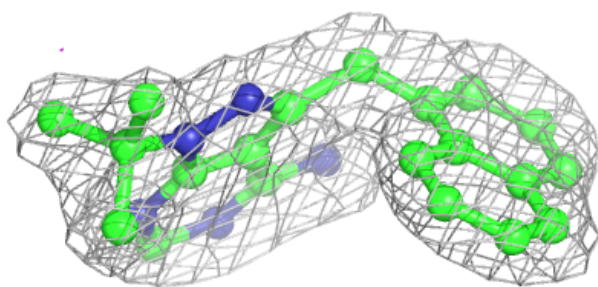
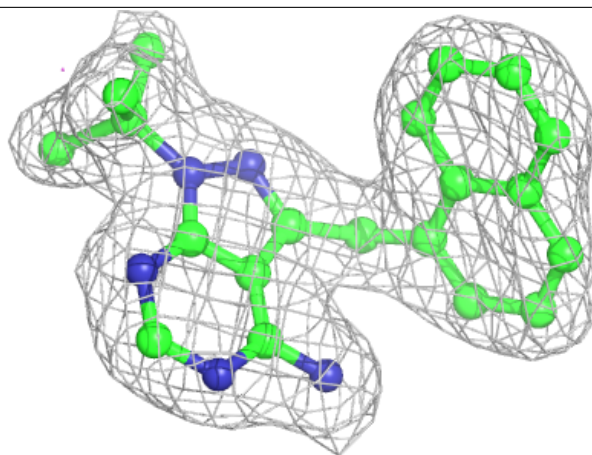
Electron density around 0JN I 302:

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and green (positive)



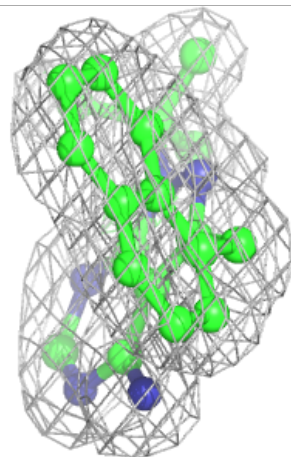
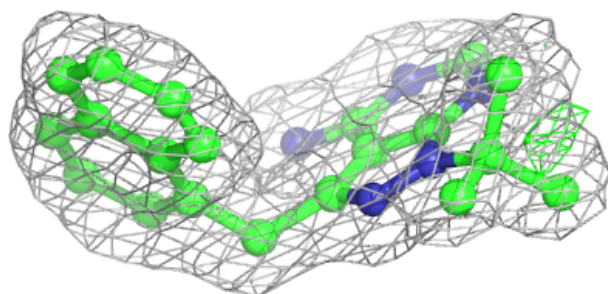
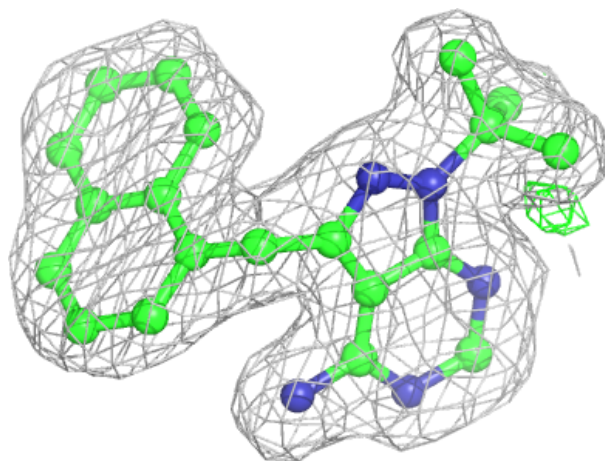
Electron density around 0JN D 302:

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and green (positive)



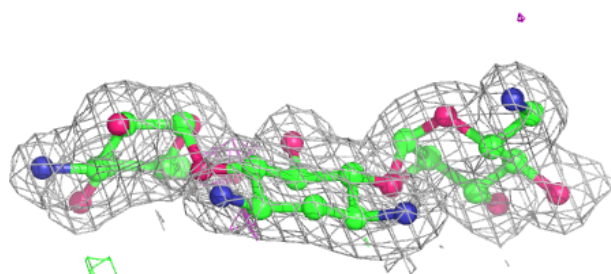
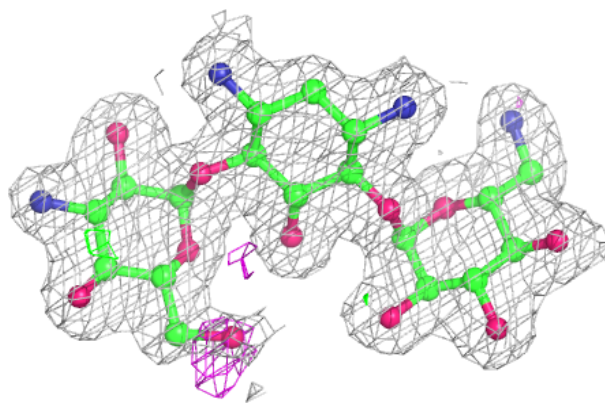
Electron density around 0JN B 302:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

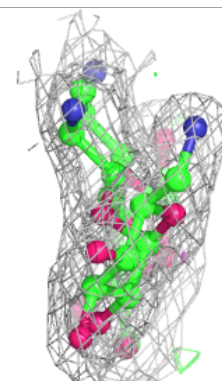
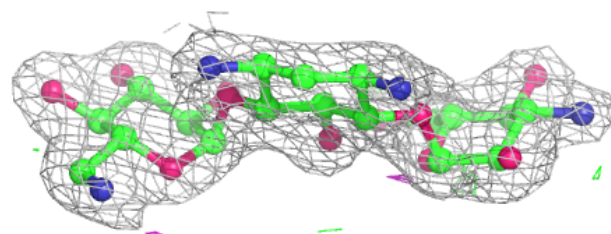
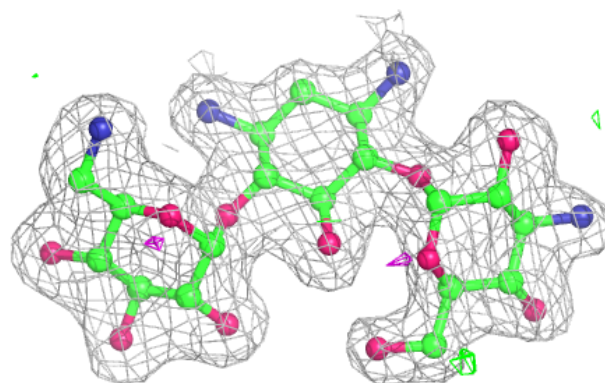


Electron density around KAN L 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

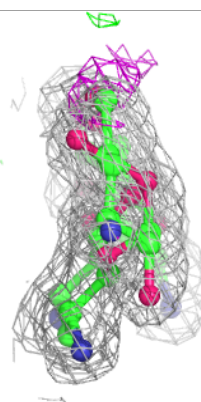
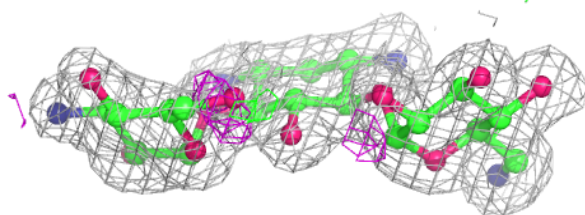
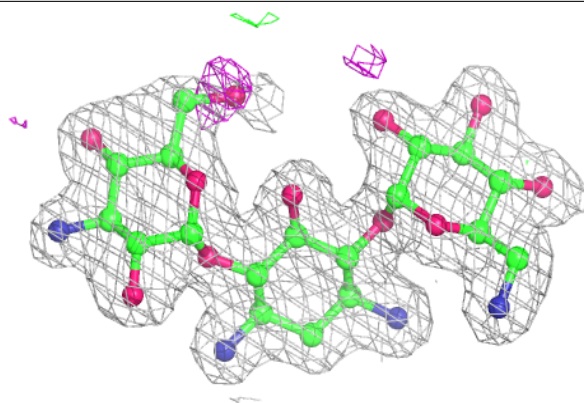
**Electron density around KAN K 301:**

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and green (positive)

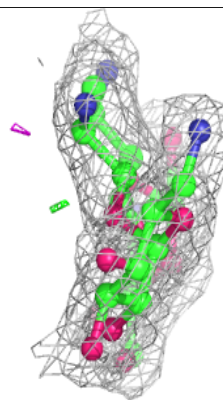
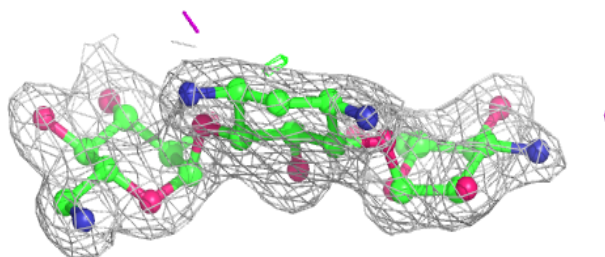
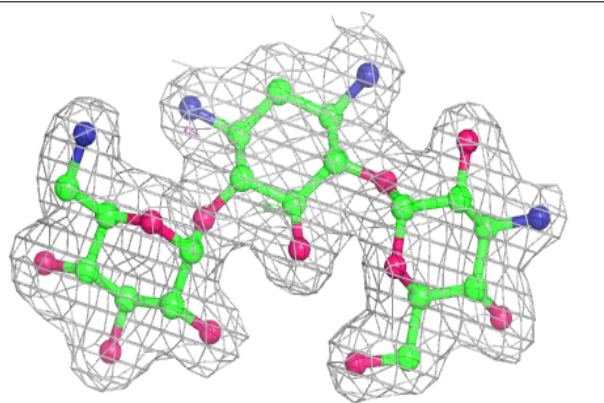


Electron density around KAN E 301:

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

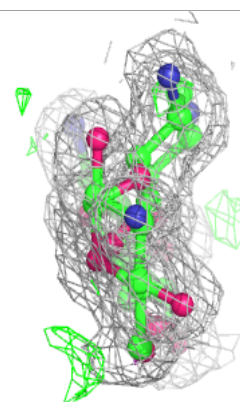
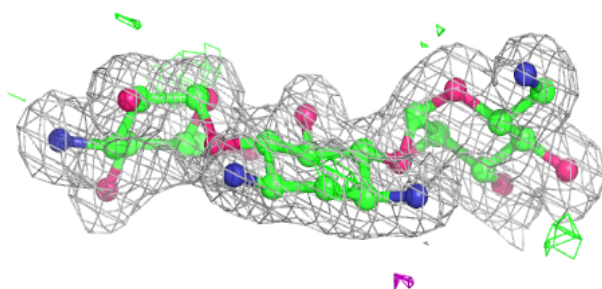
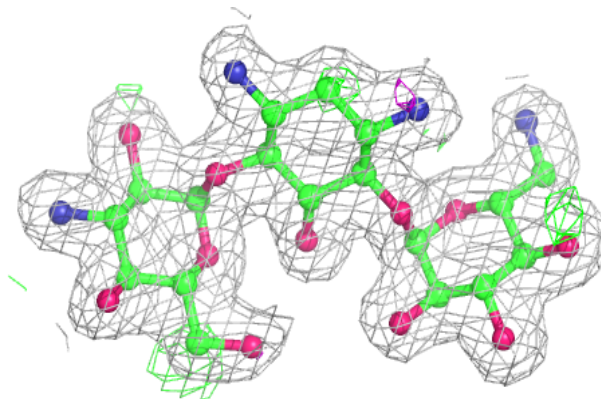
**Electron density around KAN D 301:**

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

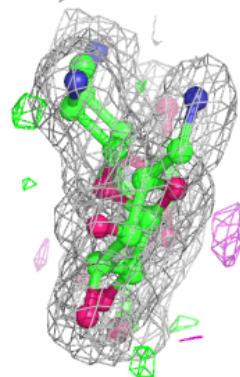
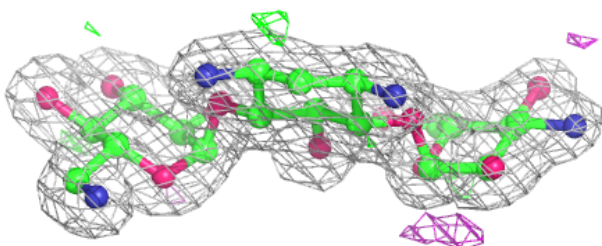
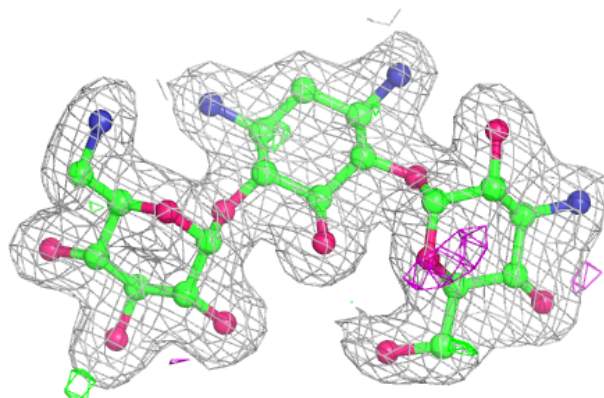


Electron density around KAN J 301:

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

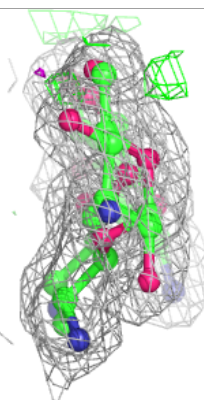
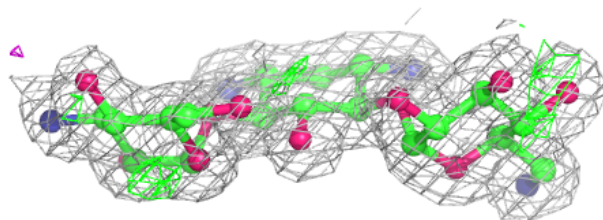
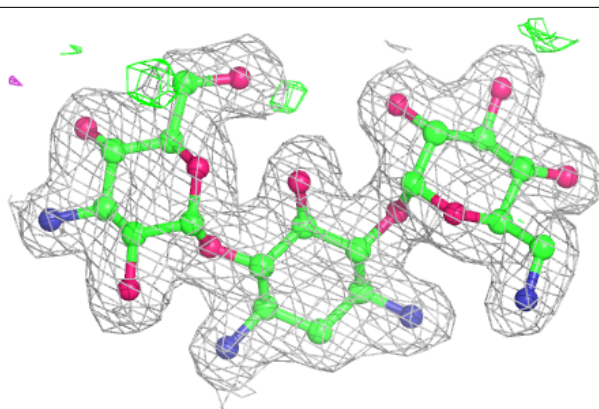
**Electron density around KAN B 301:**

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

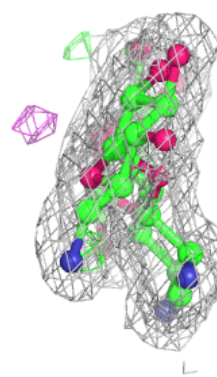
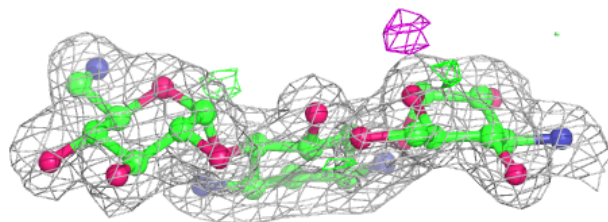
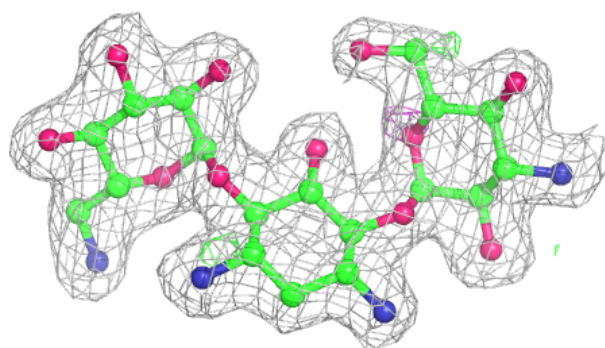


Electron density around KAN I 301:

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

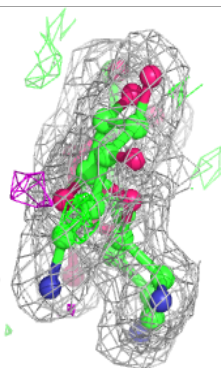
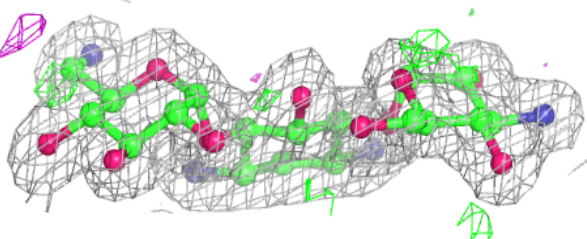
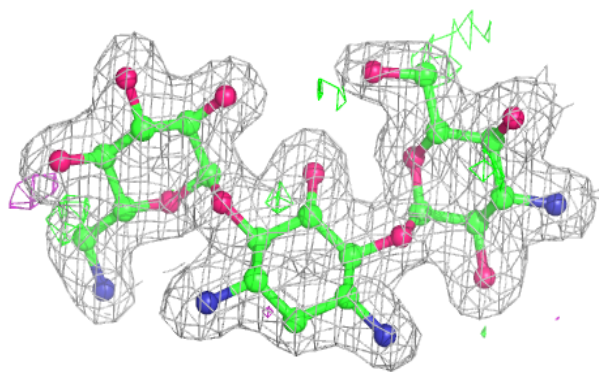
**Electron density around KAN F 301:**

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

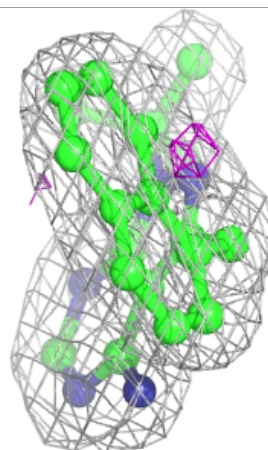
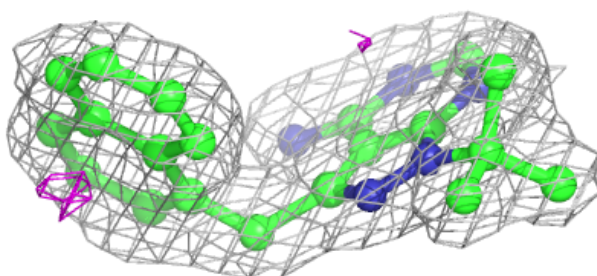
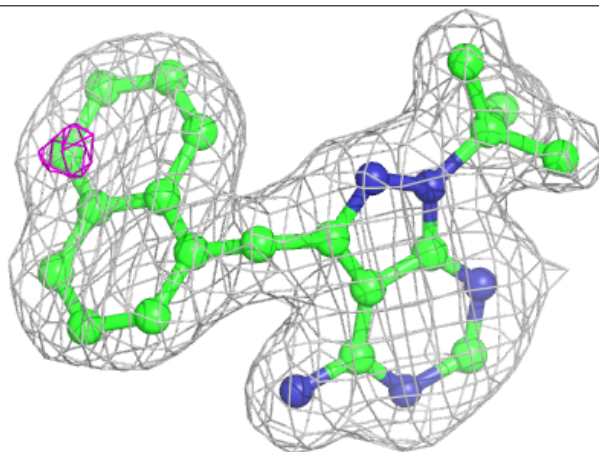


Electron density around KAN C 301:

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

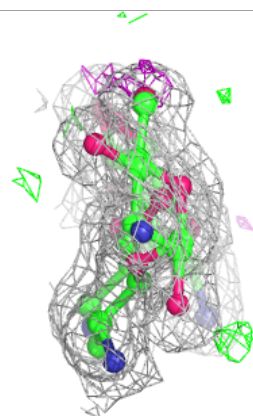
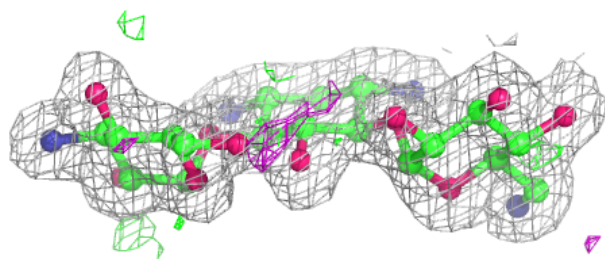
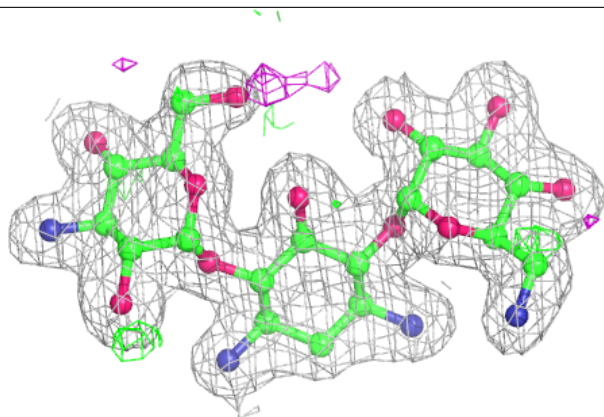
**Electron density around 0JN H 302:**

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

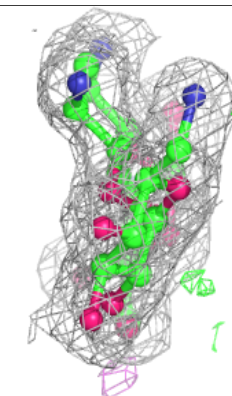
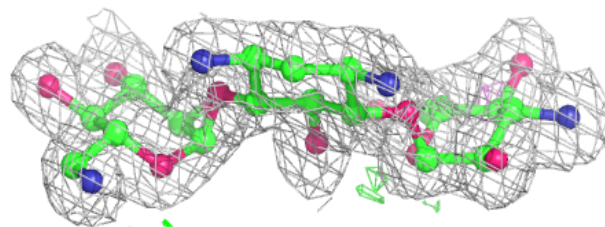
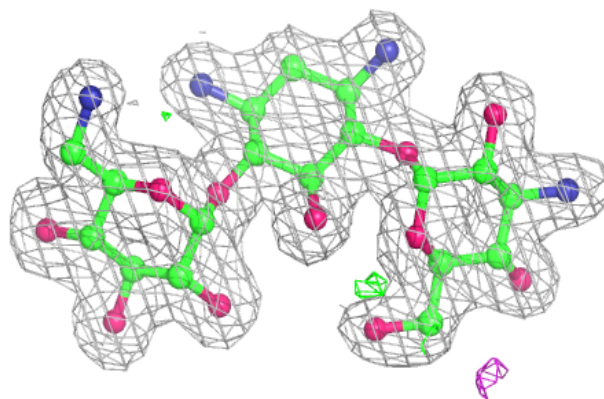


Electron density around KAN G 301:

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

**Electron density around KAN 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)



6.5 Other polymers

There are no such residues in this entry.