



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 06:06 AM EDT

PDB ID : 6N92
Title : Methylmalonyl-CoA decarboxylase in complex with 2-nitronate-propionyl-CoA
Authors : Stunkard, L.M.; Dixon, A.D.; Huth, T.J.; Lohman, J.R.
Deposited on : 2018-11-30
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

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 1.70 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15563 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.

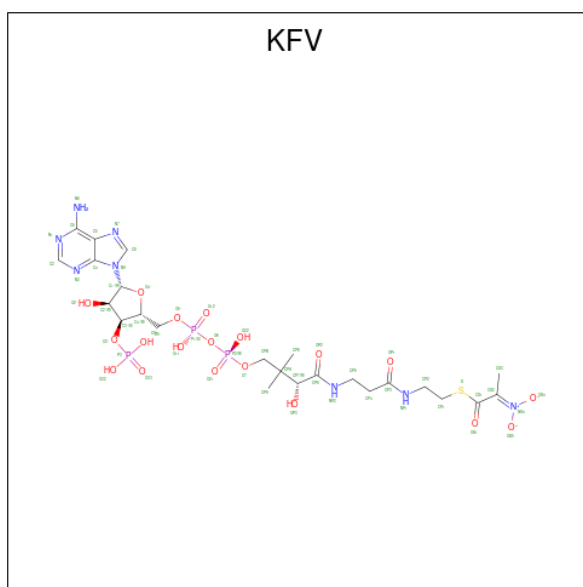
- Molecule 1 is a protein called Methylmalonyl-CoA decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	260	2152	1380	365	394	13	0	20	0
1	B	260	2141	1374	361	393	13	0	17	0
1	C	260	2139	1372	364	391	12	0	18	0
1	D	260	2136	1372	358	393	13	0	17	0
1	E	260	2128	1366	357	393	12	0	16	0
1	F	260	2160	1391	364	392	13	0	21	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	engineered mutation	UNP P52045
B	2	ALA	SER	engineered mutation	UNP P52045
C	2	ALA	SER	engineered mutation	UNP P52045
D	2	ALA	SER	engineered mutation	UNP P52045
E	2	ALA	SER	engineered mutation	UNP P52045
F	2	ALA	SER	engineered mutation	UNP P52045

- Molecule 2 is [1-[2-[3-[[2 {R}]-4-[[[2 {R},3 {S},4 {R},5 {R}]]-5-(6-aminopurin-9-yl)-4-oxidanyl-3-phosphonooxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-3,3-dimethyl-2-oxidanyl-butanoyl]amino]propanoylamino]ethylsulfanyl]-1-oxidanylidene-propan-2-ylidene]-bis(oxidanidyl)azanium (three-letter code: KfV) (formula: C₂₄H₃₈N₈O₁₉P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
2	A	1	Total	C	N	O	P	S	0	0
			55	24	8	19	3	1		
2	B	1	Total	C	N	O	P	S	0	1
			87	35	13	32	6	1		
2	C	1	Total	C	N	O	P	S	0	0
			55	24	8	19	3	1		
2	C	1	Total	C	N	O	P		0	1
			31	10	5	13	3			
2	D	1	Total	C	N	O	P	S	0	1
			96	42	14	32	6	2		
2	E	1	Total	C	N	O	P	S	0	0
			55	24	8	19	3	1		
2	E	1	Total	C	N	O	P		0	1
			31	10	5	13	3			
2	F	1	Total	C	N	O	P	S	0	1
			110	48	16	38	6	2		
2	F	1	Total	C	N	O	P		0	1
			31	10	5	13	3			

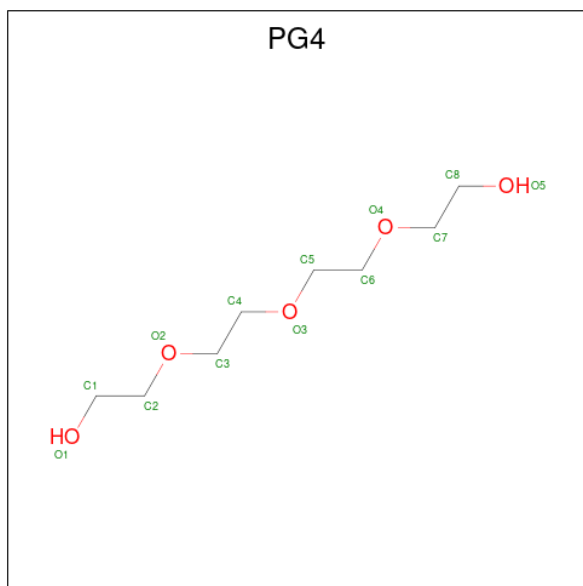
- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		
3	D	1	Total	Ni	0	0
			1	1		
3	F	1	Total	Ni	0	0
			1	1		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

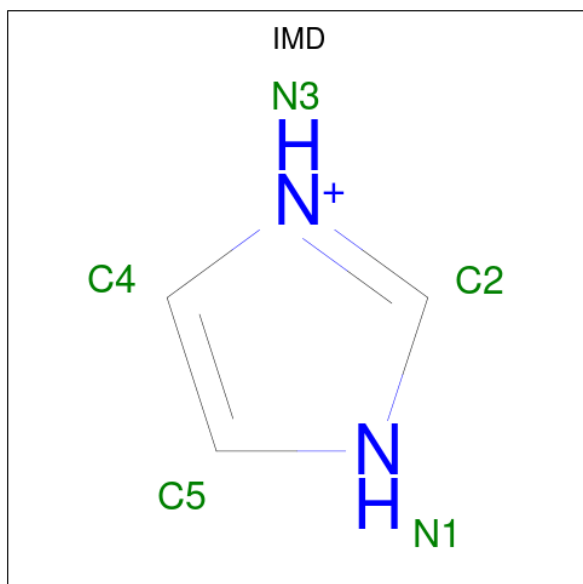
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total K 1 1	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



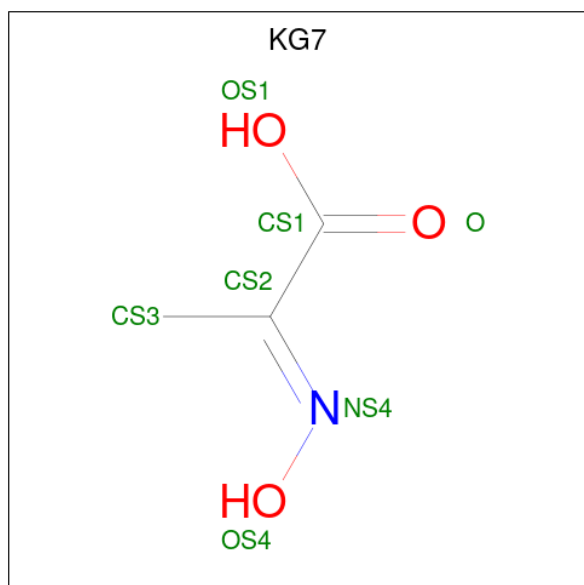
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 13 8 5	0	0

- Molecule 6 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	N	0	0
			5	3	2		
6	F	1	Total	C	N	0	0
			5	3	2		

- Molecule 7 is (2E)-2-(hydroxyimino)propanoic acid (three-letter code: KG7) (formula: $C_3H_5NO_3$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	367	Total	O	0	18
			382	382		
8	B	330	Total	O	0	14
			340	340		
8	C	353	Total	O	0	19
			367	367		
8	D	326	Total	O	0	10
			333	333		
8	E	332	Total	O	0	15
			342	342		
8	F	348	Total	O	0	19
			358	358		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.01Å 114.32Å 194.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.36 – 1.70	Depositor
% Data completeness (in resolution range)	97.5 (29.36-1.70)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.151 , 0.184	Depositor
Wilson B-factor (Å ²)	14.8	Xtrriage
Anisotropy	0.015	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	15563	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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
2	KFV	E	302[A]	-	28,33,57	1.12	2 (7%)	35,52,85	1.53	7 (20%)
2	KFV	F	303[A]	-	28,33,57	1.15	2 (7%)	35,52,85	1.58	6 (17%)
6	IMD	F	305	3	3,5,5	0.28	0	4,5,5	0.50	0
2	KFV	C	301	-	46,57,57	1.32	6 (13%)	55,85,85	2.85	17 (30%)
2	KFV	E	301	-	46,57,57	1.08	4 (8%)	55,85,85	3.12	12 (21%)
7	KG7	F	304	3	6,6,6	2.34	2 (33%)	7,7,7	2.32	4 (57%)
2	KFV	F	301[A]	-	46,57,57	1.12	2 (4%)	55,85,85	3.78	13 (23%)
2	KFV	C	303[A]	-	28,33,57	1.30	2 (7%)	35,52,85	1.83	10 (28%)
2	KFV	B	301[A]	-	46,57,57	1.28	6 (13%)	55,85,85	3.51	21 (38%)
2	KFV	B	301[B]	-	46,57,57	1.28	5 (10%)	55,85,85	3.71	18 (32%)
6	IMD	D	303	-	3,5,5	0.29	0	4,5,5	0.60	0
5	PG4	C	304	4	12,12,12	0.38	0	11,11,11	0.29	0
2	KFV	F	301[B]	-	46,57,57	0.97	2 (4%)	55,85,85	2.10	12 (21%)
2	KFV	D	302[A]	-	41,50,57	1.02	2 (4%)	52,75,85	3.30	18 (34%)
2	KFV	D	302[B]	-	41,50,57	0.97	2 (4%)	52,75,85	1.96	12 (23%)
2	KFV	A	301	-	46,57,57	1.25	7 (15%)	55,85,85	1.42	9 (16%)

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	KFV	E	302[A]	-	-	1/17/37/75	0/3/3/3
2	KFV	F	303[A]	-	-	5/17/37/75	0/3/3/3
6	IMD	F	305	3	-	-	0/1/1/1
2	KFV	C	301	-	-	7/47/75/75	0/3/3/3
2	KFV	E	301	-	-	5/47/75/75	0/3/3/3
7	KG7	F	304	3	-	0/6/6/6	-
2	KFV	F	301[A]	-	-	10/47/75/75	0/3/3/3
2	KFV	C	303[A]	-	-	8/17/37/75	0/3/3/3
2	KFV	B	301[A]	-	-	12/47/75/75	0/3/3/3
2	KFV	B	301[B]	-	-	15/47/75/75	0/3/3/3
6	IMD	D	303	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PG4	C	304	4	-	3/10/10/10	-
2	KFV	F	301[B]	-	-	16/47/75/75	0/3/3/3
2	KFV	D	302[A]	-	-	11/44/64/75	0/3/3/3
2	KFV	D	302[B]	-	-	21/44/64/75	0/3/3/3
2	KFV	A	301	-	-	0/47/75/75	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	304	KG7	CS3-CS2	4.59	1.58	1.49
2	F	301[A]	KFV	CS1-S	-3.91	1.67	1.77
2	E	301	KFV	O4'-C1'	3.75	1.46	1.41
2	C	303[A]	KFV	C5-C4	3.49	1.50	1.40
2	C	301	KFV	P3-O3'	3.15	1.65	1.59
2	C	303[A]	KFV	C2-N3	3.15	1.37	1.32
2	F	303[A]	KFV	C5-C4	3.08	1.49	1.40
2	D	302[A]	KFV	O4'-C1'	3.08	1.45	1.41
2	A	301	KFV	O4'-C1'	3.07	1.45	1.41
2	A	301	KFV	P3-O3'	3.06	1.65	1.59
2	C	301	KFV	CS3-CS2	3.05	1.56	1.49
2	A	301	KFV	C5-C4	3.00	1.48	1.40
2	B	301[A]	KFV	CS1-S	-2.92	1.70	1.77
2	B	301[B]	KFV	CS1-S	-2.92	1.70	1.77
2	A	301	KFV	CS1-S	-2.91	1.70	1.77
2	C	301	KFV	CS1-S	-2.86	1.70	1.77
2	E	302[A]	KFV	C5-C4	2.79	1.48	1.40
2	E	301	KFV	CS1-S	-2.76	1.70	1.77
2	F	301[B]	KFV	CS1-S	-2.75	1.70	1.77
2	E	302[A]	KFV	P3-O3'	2.67	1.64	1.59
2	E	301	KFV	C5-C4	2.67	1.48	1.40
2	C	301	KFV	C2-N3	2.67	1.36	1.32
2	B	301[A]	KFV	C5-C4	2.64	1.47	1.40
2	D	302[B]	KFV	C5-C4	2.61	1.47	1.40
7	F	304	KG7	O-CS1	2.60	1.29	1.22
2	F	301[A]	KFV	C5-C4	2.52	1.47	1.40
2	B	301[B]	KFV	P2-O7	2.50	1.69	1.59
2	A	301	KFV	C2-N3	2.41	1.36	1.32
2	B	301[A]	KFV	CS3-CS2	2.30	1.54	1.49
2	B	301[B]	KFV	CS3-CS2	2.30	1.54	1.49
2	B	301[A]	KFV	CP8-CPA	2.22	1.58	1.53
2	B	301[B]	KFV	CP8-CPA	2.22	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	302[A]	KFV	CP3-NP1	2.18	1.38	1.33
2	A	301	KFV	C8-N7	2.17	1.38	1.34
2	F	301[B]	KFV	C5-C4	2.14	1.46	1.40
2	F	303[A]	KFV	C2'-C1'	-2.11	1.50	1.53
2	A	301	KFV	C2'-C1'	-2.10	1.50	1.53
2	D	302[B]	KFV	C2-N3	2.07	1.35	1.32
2	C	301	KFV	O7-CPB	-2.07	1.37	1.43
2	B	301[A]	KFV	CS2-CS1	2.06	1.52	1.46
2	B	301[B]	KFV	CS2-CS1	2.06	1.52	1.46
2	C	301	KFV	C5-C4	2.04	1.46	1.40
2	E	301	KFV	P3-O3'	2.02	1.63	1.59
2	B	301[A]	KFV	O4'-C1'	2.01	1.43	1.41

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301[A]	KFV	CP8-CPA-CP7	-15.89	81.26	108.82
2	B	301[B]	KFV	CP8-CPA-CP7	-15.89	81.26	108.82
2	F	301[A]	KFV	CP8-CPA-CPB	-13.05	86.95	108.23
2	D	302[A]	KFV	CP8-CPA-CPB	-12.89	87.21	108.23
2	F	301[A]	KFV	CP8-CPA-CP9	-12.67	83.35	109.17
2	C	301	KFV	CP8-CPA-CPB	-12.30	88.18	108.23
2	F	301[A]	KFV	CP8-CPA-CP7	-11.54	88.82	108.82
2	E	301	KFV	CP8-CPA-CPB	-10.67	90.83	108.23
2	E	301	KFV	CP1-S-CS1	10.15	112.56	99.80
2	F	301[A]	KFV	CP1-S-CS1	10.14	112.54	99.80
2	B	301[A]	KFV	CP8-CPA-CP9	-9.85	89.08	109.17
2	B	301[B]	KFV	CP8-CPA-CP9	-9.85	89.08	109.17
2	B	301[B]	KFV	CP8-CPA-CPB	-9.41	92.88	108.23
2	D	302[A]	KFV	CP9-CPA-CPB	9.20	123.23	108.23
2	B	301[B]	KFV	O7-CPB-CPA	8.84	124.76	110.55
2	F	301[A]	KFV	CP9-CPA-CP7	8.73	123.95	108.82
2	B	301[A]	KFV	CP9-CPA-CP7	8.45	123.48	108.82
2	B	301[B]	KFV	CP9-CPA-CP7	8.45	123.48	108.82
2	E	301	KFV	CP8-CPA-CP9	-8.32	92.20	109.17
2	E	301	KFV	CP9-CPA-CPB	8.32	121.80	108.23
2	B	301[A]	KFV	CP8-CPA-CPB	-8.21	94.84	108.23
2	D	302[A]	KFV	CP8-CPA-CP9	-8.05	92.75	109.17
2	C	301	KFV	CP8-CPA-CP7	-7.84	95.23	108.82
2	F	301[B]	KFV	CP1-S-CS1	7.72	109.50	99.80
2	C	301	KFV	CP9-CPA-CP7	7.08	121.10	108.82
2	E	301	KFV	CP8-CPA-CP7	-6.92	96.82	108.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	302[A]	KFV	CP8-CPA-CP7	-6.71	97.19	108.82
2	E	301	KFV	CP9-CPA-CP7	6.66	120.36	108.82
2	C	301	KFV	CP8-CPA-CP9	-6.54	95.84	109.17
2	F	301[A]	KFV	P2-O6-P1	-6.53	110.41	132.83
2	D	302[B]	KFV	CP5-CP4-CP3	-6.04	102.30	112.36
2	D	302[A]	KFV	CP4-CP3-NP1	5.83	126.23	116.42
2	C	301	KFV	OP3-CP7-CPA	-5.44	97.45	110.25
2	B	301[B]	KFV	CP9-CPA-CPB	5.36	116.98	108.23
2	D	302[B]	KFV	P2-O6-P1	-5.20	114.97	132.83
2	D	302[A]	KFV	OP1-CP3-CP4	-5.14	112.62	122.02
2	F	301[B]	KFV	C1'-N9-C4	-4.95	117.95	126.64
2	C	303[A]	KFV	O4'-C1'-C2'	-4.83	99.87	106.93
2	D	302[B]	KFV	OP1-CP3-CP4	-4.68	113.45	122.02
2	B	301[A]	KFV	P2-O6-P1	-4.60	117.03	132.83
2	F	301[B]	KFV	N3-C2-N1	-4.54	121.59	128.68
2	F	301[B]	KFV	P2-O6-P1	-4.52	117.30	132.83
2	F	303[A]	KFV	P1-O6-P2	-4.51	117.36	132.83
2	D	302[A]	KFV	P2-O6-P1	-4.44	117.60	132.83
2	B	301[A]	KFV	CP4-CP5-NP2	4.39	120.77	111.90
2	B	301[B]	KFV	CP4-CP5-NP2	4.39	120.77	111.90
2	D	302[A]	KFV	CP1-CP2-NP1	4.18	121.85	112.31
2	F	301[A]	KFV	CP9-CPA-CPB	4.04	114.82	108.23
2	B	301[A]	KFV	OP3-CP7-CPA	-4.01	100.81	110.25
2	B	301[B]	KFV	OP3-CP7-CPA	-4.01	100.81	110.25
2	F	301[B]	KFV	CP1-CP2-NP1	3.97	120.75	112.42
2	D	302[B]	KFV	CP4-CP3-NP1	3.96	123.09	116.42
2	F	301[B]	KFV	CP5-CP4-CP3	-3.96	105.77	112.36
2	E	301	KFV	OP3-CP7-CPA	-3.93	101.00	110.25
2	A	301	KFV	CP9-CPA-CP7	3.88	115.56	108.82
2	F	301[B]	KFV	CP8-CPA-CP7	-3.87	102.11	108.82
2	F	301[A]	KFV	N3-C2-N1	-3.77	122.79	128.68
2	F	303[A]	KFV	N3-C2-N1	-3.72	122.87	128.68
2	E	302[A]	KFV	N3-C2-N1	-3.61	123.04	128.68
2	D	302[B]	KFV	CP7-CP6-NP2	-3.56	109.50	116.58
2	C	303[A]	KFV	O11-P1-O5'	-3.51	91.44	107.75
2	D	302[A]	KFV	CP9-CPA-CP7	3.49	114.88	108.82
2	B	301[A]	KFV	N3-C2-N1	-3.40	123.36	128.68
2	C	301	KFV	O32-P3-O31	3.39	120.60	107.64
2	B	301[A]	KFV	O11-P1-O5'	3.37	123.40	107.75
7	F	304	KG7	OS4-NS4-CS2	3.35	123.17	112.28
2	F	303[A]	KFV	C1'-N9-C4	-3.33	120.79	126.64
2	B	301[A]	KFV	CP5-CP4-CP3	-3.27	106.91	112.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301[B]	KFV	CP5-CP4-CP3	-3.27	106.91	112.36
2	C	303[A]	KFV	O7-P2-O6	3.24	115.50	104.64
2	E	301	KFV	N3-C2-N1	-3.11	123.81	128.68
2	F	303[A]	KFV	C2-N1-C6	3.10	124.06	118.75
2	D	302[A]	KFV	CP4-CP5-NP2	3.09	118.14	111.90
2	C	303[A]	KFV	O4'-C4'-C5'	3.06	119.44	109.37
2	C	303[A]	KFV	N3-C2-N1	-3.06	123.89	128.68
2	D	302[A]	KFV	N3-C2-N1	-3.05	123.91	128.68
2	C	301	KFV	O7-CPB-CPA	-3.05	105.65	110.55
2	E	302[A]	KFV	C4-C5-N7	-3.04	106.23	109.40
2	B	301[A]	KFV	OP3-CP7-CP6	-3.03	94.82	109.42
2	B	301[B]	KFV	OP3-CP7-CP6	-3.03	94.82	109.42
7	F	304	KG7	CS1-CS2-NS4	3.02	117.80	114.59
2	B	301[B]	KFV	C4-C5-N7	-3.01	106.26	109.40
2	D	302[B]	KFV	CP4-CP5-NP2	-3.01	105.82	111.90
2	E	302[A]	KFV	O3'-C3'-C2'	-3.01	100.78	111.68
2	C	303[A]	KFV	P1-O5'-C5'	-2.99	104.12	121.68
2	B	301[B]	KFV	O3'-C3'-C2'	-2.99	100.84	111.68
2	F	303[A]	KFV	C4-C5-N7	-2.99	106.28	109.40
2	F	301[B]	KFV	C2-N1-C6	2.96	123.81	118.75
2	A	301	KFV	C1'-N9-C4	-2.92	121.52	126.64
2	D	302[B]	KFV	N3-C2-N1	-2.89	124.16	128.68
2	F	301[B]	KFV	CP4-CP3-NP1	-2.88	111.58	116.42
2	E	302[A]	KFV	C1'-N9-C4	-2.85	121.63	126.64
2	D	302[B]	KFV	CP5-NP2-CP6	-2.84	117.51	122.59
2	A	301	KFV	CP1-S-CS1	2.84	103.36	99.80
2	B	301[A]	KFV	CP9-CPA-CPB	2.84	112.86	108.23
2	C	301	KFV	CP2-NP1-CP3	2.82	128.07	122.84
7	F	304	KG7	OS1-CS1-CS2	2.77	122.37	116.35
2	E	302[A]	KFV	C2-N1-C6	2.77	123.49	118.75
2	A	301	KFV	N3-C2-N1	-2.67	124.51	128.68
2	F	301[A]	KFV	CP2-NP1-CP3	-2.66	117.89	122.84
2	B	301[A]	KFV	CP1-S-CS1	2.65	103.13	99.80
2	B	301[B]	KFV	CP1-S-CS1	2.65	103.13	99.80
2	B	301[B]	KFV	N3-C2-N1	-2.63	124.56	128.68
2	F	301[B]	KFV	CP4-CP5-NP2	-2.63	106.59	111.90
2	C	301	KFV	CP4-CP5-NP2	2.59	117.12	111.90
2	D	302[B]	KFV	N6-C6-N1	2.56	123.89	118.57
2	D	302[A]	KFV	O32-P3-O31	2.54	117.35	107.64
2	F	301[A]	KFV	CP7-CP6-NP2	2.53	121.62	116.58
2	D	302[A]	KFV	C1'-N9-C4	-2.50	122.25	126.64
2	D	302[A]	KFV	C4-C5-N7	-2.49	106.81	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301[A]	KFV	C2-N1-C6	2.46	122.96	118.75
2	B	301[B]	KFV	P2-O6-P1	-2.44	124.44	132.83
2	B	301[A]	KFV	CS3-CS2-CS1	-2.44	113.84	118.35
2	B	301[B]	KFV	CS3-CS2-CS1	-2.44	113.84	118.35
2	D	302[B]	KFV	O4'-C1'-C2'	-2.43	103.38	106.93
2	C	303[A]	KFV	C5'-C4'-C3'	-2.42	106.39	114.40
2	E	302[A]	KFV	O2'-C2'-C3'	-2.42	104.31	111.17
2	C	301	KFV	N3-C2-N1	-2.39	124.94	128.68
2	D	302[A]	KFV	O4'-C1'-C2'	2.39	110.41	106.93
2	E	301	KFV	C1'-N9-C4	-2.38	122.46	126.64
2	B	301[A]	KFV	C4-C5-N7	-2.37	106.93	109.40
2	F	303[A]	KFV	O7-P2-O6	2.34	112.49	104.64
2	E	301	KFV	OP1-CP3-NP1	2.33	127.42	123.01
2	A	301	KFV	P2-O6-P1	-2.33	124.83	132.83
2	A	301	KFV	OP1-CP3-CP4	-2.31	117.79	122.02
2	C	303[A]	KFV	C4-C5-N7	-2.31	106.99	109.40
2	A	301	KFV	CP5-CP4-CP3	-2.31	108.52	112.36
2	C	301	KFV	CP9-CPA-CPB	2.29	111.97	108.23
2	B	301[A]	KFV	CP7-CP6-NP2	2.29	121.14	116.58
2	B	301[B]	KFV	CP7-CP6-NP2	2.29	121.14	116.58
2	C	301	KFV	O4'-C1'-C2'	-2.28	103.59	106.93
2	C	301	KFV	O22-P2-O21	2.27	123.48	112.24
2	A	301	KFV	O4'-C1'-C2'	2.27	110.24	106.93
2	C	301	KFV	CS3-CS2-CS1	-2.26	114.17	118.35
7	F	304	KG7	O-CS1-CS2	-2.25	118.50	121.38
2	E	301	KFV	CP2-NP1-CP3	2.25	127.02	122.84
2	E	302[A]	KFV	O22-P2-O6	2.25	112.17	104.64
2	D	302[B]	KFV	CP1-CP2-NP1	2.23	117.39	112.31
2	A	301	KFV	N6-C6-N1	2.21	123.17	118.57
2	F	301[A]	KFV	O5'-C5'-C4'	2.21	116.58	108.99
2	D	302[A]	KFV	OP2-CP6-CP7	-2.19	114.38	121.06
2	B	301[A]	KFV	P1-O5'-C5'	2.19	134.51	121.68
2	C	301	KFV	N6-C6-N1	2.18	123.10	118.57
2	B	301[A]	KFV	O4'-C4'-C5'	2.18	116.54	109.37
2	F	301[B]	KFV	CP8-CPA-CPB	2.18	111.78	108.23
2	B	301[A]	KFV	O4'-C4'-C3'	-2.17	100.23	104.87
2	C	303[A]	KFV	O2'-C2'-C1'	2.16	118.84	110.85
2	F	301[A]	KFV	C4-C5-N7	-2.16	107.15	109.40
2	D	302[A]	KFV	O2'-C2'-C3'	2.10	117.13	111.17
2	B	301[A]	KFV	OP2-CP6-NP2	-2.09	118.51	122.99
2	B	301[B]	KFV	OP2-CP6-NP2	-2.09	118.51	122.99
2	E	301	KFV	C4-C5-N7	-2.08	107.23	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	KFV	O11-P1-O5'	2.06	117.33	107.75
2	D	302[B]	KFV	O4'-C4'-C5'	2.06	116.17	109.37
2	F	301[B]	KFV	CP2-NP1-CP3	2.05	126.64	122.84
2	D	302[A]	KFV	O32-P3-O3'	2.03	115.10	105.99
2	C	303[A]	KFV	O5'-C5'-C4'	2.02	115.95	108.99
2	B	301[A]	KFV	O2'-C2'-C3'	2.02	116.90	111.17
2	C	301	KFV	C4-C5-N7	-2.00	107.31	109.40

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301[A]	KFV	C5'-O5'-P1-O11
2	B	301[A]	KFV	CP7-CPA-CPB-O7
2	B	301[A]	KFV	OP3-CP7-CPA-CPB
2	B	301[A]	KFV	CP6-CP7-CPA-CPB
2	B	301[A]	KFV	OP3-CP7-CPA-CP9
2	B	301[A]	KFV	CP6-CP7-CPA-CP9
2	B	301[B]	KFV	C3'-O3'-P3-O33
2	B	301[B]	KFV	CPB-O7-P2-O21
2	B	301[B]	KFV	CPB-O7-P2-O22
2	B	301[B]	KFV	CP9-CPA-CPB-O7
2	B	301[B]	KFV	OP3-CP7-CPA-CPB
2	B	301[B]	KFV	CP6-CP7-CPA-CPB
2	B	301[B]	KFV	OP3-CP7-CPA-CP9
2	B	301[B]	KFV	CP6-CP7-CPA-CP9
2	C	301	KFV	C5'-O5'-P1-O11
2	C	301	KFV	C5'-O5'-P1-O12
2	C	301	KFV	CP7-CPA-CPB-O7
2	C	301	KFV	OP3-CP7-CPA-CP9
2	C	301	KFV	CP6-CP7-CPA-CP9
2	C	301	KFV	CP2-CP1-S-CS1
2	C	303[A]	KFV	C3'-O3'-P3-O33
2	D	302[A]	KFV	C3'-O3'-P3-O31
2	D	302[A]	KFV	P1-O6-P2-O7
2	D	302[A]	KFV	CP7-CPA-CPB-O7
2	D	302[A]	KFV	OP3-CP7-CPA-CP9
2	D	302[A]	KFV	CP6-CP7-CPA-CP9
2	D	302[A]	KFV	OP2-CP6-CP7-OP3
2	D	302[A]	KFV	S-CP1-CP2-NP1
2	D	302[B]	KFV	C3'-O3'-P3-O33
2	D	302[B]	KFV	C5'-O5'-P1-O11

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Mol	Chain	Res	Type	Atoms
2	D	302[B]	KFV	C5'-O5'-P1-O6
2	D	302[B]	KFV	CP7-CPA-CPB-O7
2	D	302[B]	KFV	OP3-CP7-CPA-CPB
2	D	302[B]	KFV	CP6-CP7-CPA-CPB
2	D	302[B]	KFV	OP3-CP7-CPA-CP9
2	D	302[B]	KFV	CP6-CP7-CPA-CP9
2	D	302[B]	KFV	OP3-CP7-CPA-CP8
2	D	302[B]	KFV	CP6-CP7-CPA-CP8
2	D	302[B]	KFV	CP7-CP6-NP2-CP5
2	D	302[B]	KFV	S-CP1-CP2-NP1
2	E	301	KFV	CP7-CPA-CPB-O7
2	E	301	KFV	OP3-CP7-CPA-CP9
2	E	301	KFV	CP6-CP7-CPA-CP9
2	E	302[A]	KFV	C3'-O3'-P3-O32
2	F	301[A]	KFV	C5'-O5'-P1-O11
2	F	301[A]	KFV	C5'-O5'-P1-O12
2	F	301[A]	KFV	C5'-O5'-P1-O6
2	F	301[A]	KFV	CPA-CPB-O7-P2
2	F	301[A]	KFV	CP7-CPA-CPB-O7
2	F	301[A]	KFV	OP3-CP7-CPA-CPB
2	F	301[A]	KFV	CP6-CP7-CPA-CPB
2	F	301[B]	KFV	O4'-C4'-C5'-O5'
2	F	301[B]	KFV	C4'-C5'-O5'-P1
2	F	301[B]	KFV	CP1-CP2-NP1-CP3
2	F	301[B]	KFV	S-CP1-CP2-NP1
2	F	301[B]	KFV	OS1-CS1-S-CP1
2	D	302[B]	KFV	CP4-CP5-NP2-CP6
2	F	301[B]	KFV	CP4-CP5-NP2-CP6
2	D	302[B]	KFV	O4'-C4'-C5'-O5'
2	F	301[B]	KFV	C3'-C4'-C5'-O5'
2	C	303[A]	KFV	C4'-C5'-O5'-P1
2	C	303[A]	KFV	C3'-C4'-C5'-O5'
2	D	302[B]	KFV	C3'-C4'-C5'-O5'
2	D	302[A]	KFV	C4'-C3'-O3'-P3
2	B	301[B]	KFV	CP8-CPA-CPB-O7
2	E	301	KFV	CP8-CPA-CPB-O7
2	F	301[A]	KFV	CP8-CPA-CPB-O7
2	D	302[A]	KFV	C2'-C3'-O3'-P3
2	C	303[A]	KFV	O4'-C4'-C5'-O5'
2	F	303[A]	KFV	O4'-C4'-C5'-O5'
5	C	304	PG4	O3-C5-C6-O4
2	D	302[B]	KFV	CP8-CPA-CPB-O7

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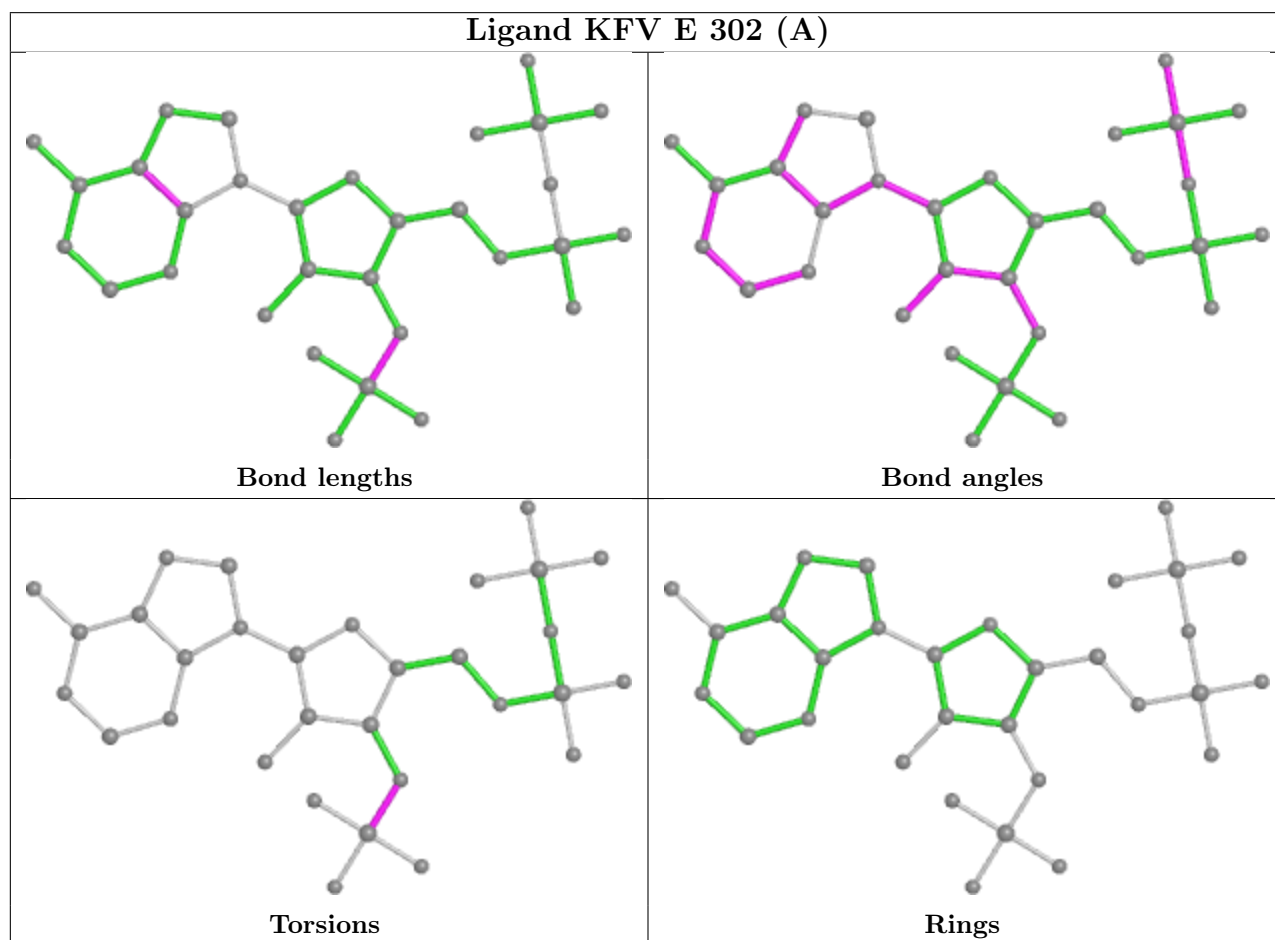
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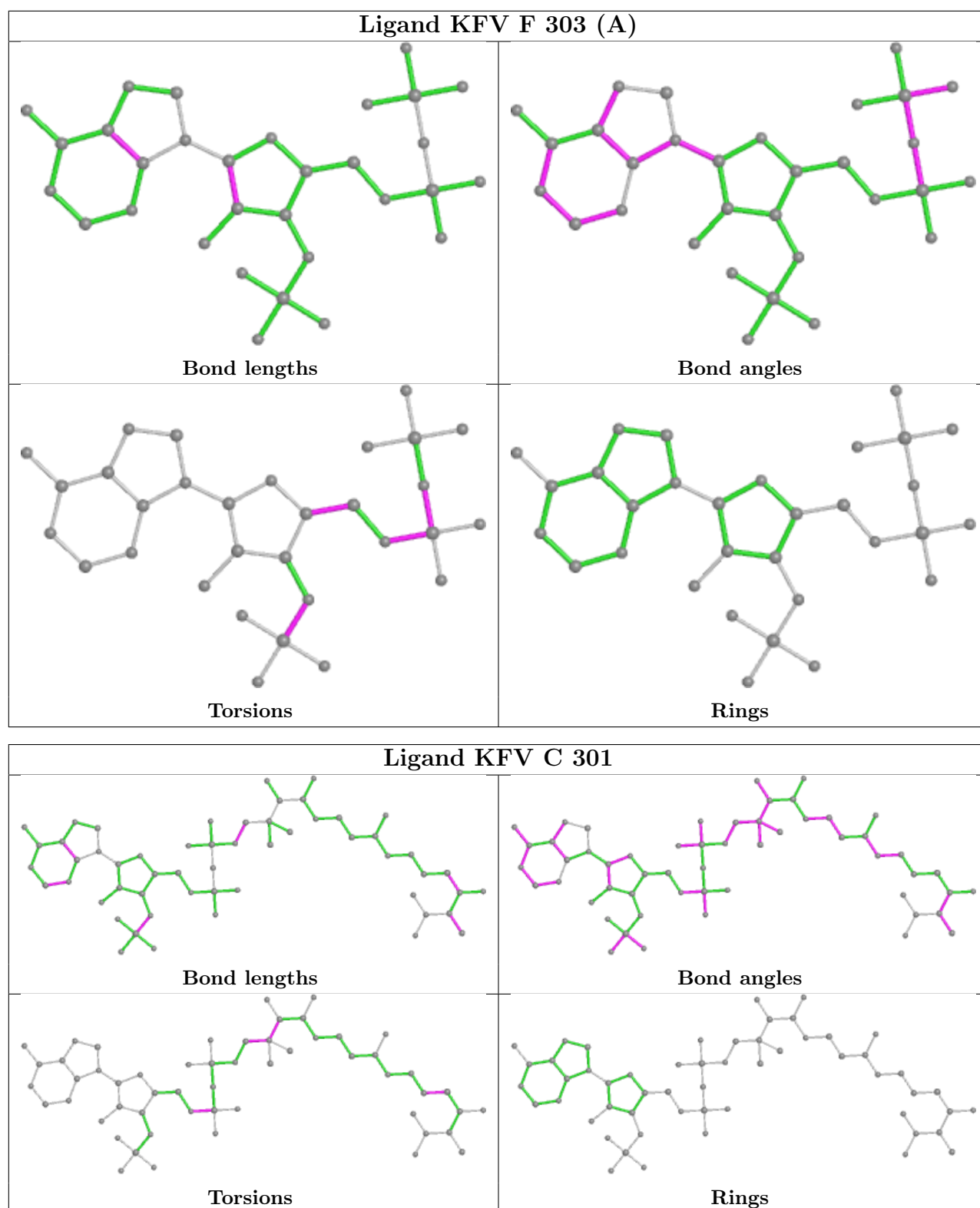
Mol	Chain	Res	Type	Atoms
2	B	301[B]	KFV	C2'-C3'-O3'-P3
2	F	301[A]	KFV	OS1-CS1-S-CP1
2	F	303[A]	KFV	C3'-C4'-C5'-O5'
2	B	301[B]	KFV	C4'-C3'-O3'-P3
2	B	301[B]	KFV	P2-O6-P1-O5'
2	E	301	KFV	P1-O6-P2-O7
2	F	303[A]	KFV	P2-O6-P1-O5'
2	D	302[A]	KFV	NP2-CP6-CP7-OP3
2	F	303[A]	KFV	C3'-O3'-P3-O33
2	F	301[A]	KFV	CP6-CP7-CPA-CP8
2	B	301[A]	KFV	C5'-O5'-P1-O6
2	B	301[B]	KFV	CPB-O7-P2-O6
2	F	301[B]	KFV	C3'-O3'-P3-O31
2	F	301[B]	KFV	C3'-O3'-P3-O32
2	C	303[A]	KFV	P2-O6-P1-O12
2	B	301[A]	KFV	C5'-O5'-P1-O12
2	B	301[A]	KFV	C3'-C4'-C5'-O5'
2	B	301[A]	KFV	O4'-C4'-C5'-O5'
2	D	302[A]	KFV	CP8-CPA-CPB-O7
2	F	301[B]	KFV	CP9-CPA-CPB-O7
2	F	301[B]	KFV	CP8-CPA-CPB-O7
5	C	304	PG4	C8-C7-O4-C6
2	B	301[B]	KFV	P1-O6-P2-O22
2	D	302[B]	KFV	C4'-C5'-O5'-P1
2	F	301[B]	KFV	OP2-CP6-CP7-CPA
5	C	304	PG4	O1-C1-C2-O2
2	B	301[A]	KFV	CP8-CPA-CPB-O7
2	D	302[B]	KFV	CP9-CPA-CPB-O7
2	F	301[B]	KFV	NP2-CP6-CP7-CPA
2	B	301[A]	KFV	CP2-CP1-S-CS1
2	B	301[B]	KFV	CP2-CP1-S-CS1
2	D	302[B]	KFV	CP1-CP2-NP1-CP3
2	C	301	KFV	C5'-O5'-P1-O6
2	C	303[A]	KFV	C3'-O3'-P3-O31
2	F	303[A]	KFV	C5'-O5'-P1-O6
2	C	303[A]	KFV	P2-O6-P1-O11
2	F	301[B]	KFV	P1-O6-P2-O21
2	F	301[B]	KFV	P1-O6-P2-O22
2	D	302[B]	KFV	CPA-CPB-O7-P2
2	C	303[A]	KFV	C5'-O5'-P1-O12
2	F	301[B]	KFV	CPB-O7-P2-O22
2	D	302[B]	KFV	OP2-CP6-NP2-CP5

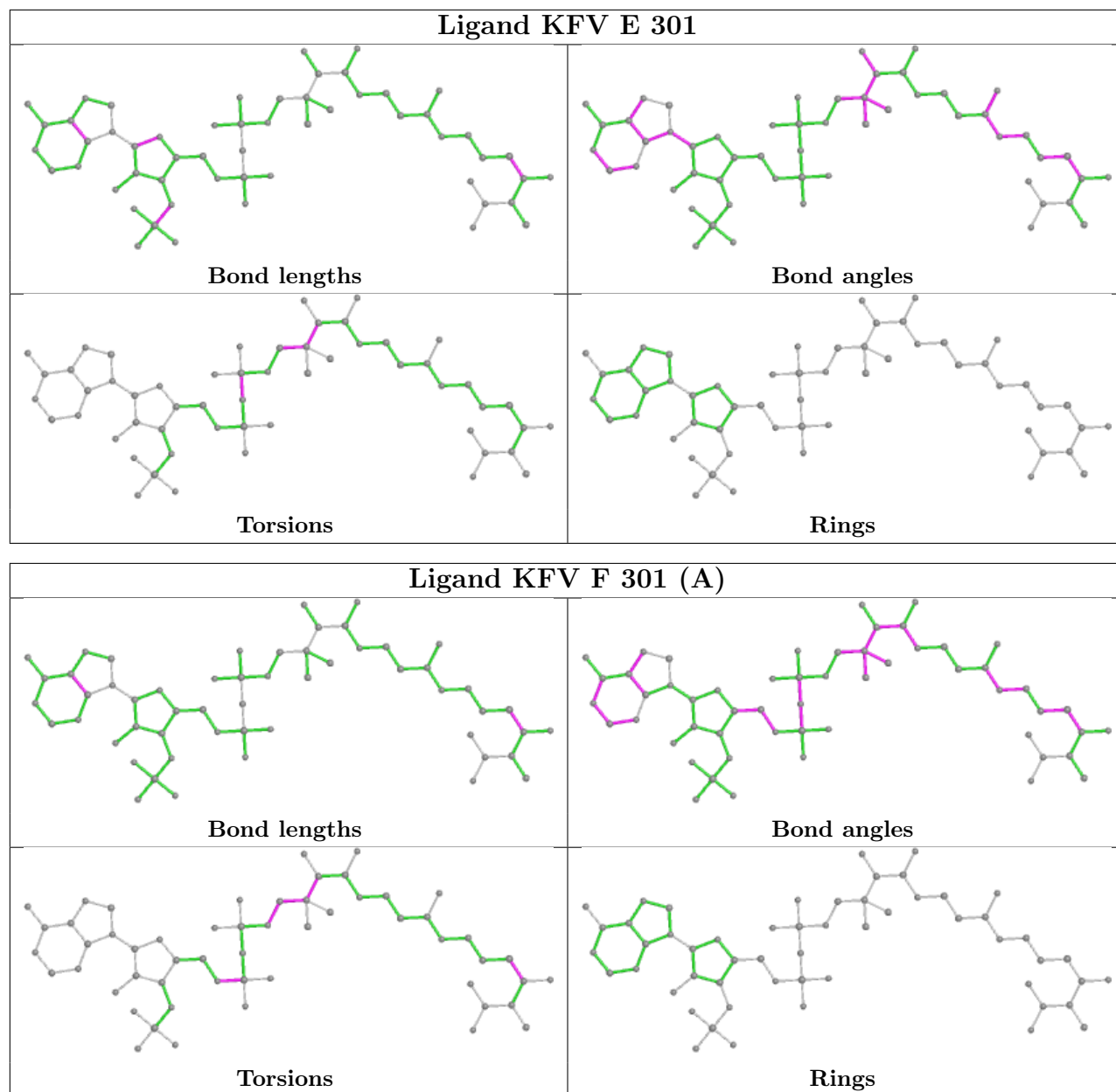
There are no ring outliers.

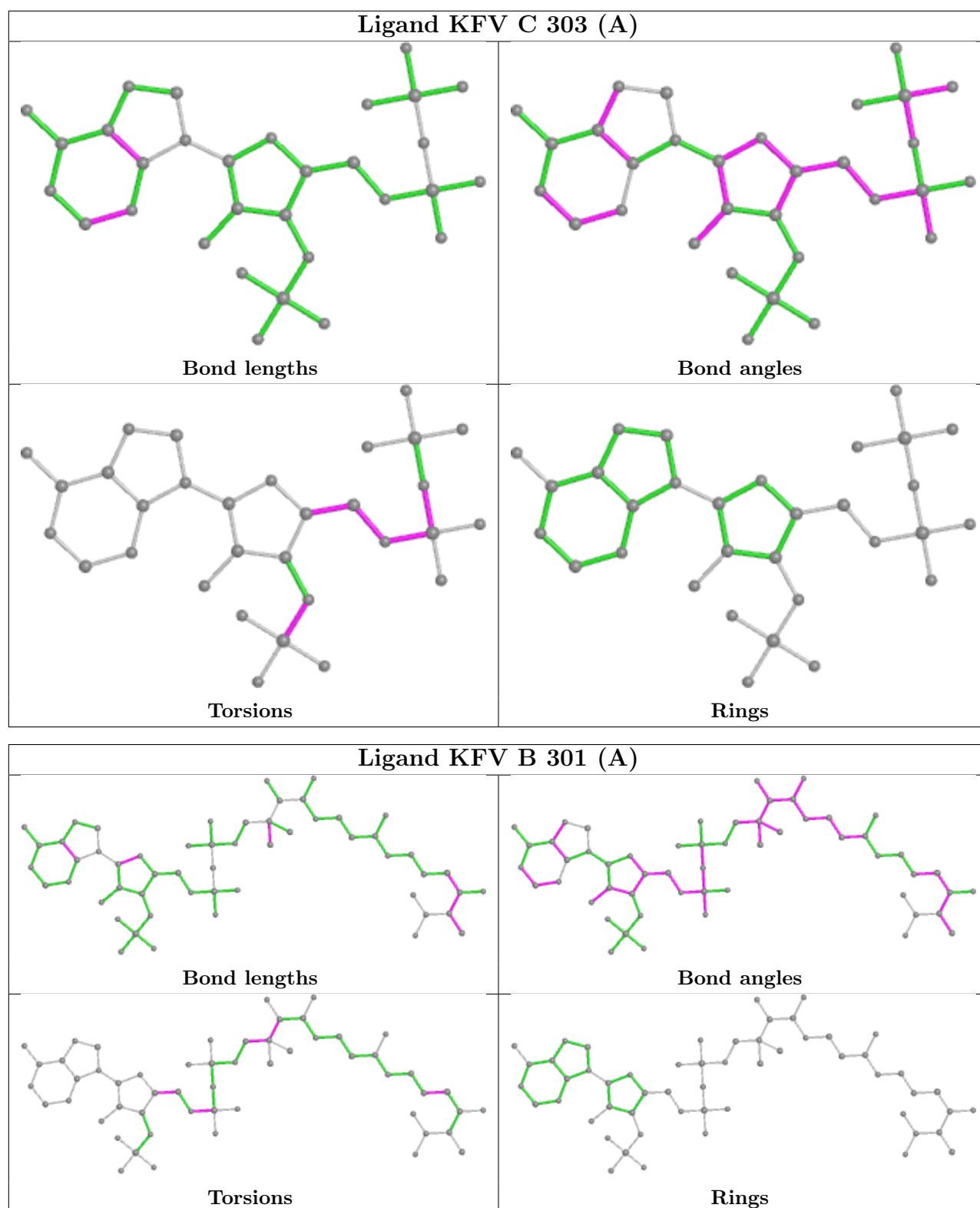
No monomer is involved in short contacts.

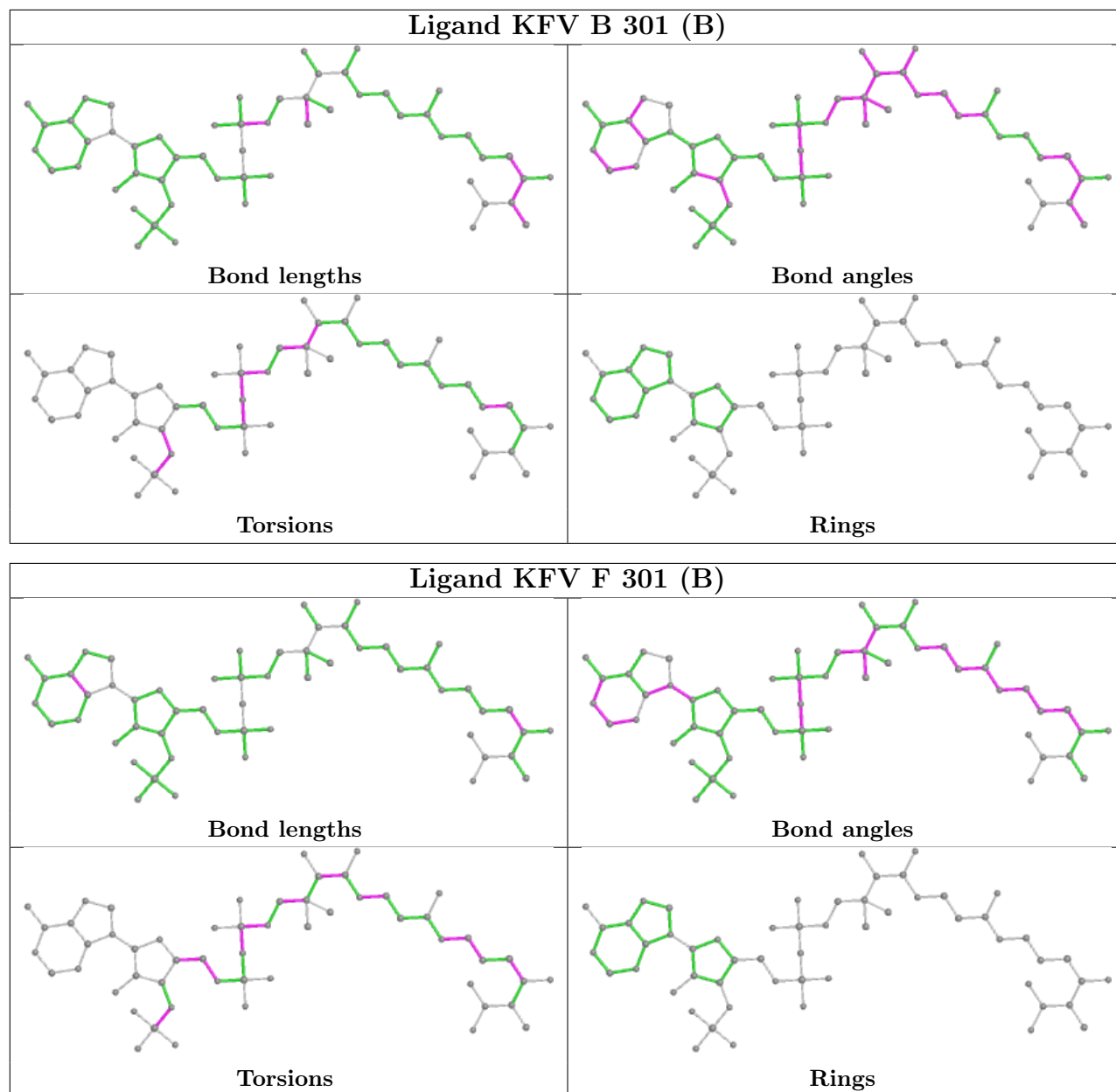
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

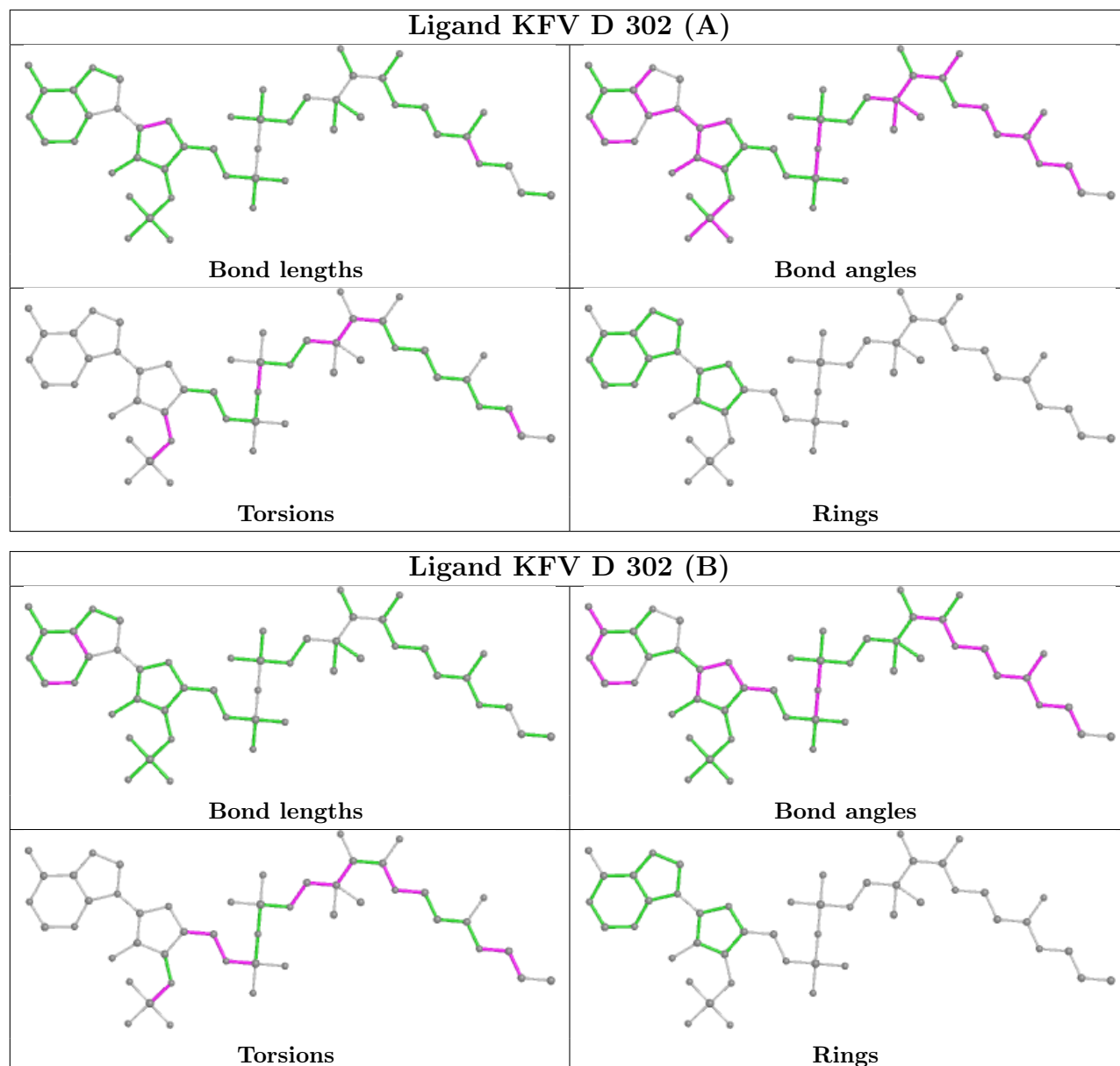


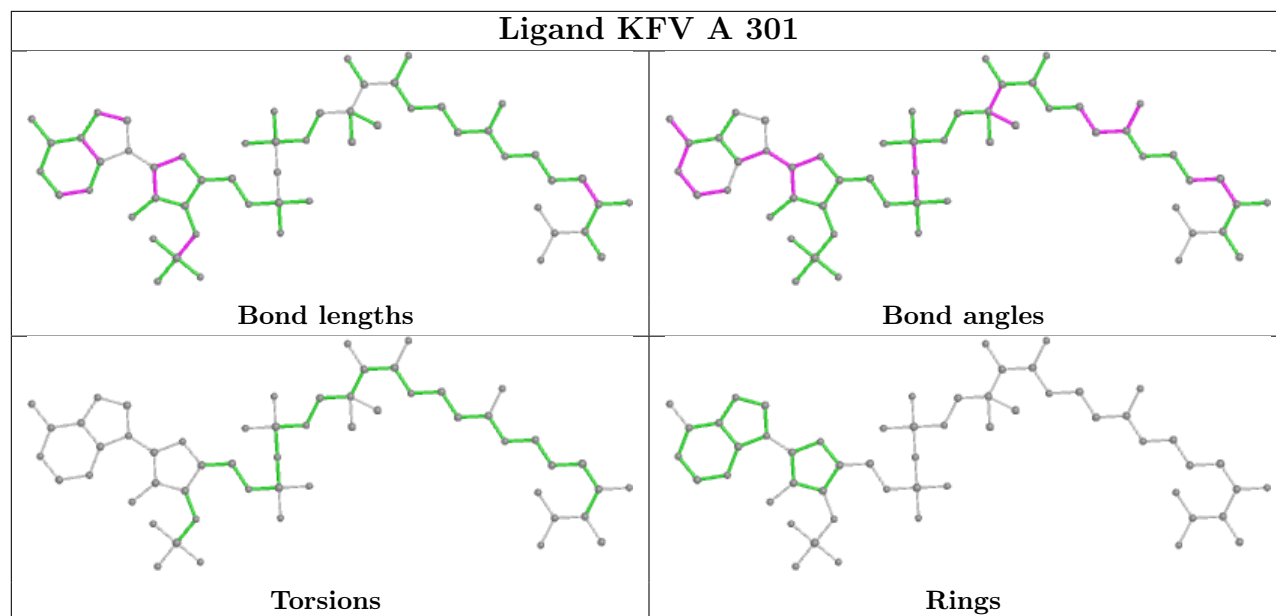












4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.