



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:28 PM UTC

PDB ID : 4FEW / pdb_00004few
Title : Crystal structure of the aminoglycoside phosphotransferase APH(3')-Ia, with substrate kanamycin and small molecule inhibitor pyrazolopyrimidine PP2
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 : 1.98 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>.

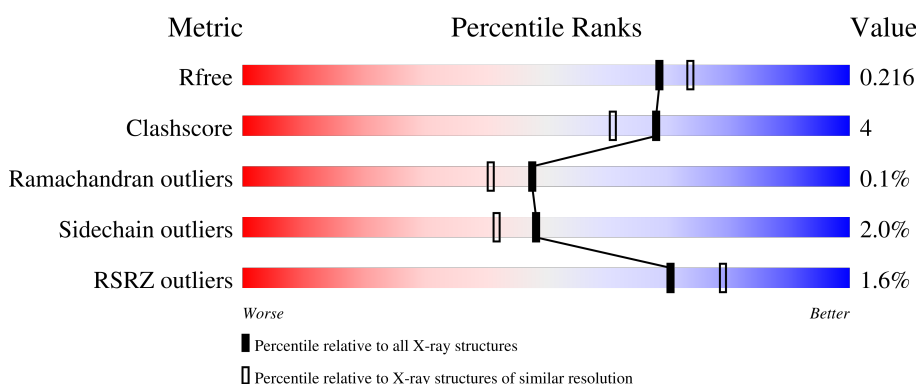
The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

i

X-RAY DIFFRACTION

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}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	90% 7% ..
1	B	272	85% 9% • 6%
1	C	272	86% 7% • 7%
1	D	272	89% 8% ..
1	E	272	88% 5% 7%

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Mol	Chain	Length	Quality of chain
1	F	272	2% 85% 12%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14307 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.

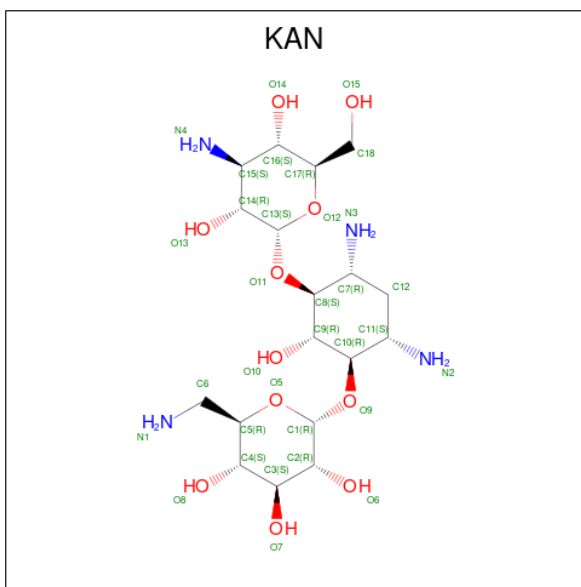
- Molecule 1 is a protein called Aminoglycoside 3'-phosphotransferase AphA1-IAB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	Se	0	1	0
			2143	1365	371	396	5	6			
1	B	256	Total	C	N	O	S	Se	0	0	0
			2071	1323	359	378	5	6			
1	C	254	Total	C	N	O	S	Se	0	5	0
			2081	1331	358	382	4	6			
1	D	266	Total	C	N	O	S	Se	0	5	0
			2176	1385	378	401	5	7			
1	E	254	Total	C	N	O	S	Se	0	4	0
			2077	1326	358	383	4	6			
1	F	266	Total	C	N	O	S	Se	0	4	0
			2178	1387	384	395	5	7			

There are 6 discrepancies between the modelled and reference sequences:

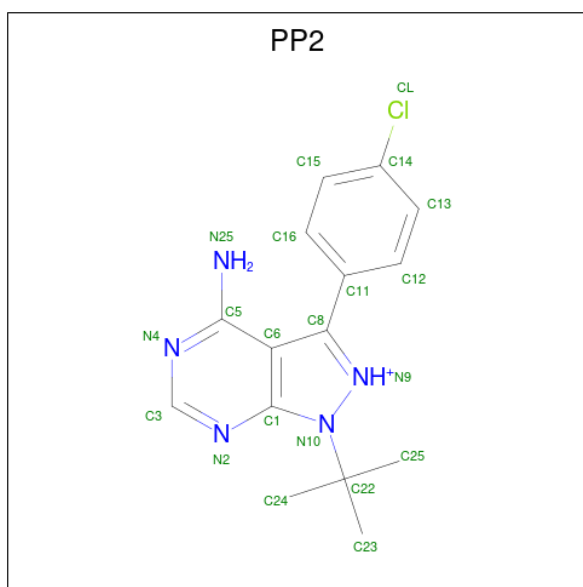
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP B0VD92
B	0	GLY	-	expression tag	UNP B0VD92
C	0	GLY	-	expression tag	UNP B0VD92
D	0	GLY	-	expression tag	UNP B0VD92
E	0	GLY	-	expression tag	UNP B0VD92
F	0	GLY	-	expression tag	UNP B0VD92

- Molecule 2 is KANAMYCIN A (CCD ID: 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		

- Molecule 3 is 1-TERT-BUTYL-3-(4-CHLORO-PHENYL)-1H-PYRAZOLO[3,4-D]PYRIMIDIN-4-YLAMINE (CCD ID: PP2) (formula: $C_{15}H_{17}ClN_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			21	15	1	5		
3	B	1	Total	C	Cl	N	0	0
			21	15	1	5		
3	C	1	Total	C	Cl	N	0	1
			42	30	2	10		
3	D	1	Total	C	Cl	N	0	0
			21	15	1	5		
3	E	1	Total	C	Cl	N	0	0
			21	15	1	5		
3	F	1	Total	C	Cl	N	0	0
			21	15	1	5		

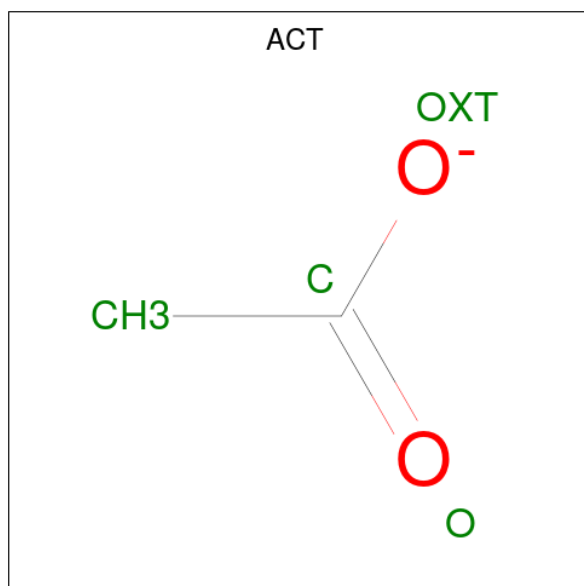
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		
4	D	2	Total	Na	0	0
			2	2		
4	E	1	Total	Na	0	0
			1	1		
4	F	2	Total	Na	0	0
			2	2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

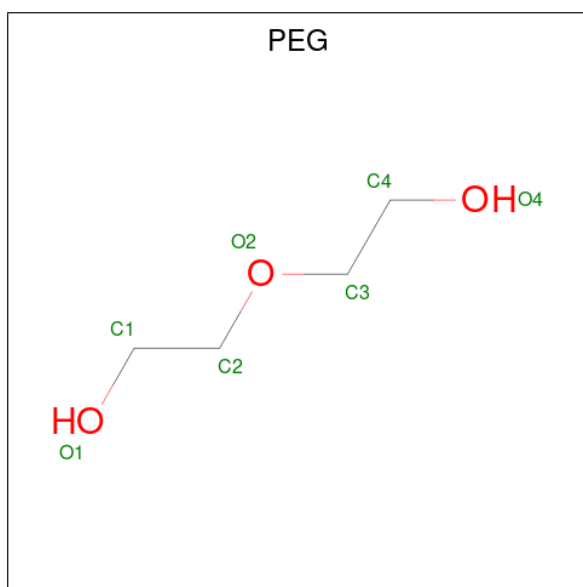
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	231	Total	O	0	6
			237	237		
8	B	139	Total	O	0	3
			142	142		
8	C	193	Total	O	0	1
			194	194		
8	D	214	Total	O	0	3
			217	217		
8	E	189	Total	O	0	2
			191	191		
8	F	204	Total	O	0	5
			209	209		

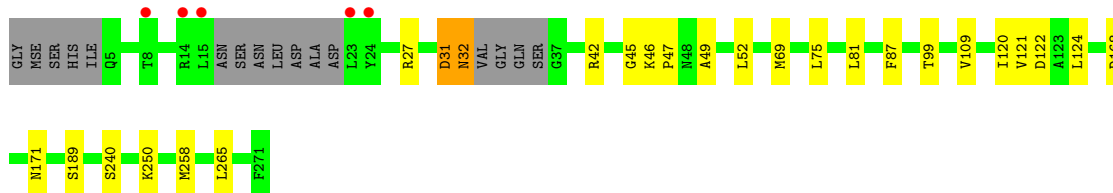
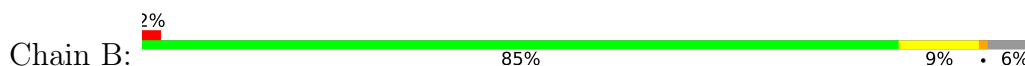
3 Residue-property plots [i](#)

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.

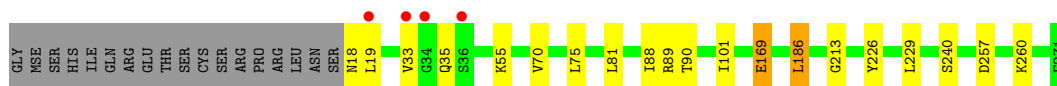
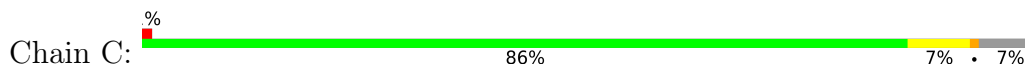
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



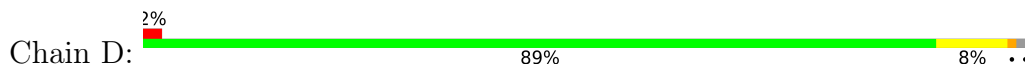
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB



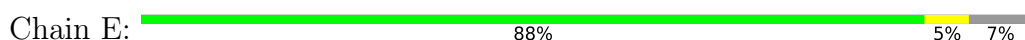
- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

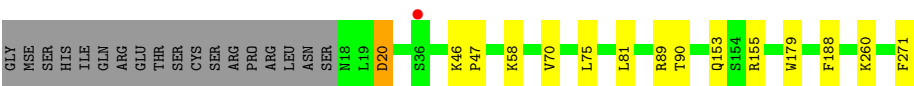


- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB

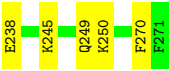
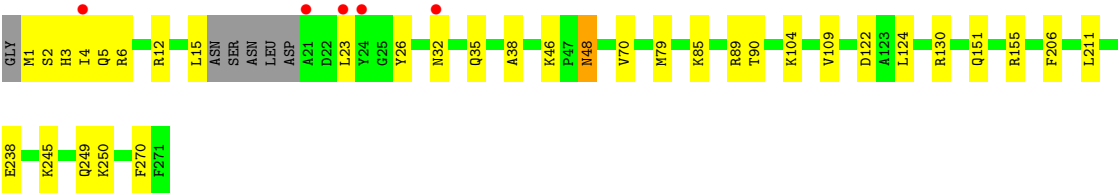
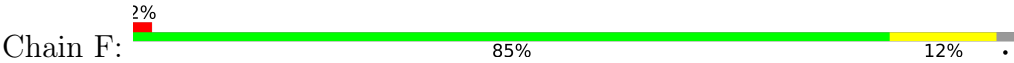


- Molecule 1: Aminoglycoside 3'-phosphotransferase AphA1-IAB





● 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	57.28Å 93.58Å 96.40Å 61.22° 73.18° 87.35°	Depositor
Resolution (Å)	23.90 – 1.98 23.90 – 1.98	Depositor EDS
% Data completeness (in resolution range)	92.2 (23.90-1.98) 92.4 (23.90-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.157 , 0.216 0.159 , 0.216	Depositor DCC
R_{free} test set	5736 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,-h-k+l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14307	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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: CL, PEG, NA, ACT, KAN, PP2

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	0.47	0/2195	0.74	0/2969
1	B	0.42	0/2118	0.72	0/2860
1	C	0.47	0/2135	0.72	0/2888
1	D	0.46	0/2234	0.74	2/3017 (0.1%)
1	E	0.46	0/2128	0.75	0/2878
1	F	0.46	0/2232	0.74	0/3010
All	All	0.46	0/13042	0.74	2/17622 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	23	LEU	N-CA-C	-6.90	104.48	113.17
1	D	240	SER	N-CA-C	5.09	112.71	108.13

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	2143	0	2082	14	0
1	B	2071	0	2013	16	0
1	C	2081	0	2023	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2176	0	2117	14	0
1	E	2077	0	2011	9	0
1	F	2178	0	2133	18	0
2	A	33	0	36	0	0
2	B	33	0	36	0	0
2	C	33	0	36	0	0
2	D	33	0	36	0	0
2	E	33	0	36	0	0
2	F	33	0	36	0	0
3	A	21	0	17	2	0
3	B	21	0	17	2	0
3	C	42	0	34	6	0
3	D	21	0	17	2	0
3	E	21	0	17	3	0
3	F	21	0	17	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
5	A	1	0	0	0	0
6	A	4	0	3	0	0
6	B	4	0	3	0	0
6	D	8	0	6	0	0
6	E	4	0	3	0	0
6	F	4	0	3	0	0
7	C	7	0	8	0	0
7	F	7	0	8	0	0
8	A	237	0	0	3	0
8	B	142	0	0	1	0
8	C	194	0	0	1	0
8	D	217	0	0	1	0
8	E	191	0	0	1	0
8	F	209	0	0	0	0
All	All	14307	0	12748	93	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 (93) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:302[A]:PP2:H3	3:C:302[A]:PP2:H12	1.10	1.16
3:D:302:PP2:H3	3:D:302:PP2:H12	1.05	1.15
3:A:302:PP2:H3	3:A:302:PP2:H12	1.05	1.12
3:F:302:PP2:H3	3:F:302:PP2:H12	1.01	1.11
3:C:302[B]:PP2:H3	3:C:302[B]:PP2:H12	1.11	1.11
3:B:302:PP2:H3	3:B:302:PP2:H12	1.09	1.08
3:E:302:PP2:H3	3:E:302:PP2:H12	1.15	1.06
3:F:302:PP2:H12	3:F:302:PP2:N25	1.82	0.94
3:D:302:PP2:H12	3:D:302:PP2:N25	1.85	0.91
3:A:302:PP2:H12	3:A:302:PP2:N25	1.88	0.88
3:C:302[B]:PP2:H12	3:C:302[B]:PP2:N25	1.91	0.86
3:B:302:PP2:H12	3:B:302:PP2:N25	1.92	0.85
3:C:302[A]:PP2:H12	3:C:302[A]:PP2:N25	1.91	0.84
3:E:302:PP2:H12	3:E:302:PP2:N25	1.92	0.84
1:F:89[A]:ARG:NH1	1:F:90:THR:O	2.21	0.74
1:D:256:PRO:HB2	1:D:258:MSE:HE3	1.72	0.72
3:E:302:PP2:H3	3:E:302:PP2:C12	2.00	0.69
1:E:89[B]:ARG:NH1	1:E:90:THR:O	2.27	0.67
1:C:89[A]:ARG:NH1	1:C:90:THR:O	2.28	0.66
1:C:260:LYS:NZ	8:C:558:HOH:O	2.29	0.62
1:C:19:LEU:HD22	1:C:88:ILE:HD12	1.82	0.61
1:C:186:LEU:HD23	1:C:186:LEU:H	1.67	0.60
1:F:79:MSE:SE	1:F:130:ARG:HG2	2.52	0.60
1:B:46:LYS:HD2	1:B:47:PRO:HD2	1.82	0.60
1:F:32:ASN:HB2	1:F:35:GLN:HB2	1.84	0.60
1:E:58:LYS:NZ	8:E:583:HOH:O	2.30	0.59
1:F:155[A]:ARG:NH1	1:F:270:PHE:O	2.35	0.59
1:B:27:ARG:HG3	1:B:45:GLY:HA3	1.85	0.57
1:A:30:ARG:NH1	8:A:599:HOH:O	2.30	0.57
1:F:151:GLN:O	1:F:155[A]:ARG:HG3	2.06	0.55
1:A:124:LEU:HD22	1:A:204:LEU:HD13	1.88	0.55
1:E:70:VAL:HG11	1:F:70:VAL:HG11	1.88	0.55
1:D:4:ILE:HG23	1:D:6:ARG:HG3	1.89	0.54
1:E:20:ASP:OD1	1:E:20:ASP:N	2.40	0.54
1:F:124:LEU:HD23	1:F:211:LEU:HD11	1.90	0.53
1:A:166:PHE:HZ	1:A:175[B]:VAL:HG12	1.75	0.52
1:A:6:ARG:HH11	1:A:6:ARG:HB3	1.75	0.52
1:C:75:LEU:HB3	1:C:81:LEU:HD11	1.90	0.52
1:A:7:GLU:OE2	1:B:42:ARG:NH1	2.41	0.51
1:F:109:VAL:HG21	1:F:206:PHE:HB2	1.93	0.51
1:A:6:ARG:HB3	1:A:6:ARG:NH1	2.25	0.51
1:C:70[A]:VAL:HG11	1:D:70[A]:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:ASP:OD1	1:F:250:LYS:HG3	2.11	0.49
1:D:256:PRO:HB2	1:D:258:MSE:CE	2.40	0.48
3:C:302[A]:PP2:H15	1:D:5:GLN:OE1	2.12	0.48
1:D:124:LEU:HD22	1:D:204:LEU:HD13	1.95	0.48
1:A:188:PHE:CD1	1:A:260:LYS:HE2	2.49	0.48
1:C:169:GLU:HA	1:F:1:MSE:HE3	1.96	0.48
1:D:122:ASP:OD1	1:D:250:LYS:HG3	2.13	0.47
1:F:12:ARG:HH21	1:F:15:LEU:HD11	1.79	0.47
1:C:257:ASP:CG	1:C:260:LYS:HG3	2.40	0.47
1:E:75:LEU:HB3	1:E:81:LEU:HD11	1.96	0.47
1:D:89:ARG:NH1	1:D:90:THR:O	2.46	0.46
1:D:258:MSE:HA	1:D:258:MSE:HE2	1.96	0.46
1:E:188:PHE:CD1	1:E:260:LYS:HE2	2.50	0.46
1:A:175[A]:VAL:HG23	8:A:411:HOH:O	2.15	0.46
1:B:52:LEU:HD23	1:B:99:THR:HA	1.98	0.46
1:A:27:ARG:HE	1:A:27:ARG:HB3	1.30	0.46
1:D:56:HIS:HB2	1:D:95:TRP:CZ3	2.51	0.46
1:F:12:ARG:NH2	1:F:15:LEU:HD11	2.31	0.45
1:D:21:ALA:HA	1:D:24:TYR:CZ	2.51	0.45
1:D:148:ARG:HD2	8:D:600:HOH:O	2.16	0.45
1:B:69:MSE:HG3	1:B:87:PHE:CG	2.51	0.44
1:A:19:LEU:O	1:A:23:LEU:HG	2.17	0.44
1:F:26:TYR:CE2	1:F:46:LYS:HD3	2.53	0.44
1:D:70[B]:VAL:HG12	1:D:141:PHE:HZ	1.83	0.43
1:B:121:VAL:HA	1:B:124:LEU:HD12	2.00	0.43
1:C:101:ILE:HD13	1:C:213:GLY:HA3	2.01	0.43
1:B:31:ASP:HA	1:B:32:ASN:HA	1.72	0.42
1:C:169:GLU:CD	1:C:169:GLU:H	2.25	0.42
1:F:245:LYS:HE2	1:F:249:GLN:NE2	2.34	0.42
1:A:75:LEU:HB3	1:A:81:LEU:HD11	2.01	0.42
1:A:245:LYS:NZ	8:A:582:HOH:O	2.42	0.42
1:F:32:ASN:ND2	1:F:38:ALA:O	2.33	0.42
1:B:122:ASP:OD1	1:B:250:LYS:HG3	2.19	0.42
1:E:155:ARG:HH21	1:E:271:PHE:HA	1.85	0.42
1:B:265:LEU:HD23	1:B:265:LEU:HA	1.79	0.41
1:C:55:LYS:HE3	3:C:302[B]:PP2:H15	2.01	0.41
1:E:46:LYS:HA	1:E:47:PRO:HD2	1.95	0.41
1:B:46:LYS:HG2	1:B:49:ALA:HB3	2.02	0.41
1:D:23:LEU:HD12	1:D:23:LEU:HA	1.82	0.41
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.92	0.41
1:B:69:MSE:HE3	1:B:69:MSE:HB3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:ILE:HG23	1:F:6[B]:ARG:HG3	2.02	0.41
1:B:75:LEU:HB3	1:B:81:LEU:HD11	2.03	0.41
1:B:168:ASP:O	1:B:171:ASN:HB2	2.21	0.41
1:B:258:MSE:HE3	8:B:520:HOH:O	2.20	0.41
1:E:153:GLN:HB2	1:E:179:TRP:CH2	2.55	0.41
1:F:2:SER:HB2	1:F:3:HIS:CD2	2.56	0.41
1:B:109:VAL:HG12	1:B:120:ILE:HD11	2.03	0.41
1:A:89:ARG:HB3	1:B:87:PHE:HB3	2.03	0.40
1:F:48:ASN:OD1	1:F:48:ASN:N	2.54	0.40
1:C:226:TYR:HA	1:C:229:LEU:HB2	2.04	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	265/272 (97%)	257 (97%)	7 (3%)	1 (0%)	30	20
1	B	250/272 (92%)	247 (99%)	3 (1%)	0	100	100
1	C	257/272 (94%)	251 (98%)	6 (2%)	0	100	100
1	D	267/272 (98%)	263 (98%)	4 (2%)	0	100	100
1	E	256/272 (94%)	246 (96%)	10 (4%)	0	100	100
1	F	266/272 (98%)	260 (98%)	6 (2%)	0	100	100
All	All	1561/1632 (96%)	1524 (98%)	36 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	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	234/231 (101%)	228 (97%)	6 (3%)	40	32
1	B	225/231 (97%)	221 (98%)	4 (2%)	51	46
1	C	226/231 (98%)	220 (97%)	6 (3%)	39	31
1	D	238/231 (103%)	234 (98%)	4 (2%)	53	48
1	E	225/231 (97%)	224 (100%)	1 (0%)	84	82
1	F	237/231 (103%)	230 (97%)	7 (3%)	36	27
All	All	1385/1386 (100%)	1357 (98%)	28 (2%)	48	42

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	16	ASN
1	A	20	ASP
1	A	27	ARG
1	A	33	VAL
1	A	216	ASP
1	B	31	ASP
1	B	32	ASN
1	B	189	SER
1	B	240	SER
1	C	18	ASN
1	C	33	VAL
1	C	35	GLN
1	C	169	GLU
1	C	186	LEU
1	C	240	SER
1	D	2	SER
1	D	4	ILE
1	D	110	LEU
1	D	238	GLU
1	E	20	ASP
1	F	5	GLN

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Mol	Chain	Res	Type
1	F	23	LEU
1	F	48	ASN
1	F	85[A]	LYS
1	F	85[B]	LYS
1	F	104	LYS
1	F	238	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	255	ASN
1	A	259	ASN
1	B	86	HIS
1	B	138	ASN
1	B	158	ASN
1	C	35	GLN
1	C	73	ASN
1	C	259	ASN
1	D	73	ASN
1	D	138	ASN
1	D	262	GLN
1	E	73	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 29 ligands modelled in this entry, 8 are monoatomic - leaving 21 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	PP2	E	302	-	23,23,23	2.13	3 (13%)	32,35,35	2.46	10 (31%)
7	PEG	C	303	-	6,6,6	1.13	0	5,5,5	1.50	0
3	PP2	A	302	-	23,23,23	2.27	4 (17%)	32,35,35	2.22	10 (31%)
2	KAN	A	301	-	34,35,35	0.86	2 (5%)	47,52,52	1.27	6 (12%)
2	KAN	B	301	-	34,35,35	0.63	0	47,52,52	1.34	6 (12%)
3	PP2	D	302	-	23,23,23	2.13	3 (13%)	32,35,35	2.47	12 (37%)
3	PP2	B	302	-	23,23,23	2.19	3 (13%)	32,35,35	2.32	9 (28%)
6	ACT	E	304	4	3,3,3	0.77	0	3,3,3	1.25	0
2	KAN	D	301	-	34,35,35	0.82	1 (2%)	47,52,52	1.38	7 (14%)
2	KAN	E	301	-	34,35,35	0.91	1 (2%)	47,52,52	1.50	5 (10%)
7	PEG	F	306	-	6,6,6	1.06	0	5,5,5	1.68	2 (40%)
2	KAN	F	301	-	34,35,35	0.88	1 (2%)	47,52,52	1.41	6 (12%)
6	ACT	A	305	4	3,3,3	0.87	0	3,3,3	1.31	0
2	KAN	C	301	-	34,35,35	0.81	1 (2%)	47,52,52	1.43	8 (17%)
6	ACT	D	306	4	3,3,3	0.84	0	3,3,3	1.39	0
6	ACT	B	304	4	3,3,3	0.83	0	3,3,3	1.32	0
6	ACT	F	305	4	3,3,3	0.85	0	3,3,3	1.36	0
3	PP2	C	302[A]	-	23,23,23	2.22	2 (8%)	32,35,35	2.58	12 (37%)
6	ACT	D	305	-	3,3,3	0.87	0	3,3,3	1.49	0
3	PP2	C	302[B]	-	23,23,23	2.25	3 (13%)	32,35,35	2.47	11 (34%)
3	PP2	F	302	-	23,23,23	2.17	3 (13%)	32,35,35	2.47	9 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PP2	E	302	-	-	0/10/10/10	0/3/3/3
3	PP2	A	302	-	-	3/10/10/10	0/3/3/3
2	KAN	A	301	-	-	2/12/72/72	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KAN	F	301	-	-	2/12/72/72	0/3/3/3
2	KAN	B	301	-	-	1/12/72/72	0/3/3/3
7	PEG	F	306	-	-	1/4/4/4	-
3	PP2	D	302	-	-	3/10/10/10	0/3/3/3
3	PP2	B	302	-	-	3/10/10/10	0/3/3/3
7	PEG	C	303	-	-	1/4/4/4	-
2	KAN	D	301	-	-	1/12/72/72	0/3/3/3
3	PP2	C	302[A]	-	-	2/10/10/10	0/3/3/3
2	KAN	C	301	-	-	2/12/72/72	0/3/3/3
3	PP2	C	302[B]	-	-	1/10/10/10	0/3/3/3
3	PP2	F	302	-	-	2/10/10/10	0/3/3/3
2	KAN	E	301	-	-	2/12/72/72	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	PP2	N10-N9	-7.74	1.23	1.39
3	C	302[A]	PP2	N10-N9	-7.70	1.23	1.39
3	F	302	PP2	N10-N9	-7.66	1.23	1.39
3	A	302	PP2	N10-N9	-7.61	1.24	1.39
3	C	302[B]	PP2	N10-N9	-7.58	1.24	1.39
3	E	302	PP2	N10-N9	-7.58	1.24	1.39
3	D	302	PP2	N10-N9	-7.55	1.24	1.39
3	A	302	PP2	C11-C8	-6.62	1.39	1.49
3	C	302[B]	PP2	C11-C8	-6.50	1.40	1.49
3	C	302[A]	PP2	C11-C8	-6.39	1.40	1.49
3	F	302	PP2	C11-C8	-5.94	1.40	1.49
3	B	302	PP2	C11-C8	-5.79	1.41	1.49
3	D	302	PP2	C11-C8	-5.60	1.41	1.49
3	E	302	PP2	C11-C8	-5.34	1.41	1.49
3	E	302	PP2	C1-N10	-3.08	1.33	1.35
2	F	301	KAN	C14-C15	-2.65	1.50	1.53
3	B	302	PP2	C1-N10	-2.44	1.33	1.35
2	E	301	KAN	O5-C1	2.39	1.48	1.41
3	F	302	PP2	C1-N10	-2.32	1.33	1.35
3	C	302[B]	PP2	C1-N10	-2.30	1.33	1.35
2	A	301	KAN	O5-C5	2.26	1.49	1.44
3	D	302	PP2	C1-N10	-2.23	1.33	1.35
2	D	301	KAN	C16-C15	-2.22	1.50	1.53
2	C	301	KAN	O5-C1	2.13	1.47	1.41
2	A	301	KAN	O11-C13	2.12	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	PP2	C1-N10	-2.02	1.34	1.35
3	A	302	PP2	C6-C5	-2.01	1.40	1.42

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302[A]	PP2	C6-C1-N2	-7.35	119.17	126.97
3	C	302[B]	PP2	C6-C1-N2	-6.64	119.93	126.97
3	F	302	PP2	C6-C1-N2	-6.39	120.19	126.97
3	D	302	PP2	C6-C1-N2	-6.34	120.24	126.97
3	E	302	PP2	C6-C8-N9	-6.11	106.00	110.19
3	E	302	PP2	C6-C1-N2	-6.09	120.51	126.97
3	B	302	PP2	C6-C1-N2	-5.98	120.63	126.97
3	A	302	PP2	C6-C1-N2	-5.92	120.69	126.97
3	B	302	PP2	C6-C8-N9	-5.26	106.58	110.19
3	F	302	PP2	N4-C3-N2	-5.18	120.75	128.58
2	E	301	KAN	O5-C5-C6	5.11	115.89	106.07
3	C	302[B]	PP2	N4-C3-N2	-5.05	120.94	128.58
3	C	302[A]	PP2	N4-C3-N2	-4.99	121.03	128.58
3	D	302	PP2	C6-C8-N9	-4.97	106.78	110.19
3	A	302	PP2	N4-C3-N2	-4.88	121.20	128.58
3	B	302	PP2	N4-C3-N2	-4.84	121.26	128.58
3	D	302	PP2	N4-C3-N2	-4.77	121.36	128.58
3	F	302	PP2	C11-C8-N9	4.76	125.11	118.91
3	E	302	PP2	N4-C3-N2	-4.70	121.47	128.58
3	F	302	PP2	C6-C8-N9	-4.67	106.99	110.19
3	D	302	PP2	C11-C8-N9	4.65	124.96	118.91
3	C	302[A]	PP2	N2-C1-N10	4.60	132.73	125.48
3	E	302	PP2	N2-C1-N10	4.59	132.72	125.48
3	A	302	PP2	N2-C1-N10	4.56	132.67	125.48
3	E	302	PP2	C11-C8-N9	4.42	124.66	118.91
3	F	302	PP2	N2-C1-N10	4.35	132.34	125.48
3	B	302	PP2	N2-C1-N10	4.35	132.34	125.48
3	D	302	PP2	N2-C1-N10	4.27	132.21	125.48
3	C	302[B]	PP2	N2-C1-N10	4.22	132.14	125.48
3	C	302[B]	PP2	C11-C8-N9	4.22	124.39	118.91
3	A	302	PP2	C6-C8-N9	-4.21	107.30	110.19
3	C	302[A]	PP2	C3-N2-C1	4.15	121.97	111.83
3	C	302[B]	PP2	C3-N2-C1	4.02	121.65	111.83
3	C	302[A]	PP2	C11-C8-N9	3.99	124.10	118.91
3	F	302	PP2	C3-N2-C1	3.86	121.25	111.83
3	D	302	PP2	C3-N2-C1	3.68	120.81	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	PP2	C11-C8-N9	3.65	123.66	118.91
3	C	302[B]	PP2	C22-N10-N9	3.62	124.37	117.90
3	C	302[A]	PP2	C22-N10-N9	3.61	124.35	117.90
2	D	301	KAN	O11-C8-C9	3.56	116.29	107.23
3	E	302	PP2	C3-N2-C1	3.52	120.44	111.83
3	B	302	PP2	C3-N2-C1	3.51	120.41	111.83
3	C	302[A]	PP2	C6-C8-N9	-3.51	107.78	110.19
2	C	301	KAN	C17-C16-C15	-3.48	106.83	110.67
3	C	302[B]	PP2	C6-C8-N9	-3.46	107.81	110.19
2	A	301	KAN	O11-C8-C9	3.43	115.96	107.23
3	A	302	PP2	C11-C8-N9	3.43	123.37	118.91
2	E	301	KAN	O11-C8-C9	3.42	115.93	107.23
3	A	302	PP2	C3-N2-C1	3.41	120.16	111.83
2	D	301	KAN	C6-C5-C4	-3.40	104.85	112.80
2	C	301	KAN	O5-C5-C6	3.37	112.55	106.07
2	C	301	KAN	O11-C8-C9	3.31	115.63	107.23
2	F	301	KAN	O11-C8-C9	3.29	115.60	107.23
3	F	302	PP2	C22-N10-N9	3.26	123.73	117.90
2	B	301	KAN	O11-C8-C9	3.21	115.39	107.23
3	C	302[B]	PP2	C6-C8-C11	-3.12	127.58	131.28
2	F	301	KAN	C6-C5-C4	-3.11	105.53	112.80
3	D	302	PP2	C22-N10-N9	3.10	123.44	117.90
3	B	302	PP2	C22-N10-N9	3.08	123.40	117.90
2	F	301	KAN	O5-C5-C6	3.05	111.93	106.07
2	D	301	KAN	C18-C17-C16	-2.98	105.70	113.02
3	B	302	PP2	C12-C11-C8	2.95	124.29	120.64
2	E	301	KAN	C13-C14-C15	2.95	114.36	110.40
3	C	302[A]	PP2	C1-C6-C8	-2.85	102.75	104.74
3	F	302	PP2	C6-C8-C11	-2.85	127.90	131.28
3	C	302[A]	PP2	C16-C11-C8	-2.84	117.13	120.64
3	E	302	PP2	C22-N10-N9	2.82	122.94	117.90
3	C	302[A]	PP2	C6-C8-C11	-2.80	127.96	131.28
3	A	302	PP2	C22-N10-N9	2.77	122.86	117.90
3	C	302[B]	PP2	C1-C6-C8	-2.77	102.81	104.74
2	B	301	KAN	C13-C14-C15	2.75	114.10	110.40
2	F	301	KAN	C17-C16-C15	-2.75	107.63	110.67
2	B	301	KAN	C1-O9-C10	-2.63	111.75	117.98
3	C	302[B]	PP2	C16-C11-C8	-2.59	117.43	120.64
3	D	302	PP2	C6-C8-C11	-2.57	128.23	131.28
2	B	301	KAN	C6-C5-C4	-2.54	106.85	112.80
2	A	301	KAN	O5-C5-C6	2.52	110.92	106.07
2	A	301	KAN	O12-C17-C18	2.52	112.69	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	KAN	C13-C14-C15	2.51	113.77	110.40
3	C	302[A]	PP2	C12-C11-C8	2.50	123.73	120.64
2	E	301	KAN	C6-C5-C4	-2.50	106.96	112.80
3	C	302[B]	PP2	C12-C11-C8	2.46	123.68	120.64
2	C	301	KAN	C6-C5-C4	-2.46	107.06	112.80
2	D	301	KAN	C17-C16-C15	-2.41	108.00	110.67
3	D	302	PP2	C15-C14-CL	2.38	122.87	119.36
3	F	302	PP2	C15-C14-CL	2.37	122.86	119.36
2	B	301	KAN	C16-C15-C14	-2.36	105.93	111.06
2	F	301	KAN	C10-C9-C8	2.34	113.86	109.11
2	A	301	KAN	C16-C15-C14	-2.33	106.01	111.06
3	A	302	PP2	C12-C11-C8	2.32	123.50	120.64
3	A	302	PP2	C16-C11-C8	-2.29	117.80	120.64
3	C	302[A]	PP2	C5-C6-C1	2.28	117.44	115.74
2	D	301	KAN	C13-C14-C15	2.26	113.44	110.40
2	D	301	KAN	O14-C16-C15	-2.25	106.17	110.22
2	E	301	KAN	C17-C16-C15	-2.25	108.18	110.67
3	B	302	PP2	C16-C11-C8	-2.22	117.89	120.64
2	B	301	KAN	O5-C5-C6	2.21	110.31	106.07
2	A	301	KAN	C6-C5-C4	-2.20	107.66	112.80
3	E	302	PP2	C15-C14-C13	-2.19	118.52	121.24
3	E	302	PP2	C15-C14-CL	2.18	122.57	119.36
2	F	301	KAN	C14-C15-N4	-2.16	106.63	111.05
2	A	301	KAN	C17-C16-C15	-2.16	108.28	110.67
7	F	306	PEG	O2-C2-C1	2.15	119.61	110.11
2	C	301	KAN	O11-C13-C14	-2.14	102.81	108.09
7	F	306	PEG	O2-C3-C4	2.13	119.52	110.11
3	D	302	PP2	C25-C22-N10	2.06	111.81	108.87
3	A	302	PP2	C3-N4-C5	2.06	122.11	118.73
2	C	301	KAN	O9-C10-C9	2.05	112.44	107.23
3	D	302	PP2	C15-C14-C13	-2.04	118.71	121.24
2	C	301	KAN	O13-C14-C15	2.03	113.87	110.22
3	D	302	PP2	C1-C6-C8	-2.03	103.32	104.74
2	D	301	KAN	C10-C9-C8	2.02	113.20	109.11
3	E	302	PP2	C6-C8-C11	-2.01	128.89	131.28

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	306	PEG	C1-C2-O2-C3
7	C	303	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	D	301	KAN	C9-C8-O11-C13
3	A	302	PP2	C12-C11-C8-C6
3	B	302	PP2	C12-C11-C8-C6
2	E	301	KAN	C9-C8-O11-C13
2	C	301	KAN	C9-C8-O11-C13
2	A	301	KAN	C9-C8-O11-C13
2	F	301	KAN	C9-C8-O11-C13
3	D	302	PP2	C12-C11-C8-C6
3	F	302	PP2	C12-C11-C8-C6
3	A	302	PP2	C16-C11-C8-C6
3	B	302	PP2	C16-C11-C8-C6
2	B	301	KAN	C9-C8-O11-C13
2	C	301	KAN	C9-C10-O9-C1
2	E	301	KAN	C9-C10-O9-C1
3	C	302[A]	PP2	C12-C11-C8-C6
3	C	302[B]	PP2	C12-C11-C8-C6
2	F	301	KAN	C9-C10-O9-C1
3	D	302	PP2	C16-C11-C8-C6
3	F	302	PP2	C16-C11-C8-C6
2	A	301	KAN	C9-C10-O9-C1
3	A	302	PP2	C12-C11-C8-N9
3	B	302	PP2	C12-C11-C8-N9
3	D	302	PP2	C12-C11-C8-N9
3	C	302[A]	PP2	C16-C11-C8-C6

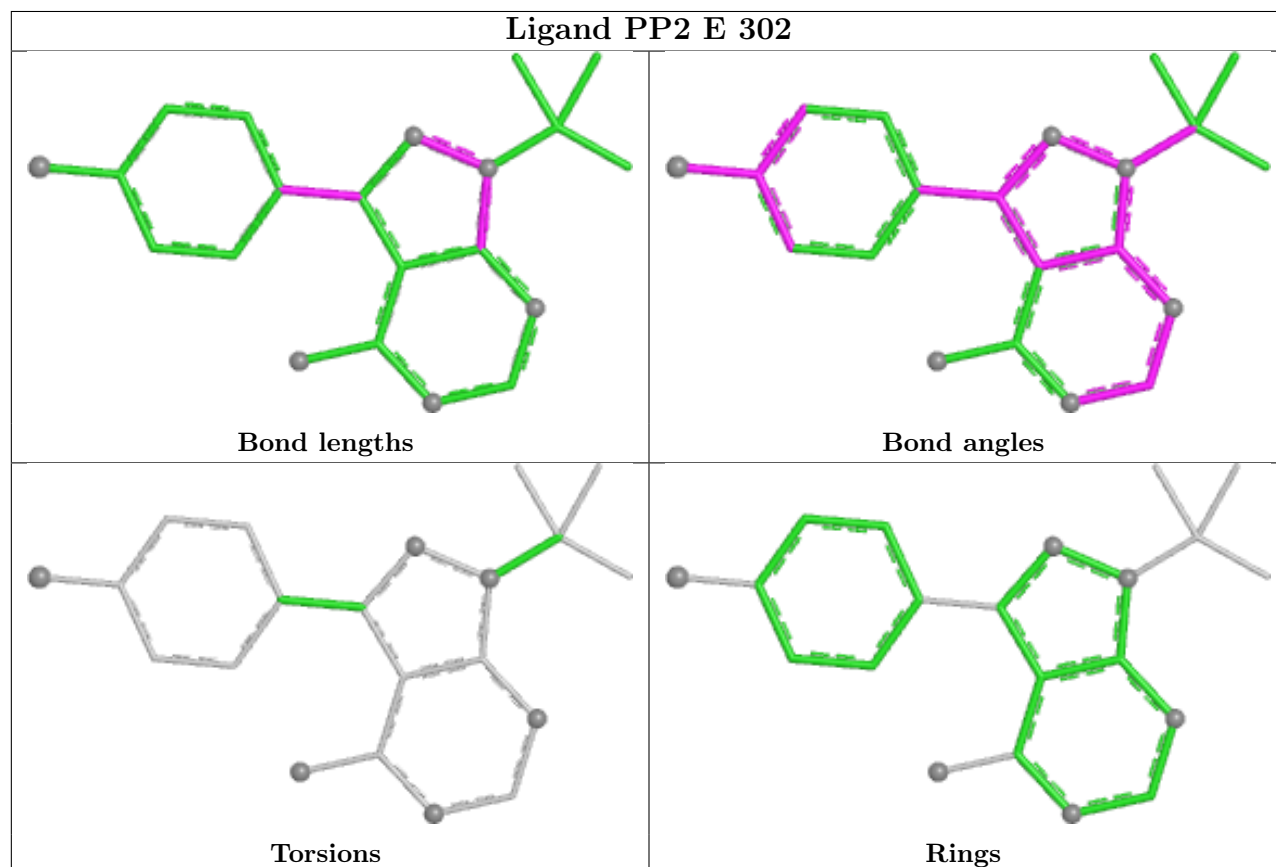
There are no ring outliers.

7 monomers are involved in 17 short contacts:

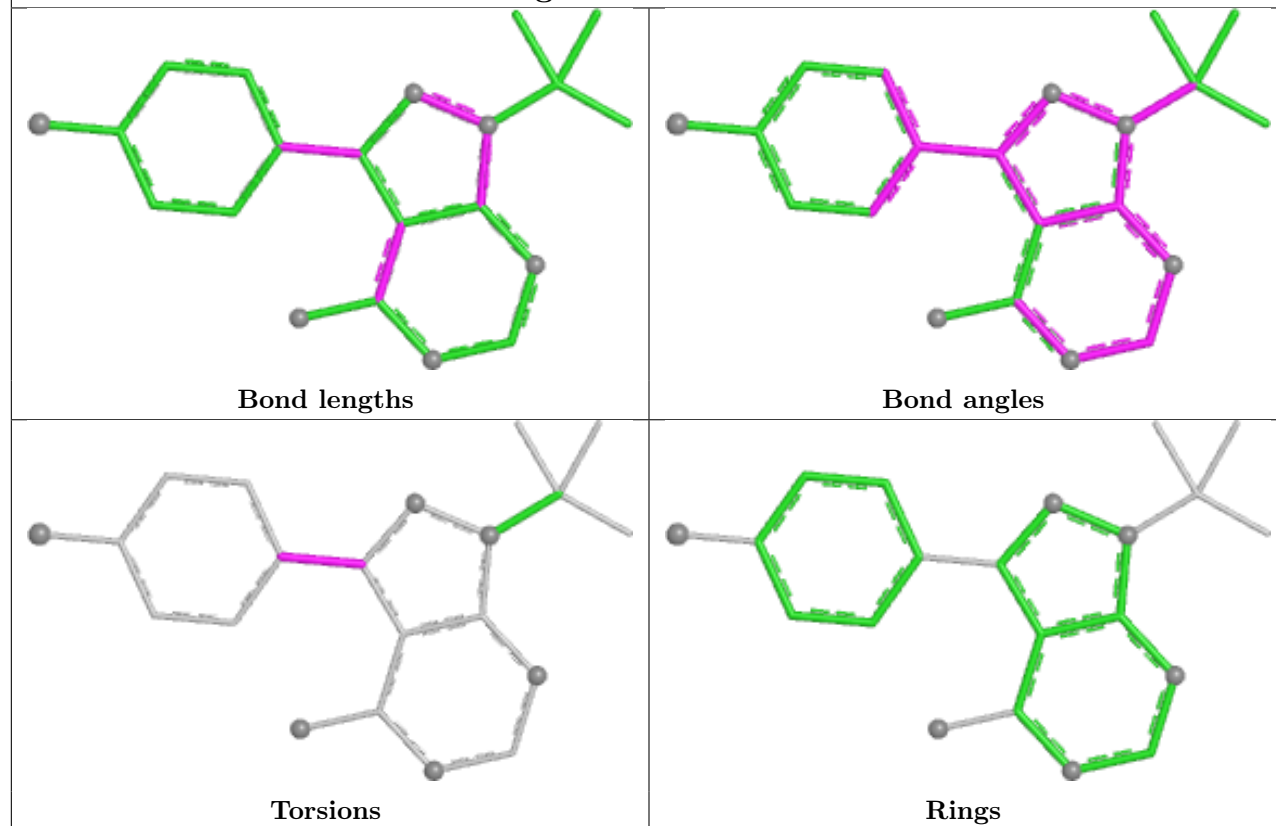
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	302	PP2	3	0
3	A	302	PP2	2	0
3	D	302	PP2	2	0
3	B	302	PP2	2	0
3	C	302[A]	PP2	3	0
3	C	302[B]	PP2	3	0
3	F	302	PP2	2	0

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

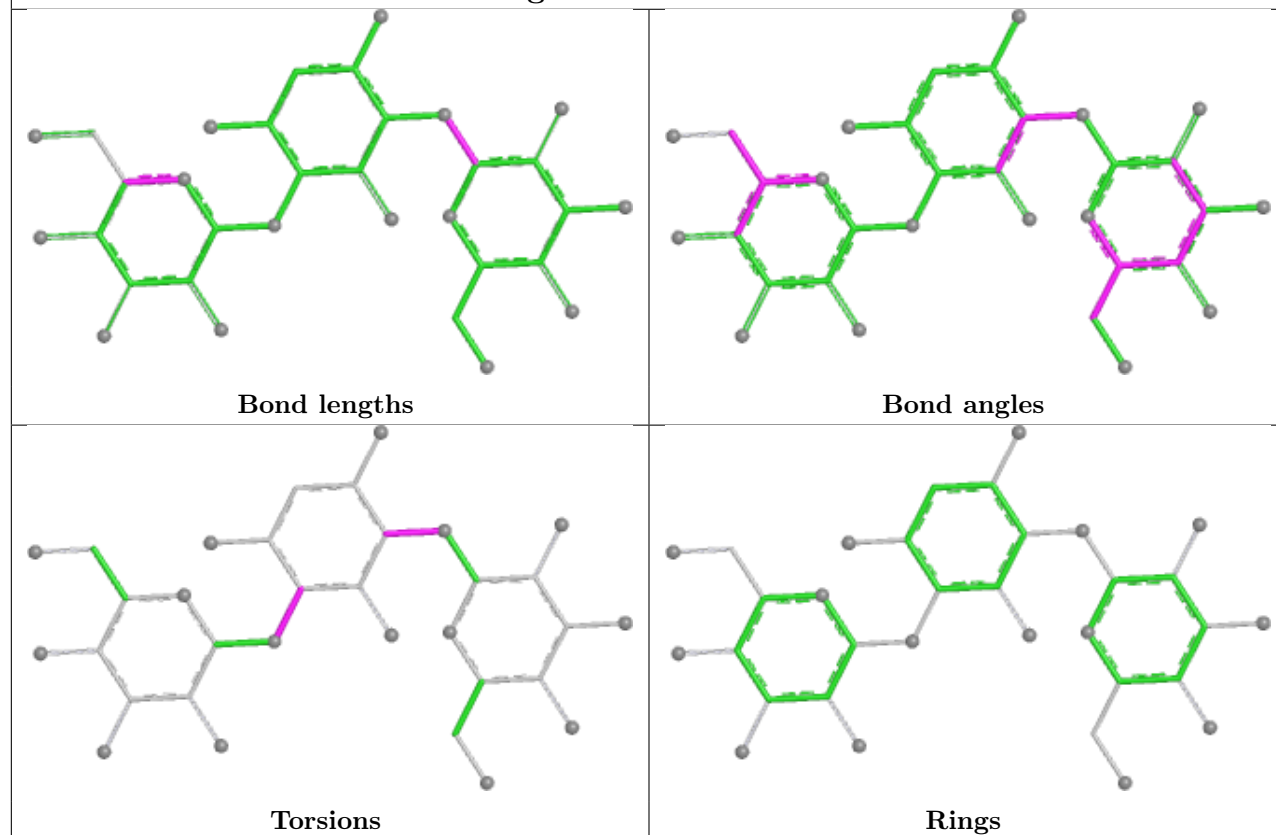
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

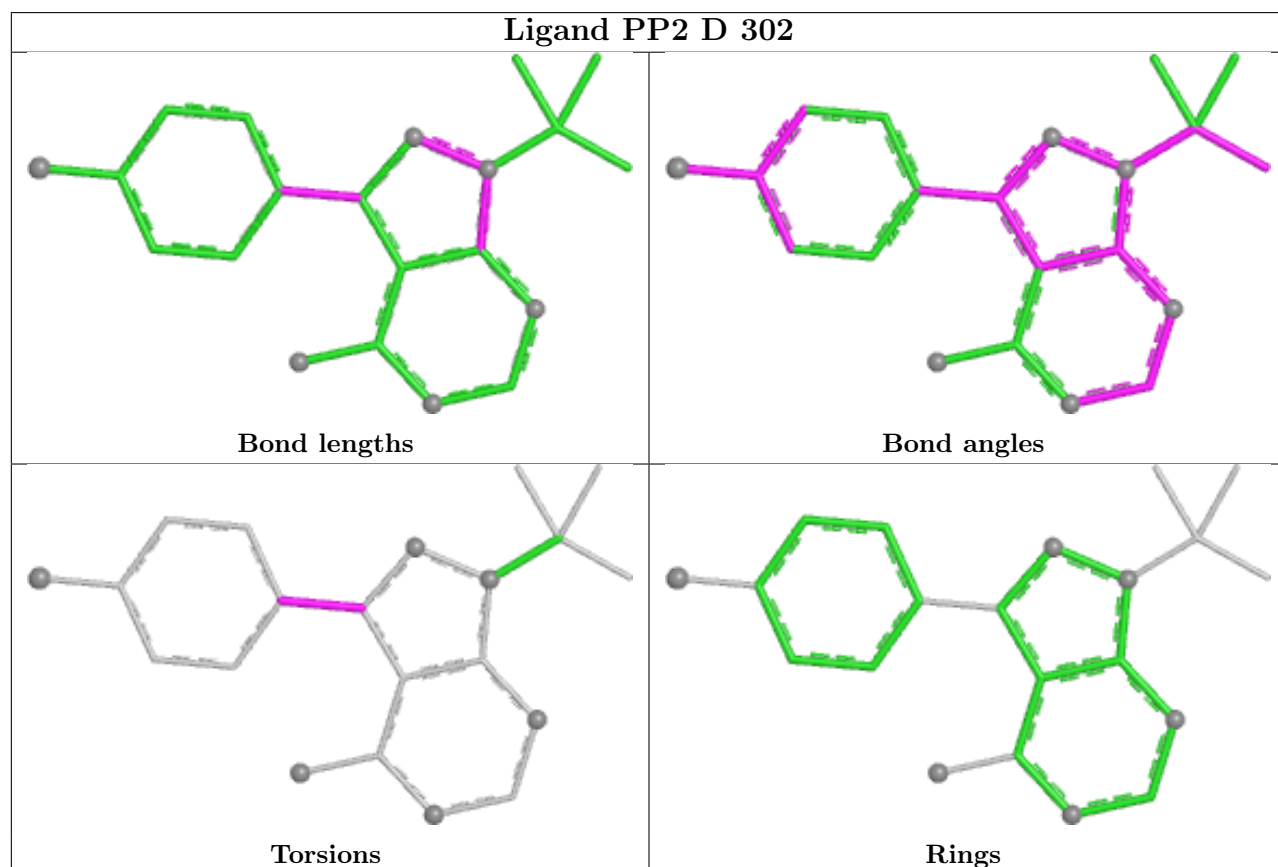
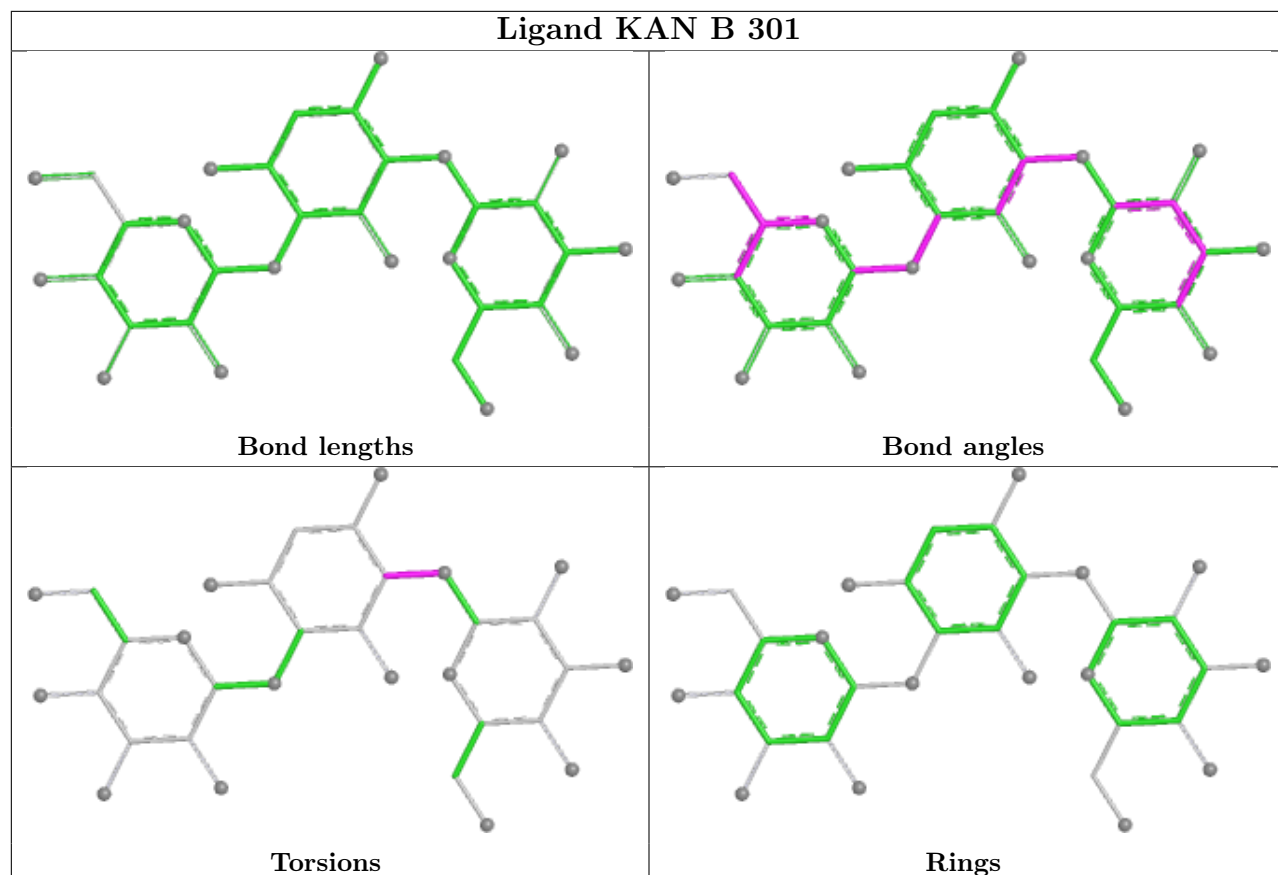


Ligand PP2 A 302

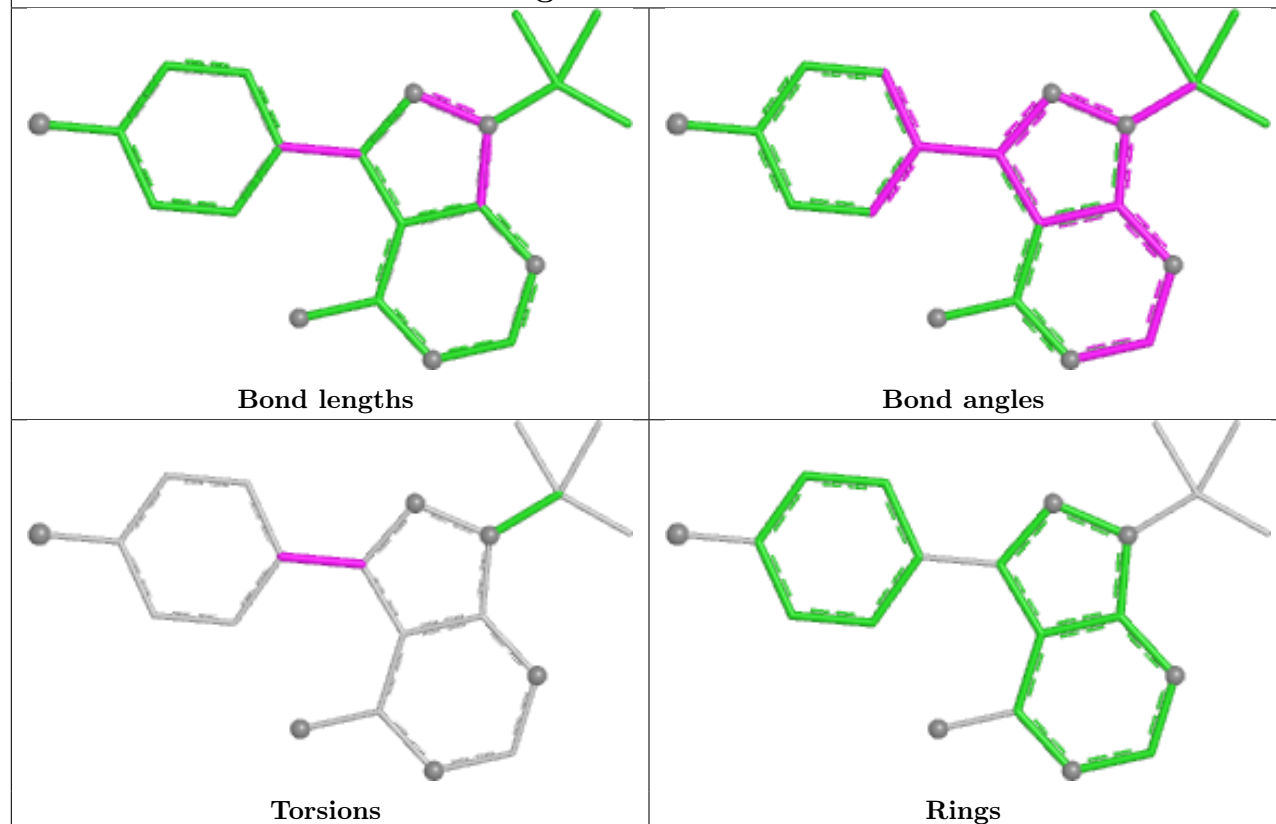


Ligand KAN A 301

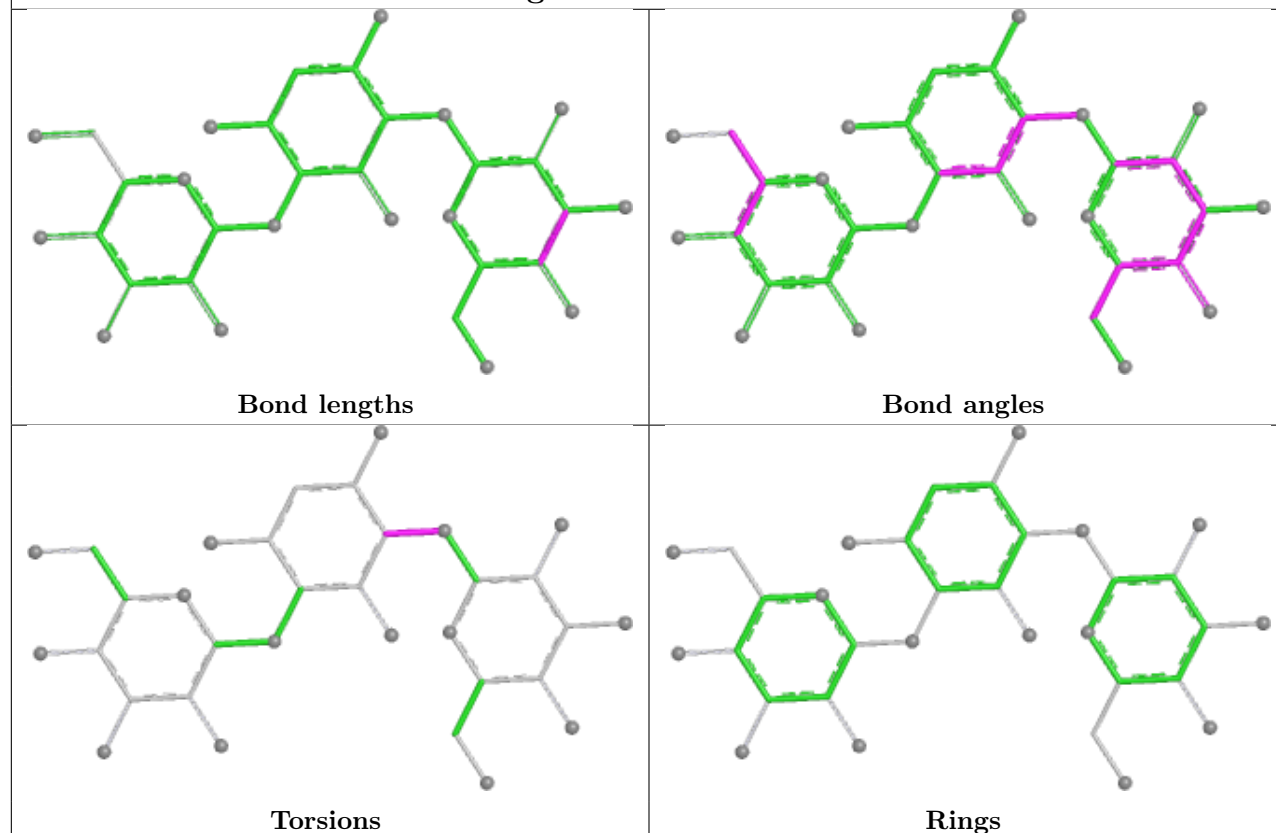


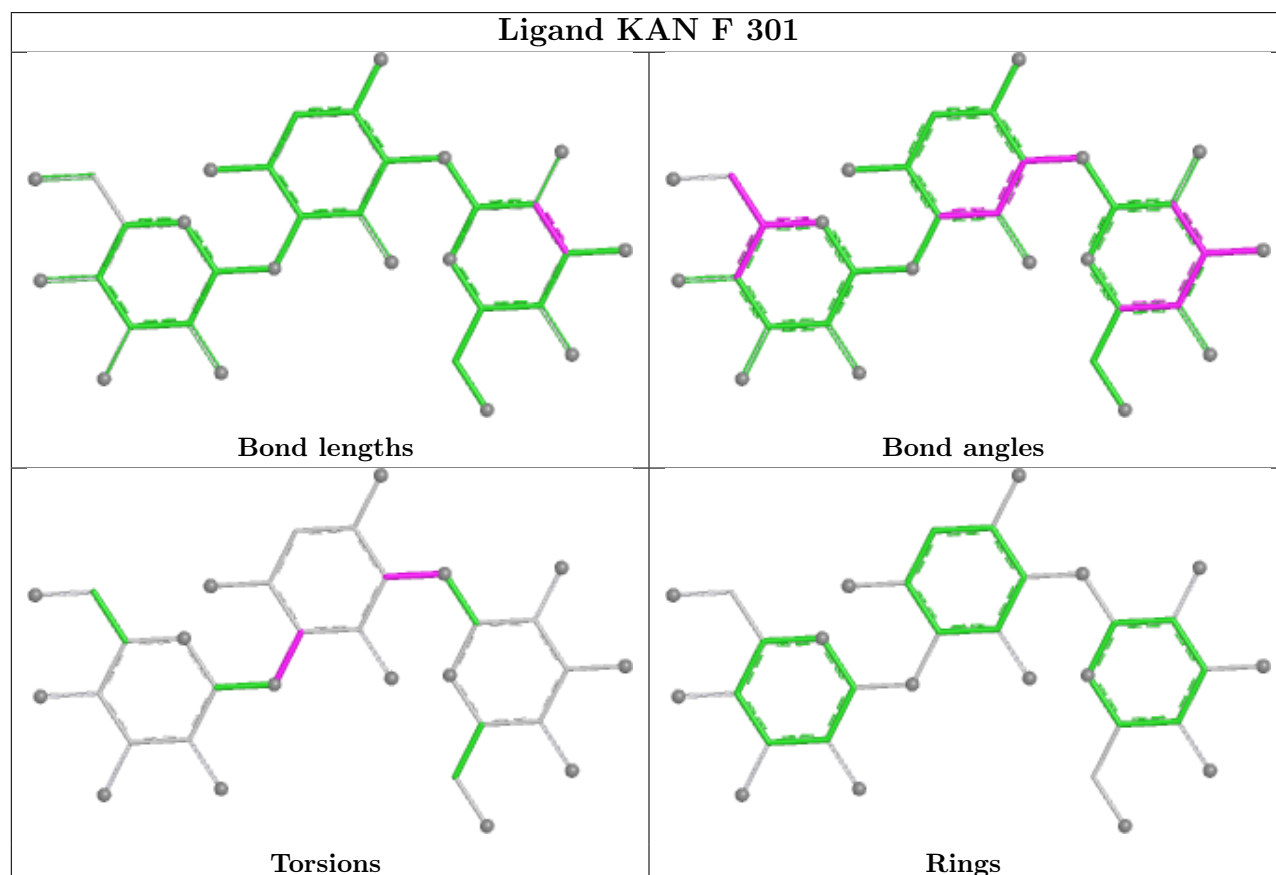
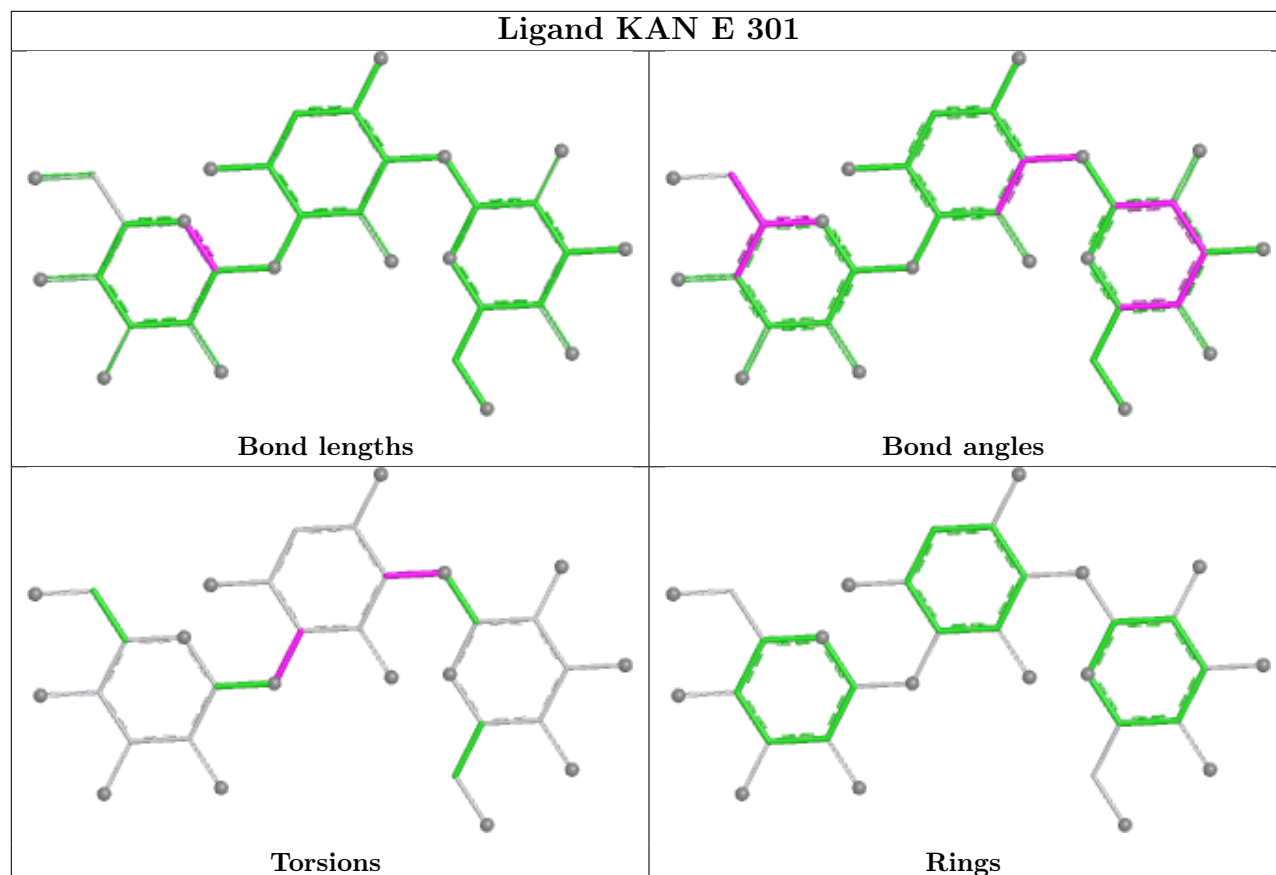


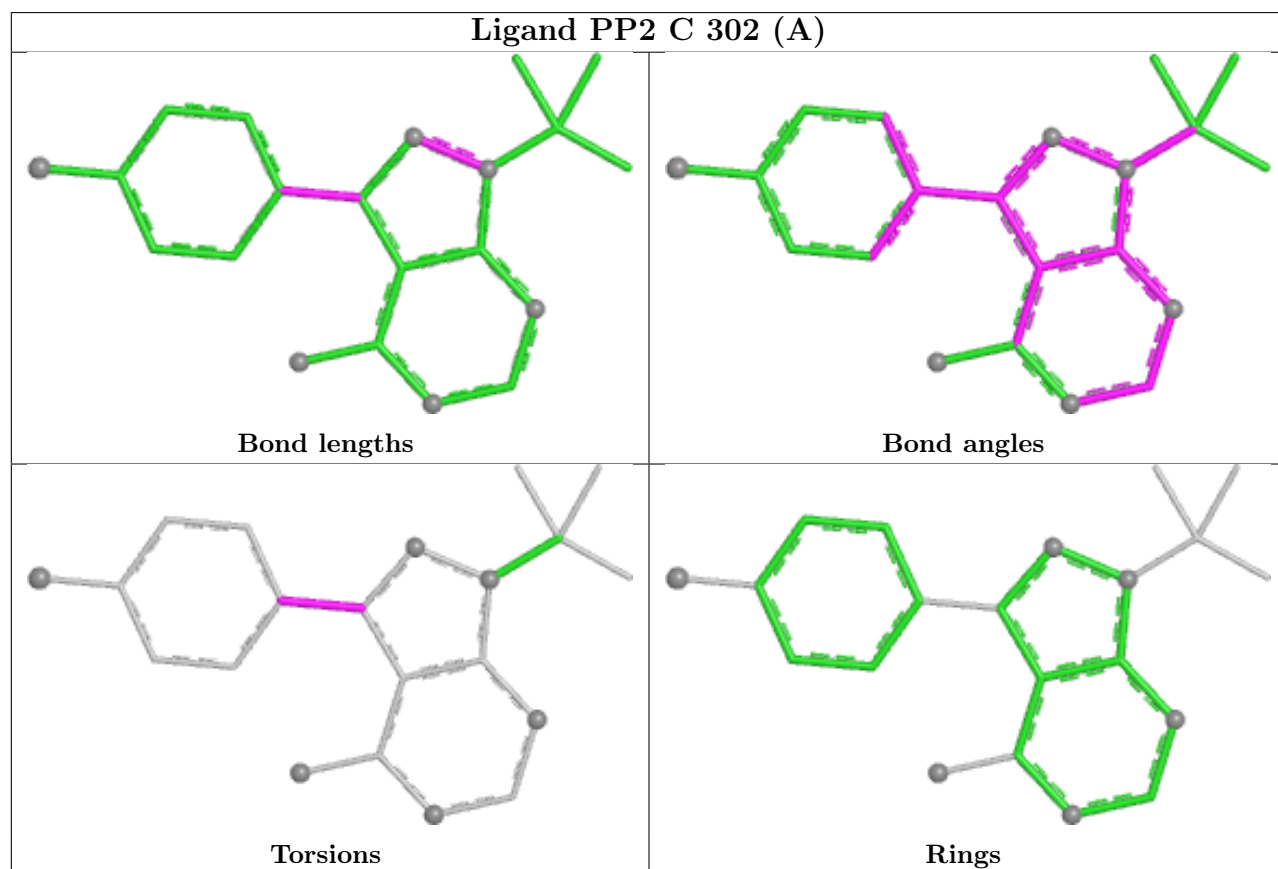
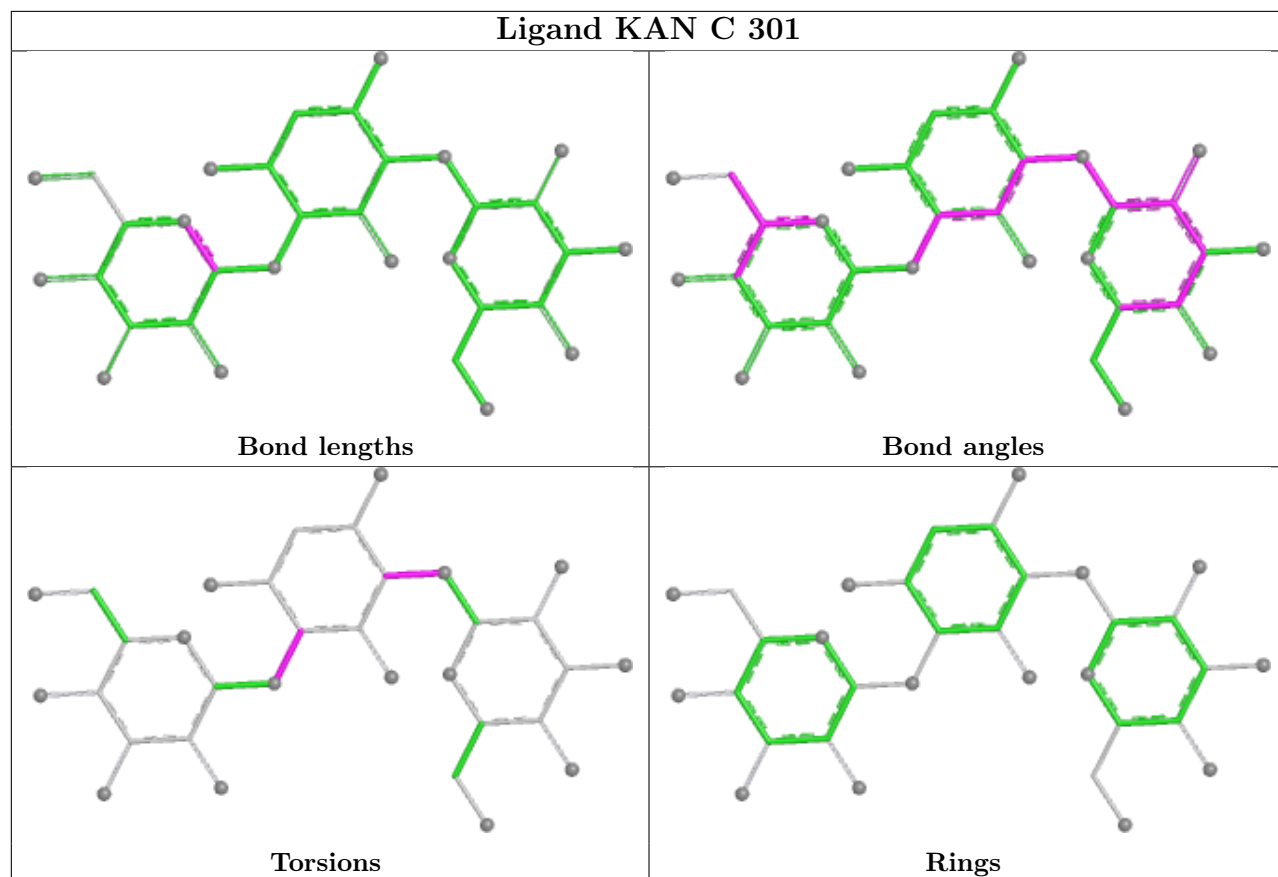
Ligand PP2 B 302



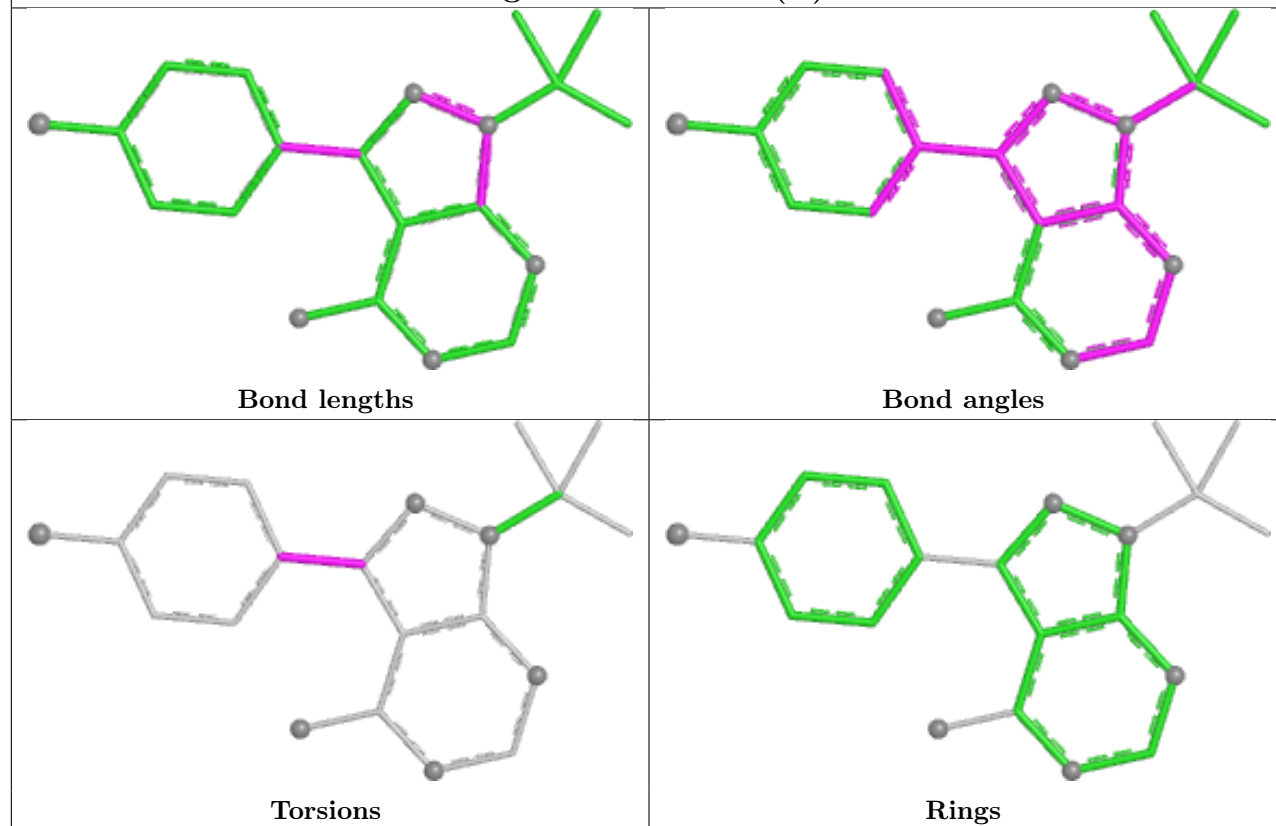
Ligand KAN D 301



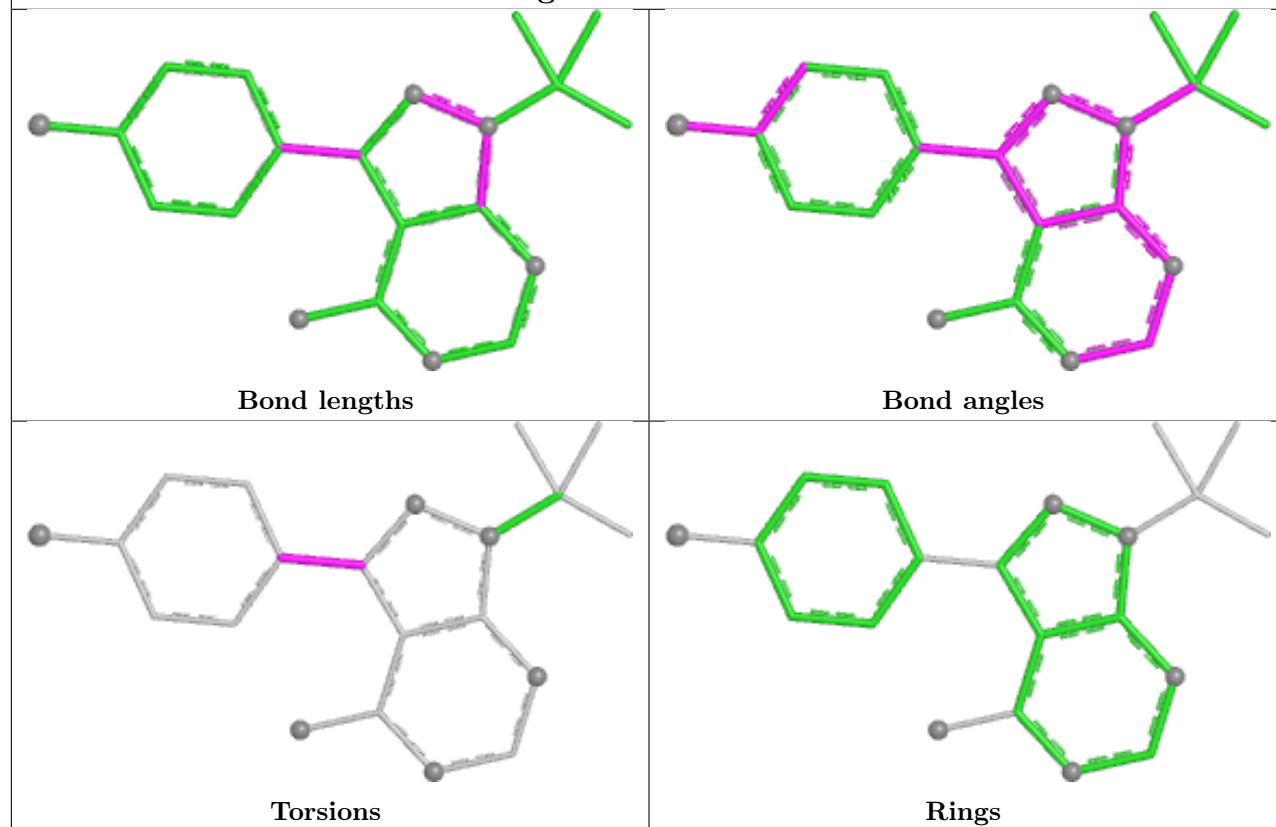




Ligand PP2 C 302 (B)



Ligand PP2 F 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	260/272 (95%)	-0.34	4 (1%)	72	80	15, 29, 87, 112	1 (0%)
1	B	250/272 (91%)	-0.09	5 (2%)	65	74	20, 39, 87, 121	0
1	C	248/272 (91%)	-0.38	4 (1%)	70	79	10, 27, 60, 104	5 (2%)
1	D	259/272 (95%)	-0.36	5 (1%)	66	75	13, 29, 80, 121	5 (1%)
1	E	248/272 (91%)	-0.38	1 (0%)	88	92	15, 29, 57, 109	4 (1%)
1	F	259/272 (95%)	-0.32	5 (1%)	66	75	15, 29, 79, 116	4 (1%)
All	All	1524/1632 (93%)	-0.31	24 (1%)	70	79	10, 30, 75, 121	19 (1%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	34	GLY	5.2
1	C	36	SER	3.7
1	A	33	VAL	3.7
1	B	8	THR	3.7
1	C	33	VAL	3.3
1	A	15	LEU	3.3
1	E	36	SER	3.3
1	D	4	ILE	3.0
1	A	34	GLY	2.9
1	F	24	TYR	2.7
1	D	3	HIS	2.6
1	F	23	LEU	2.5
1	D	24	TYR	2.5
1	F	21	ALA	2.4
1	D	23	LEU	2.4
1	D	32	ASN	2.4
1	B	14	ARG	2.3
1	F	4	ILE	2.3
1	B	23	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	19	LEU	2.3
1	B	15	LEU	2.2
1	F	32	ASN	2.2
1	A	21	ALA	2.2
1	B	24	TYR	2.1

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 oligosaccharides 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
6	ACT	D	306	4/4	0.59	0.15	44,60,61,66	0
6	ACT	F	305	4/4	0.69	0.18	61,75,101,107	0
7	PEG	C	303	7/7	0.81	0.16	38,60,89,127	0
6	ACT	D	305	4/4	0.85	0.11	32,38,46,75	0
6	ACT	A	305	4/4	0.85	0.09	27,40,47,49	0
6	ACT	B	304	4/4	0.86	0.10	31,59,67,91	0
4	NA	B	303	1/1	0.88	0.10	44,44,44,44	0
3	PP2	F	302	21/21	0.89	0.13	16,38,75,133	21
7	PEG	F	306	7/7	0.91	0.14	35,42,68,114	0
4	NA	D	304	1/1	0.92	0.06	40,40,40,40	0
3	PP2	B	302	21/21	0.92	0.10	19,37,63,143	21
4	NA	D	303	1/1	0.94	0.06	22,22,22,22	1
3	PP2	D	302	21/21	0.94	0.10	10,24,51,82	21
6	ACT	E	304	4/4	0.94	0.08	37,47,51,99	0
2	KAN	B	301	33/33	0.95	0.06	25,28,36,38	0
3	PP2	E	302	21/21	0.95	0.09	11,20,39,60	21
4	NA	F	304	1/1	0.95	0.05	37,37,37,37	0
5	CL	A	304	1/1	0.95	0.07	45,45,45,45	0

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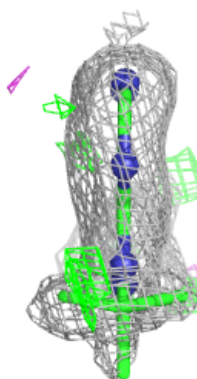
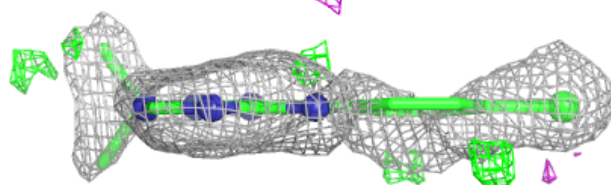
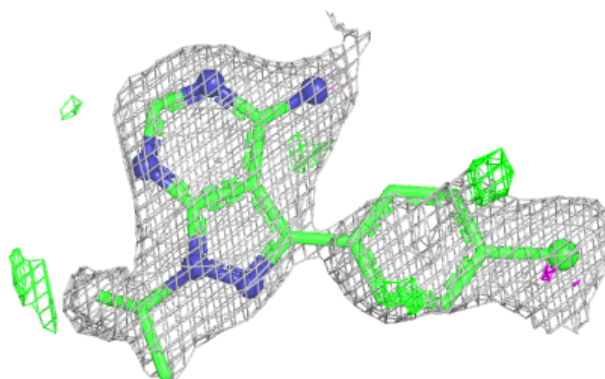
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	KAN	E	301	33/33	0.95	0.06	30,33,37,38	0
2	KAN	A	301	33/33	0.95	0.06	17,23,33,36	0
3	PP2	A	302	21/21	0.96	0.08	15,30,81,115	21
2	KAN	C	301	33/33	0.96	0.05	22,25,35,38	0
2	KAN	F	301	33/33	0.96	0.05	13,19,26,27	0
3	PP2	C	302[A]	21/21	0.97	0.07	3,22,47,104	21
3	PP2	C	302[B]	21/21	0.97	0.07	0,21,75,103	21
4	NA	A	303	1/1	0.97	0.04	32,32,32,32	0
2	KAN	D	301	33/33	0.97	0.04	17,21,25,25	0
4	NA	F	303	1/1	0.98	0.05	23,23,23,23	1
4	NA	E	303	1/1	0.99	0.03	35,35,35,35	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.

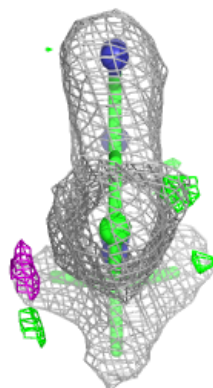
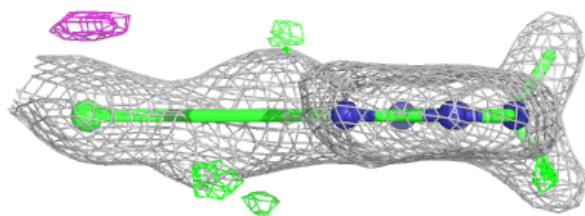
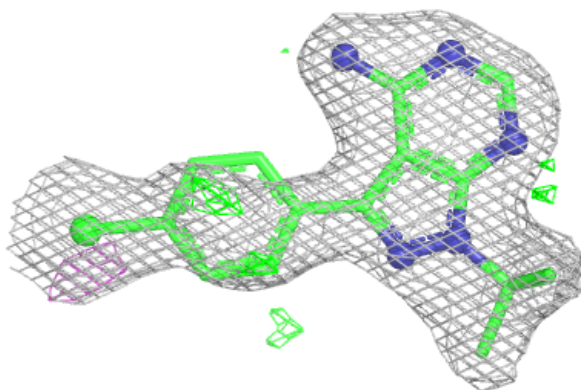
Electron density around PP2 F 302:

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

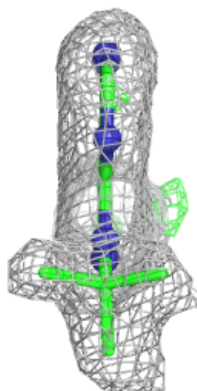
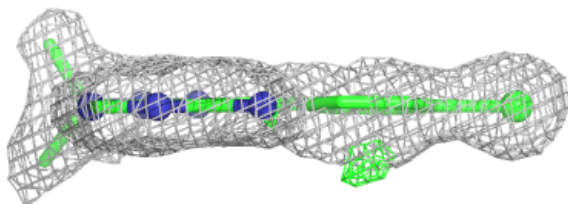
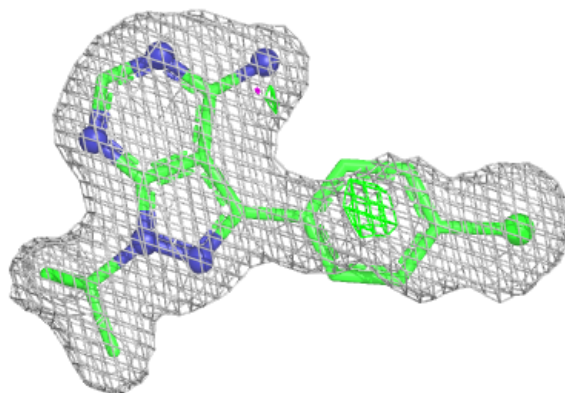


Electron density around PP2 B 302:

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

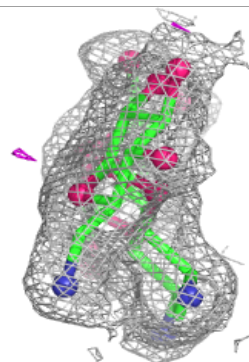
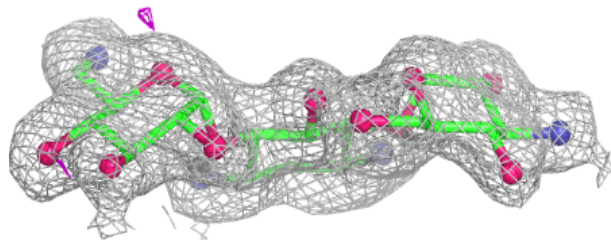
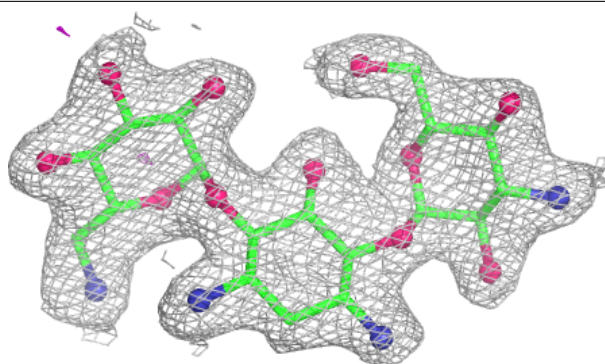
**Electron density around PP2 D 302:**

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and green (positive)

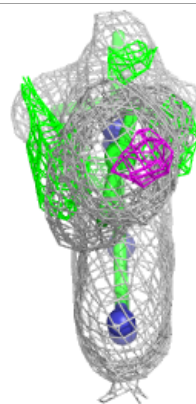
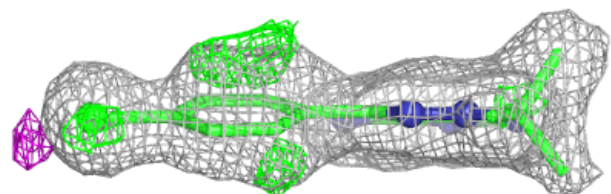
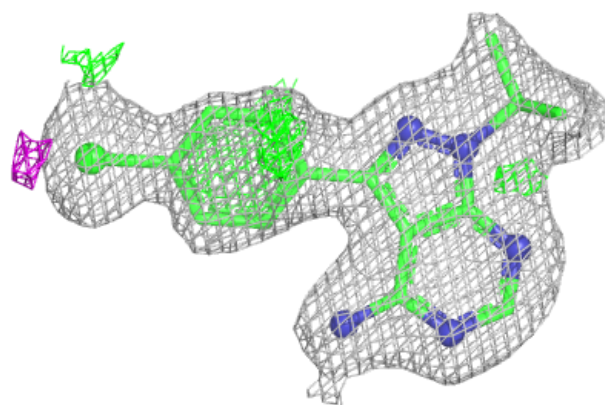


Electron density around KAN B 301:

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and green (positive)

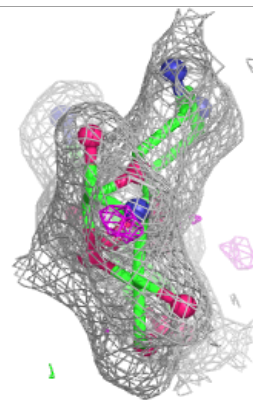
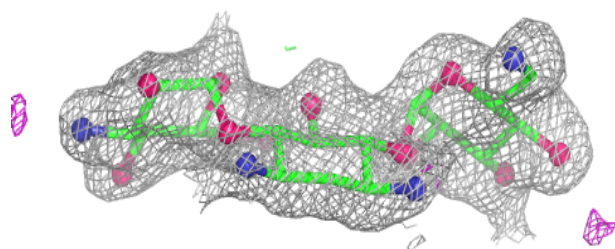
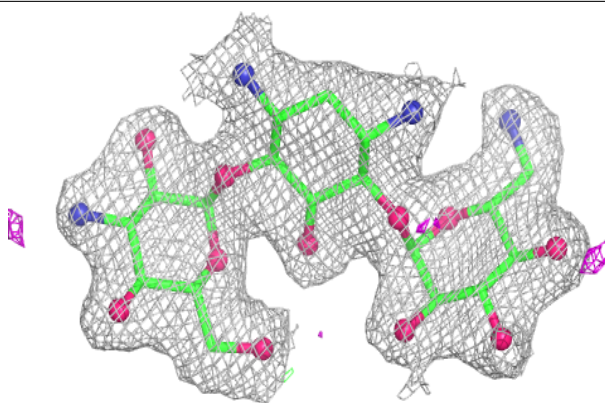
**Electron density around PP2 E 302:**

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and green (positive)

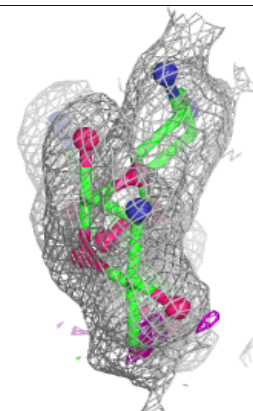
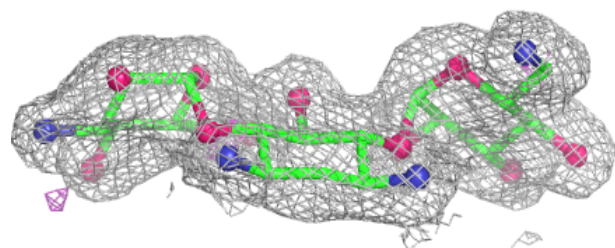
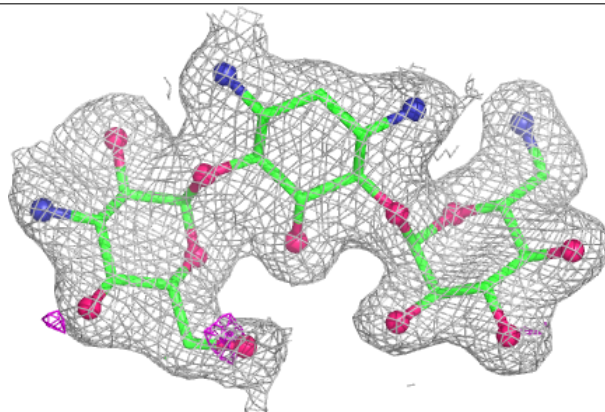


Electron density around KAN E 301:

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and green (positive)

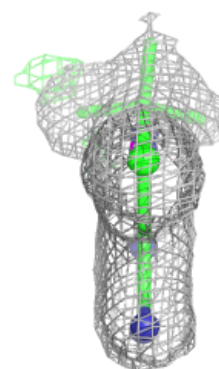
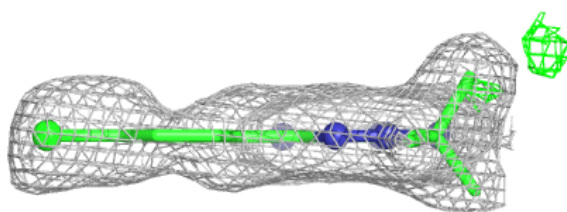
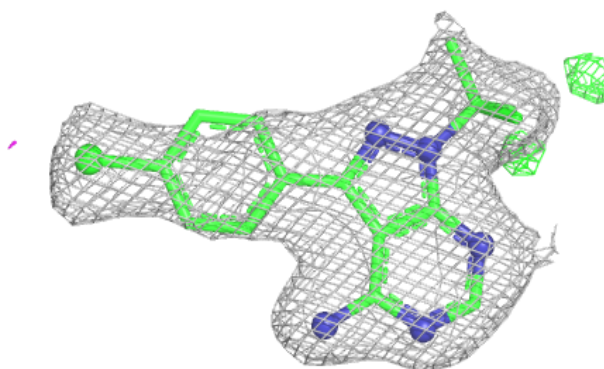
**Electron density around KAN A 301:**

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and green (positive)

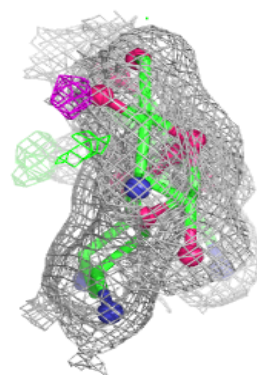
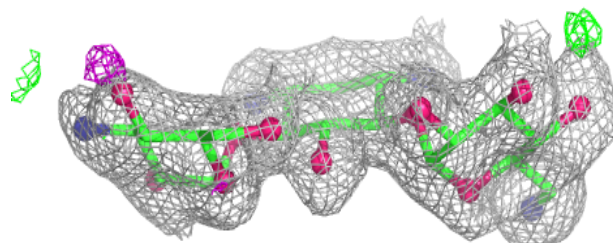
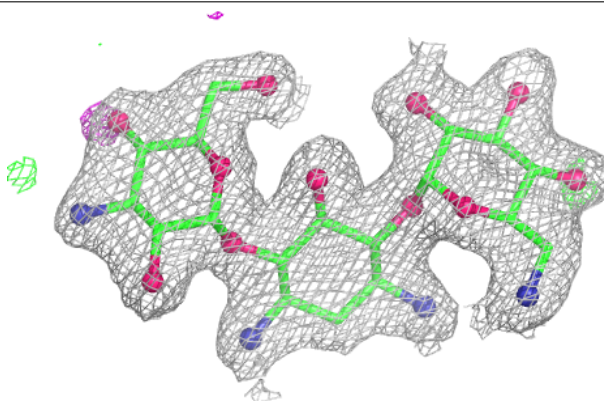


Electron density around PP2 A 302:

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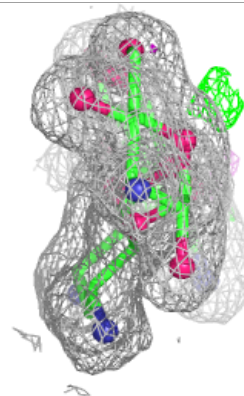
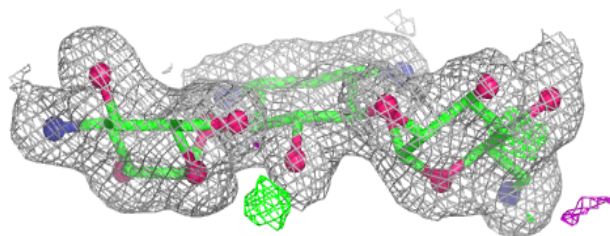
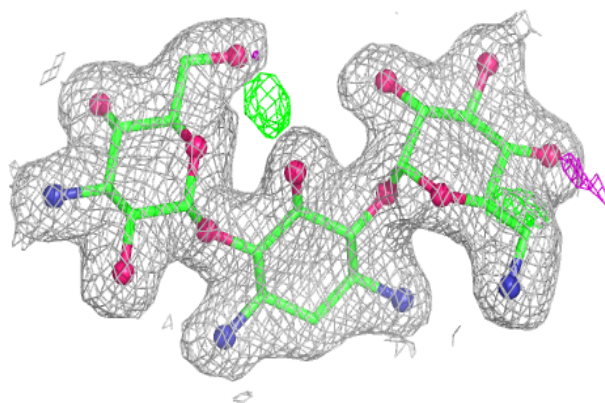
**Electron density around KAN C 301:**

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



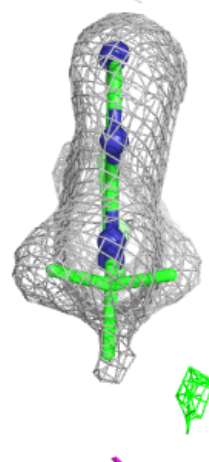
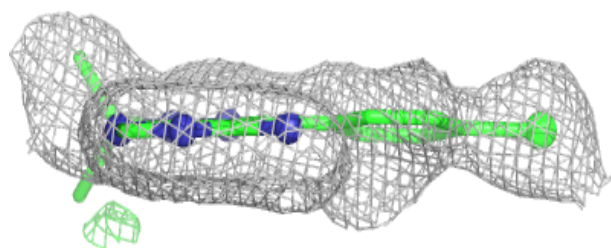
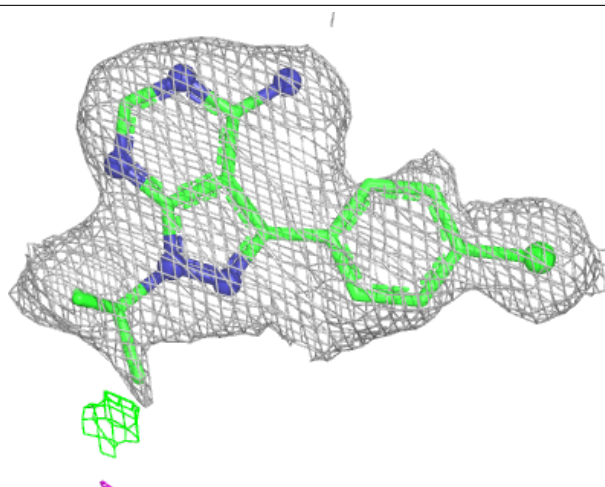
Electron density around KAN F 301:

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



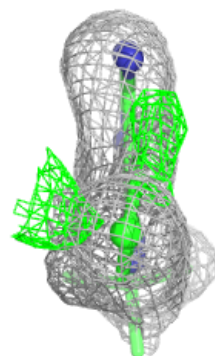
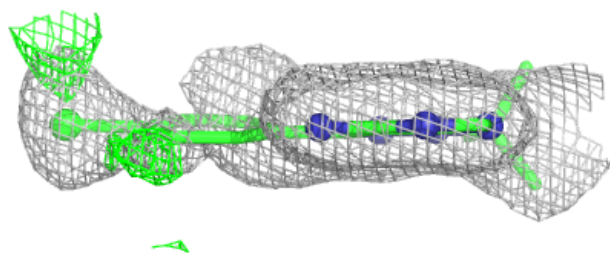
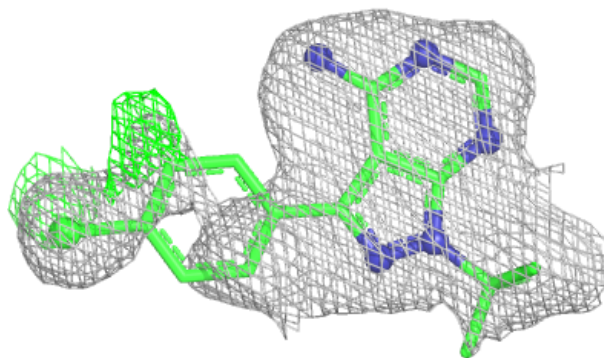
Electron density around PP2 C 302 (A):

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

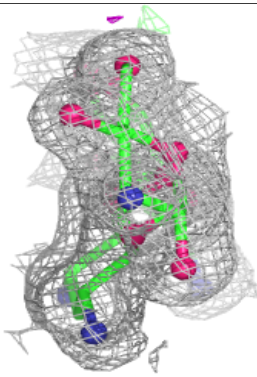
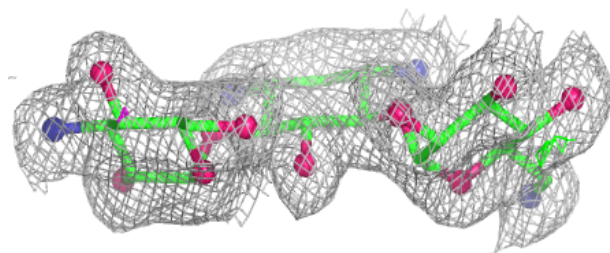
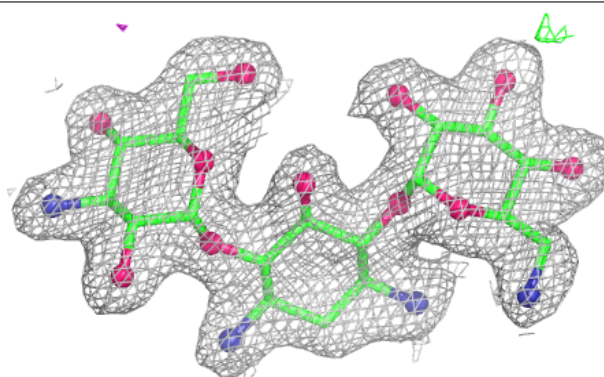


Electron density around PP2 C 302 (B):

$2mF_o-DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.