



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 02:26 AM EDT

PDB ID : 6N94
Title : Methylmalonyl-CoA decarboxylase in complex with 2-nitronate-propionyl-amino(dethia)-CoA
Authors : Stunkard, L.M.; Dixon, A.D.; Huth, T.J.; Lohman, J.R.
Deposited on : 2018-11-30
Resolution : 1.75 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 1.75 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 [i](#)

There are 9 unique types of molecules in this entry. The entry contains 15267 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.

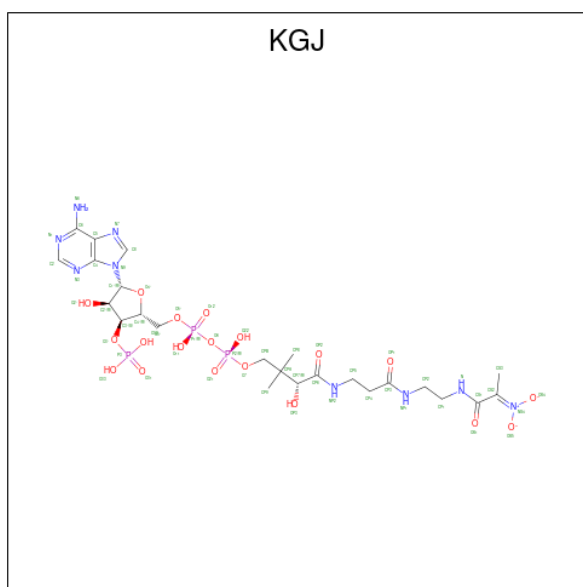
- Molecule 1 is a protein called Methylmalonyl-CoA decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	260	2153	1379	366	395	13	0	20	0
1	B	260	2139	1377	361	389	12	0	18	0
1	C	260	2136	1369	363	392	12	0	16	0
1	D	260	2110	1351	355	391	13	0	15	0
1	E	260	2135	1368	360	395	12	0	17	0
1	F	260	2150	1381	365	392	12	0	19	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-phosphonoxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-3,3-dimethyl-2-oxidanyl-butanoyl]amino]propanoylamino]ethylamino]-1-oxidanylidene-prop an-2-ylidene]-bis(oxidanidyl)azanum (three-letter code: KGJ) (formula: C₂₄H₃₉N₉O₁₉P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			55	24	9	19	3		
2	B	1	Total	C	N	O	P	0	0
			55	24	9	19	3		
2	C	1	Total	C	N	O	P	0	0
			55	24	9	19	3		
2	C	1	Total	C	N	O	P	0	1
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	1
			82	34	14	29	5		
2	E	1	Total	C	N	O	P	0	1
			82	34	14	29	5		
2	E	1	Total	C	N	O	P	0	1
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	1
			82	34	14	29	5		
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		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

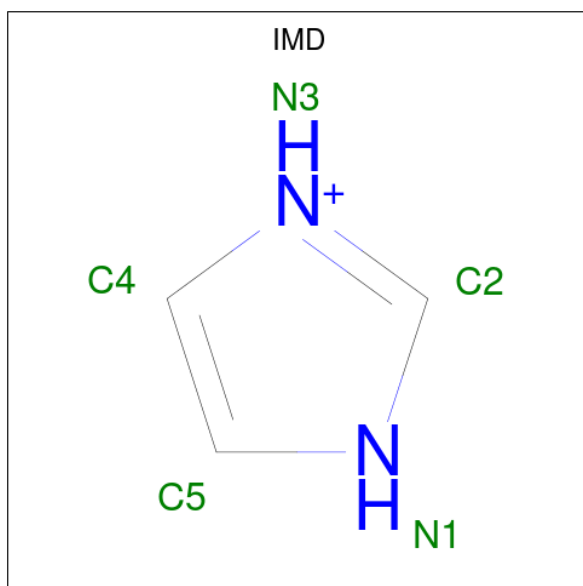
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total K 1 1	0	0
5	F	1	Total K 1 1	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



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

- Molecule 7 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



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

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	1	Total	C O	0	0
			10	6 4		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	337	Total	O	0	14
			349	349		
9	B	280	Total	O	0	9
			286	286		
9	C	308	Total	O	0	17
			321	321		
9	D	300	Total	O	0	12
			309	309		
9	E	311	Total	O	0	18
			322	322		
9	F	299	Total	O	0	12
			307	307		

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	87.05Å 114.82Å 193.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.29 – 1.75	Depositor
% Data completeness (in resolution range)	94.0 (29.29-1.75)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.75Å)	Xtrriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.146 , 0.178	Depositor
Wilson B-factor (Å ²)	20.3	Xtrriage
Anisotropy	0.035	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	15267	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 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	KGJ	B	301	-	45,57,57	1.77	5 (11%)	57,85,85	3.07	18 (31%)
2	KGJ	F	301[A]	-	45,57,57	1.43	3 (6%)	57,85,85	1.65	13 (22%)
2	KGJ	C	302[A]	-	28,33,57	1.07	2 (7%)	35,52,85	1.35	3 (8%)
7	IMD	D	303	-	3,5,5	0.27	0	4,5,5	0.67	0
2	KGJ	D	302[B]	-	45,57,57	1.69	3 (6%)	57,85,85	1.27	6 (10%)
4	PEG	B	302	-	6,6,6	0.19	0	5,5,5	0.12	0
2	KGJ	F	301[B]	-	45,57,57	1.49	2 (4%)	57,85,85	1.48	10 (17%)
2	KGJ	C	301	-	45,57,57	1.56	4 (8%)	57,85,85	1.19	5 (8%)
4	PEG	C	304	-	6,6,6	0.17	0	5,5,5	0.16	0
8	PGE	F	304	5	9,9,9	0.29	0	8,8,8	0.24	0
2	KGJ	F	302[A]	-	28,33,57	1.13	2 (7%)	35,52,85	1.60	6 (17%)
2	KGJ	A	301	-	45,57,57	1.69	5 (11%)	57,85,85	1.62	13 (22%)
2	KGJ	E	301[A]	-	45,57,57	1.52	5 (11%)	57,85,85	1.52	7 (12%)
6	PG4	C	305	5	12,12,12	0.29	0	11,11,11	0.25	0
2	KGJ	E	302[A]	-	28,33,57	1.11	1 (3%)	35,52,85	1.38	6 (17%)
2	KGJ	E	301[B]	-	45,57,57	1.56	5 (11%)	57,85,85	1.07	4 (7%)
2	KGJ	D	302[A]	-	45,57,57	1.67	3 (6%)	57,85,85	1.37	6 (10%)

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	KGJ	B	301	-	-	9/51/75/75	0/3/3/3
2	KGJ	F	301[A]	-	-	6/51/75/75	0/3/3/3
2	KGJ	C	302[A]	-	-	7/17/37/75	0/3/3/3
7	IMD	D	303	-	-	-	0/1/1/1
2	KGJ	D	302[B]	-	-	1/51/75/75	0/3/3/3
4	PEG	B	302	-	-	2/4/4/4	-
2	KGJ	F	301[B]	-	-	6/51/75/75	0/3/3/3
2	KGJ	C	301	-	-	0/51/75/75	0/3/3/3
4	PEG	C	304	-	-	2/4/4/4	-
8	PGE	F	304	5	-	1/7/7/7	-
2	KGJ	F	302[A]	-	-	4/17/37/75	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KGJ	A	301	-	-	1/51/75/75	0/3/3/3
2	KGJ	E	301[A]	-	-	4/51/75/75	0/3/3/3
6	PG4	C	305	5	-	3/10/10/10	-
2	KGJ	E	302[A]	-	-	4/17/37/75	0/3/3/3
2	KGJ	E	301[B]	-	-	3/51/75/75	0/3/3/3
2	KGJ	D	302[A]	-	-	5/51/75/75	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	302[A]	KGJ	CS1-N	9.21	1.49	1.33
2	D	302[B]	KGJ	CS1-N	9.21	1.49	1.33
2	B	301	KGJ	CS1-N	9.18	1.49	1.33
2	C	301	KGJ	CS1-N	8.17	1.47	1.33
2	A	301	KGJ	CS1-N	8.12	1.47	1.33
2	E	301[A]	KGJ	CS1-N	8.10	1.47	1.33
2	E	301[B]	KGJ	CS1-N	8.10	1.47	1.33
2	F	301[A]	KGJ	CS1-N	7.78	1.47	1.33
2	F	301[B]	KGJ	CS1-N	7.78	1.47	1.33
2	A	301	KGJ	O4'-C1'	4.96	1.48	1.41
2	D	302[A]	KGJ	O4'-C1'	3.01	1.45	1.41
2	B	301	KGJ	O4'-C1'	2.99	1.45	1.41
2	A	301	KGJ	P3-O3'	2.93	1.64	1.59
2	E	302[A]	KGJ	C5-C4	2.77	1.48	1.40
2	D	302[B]	KGJ	O4'-C1'	2.77	1.44	1.41
2	F	301[B]	KGJ	C5-C4	2.75	1.48	1.40
2	C	301	KGJ	P3-O3'	2.63	1.64	1.59
2	F	302[A]	KGJ	C5-C4	2.62	1.47	1.40
2	A	301	KGJ	C5-C4	2.58	1.47	1.40
2	B	301	KGJ	CS3-CS2	2.54	1.54	1.49
2	F	302[A]	KGJ	P2-O7	2.52	1.64	1.54
2	C	302[A]	KGJ	C5-C4	2.49	1.47	1.40
2	B	301	KGJ	OS1-CS1	-2.39	1.19	1.23
2	E	301[A]	KGJ	C5-C4	2.33	1.47	1.40
2	C	301	KGJ	C5-C4	2.31	1.47	1.40
2	A	301	KGJ	C2-N1	2.28	1.38	1.33
2	E	301[B]	KGJ	C5-C4	2.25	1.46	1.40
2	E	301[A]	KGJ	OS1-CS1	-2.25	1.19	1.23
2	E	301[B]	KGJ	OS1-CS1	-2.25	1.19	1.23
2	C	302[A]	KGJ	C2-N3	2.24	1.35	1.32
2	C	301	KGJ	C5-N7	-2.15	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301[A]	KGJ	C5-C4	2.11	1.46	1.40
2	D	302[A]	KGJ	P3-O33	-2.05	1.46	1.54
2	B	301	KGJ	CP8-CPA	2.05	1.58	1.53
2	D	302[B]	KGJ	C5-C4	2.04	1.46	1.40
2	E	301[A]	KGJ	CS3-CS2	2.04	1.53	1.49
2	E	301[B]	KGJ	CS3-CS2	2.04	1.53	1.49
2	F	301[A]	KGJ	C2'-C1'	-2.04	1.50	1.53
2	E	301[A]	KGJ	CP2-NP1	-2.01	1.41	1.46
2	E	301[B]	KGJ	CP2-NP1	-2.01	1.41	1.46

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	KGJ	CP8-CPA-CPB	-12.23	88.29	108.23
2	B	301	KGJ	CP9-CPA-CPB	9.82	124.26	108.23
2	B	301	KGJ	CP8-CPA-CP7	-9.67	92.06	108.82
2	B	301	KGJ	CP8-CPA-CP9	-7.25	94.39	109.17
2	E	301[A]	KGJ	P2-O6-P1	-5.77	113.03	132.83
2	F	301[A]	KGJ	P2-O6-P1	-5.21	114.94	132.83
2	D	302[A]	KGJ	P2-O6-P1	-4.81	116.34	132.83
2	F	301[B]	KGJ	O5'-C5'-C4'	4.39	124.10	108.99
2	A	301	KGJ	N3-C2-N1	-4.21	122.09	128.68
2	F	301[A]	KGJ	N3-C2-N1	-4.15	122.20	128.68
2	F	302[A]	KGJ	N3-C2-N1	-4.12	122.24	128.68
2	B	301	KGJ	N3-C2-N1	-4.09	122.28	128.68
2	C	302[A]	KGJ	N3-C2-N1	-3.98	122.46	128.68
2	D	302[A]	KGJ	CP9-CPA-CP7	3.92	115.61	108.82
2	D	302[B]	KGJ	CP9-CPA-CP7	3.92	115.61	108.82
2	E	301[A]	KGJ	N3-C2-N1	-3.88	122.62	128.68
2	B	301	KGJ	P2-O6-P1	-3.87	119.53	132.83
2	F	302[A]	KGJ	P1-O6-P2	-3.87	119.56	132.83
2	A	301	KGJ	O4'-C1'-C2'	3.86	112.57	106.93
2	A	301	KGJ	C1'-N9-C4	-3.75	120.05	126.64
2	D	302[A]	KGJ	N3-C2-N1	-3.72	122.87	128.68
2	F	302[A]	KGJ	C1'-N9-C4	-3.70	120.14	126.64
2	B	301	KGJ	OP3-CP7-CPA	-3.68	101.59	110.25
2	F	302[A]	KGJ	O22-P2-O6	3.60	116.70	104.64
2	E	302[A]	KGJ	N3-C2-N1	-3.51	123.19	128.68
2	B	301	KGJ	CP9-CPA-CP7	3.22	114.41	108.82
2	F	301[A]	KGJ	O7-P2-O21	-3.18	96.64	109.07
2	F	301[B]	KGJ	O7-P2-O21	-3.18	96.64	109.07
2	B	301	KGJ	CP5-CP4-CP3	-3.15	107.12	112.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	302[A]	KGJ	P1-O6-P2	-3.12	122.14	132.83
2	F	301[B]	KGJ	N3-C2-N1	-3.07	123.87	128.68
2	B	301	KGJ	C5-C6-N6	-3.04	115.72	120.35
2	E	301[B]	KGJ	N3-C2-N1	-2.99	124.00	128.68
2	E	301[A]	KGJ	CP5-CP4-CP3	-2.97	107.40	112.36
2	E	301[B]	KGJ	CP5-CP4-CP3	-2.97	107.40	112.36
2	A	301	KGJ	O5'-P1-O12	-2.91	97.71	109.07
2	E	301[A]	KGJ	C2-N1-C6	2.88	123.68	118.75
2	A	301	KGJ	C2-N1-C6	2.86	123.64	118.75
2	E	302[A]	KGJ	C4-C5-N7	-2.86	106.42	109.40
2	F	301[A]	KGJ	C1'-N9-C4	-2.85	121.64	126.64
2	F	302[A]	KGJ	C2-N1-C6	2.80	123.54	118.75
2	A	301	KGJ	O3'-P3-O31	-2.75	98.78	109.39
2	D	302[B]	KGJ	N3-C2-N1	-2.75	124.39	128.68
2	F	301[A]	KGJ	OP1-CP3-CP4	-2.74	117.00	122.02
2	F	301[B]	KGJ	OP1-CP3-CP4	-2.74	117.00	122.02
2	C	301	KGJ	N3-C2-N1	-2.69	124.47	128.68
2	A	301	KGJ	N6-C6-N1	2.68	124.14	118.57
2	B	301	KGJ	O7-CPB-CPA	-2.67	106.25	110.55
2	D	302[B]	KGJ	O4'-C4'-C5'	2.64	118.06	109.37
2	E	301[A]	KGJ	O32-P3-O3'	2.63	117.76	105.99
2	D	302[A]	KGJ	N6-C6-N1	2.62	124.01	118.57
2	A	301	KGJ	O7-CPB-CPA	-2.61	106.35	110.55
2	D	302[B]	KGJ	N6-C6-N1	2.59	123.95	118.57
2	C	302[A]	KGJ	P1-O6-P2	-2.58	123.96	132.83
2	B	301	KGJ	C1'-N9-C4	-2.58	122.11	126.64
2	F	301[A]	KGJ	C2-N1-C6	2.56	123.13	118.75
2	C	301	KGJ	P2-O6-P1	-2.56	124.05	132.83
2	E	301[A]	KGJ	N6-C6-N1	2.52	123.81	118.57
2	D	302[A]	KGJ	CP2-CP1-N	-2.50	103.14	111.44
2	D	302[B]	KGJ	CP2-CP1-N	-2.50	103.14	111.44
2	F	302[A]	KGJ	C4-C5-N7	-2.49	106.81	109.40
2	B	301	KGJ	OS1-CS1-CS2	-2.47	117.29	120.41
2	F	301[A]	KGJ	CP5-CP4-CP3	-2.45	108.27	112.36
2	F	301[B]	KGJ	CP5-CP4-CP3	-2.45	108.27	112.36
2	C	301	KGJ	CP7-CP6-NP2	2.45	121.45	116.58
2	C	301	KGJ	C2-N1-C6	2.44	122.93	118.75
2	C	302[A]	KGJ	C2-N1-C6	2.44	122.92	118.75
2	B	301	KGJ	O5'-C5'-C4'	-2.41	100.68	108.99
2	F	301[A]	KGJ	C4-C5-N7	-2.35	106.95	109.40
2	F	301[B]	KGJ	C2-N1-C6	2.34	122.76	118.75
2	F	301[B]	KGJ	C4-C5-N7	-2.32	106.98	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	KGJ	O33-P3-O31	2.31	119.72	110.68
2	E	301[A]	KGJ	OS1-CS1-CS2	-2.30	117.51	120.41
2	E	301[B]	KGJ	OS1-CS1-CS2	-2.30	117.51	120.41
2	F	301[A]	KGJ	O4'-C4'-C5'	-2.28	101.87	109.37
2	A	301	KGJ	O2'-C2'-C3'	2.26	117.59	111.17
2	D	302[A]	KGJ	O3'-C3'-C2'	-2.24	103.57	111.68
2	F	301[A]	KGJ	CP8-CPA-CPB	-2.23	104.60	108.23
2	F	301[B]	KGJ	CP8-CPA-CPB	-2.23	104.60	108.23
2	B	301	KGJ	O3'-C3'-C2'	-2.23	103.62	111.68
2	D	302[B]	KGJ	C2'-C3'-C4'	2.20	107.13	103.22
2	A	301	KGJ	O33-P3-O32	2.19	116.00	107.64
2	C	301	KGJ	CP5-CP4-CP3	-2.17	108.73	112.36
2	F	301[A]	KGJ	O5'-P1-O12	-2.17	100.57	109.07
2	A	301	KGJ	CP5-CP4-CP3	-2.12	108.82	112.36
2	F	301[A]	KGJ	O33-P3-O32	2.11	115.70	107.64
2	A	301	KGJ	CP2-CP1-N	-2.11	104.44	111.44
2	B	301	KGJ	CP7-CP6-NP2	-2.11	112.39	116.58
2	E	302[A]	KGJ	O7-P2-O21	-2.09	102.52	110.68
2	F	301[B]	KGJ	O4'-C1'-C2'	-2.07	103.90	106.93
2	F	301[A]	KGJ	CP8-CPA-CP7	2.07	112.41	108.82
2	F	301[B]	KGJ	CP8-CPA-CP7	2.07	112.41	108.82
2	E	302[A]	KGJ	O7-P2-O6	2.06	111.55	104.64
2	E	301[B]	KGJ	C4-C5-N7	-2.06	107.25	109.40
2	B	301	KGJ	C2'-C3'-C4'	2.06	106.87	103.22
2	B	301	KGJ	O33-P3-O31	2.05	118.70	110.68
2	E	302[A]	KGJ	C2-N1-C6	2.03	122.23	118.75

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	KGJ	C3'-O3'-P3-O33
2	B	301	KGJ	C5'-O5'-P1-O12
2	B	301	KGJ	CP7-CPA-CPB-O7
2	B	301	KGJ	OP3-CP7-CPA-CP9
2	B	301	KGJ	CP6-CP7-CPA-CP9
2	D	302[A]	KGJ	C5'-O5'-P1-O12
2	D	302[A]	KGJ	C5'-O5'-P1-O6
2	E	301[A]	KGJ	C5'-O5'-P1-O12
2	E	301[B]	KGJ	P1-O6-P2-O7
2	F	301[A]	KGJ	C5'-O5'-P1-O6
2	F	301[B]	KGJ	C5'-O5'-P1-O11

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Mol	Chain	Res	Type	Atoms
2	F	301[B]	KGJ	C5'-O5'-P1-O12
2	F	302[A]	KGJ	C5'-O5'-P1-O11
2	F	302[A]	KGJ	C5'-O5'-P1-O12
4	C	304	PEG	O2-C3-C4-O4
2	F	301[B]	KGJ	O4'-C4'-C5'-O5'
4	B	302	PEG	O1-C1-C2-O2
2	C	302[A]	KGJ	C4'-C3'-O3'-P3
2	E	301[A]	KGJ	C4'-C3'-O3'-P3
2	D	302[A]	KGJ	CP4-CP5-NP2-CP6
2	D	302[B]	KGJ	CP4-CP5-NP2-CP6
2	C	302[A]	KGJ	C2'-C3'-O3'-P3
2	E	301[A]	KGJ	C2'-C3'-O3'-P3
4	B	302	PEG	O2-C3-C4-O4
4	C	304	PEG	O1-C1-C2-O2
2	D	302[A]	KGJ	O4'-C4'-C5'-O5'
2	D	302[A]	KGJ	C3'-C4'-C5'-O5'
2	E	301[A]	KGJ	P1-O6-P2-O7
2	B	301	KGJ	C5'-O5'-P1-O6
2	C	302[A]	KGJ	C3'-O3'-P3-O33
2	E	302[A]	KGJ	C5'-O5'-P1-O6
2	F	301[B]	KGJ	C5'-O5'-P1-O6
2	F	301[A]	KGJ	P2-O6-P1-O11
2	E	302[A]	KGJ	C5'-O5'-P1-O12
2	F	301[A]	KGJ	C5'-O5'-P1-O11
2	C	302[A]	KGJ	C3'-C4'-C5'-O5'
2	F	302[A]	KGJ	C4'-C5'-O5'-P1
2	F	301[B]	KGJ	C3'-C4'-C5'-O5'
2	B	301	KGJ	CP8-CPA-CPB-O7
2	C	302[A]	KGJ	O4'-C4'-C5'-O5'
2	A	301	KGJ	P2-O6-P1-O11
2	E	301[B]	KGJ	P2-O6-P1-O11
2	F	301[A]	KGJ	P1-O6-P2-O22
6	C	305	PG4	C4-C3-O2-C2
2	E	302[A]	KGJ	C4'-C3'-O3'-P3
8	F	304	PGE	O3-C5-C6-O4
2	B	301	KGJ	C3'-C4'-C5'-O5'
2	C	302[A]	KGJ	P1-O6-P2-O21
6	C	305	PG4	O1-C1-C2-O2
2	E	302[A]	KGJ	C2'-C3'-O3'-P3
2	F	301[A]	KGJ	CP4-CP5-NP2-CP6
2	F	301[B]	KGJ	CP4-CP5-NP2-CP6
6	C	305	PG4	C3-C4-O3-C5

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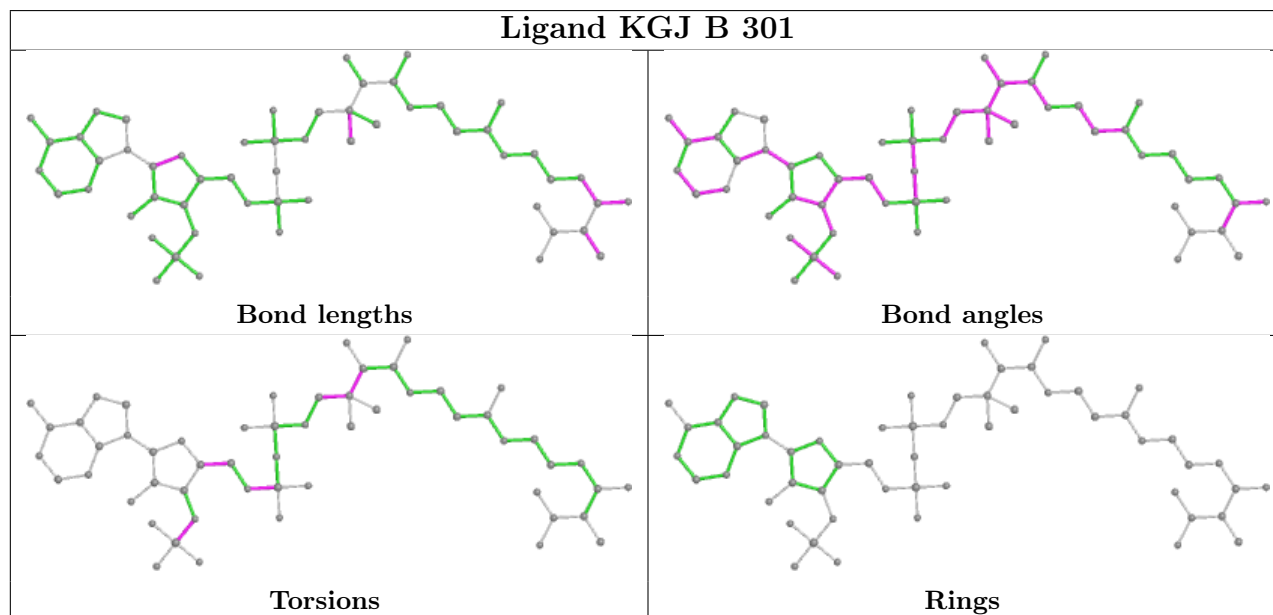
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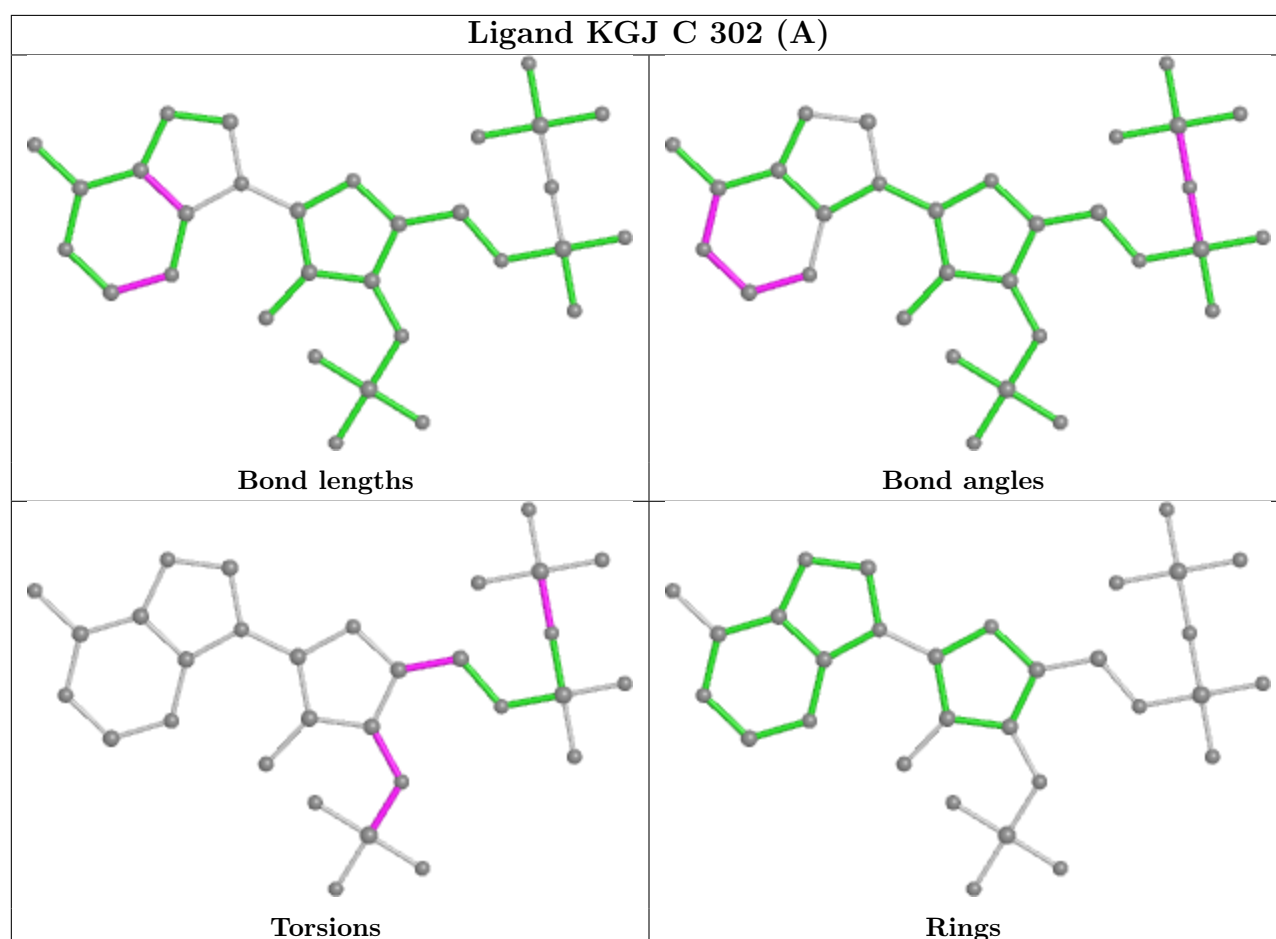
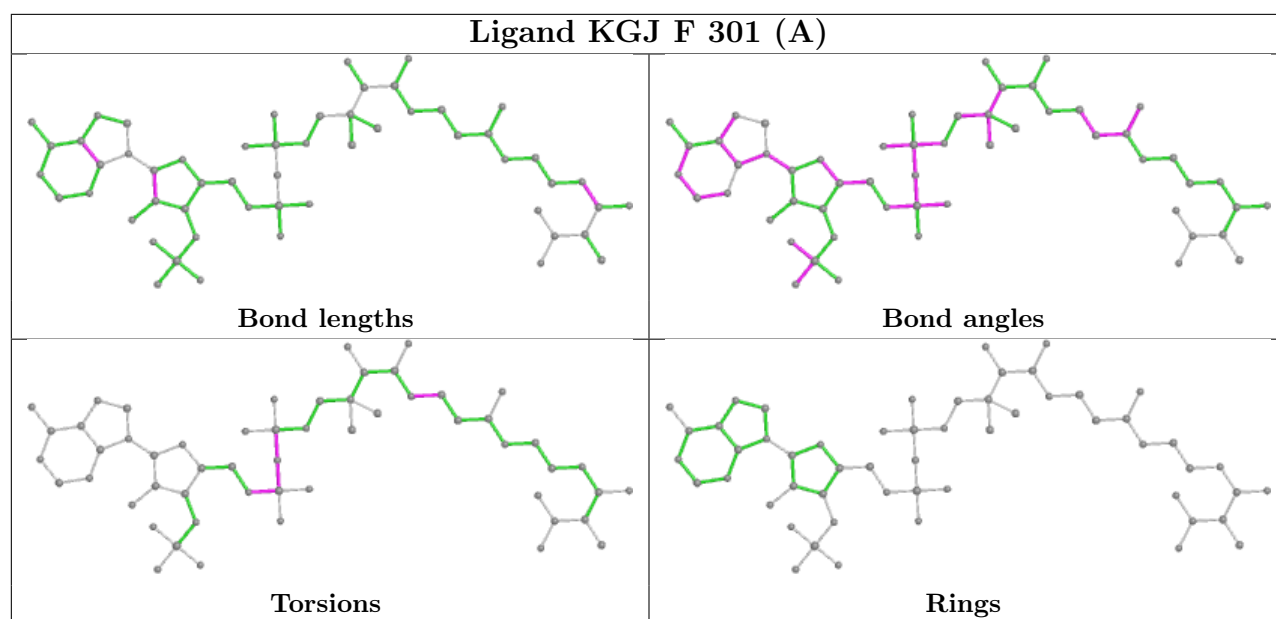
Mol	Chain	Res	Type	Atoms
2	B	301	KGJ	O4'-C4'-C5'-O5'
2	C	302[A]	KGJ	P1-O6-P2-O22
2	F	302[A]	KGJ	C5'-O5'-P1-O6
2	E	301[B]	KGJ	P2-O6-P1-O12
2	F	301[A]	KGJ	P1-O6-P2-O21

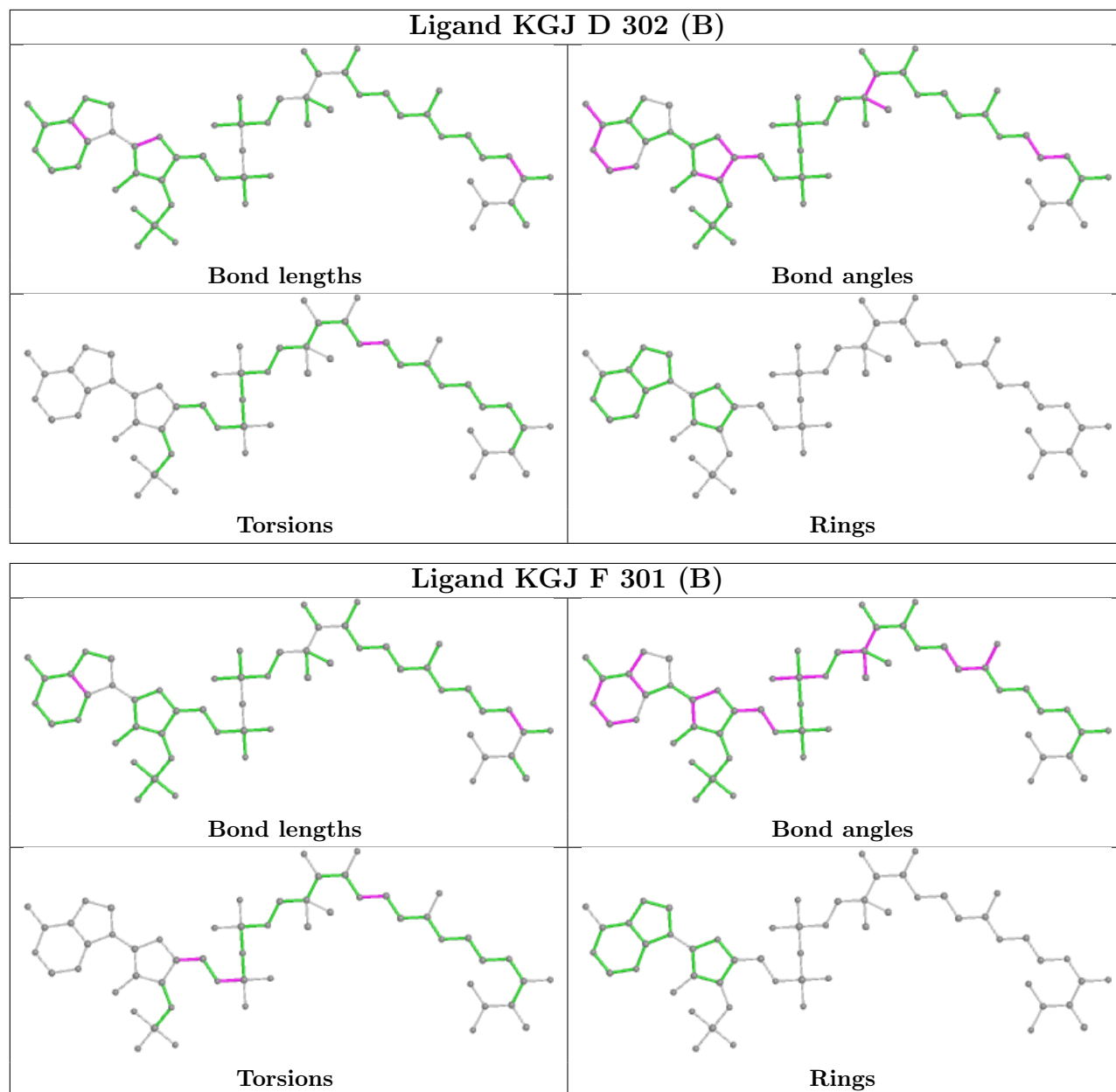
There are no ring outliers.

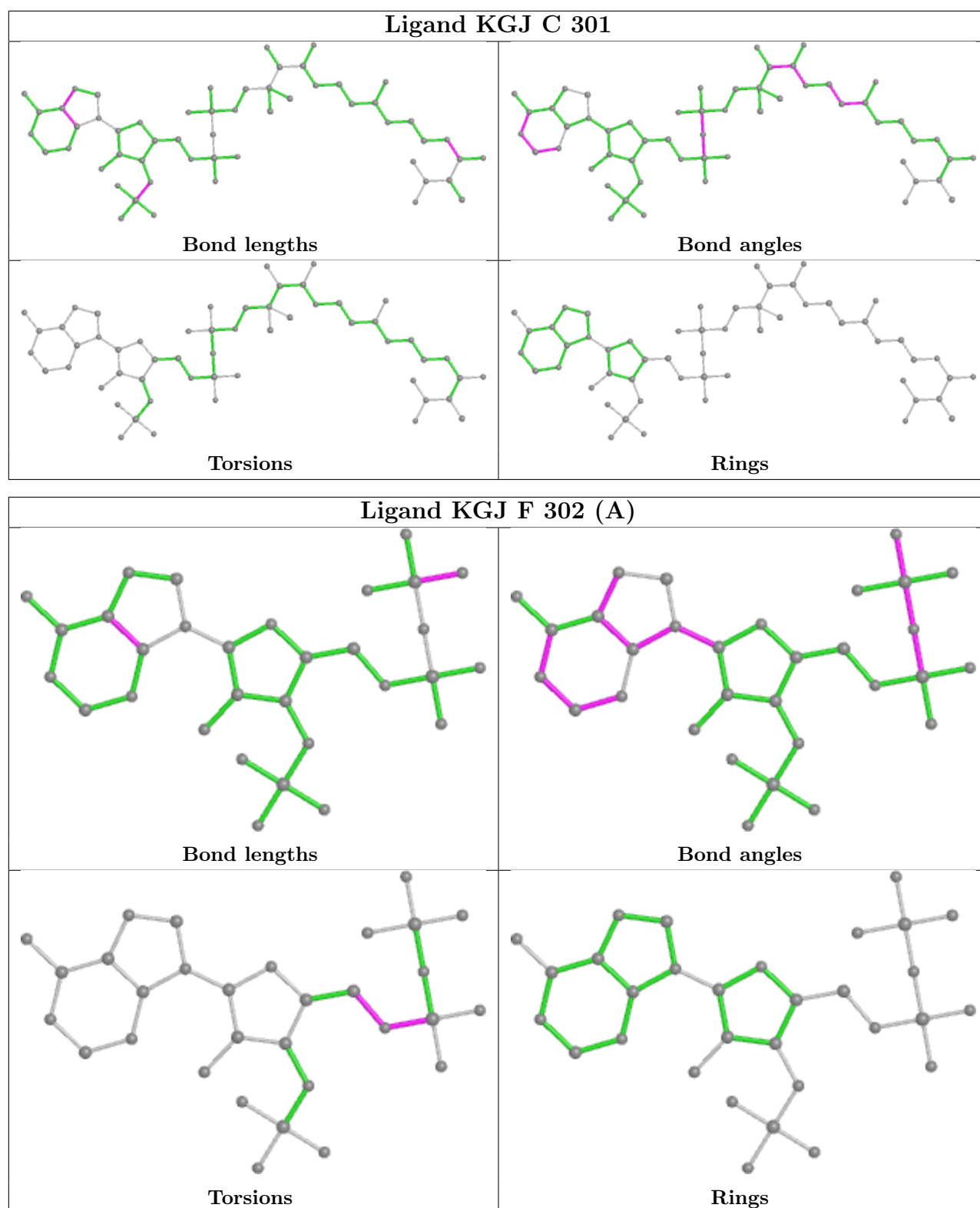
No monomer is involved in short contacts.

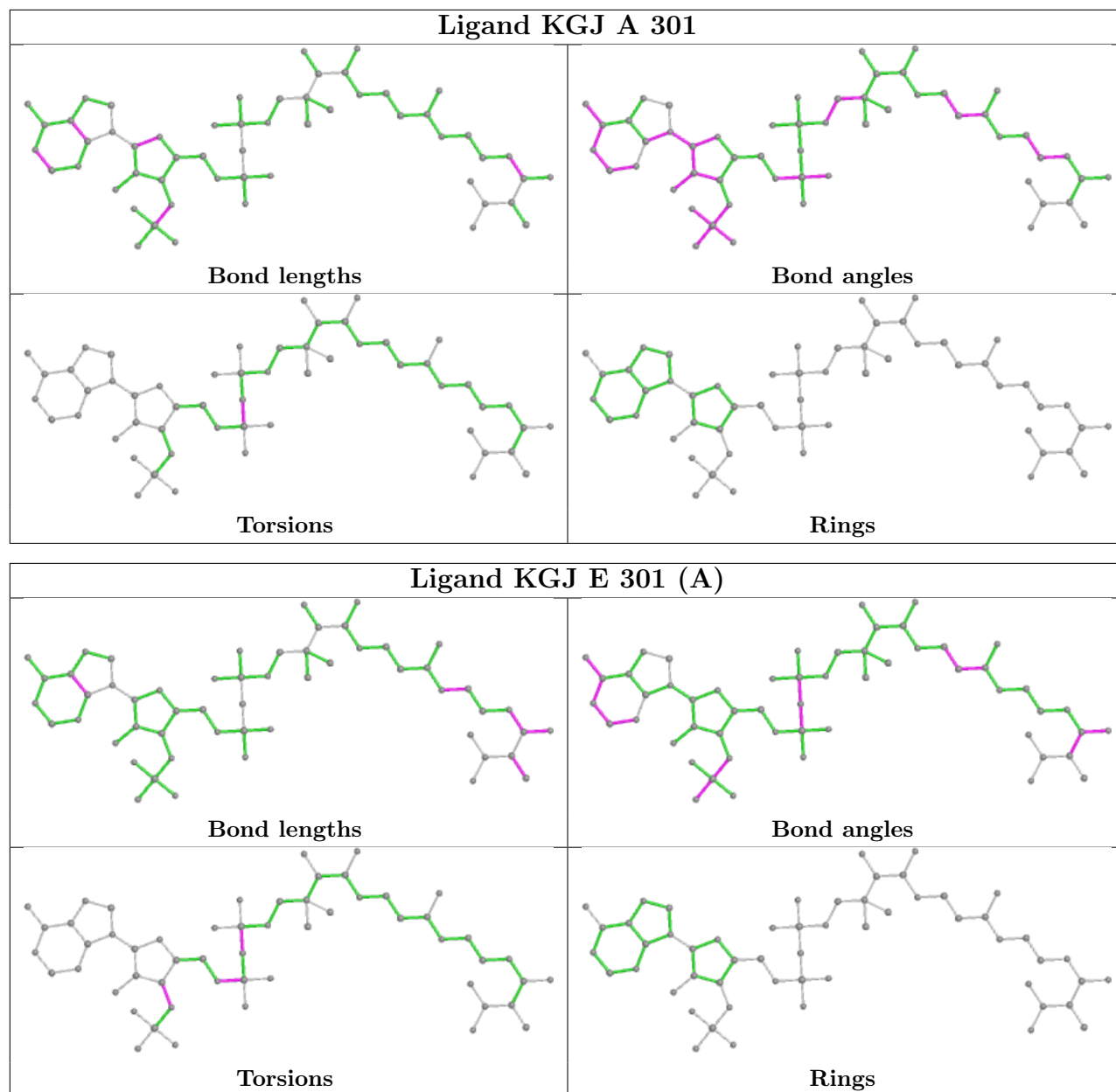
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

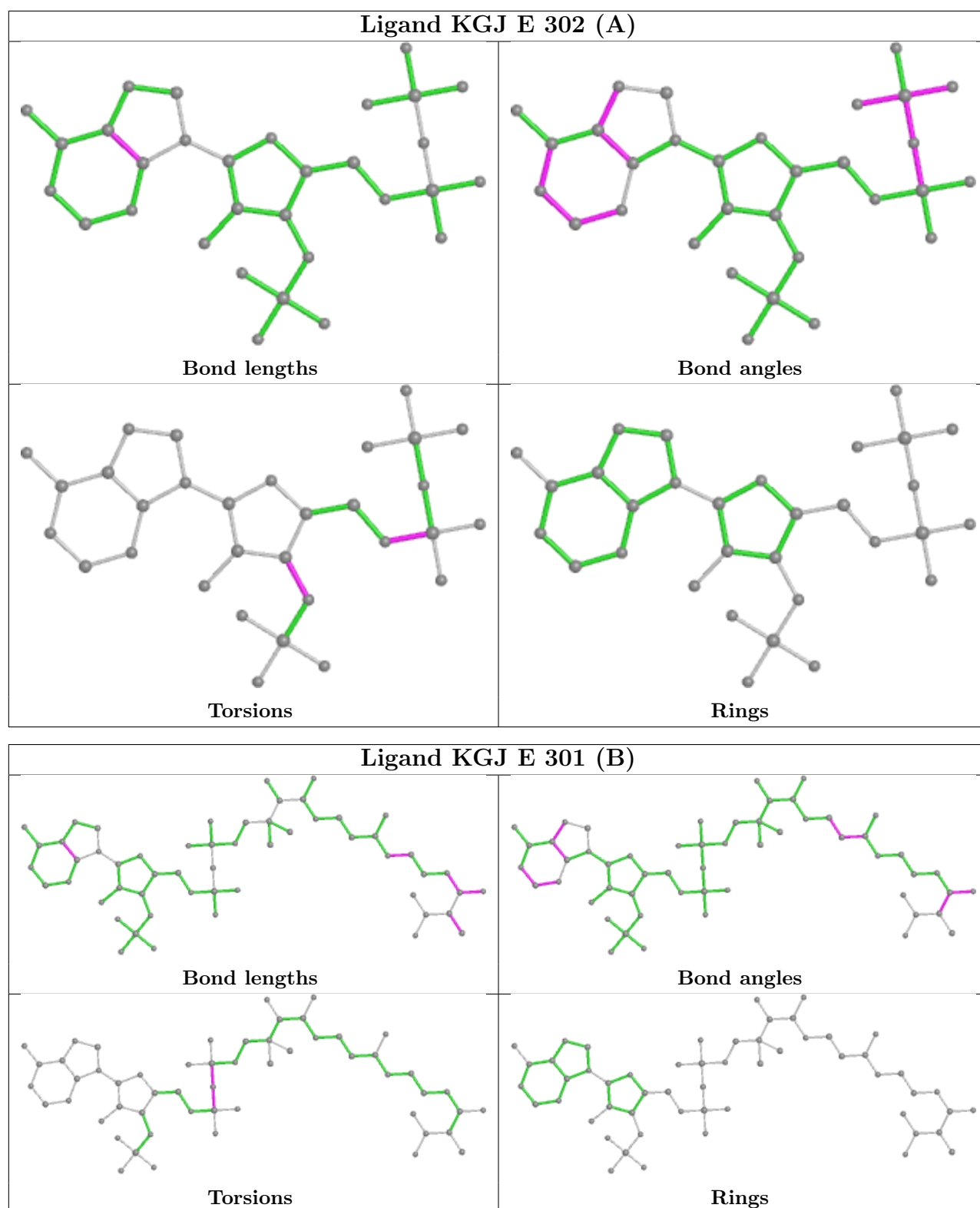


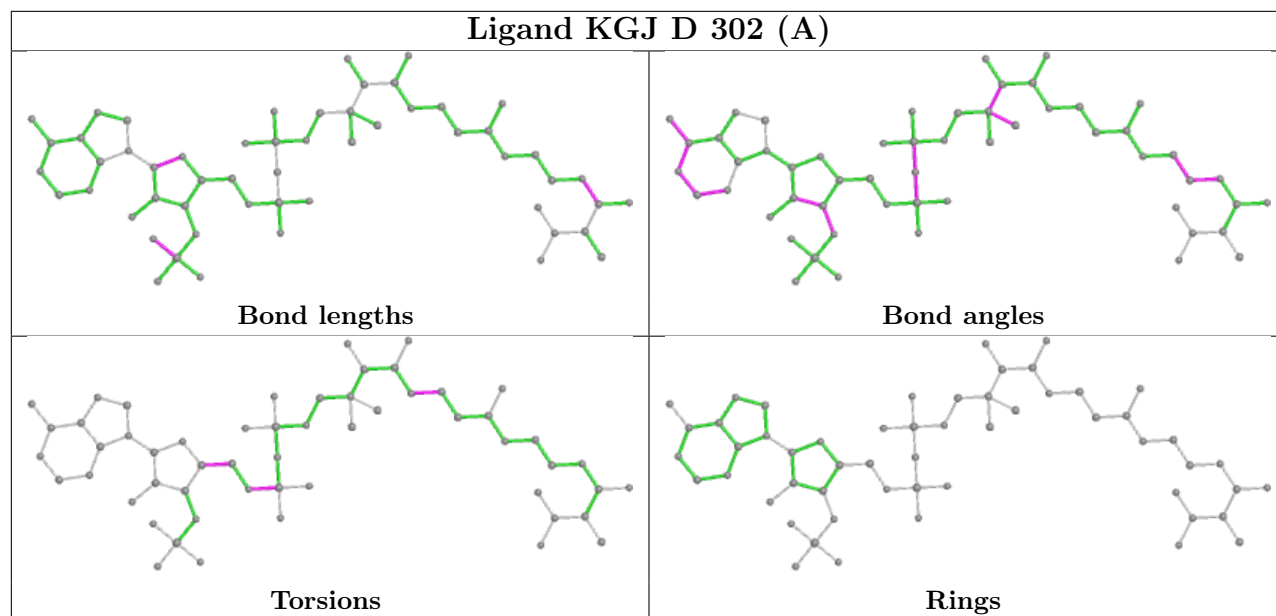












4.7 Other polymers [i](#)

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 [i](#)

5.1 Protein, DNA and RNA chains [i](#)

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

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

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

5.3 Carbohydrates [i](#)

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

5.4 Ligands [i](#)

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

5.5 Other polymers [i](#)

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