



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2023 – 06:08 PM EDT

PDB ID : 4FEU
Title : Crystal structure of the aminoglycoside phosphotransferase APH(3')-Ia, with substrate kanamycin and small molecule inhibitor anthrapyrazolone SP600125
Authors : Stogios, P.J.; Evdokimova, E.; Wawrzak, Z.; Minasov, G.; Egorova, O.; Di Leo, R.; Shakya, T.; Spanogiannopoulos, P.; Wright, G.D.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2012-05-30
Resolution : 2.37 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

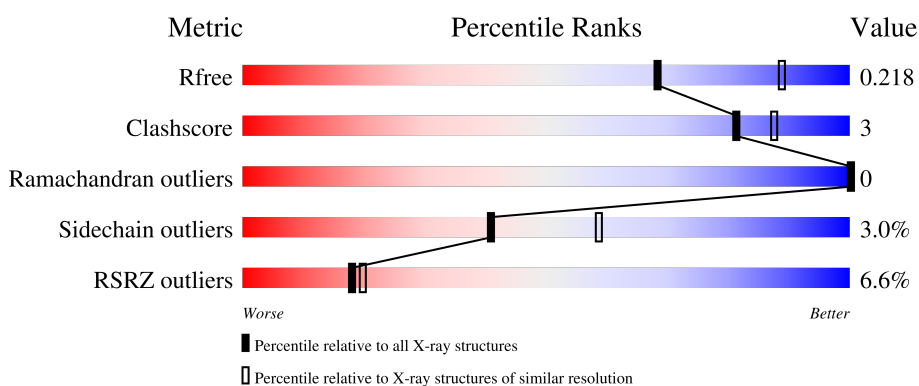
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 $\leq 5\%$. 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	
1	B	272	
1	C	272	
1	D	272	
1	E	272	

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Mol	Chain	Length	Quality of chain
1	F	272	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into three segments: a small red segment on the left labeled '3%', a large green segment in the middle labeled '86%', and a small grey segment on the right labeled '10%'. The segments are separated by thin white lines.</p>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13331 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.

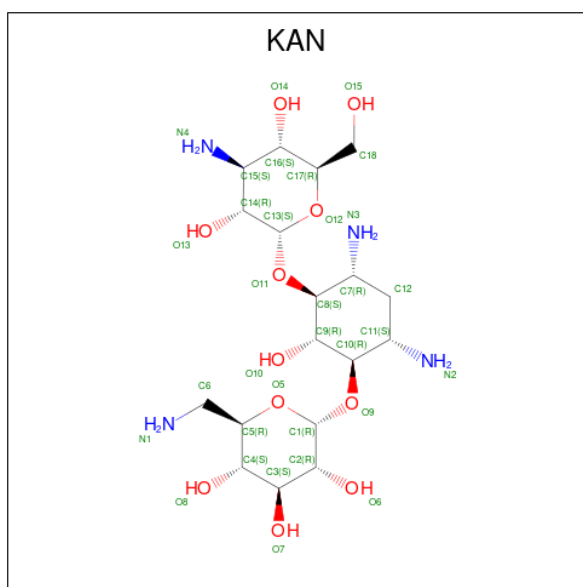
- Molecule 1 is a protein called Aminoglycoside 3'-phosphotransferase AphA1-IAB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	253	Total 2042	C 1307	N 348	O 377	S 4	Se 6	0	1	0
1	B	263	Total 2138	C 1362	N 373	O 392	S 5	Se 6	0	2	0
1	C	262	Total 2116	C 1348	N 364	O 393	S 5	Se 6	0	1	0
1	D	242	Total 1952	C 1252	N 334	O 356	S 4	Se 6	0	0	0
1	E	264	Total 2125	C 1354	N 368	O 392	S 5	Se 6	0	0	0
1	F	245	Total 2000	C 1282	N 342	O 366	S 4	Se 6	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

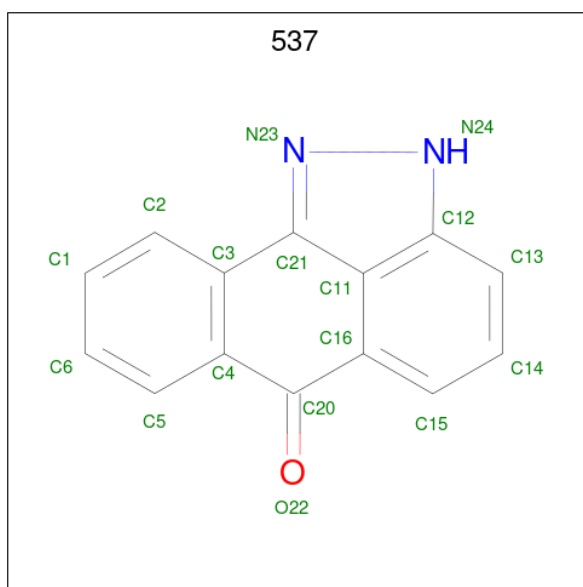
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP B0VD92
B	0	GLY	-	expression tag	UNP B0VD92
C	0	GLY	-	expression tag	UNP B0VD92
D	0	GLY	-	expression tag	UNP B0VD92
E	0	GLY	-	expression tag	UNP B0VD92
F	0	GLY	-	expression tag	UNP B0VD92

- Molecule 2 is KANAMYCIN A (three-letter code: KAN) (formula: C₁₈H₃₆N₄O₁₁).



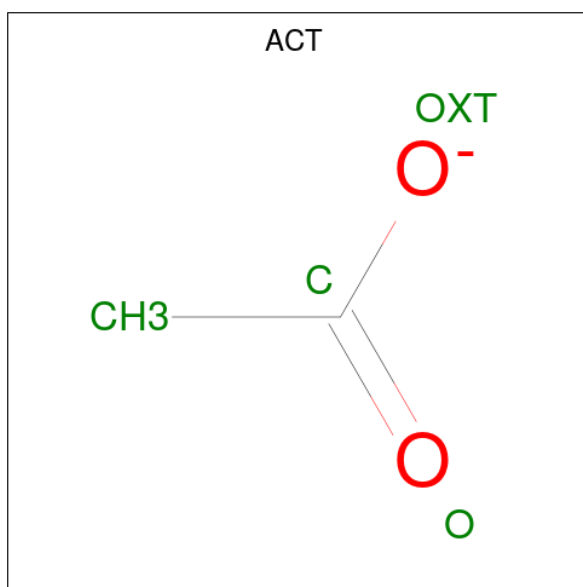
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	33	18	4	11	0	0
2	B	1	33	18	4	11	0	0
2	C	1	33	18	4	11	0	0
2	D	1	33	18	4	11	0	0
2	E	1	33	18	4	11	0	0
2	F	1	33	18	4	11	0	0

- Molecule 3 is 2,6-DIHYDROANTHRA/1,9-CD/PYRAZOL-6-ONE (three-letter code: 537) (formula: C₁₄H₈N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	14	2	1		
3	C	1	Total	C	N	O	0	0
			17	14	2	1		
3	E	1	Total	C	N	O	0	0
			17	14	2	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0

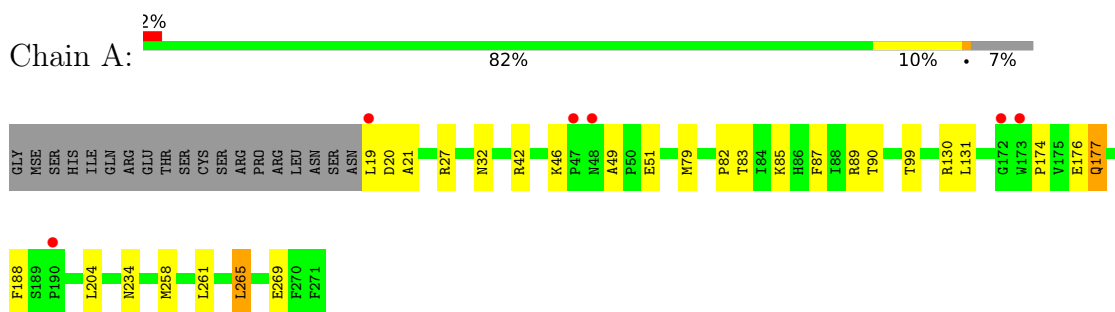
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	129	Total O 129 129	0	0
5	B	135	Total O 138 138	0	3
5	C	129	Total O 130 130	0	1
5	D	45	Total O 45 45	0	0
5	E	126	Total O 129 129	0	3
5	F	111	Total O 114 114	0	3

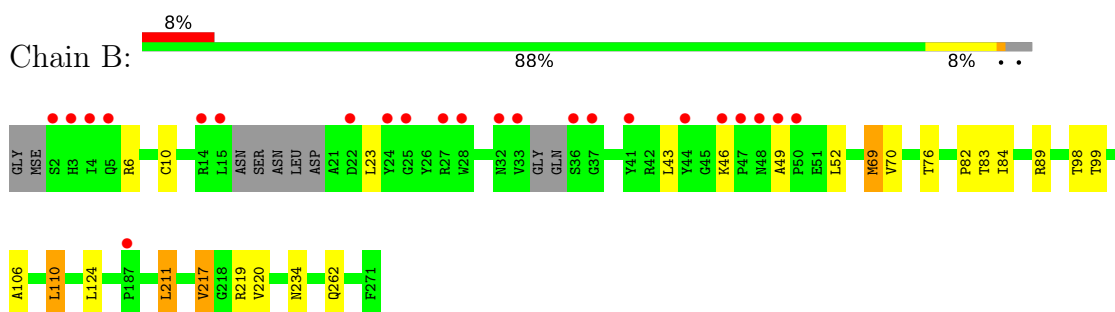
3 Residue-property plots [i](#)

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.

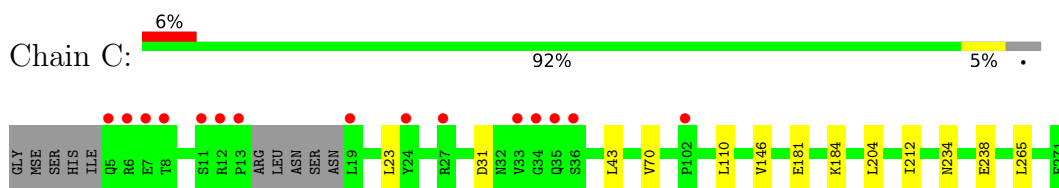
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



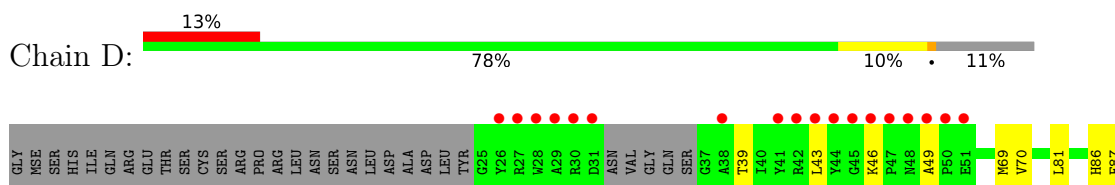
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

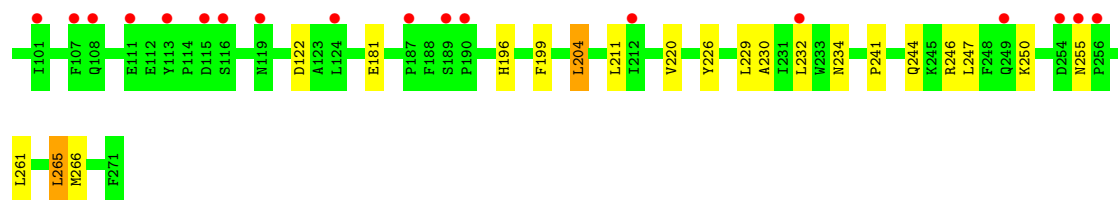


- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

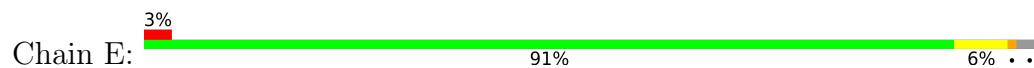


- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

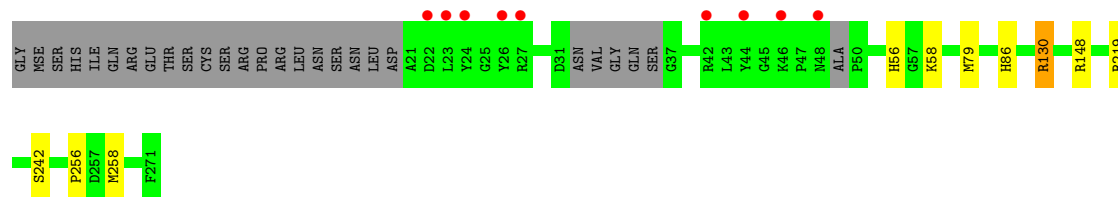
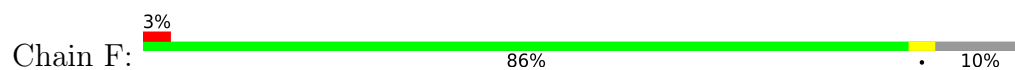




- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



- 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	57.75Å 94.16Å 96.77Å 61.21° 73.11° 87.36°	Depositor
Resolution (Å)	19.97 – 2.37 19.97 – 2.37	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.97-2.37) 98.2 (19.97-2.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.38Å)	Xtrriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.160 , 0.215 0.164 , 0.218	Depositor DCC
R_{free} test set	3406 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtrriage
Anisotropy	0.333	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.010 for -h,-k,-h-k+l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13331	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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: KAN, 537, ACT

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	0.50	0/2090	0.68	0/2828
1	B	0.49	0/2186	0.66	0/2952
1	C	0.51	0/2164	0.68	0/2925
1	D	0.48	0/1998	0.63	0/2700
1	E	0.50	0/2173	0.67	0/2937
1	F	0.49	0/2046	0.67	0/2762
All	All	0.49	0/12657	0.67	0/17104

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	2042	0	1978	16	0
1	B	2138	0	2076	15	0
1	C	2116	0	2045	6	0
1	D	1952	0	1896	19	0
1	E	2125	0	2062	10	0
1	F	2000	0	1937	6	0
2	A	33	0	36	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	A	17	0	8	0	0
3	C	17	0	8	0	0
3	E	17	0	8	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
4	C	8	0	6	0	0
4	D	4	0	3	0	0
4	F	4	0	3	0	0
5	A	129	0	0	1	0
5	B	138	0	0	1	0
5	C	130	0	0	0	0
5	D	45	0	0	0	0
5	E	129	0	0	1	0
5	F	114	0	0	1	0
All	All	13331	0	12252	64	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (64) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:MSE:SE	1:A:261:LEU:HD23	2.38	0.74
1:E:34:GLY:H	1:E:35:GLN:HG3	1.58	0.68
1:A:234:ASN:HB2	1:A:265:LEU:HD11	1.81	0.62
1:E:256:PRO:HB2	1:E:258:MSE:CE	2.34	0.58
1:B:124:LEU:HD23	1:B:211:LEU:HD21	1.85	0.57
1:C:70:VAL:HG11	1:D:70:VAL:HG11	1.87	0.56
1:C:181:GLU:HA	1:C:184:LYS:HE3	1.87	0.56
1:D:234:ASN:HB2	1:D:265:LEU:HD11	1.89	0.54
1:D:46:LYS:HB3	1:D:49:ALA:HB3	1.91	0.53
1:A:32:ASN:HB3	1:B:6:ARG:HB2	1.89	0.53
1:A:46:LYS:HB3	1:A:49:ALA:HB3	1.91	0.51
1:E:19:LEU:HD22	1:E:88:ILE:HD12	1.93	0.50
1:D:122:ASP:HA	1:D:250:LYS:HD3	1.92	0.50
1:C:234:ASN:HB2	1:C:265:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:79:MSE:SE	1:F:130:ARG:HG2	2.63	0.49
1:A:87:PHE:HB3	1:B:89:ARG:HB3	1.95	0.48
1:B:52:LEU:HD23	1:B:99:THR:HA	1.94	0.48
1:B:234:ASN:ND2	5:B:510[A]:HOH:O	2.47	0.48
1:F:219[B]:ARG:HG3	5:F:452[B]:HOH:O	2.14	0.48
1:A:174:PRO:HD2	1:A:177:GLN:HB2	1.96	0.47
1:F:56:HIS:HE1	1:F:58:LYS:HE3	1.79	0.47
1:A:32:ASN:ND2	1:E:237:GLY:O	2.48	0.46
1:D:230:ALA:HB1	1:D:265:LEU:HD13	1.97	0.46
1:B:82:PRO:HB3	1:B:99:THR:O	2.15	0.46
1:C:23:LEU:HD22	1:C:43:LEU:HD22	1.96	0.46
1:D:196:HIS:HA	1:D:220:VAL:HG22	1.99	0.45
1:E:72:LEU:HD12	1:E:81:LEU:HD23	1.99	0.45
1:E:124:LEU:HD13	1:E:232:LEU:HD11	1.98	0.44
1:E:256:PRO:HB2	1:E:258:MSE:HE2	1.99	0.44
1:B:217:VAL:HG22	1:B:220:VAL:HG21	2.00	0.44
1:D:241:PRO:HA	1:D:244:GLN:HE21	1.83	0.44
1:A:82:PRO:HB3	1:A:99:THR:O	2.18	0.43
1:B:217:VAL:HG22	1:B:220:VAL:CG2	2.48	0.43
1:D:246:ARG:HE	1:D:250:LYS:NZ	2.17	0.43
1:E:19:LEU:H	1:E:19:LEU:HD23	1.84	0.43
1:A:79:MSE:HE2	1:A:131:LEU:HB2	2.01	0.42
1:A:89:ARG:HG2	1:B:69:MSE:HE3	2.00	0.42
1:A:258:MSE:SE	1:A:261:LEU:CD2	3.14	0.42
1:E:130:ARG:NH2	5:E:445:HOH:O	2.52	0.42
1:D:204:LEU:HB3	1:D:211:LEU:HD11	2.00	0.42
1:A:89:ARG:NH1	1:A:90:THR:O	2.48	0.42
1:D:232:LEU:HD23	1:D:247:LEU:HD11	2.02	0.42
1:A:19:LEU:HG	1:A:21:ALA:H	1.85	0.42
1:A:269:GLU:OE1	2:A:301:KAN:N3	2.51	0.42
1:C:70:VAL:HG11	1:D:70:VAL:CG1	2.50	0.42
1:F:256:PRO:HB2	1:F:258:MSE:CE	2.50	0.42
1:B:10:CYS:HB2	1:E:114:PRO:HG3	2.01	0.41
1:D:181:GLU:HB2	1:D:266:MSE:HE1	2.02	0.41
1:D:204:LEU:HD22	1:D:211:LEU:HD21	2.03	0.41
1:F:256:PRO:HB2	1:F:258:MSE:HE2	2.02	0.41
1:B:43:LEU:HB2	1:B:52:LEU:HB2	2.02	0.41
1:D:230:ALA:HA	1:D:261:LEU:HD12	2.03	0.41
1:D:69:MSE:HG3	1:D:87:PHE:CG	2.55	0.41
1:C:70:VAL:CG1	1:D:70:VAL:HG11	2.50	0.41
1:A:83[B]:THR:HB	5:A:443:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LYS:HB3	1:B:49:ALA:HB3	2.02	0.41
1:B:106:ALA:O	1:B:110:LEU:HB2	2.21	0.41
1:A:42:ARG:HD2	1:A:51:GLU:OE2	2.21	0.40
1:D:199:PHE:CE2	1:D:232:LEU:HD22	2.56	0.40
1:D:69:MSE:HG3	1:D:87:PHE:CD1	2.56	0.40
1:B:83:THR:O	1:B:98:THR:HA	2.21	0.40
1:D:226:TYR:HA	1:D:229:LEU:HB2	2.02	0.40
1:B:69:MSE:HE2	1:B:84:ILE:HD13	2.04	0.40
1:F:148:ARG:HD2	1:F:219[A]:ARG:NH1	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	252/272 (93%)	244 (97%)	8 (3%)	0	100	100
1	B	259/272 (95%)	250 (96%)	9 (4%)	0	100	100
1	C	259/272 (95%)	249 (96%)	10 (4%)	0	100	100
1	D	238/272 (88%)	224 (94%)	14 (6%)	0	100	100
1	E	260/272 (96%)	251 (96%)	9 (4%)	0	100	100
1	F	241/272 (89%)	234 (97%)	7 (3%)	0	100	100
All	All	1509/1632 (92%)	1452 (96%)	57 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	221/231 (96%)	212 (96%)	9 (4%)	30	45
1	B	233/231 (101%)	224 (96%)	9 (4%)	32	48
1	C	230/231 (100%)	224 (97%)	6 (3%)	46	64
1	D	211/231 (91%)	204 (97%)	7 (3%)	38	55
1	E	231/231 (100%)	225 (97%)	6 (3%)	46	64
1	F	216/231 (94%)	213 (99%)	3 (1%)	67	81
All	All	1342/1386 (97%)	1302 (97%)	40 (3%)	41	59

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASP
1	A	27	ARG
1	A	85	LYS
1	A	130	ARG
1	A	176	GLU
1	A	177	GLN
1	A	188	PHE
1	A	204	LEU
1	A	265	LEU
1	B	23	LEU
1	B	69	MSE
1	B	70	VAL
1	B	76	THR
1	B	110	LEU
1	B	211	LEU
1	B	217	VAL
1	B	219	ARG
1	B	262	GLN
1	C	31	ASP
1	C	110	LEU
1	C	146	VAL
1	C	204	LEU
1	C	212	ILE
1	C	238	GLU
1	D	39	THR
1	D	43	LEU
1	D	81	LEU

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Mol	Chain	Res	Type
1	D	86	HIS
1	D	204	LEU
1	D	255	ASN
1	D	265	LEU
1	E	9	SER
1	E	23	LEU
1	E	33	VAL
1	E	72	LEU
1	E	116	SER
1	E	130	ARG
1	F	86	HIS
1	F	130	ARG
1	F	242	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	GLN
1	B	32	ASN
1	B	73	ASN
1	B	234	ASN
1	B	249	GLN
1	D	73	ASN
1	D	244	GLN
1	F	138	ASN
1	F	153	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACT	C	304	-	3,3,3	0.80	0	3,3,3	1.26	0
2	KAN	B	301	-	35,35,35	0.74	1 (2%)	46,52,52	1.30	6 (13%)
2	KAN	F	301	-	35,35,35	0.72	1 (2%)	46,52,52	1.09	4 (8%)
3	537	E	302	-	16,20,20	2.59	5 (31%)	23,30,30	2.74	7 (30%)
4	ACT	B	302	-	3,3,3	0.87	0	3,3,3	1.04	0
4	ACT	A	303	-	3,3,3	1.01	0	3,3,3	0.74	0
2	KAN	E	301	-	35,35,35	0.94	3 (8%)	46,52,52	1.18	7 (15%)
4	ACT	F	302	-	3,3,3	1.33	1 (33%)	3,3,3	1.12	0
3	537	A	302	-	16,20,20	2.61	4 (25%)	23,30,30	2.71	6 (26%)
2	KAN	D	301	-	35,35,35	0.79	1 (2%)	46,52,52	1.10	3 (6%)
4	ACT	D	302	-	3,3,3	1.02	0	3,3,3	1.01	0
2	KAN	C	301	-	35,35,35	0.87	2 (5%)	46,52,52	1.42	4 (8%)
2	KAN	A	301	-	35,35,35	0.74	0	46,52,52	1.14	5 (10%)
4	ACT	C	303	-	3,3,3	1.11	0	3,3,3	1.04	0
3	537	C	302	-	16,20,20	2.51	4 (25%)	23,30,30	2.62	7 (30%)

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	B	301	-	-	1/12/72/72	0/3/3/3
2	KAN	F	301	-	-	3/12/72/72	0/3/3/3
3	537	E	302	-	-	-	0/4/4/4
2	KAN	E	301	-	-	1/12/72/72	0/3/3/3
3	537	A	302	-	-	-	0/4/4/4
2	KAN	D	301	-	-	1/12/72/72	0/3/3/3
2	KAN	C	301	-	-	1/12/72/72	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KAN	A	301	-	-	1/12/72/72	0/3/3/3
3	537	C	302	-	-	-	0/4/4/4

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	302	537	N23-N24	-5.99	1.25	1.37
3	C	302	537	N23-N24	-5.97	1.25	1.37
3	A	302	537	N23-N24	-5.92	1.26	1.37
3	C	302	537	C16-C20	-5.33	1.40	1.48
3	A	302	537	C16-C20	-5.23	1.40	1.48
3	E	302	537	C16-C20	-5.13	1.41	1.48
3	A	302	537	C4-C20	-5.12	1.41	1.48
3	E	302	537	C4-C20	-4.41	1.42	1.48
3	C	302	537	C4-C20	-4.00	1.42	1.48
2	E	301	KAN	O5-C1	3.27	1.50	1.41
2	C	301	KAN	C6-C5	2.81	1.55	1.52
3	A	302	537	C16-C11	-2.54	1.38	1.42
2	F	301	KAN	C6-C5	2.39	1.55	1.52
3	E	302	537	C16-C11	-2.34	1.38	1.42
3	E	302	537	C14-C13	2.26	1.41	1.36
2	D	301	KAN	C6-C5	2.24	1.55	1.52
3	C	302	537	C16-C11	-2.21	1.39	1.42
2	C	301	KAN	O9-C1	2.15	1.47	1.41
2	E	301	KAN	O12-C13	2.06	1.47	1.41
2	E	301	KAN	C6-C5	2.04	1.54	1.52
2	B	301	KAN	C6-C5	2.02	1.54	1.52
4	F	302	ACT	OXT-C	-2.01	1.21	1.30

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	302	537	C15-C16-C20	7.96	126.40	119.61
3	A	302	537	C15-C16-C20	7.14	125.70	119.61
3	C	302	537	C15-C16-C20	6.81	125.42	119.61
3	A	302	537	C3-C21-C11	-6.15	117.43	121.92
3	C	302	537	C3-C21-C11	-5.68	117.78	121.92
3	A	302	537	C3-C21-N23	5.34	138.44	127.79
3	E	302	537	C3-C21-C11	-5.24	118.09	121.92
3	C	302	537	C3-C21-N23	4.89	137.54	127.79
3	E	302	537	C3-C21-N23	4.73	137.22	127.79
3	E	302	537	C13-C12-N24	4.70	137.84	130.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	KAN	O5-C5-C6	4.68	114.72	106.01
3	C	302	537	C13-C12-N24	4.61	137.69	130.19
2	B	301	KAN	C6-C5-C4	-4.56	104.13	113.10
3	A	302	537	C13-C12-N24	4.53	137.56	130.19
2	C	301	KAN	C6-C5-C4	-4.43	104.38	113.10
3	E	302	537	C11-C16-C20	-3.96	116.65	119.92
2	D	301	KAN	C1-O9-C10	-3.21	110.01	117.96
2	F	301	KAN	C1-O9-C10	-3.06	110.39	117.96
3	C	302	537	C11-C16-C20	-3.01	117.43	119.92
2	D	301	KAN	C6-C5-C4	-2.96	107.28	113.10
2	B	301	KAN	O5-C5-C6	2.89	111.39	106.01
2	A	301	KAN	C11-C12-C7	-2.86	105.32	111.18
2	E	301	KAN	O12-C17-C16	2.75	114.68	109.69
2	B	301	KAN	C13-O11-C8	-2.62	111.49	117.96
3	A	302	537	C11-C16-C20	-2.54	117.82	119.92
2	B	301	KAN	O11-C13-O12	-2.50	103.68	110.67
2	E	301	KAN	C18-C17-C16	-2.46	107.25	113.00
2	B	301	KAN	O9-C10-C9	2.45	113.80	107.28
3	A	302	537	C16-C11-C12	2.44	125.87	120.00
2	B	301	KAN	O11-C8-C7	-2.44	103.36	109.18
2	A	301	KAN	O9-C1-C2	2.41	114.34	108.10
2	E	301	KAN	C13-O11-C8	-2.38	112.07	117.96
2	A	301	KAN	O12-C17-C18	2.38	112.36	106.44
2	E	301	KAN	O6-C2-C3	-2.33	104.95	110.35
3	E	302	537	C16-C11-C12	2.32	125.56	120.00
2	E	301	KAN	O12-C17-C18	2.28	112.11	106.44
3	C	302	537	C2-C3-C21	-2.24	119.38	122.55
2	E	301	KAN	O5-C5-C4	2.23	113.74	109.69
3	C	302	537	C16-C11-C12	2.23	125.34	120.00
2	E	301	KAN	C1-O5-C5	2.19	117.98	113.69
3	E	302	537	C16-C20-C4	2.18	119.64	117.31
2	C	301	KAN	C13-O11-C8	-2.18	112.58	117.96
2	C	301	KAN	O9-C1-C2	2.16	113.70	108.10
2	F	301	KAN	O11-C8-C9	2.16	113.03	107.28
2	D	301	KAN	C10-C9-C8	2.15	113.43	108.96
2	F	301	KAN	O5-C5-C6	2.11	109.94	106.01
2	F	301	KAN	O5-C5-C4	2.09	113.49	109.69
2	A	301	KAN	C6-C5-C4	-2.02	109.12	113.10
2	A	301	KAN	C10-C9-C8	2.01	113.14	108.96

There are no chirality outliers.

All (8) torsion outliers are listed below:

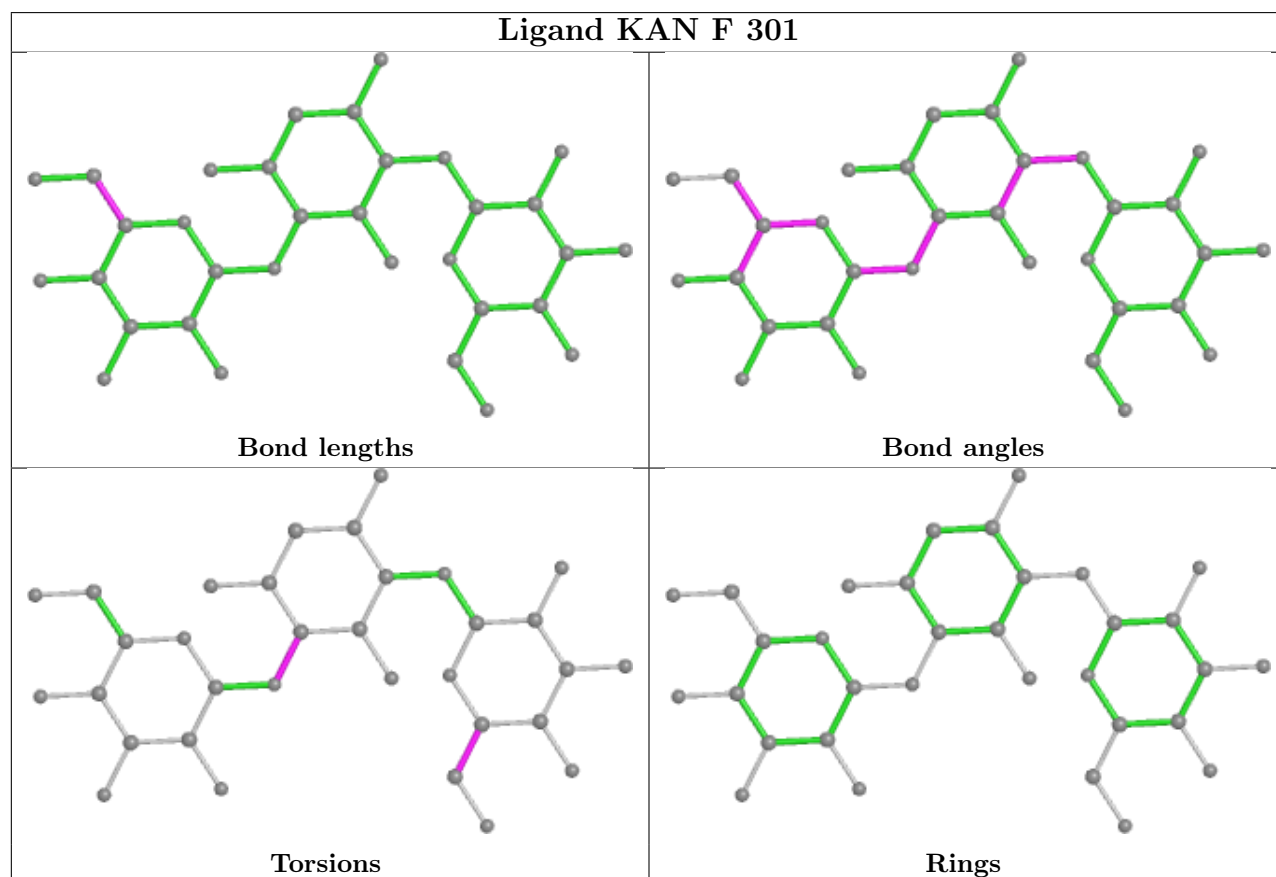
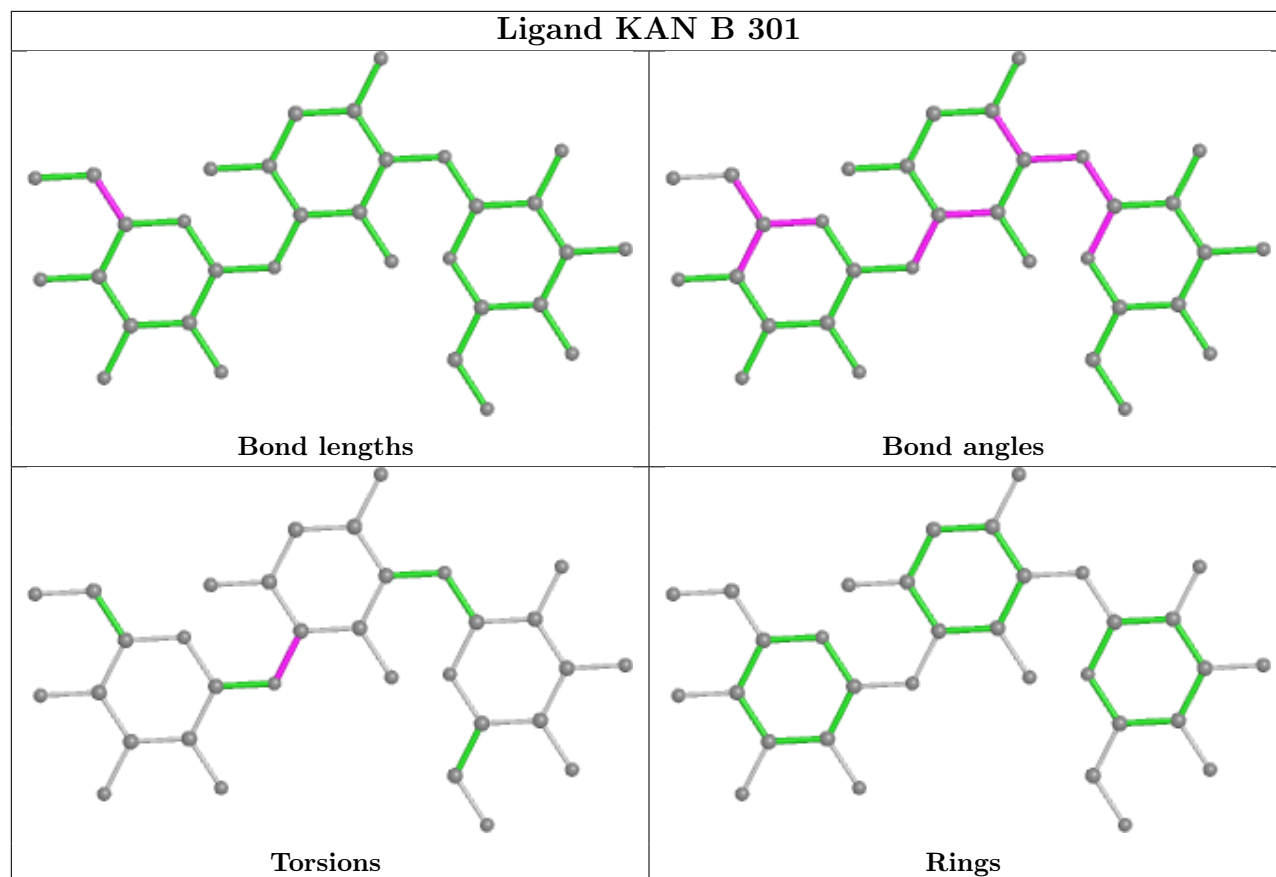
Mol	Chain	Res	Type	Atoms
2	F	301	KAN	O12-C17-C18-O15
2	F	301	KAN	C16-C17-C18-O15
2	C	301	KAN	C16-C17-C18-O15
2	D	301	KAN	O5-C1-O9-C10
2	F	301	KAN	C9-C10-O9-C1
2	B	301	KAN	C9-C10-O9-C1
2	E	301	KAN	C14-C13-O11-C8
2	A	301	KAN	C9-C10-O9-C1

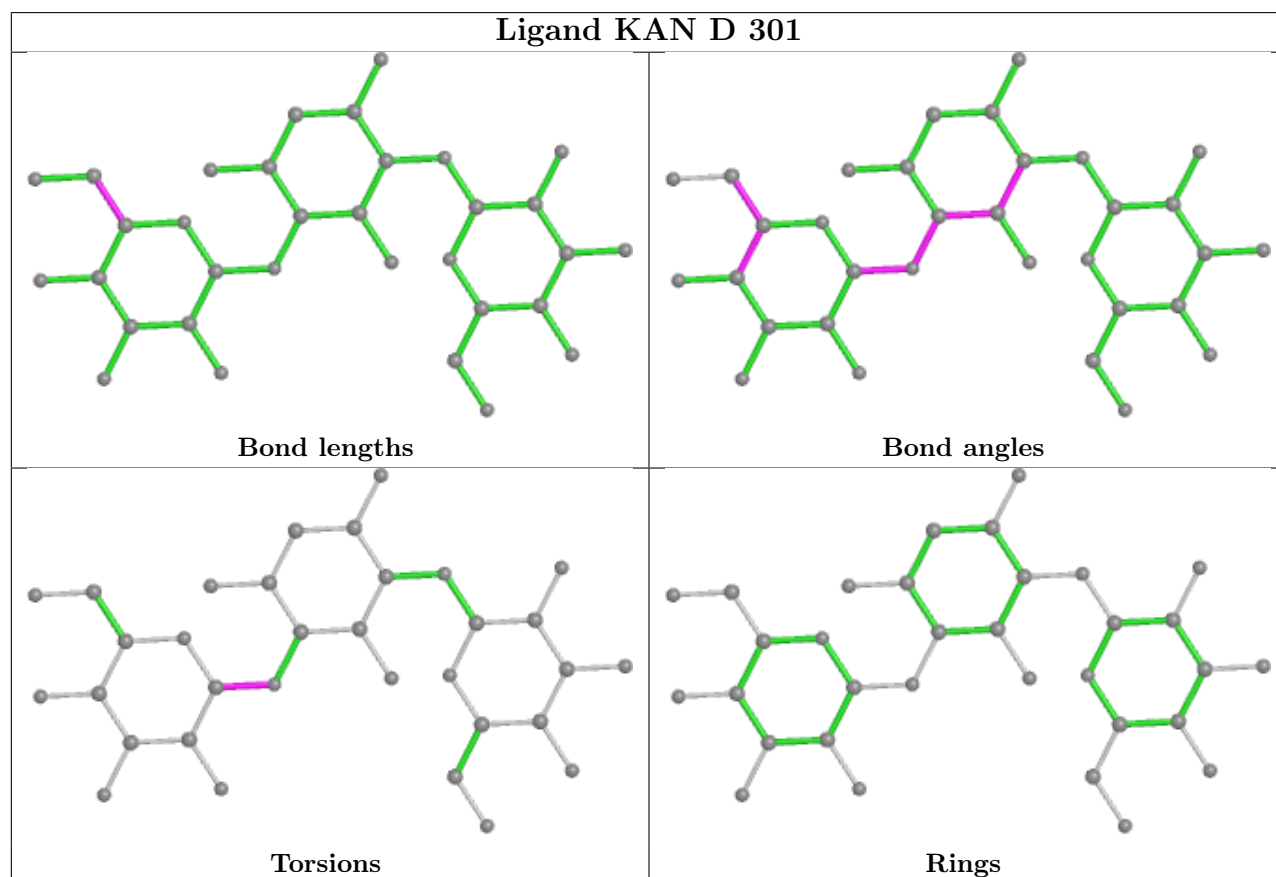
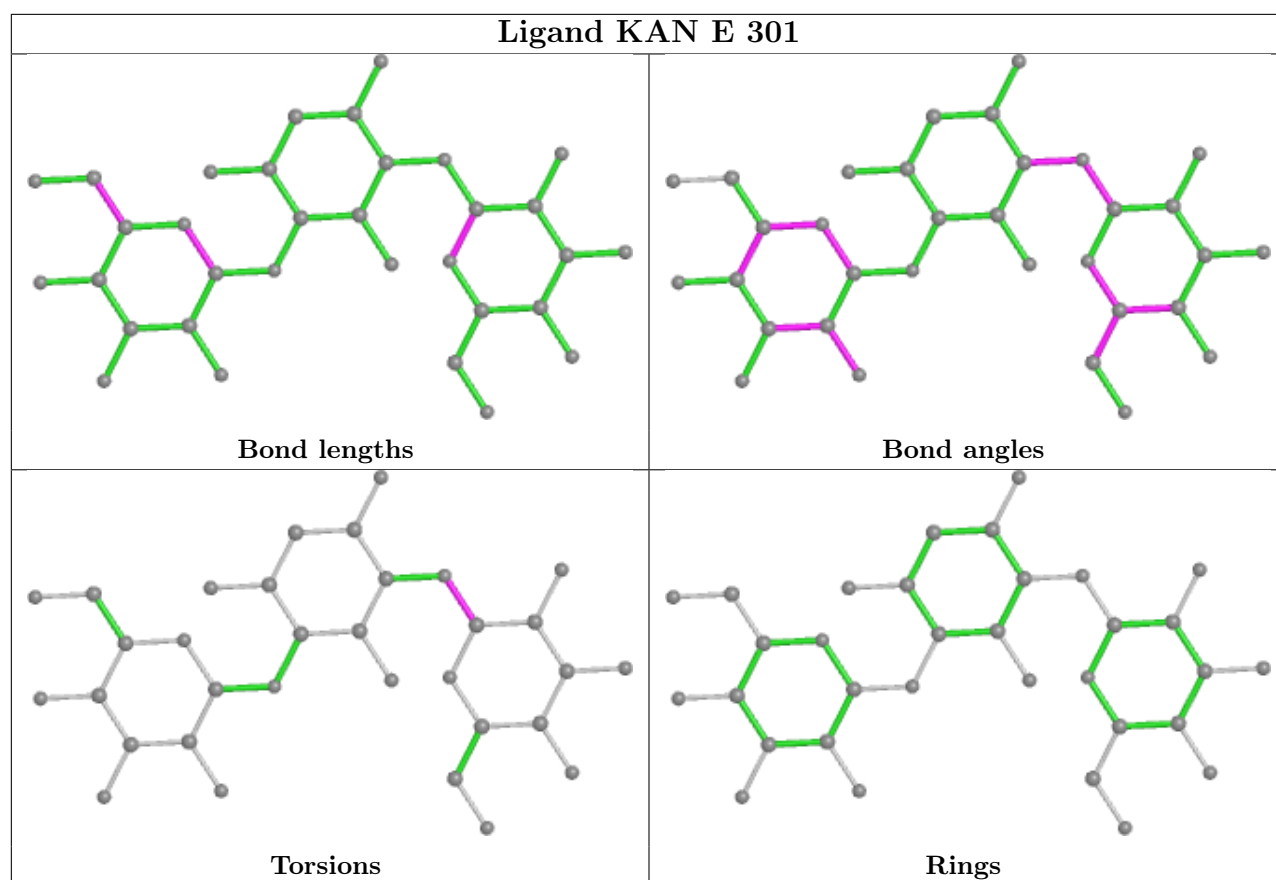
There are no ring outliers.

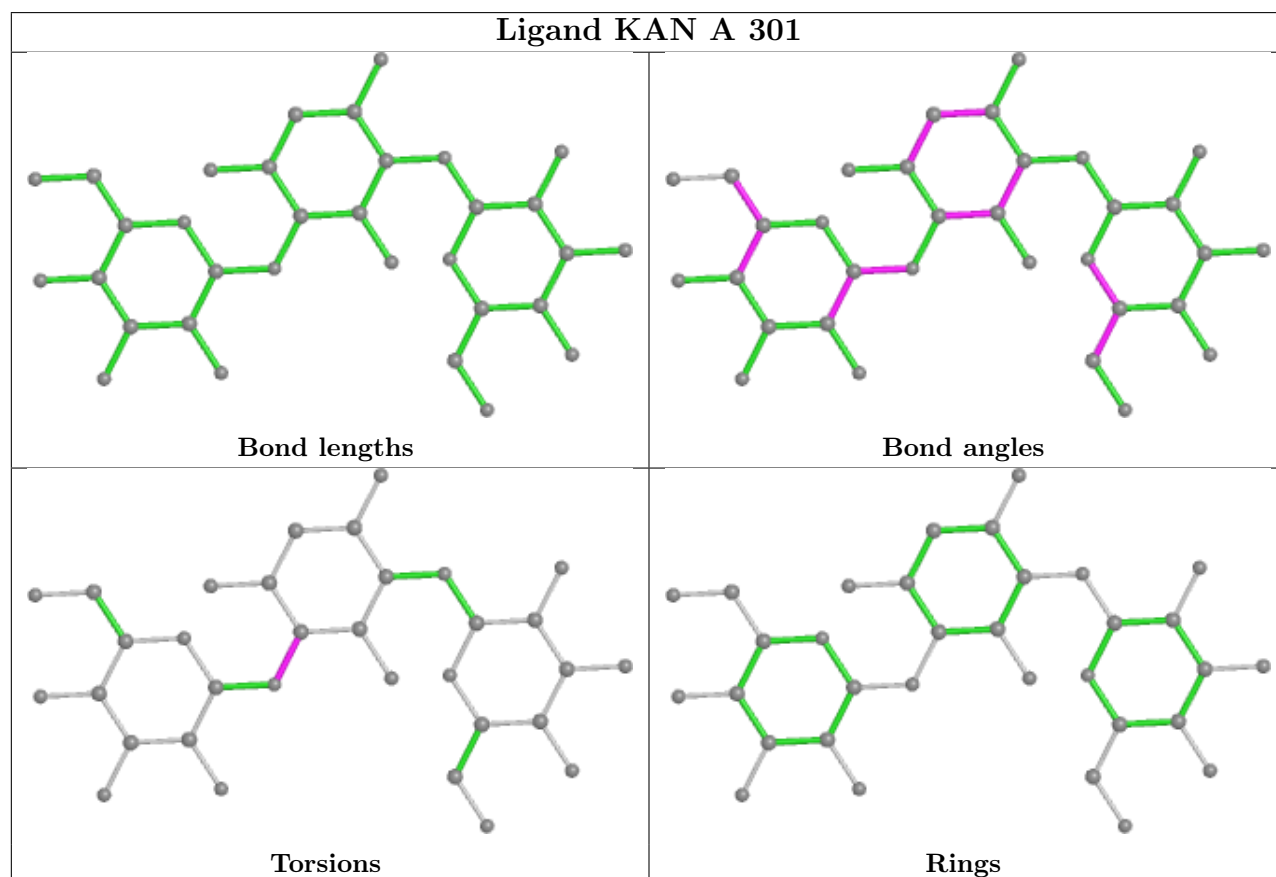
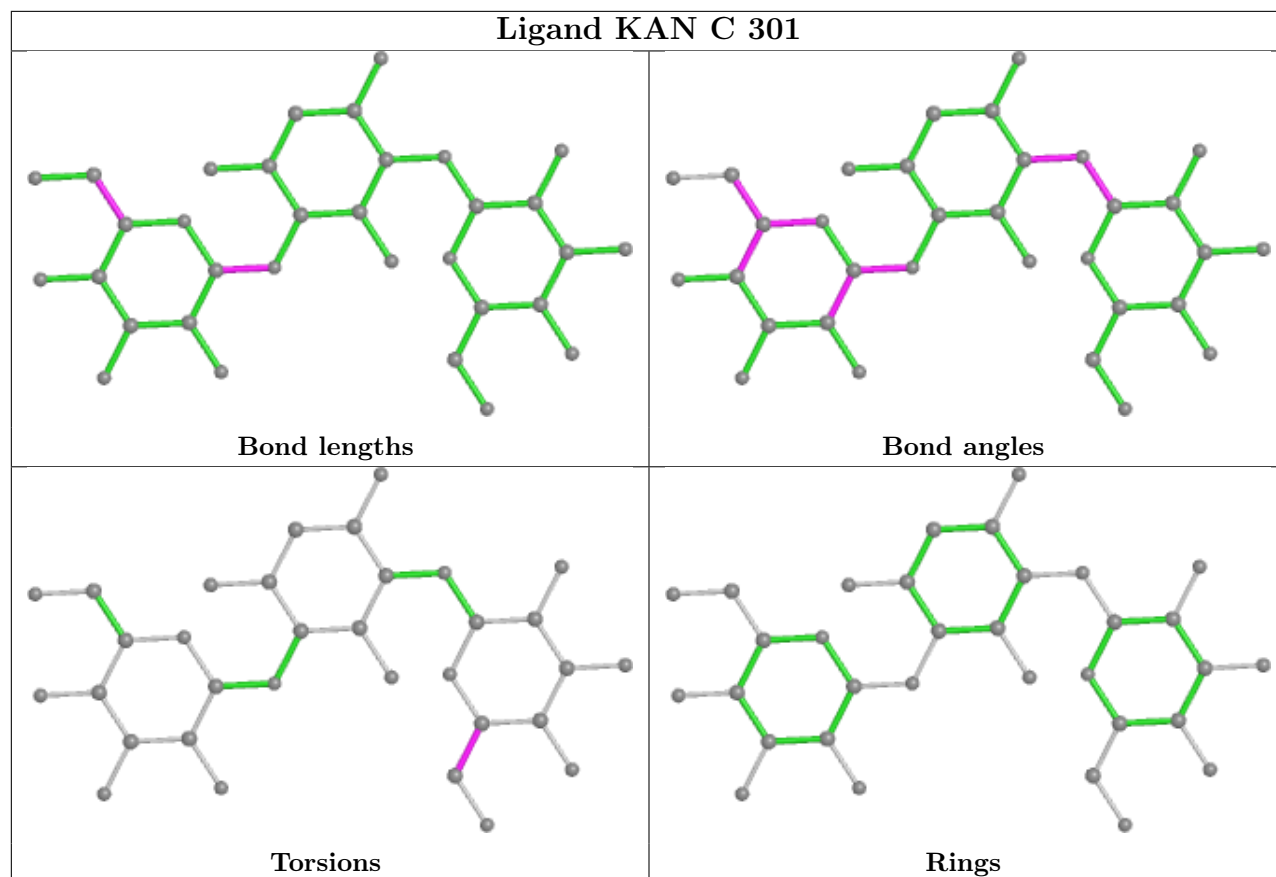
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	KAN	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.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	247/272 (90%)	-0.16	6 (2%) 59 60	27, 46, 81, 95	0
1	B	257/272 (94%)	0.04	23 (8%) 9 10	30, 48, 131, 165	0
1	C	256/272 (94%)	-0.10	15 (5%) 22 24	29, 46, 108, 153	0
1	D	236/272 (86%)	0.63	36 (15%) 2 2	41, 67, 139, 197	0
1	E	258/272 (94%)	-0.19	9 (3%) 44 47	32, 46, 77, 113	0
1	F	239/272 (87%)	-0.12	9 (3%) 40 43	30, 47, 117, 148	0
All	All	1493/1632 (91%)	0.01	98 (6%) 18 20	27, 49, 112, 197	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	41	TYR	8.6
1	D	42	ARG	7.8
1	D	29	ALA	7.7
1	D	31	ASP	6.7
1	C	19	LEU	6.6
1	D	28	TRP	6.6
1	F	24	TYR	5.8
1	C	5	GLN	5.7
1	E	14	ARG	5.7
1	B	28	TRP	5.7
1	B	47	PRO	5.5
1	D	30	ARG	5.3
1	D	43	LEU	5.3
1	B	24	TYR	5.2
1	C	24	TYR	5.1
1	D	51	GLU	5.1
1	D	38	ALA	4.9
1	C	6	ARG	4.9
1	A	47	PRO	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	36	SER	4.7
1	B	32	ASN	4.7
1	B	2	SER	4.7
1	C	7	GLU	4.6
1	F	23	LEU	4.5
1	B	48	ASN	4.5
1	F	48	ASN	4.5
1	E	36	SER	4.4
1	A	19	LEU	4.2
1	B	33	VAL	4.2
1	D	116	SER	4.0
1	D	48	ASN	4.0
1	D	26	TYR	3.9
1	F	42	ARG	3.9
1	E	33	VAL	3.9
1	D	27	ARG	3.9
1	B	44	TYR	3.8
1	D	44	TYR	3.6
1	D	47	PRO	3.6
1	B	14	ARG	3.5
1	B	15	LEU	3.5
1	F	22	ASP	3.5
1	B	37	GLY	3.5
1	C	36	SER	3.5
1	C	8	THR	3.5
1	B	4	ILE	3.4
1	F	46	LYS	3.3
1	C	35	GLN	3.2
1	B	27	ARG	3.2
1	D	115	ASP	3.1
1	D	50	PRO	3.1
1	D	124	LEU	3.1
1	E	19	LEU	3.1
1	C	34	GLY	3.0
1	A	172	GLY	3.0
1	E	34	GLY	3.0
1	D	107	PHE	3.0
1	B	22	ASP	2.9
1	F	27	ARG	2.9
1	B	3	HIS	2.9
1	C	11	SER	2.8
1	D	45	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	35	GLN	2.8
1	D	46	LYS	2.7
1	D	101	ILE	2.6
1	B	49	ALA	2.6
1	D	249	GLN	2.6
1	E	15	LEU	2.6
1	B	187	PRO	2.5
1	A	48	ASN	2.5
1	D	49	ALA	2.5
1	C	27	ARG	2.5
1	B	25	GLY	2.5
1	D	255	ASN	2.5
1	A	173	TRP	2.4
1	B	5	GLN	2.4
1	D	111	GLU	2.4
1	D	187	PRO	2.4
1	D	119	ASN	2.4
1	C	33	VAL	2.4
1	D	254	ASP	2.4
1	D	212	ILE	2.3
1	F	26	TYR	2.3
1	D	113	TYR	2.2
1	F	44	TYR	2.2
1	C	102	PRO	2.2
1	A	190	PRO	2.2
1	D	232	LEU	2.1
1	E	168	ASP	2.1
1	B	41	TYR	2.1
1	B	50	PRO	2.1
1	D	190	PRO	2.1
1	E	18	ASN	2.1
1	C	13	PRO	2.1
1	D	256	PRO	2.1
1	D	108	GLN	2.0
1	C	12	ARG	2.0
1	B	46	LYS	2.0
1	D	189	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

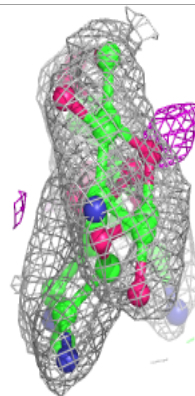
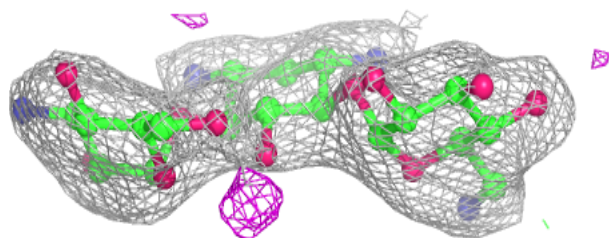
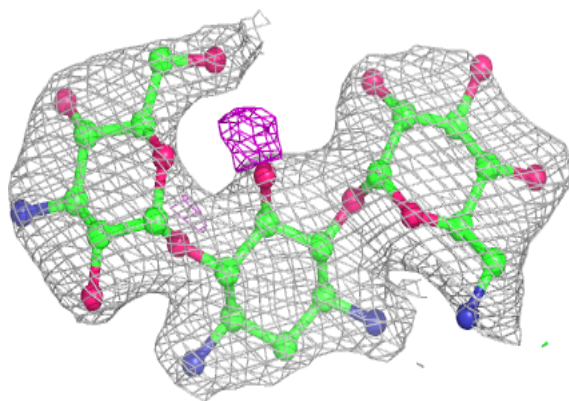
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ACT	A	303	4/4	0.85	0.23	91,91,91,92	0
4	ACT	F	302	4/4	0.91	0.16	74,74,74,74	0
4	ACT	C	303	4/4	0.93	0.13	77,77,77,77	0
4	ACT	D	302	4/4	0.93	0.17	83,83,83,83	0
2	KAN	D	301	33/33	0.93	0.18	36,57,96,300	0
4	ACT	B	302	4/4	0.94	0.09	77,77,78,78	0
4	ACT	C	304	4/4	0.94	0.17	77,78,79,79	0
2	KAN	A	301	33/33	0.95	0.10	32,47,71,91	0
2	KAN	C	301	33/33	0.96	0.09	21,41,63,99	0
2	KAN	E	301	33/33	0.96	0.09	25,39,86,142	0
2	KAN	F	301	33/33	0.96	0.09	23,37,55,111	0
2	KAN	B	301	33/33	0.97	0.08	19,34,52,112	0
3	537	A	302	17/17	0.97	0.10	32,44,83,300	0
3	537	C	302	17/17	0.97	0.09	30,42,75,96	0
3	537	E	302	17/17	0.99	0.08	26,35,65,66	0

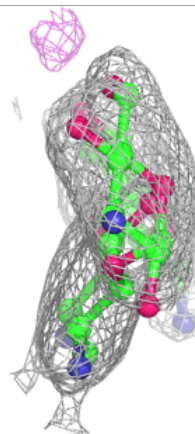
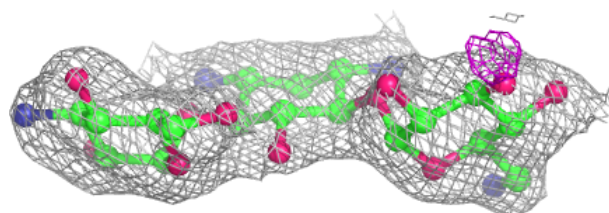
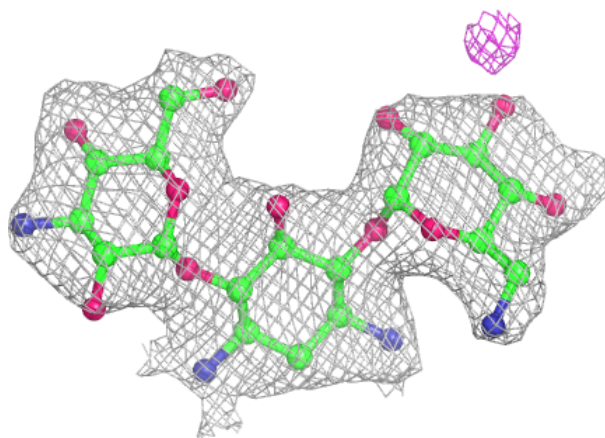
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

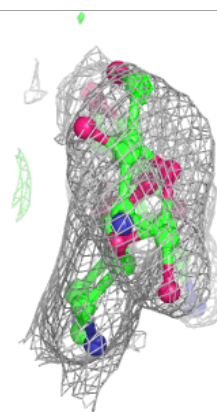
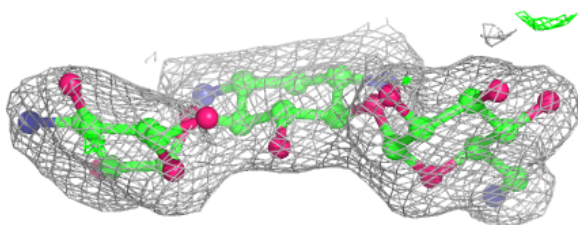
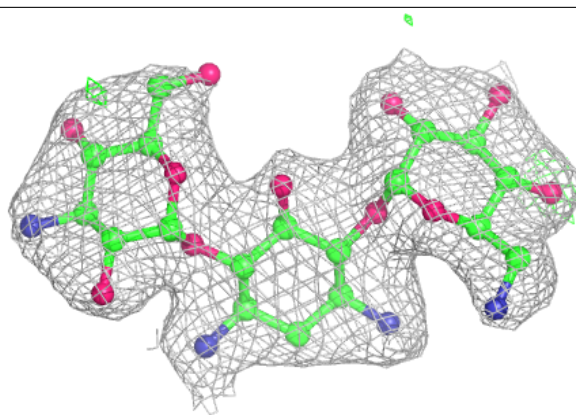
**Electron density around KAN A 301:**

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

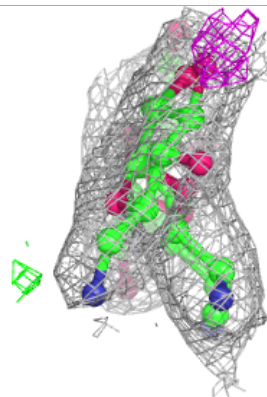
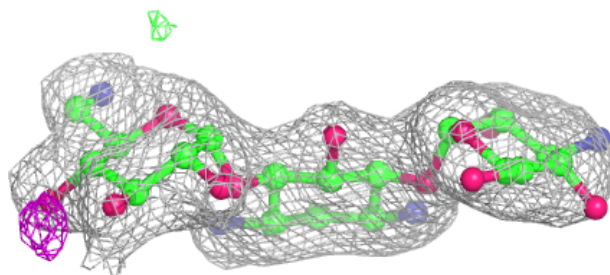
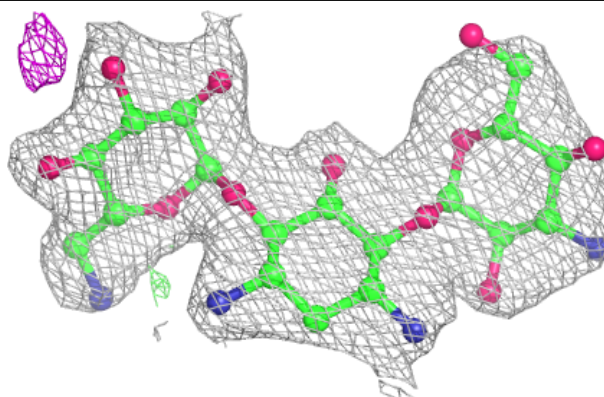


Electron density around KAN C 301:

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

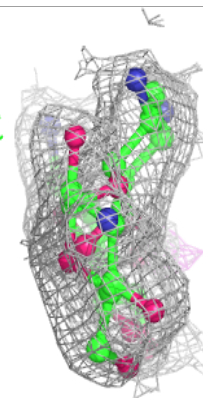
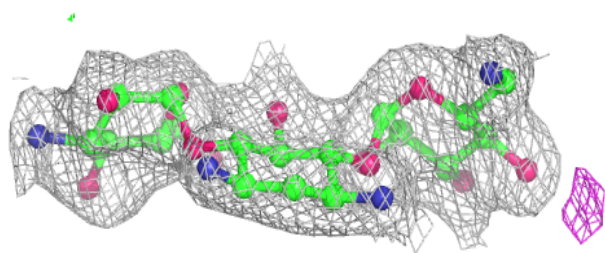
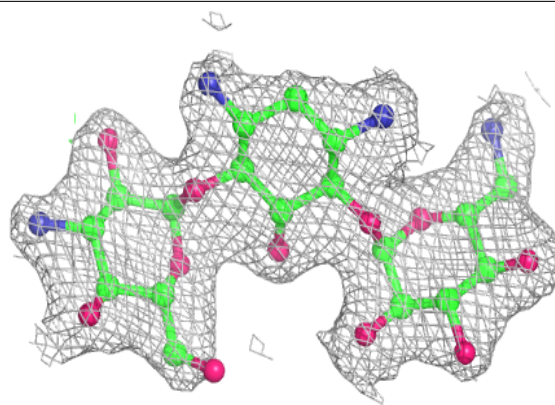
**Electron density around KAN E 301:**

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

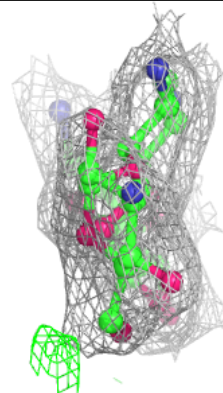
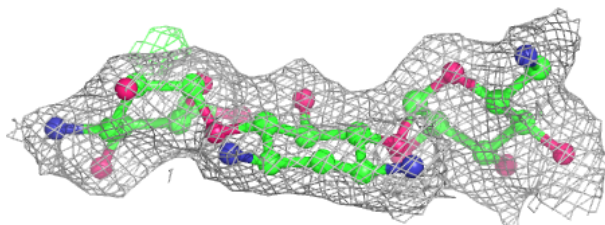
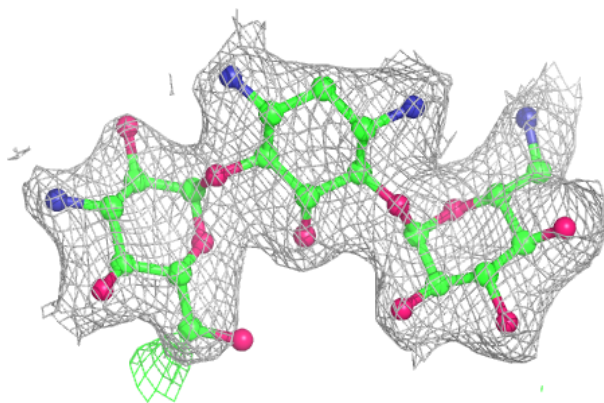


Electron density around KAN F 301:

$2mF_o-DF_c$ (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.