



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2023 – 02:11 AM EDT

PDB ID : 1KBQ
Title : Complex of Human NAD(P)H quinone Oxidoreductase with 5-methoxy-1,2-dimethyl-3-(4-nitrophenoxy-methyl)indole-4,7-dione (ES936)
Authors : Faig, M.; Bianchet, M.A.; Amzel, L.M.
Deposited on : 2001-11-06
Resolution : 1.80 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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

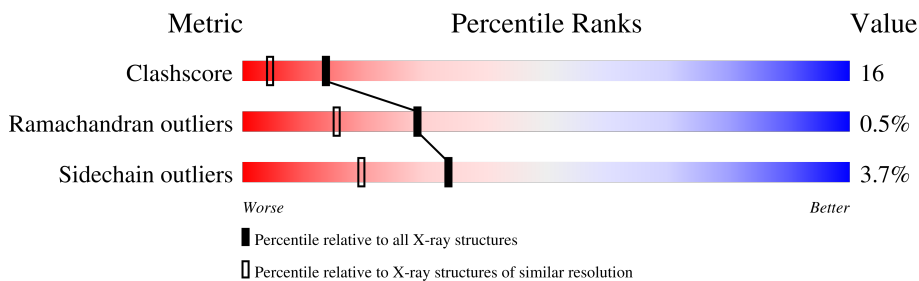
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	273	
1	B	273	
1	C	273	
1	D	273	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9494 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 NAD(P)H dehydrogenase [quinone] 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	272	Total	C	N	O	S	0	0	0
			2168	1409	364	388	7			
1	B	271	Total	C	N	O	S	0	0	0
			2164	1407	363	387	7			
1	C	271	Total	C	N	O	S	0	0	0
			2164	1407	363	387	7			
1	D	272	Total	C	N	O	S	0	0	0
			2168	1409	364	388	7			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



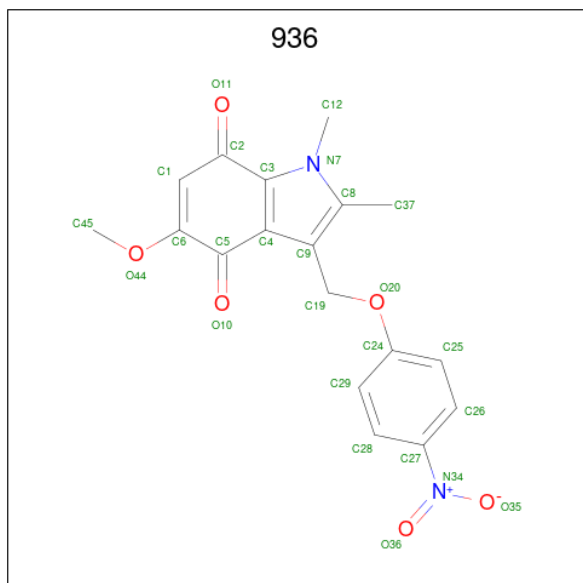
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 5-METHOXY-1,2-DIMETHYL-3-(4-NITROPHENOXYMETHYL)INDOLE-4,7-DIONE (three-letter code: 936) (formula: C₁₈H₁₆N₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total	C	N	O	0	0
			26	18	2	6		
3	B	1	Total	C	N	O	0	0
			26	18	2	6		
3	C	1	Total	C	N	O	0	0
			26	18	2	6		
3	D	1	Total	C	N	O	0	0
			26	18	2	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	129	Total	O	0	0
			129	129		
4	B	144	Total	O	0	0
			144	144		
4	C	114	Total	O	0	0
			114	114		

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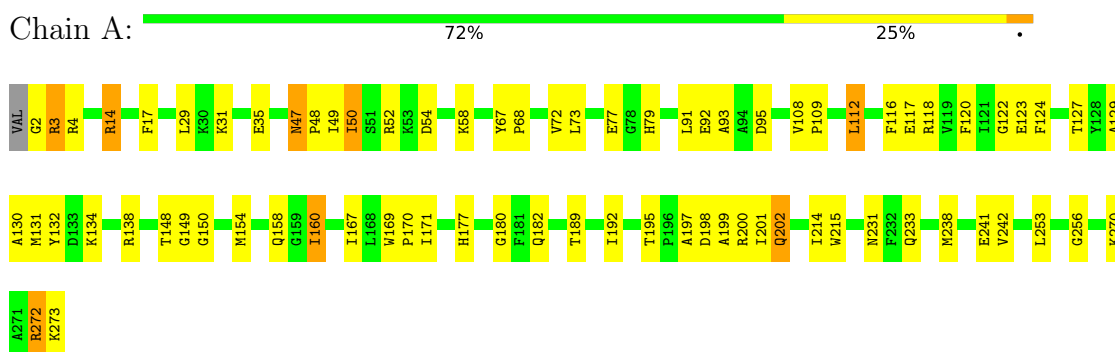
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	127	Total 127	O 127	0	0

3 Residue-property plots [i](#)

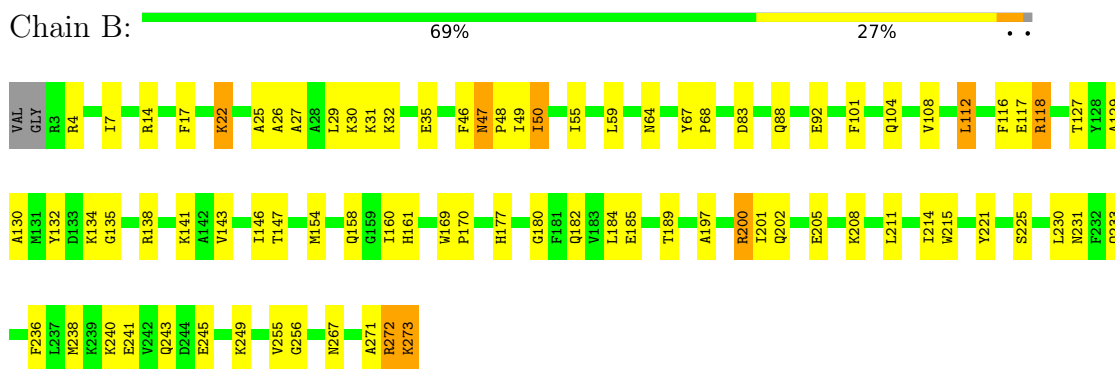
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

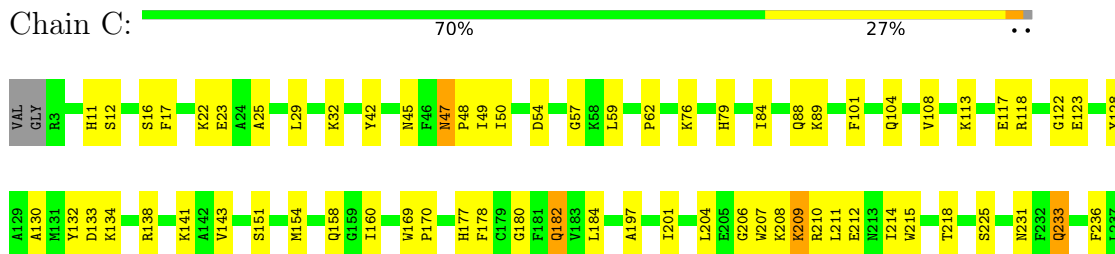
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1



- Molecule 1: NAD(P)H dehydrogenase [quinone] 1



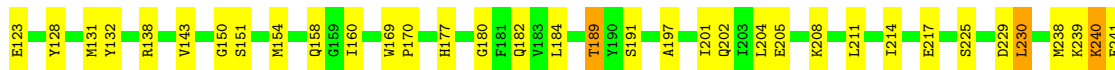
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1





● Molecule 1: NAD(P)H dehydrogenase [quinone] 1

Chain D: 71% 27%



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.48Å 56.77Å 96.91Å 77.25° 76.83° 86.90°	Depositor
Resolution (Å)	32.19 – 1.80	Depositor
% Data completeness (in resolution range)	94.6 (32.19-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	9494	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

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: FAD, 936

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	0.40	0/2226	0.64	1/3005 (0.0%)
1	B	0.41	0/2222	0.66	3/3000 (0.1%)
1	C	0.39	0/2222	0.60	1/3000 (0.0%)
1	D	0.41	0/2226	0.61	1/3005 (0.0%)
All	All	0.40	0/8896	0.63	6/12010 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	D	182	GLN	N-CA-C	-6.05	94.66	111.00
1	A	182	GLN	N-CA-C	-5.83	95.27	111.00
1	C	182	GLN	N-CA-C	-5.75	95.49	111.00
1	B	118	ARG	NE-CZ-NH2	-5.71	117.44	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2168	0	2167	71	0
1	B	2164	0	2164	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2164	0	2164	65	0
1	D	2168	0	2167	82	0
2	A	53	0	31	6	0
2	B	53	0	31	3	0
2	C	53	0	31	3	0
2	D	53	0	31	3	0
3	A	26	0	16	1	0
3	B	26	0	16	2	0
3	C	26	0	16	2	0
3	D	26	0	16	3	0
4	A	129	0	0	5	0
4	B	144	0	0	6	0
4	C	114	0	0	3	0
4	D	127	0	0	5	0
All	All	9494	0	8850	284	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 16.

The worst 5 of 284 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:VAL:CG2	1:B:112:LEU:HD13	1.94	0.97
1:B:135:GLY:O	1:B:138:ARG:HG3	1.68	0.93
1:A:14:ARG:H	1:A:14:ARG:NE	1.68	0.92
1:D:17:PHE:HB2	2:D:604:FAD:H52A	1.51	0.92
1:A:50:ILE:HG13	1:A:118:ARG:HG2	1.53	0.90

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	270/273 (99%)	255 (94%)	14 (5%)	1 (0%)	34	21
1	B	269/273 (98%)	256 (95%)	12 (4%)	1 (0%)	34	21
1	C	269/273 (98%)	255 (95%)	13 (5%)	1 (0%)	34	21
1	D	270/273 (99%)	255 (94%)	13 (5%)	2 (1%)	22	10
All	All	1078/1092 (99%)	1021 (95%)	52 (5%)	5 (0%)	29	15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	C	272	ARG
1	B	272	ARG
1	D	230	LEU
1	D	191	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	226/227 (100%)	215 (95%)	11 (5%)	25	11
1	B	226/227 (100%)	216 (96%)	10 (4%)	28	14
1	C	226/227 (100%)	220 (97%)	6 (3%)	44	31
1	D	226/227 (100%)	220 (97%)	6 (3%)	44	31
All	All	904/908 (100%)	871 (96%)	33 (4%)	34	19

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	52	ARG
1	D	158	GLN
1	D	240	LYS
1	B	22	LYS
1	B	14	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	79	HIS
1	D	158	GLN
1	D	243	GLN
1	B	172	GLN
1	B	79	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	936	B	704	-	26,28,28	3.20	13 (50%)	30,41,41	2.28	9 (30%)
3	936	A	703	-	26,28,28	3.12	11 (42%)	30,41,41	2.23	7 (23%)
2	FAD	B	602	-	53,58,58	1.97	16 (30%)	68,89,89	1.19	6 (8%)
2	FAD	C	603	-	53,58,58	2.03	19 (35%)	68,89,89	1.23	9 (13%)
2	FAD	D	604	-	53,58,58	2.04	20 (37%)	68,89,89	1.20	5 (7%)
3	936	C	701	-	26,28,28	3.16	10 (38%)	30,41,41	2.22	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	A	601	-	53,58,58	2.04	18 (33%)	68,89,89	1.20	7 (10%)
3	936	D	702	-	26,28,28	3.21	7 (26%)	30,41,41	2.35	9 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	936	B	704	-	-	3/7/27/27	0/3/3/3
3	936	A	703	-	-	3/7/27/27	0/3/3/3
2	FAD	B	602	-	-	2/30/50/50	0/6/6/6
2	FAD	C	603	-	-	3/30/50/50	0/6/6/6
2	FAD	D	604	-	-	2/30/50/50	0/6/6/6
3	936	C	701	-	-	3/7/27/27	0/3/3/3
2	FAD	A	601	-	-	2/30/50/50	0/6/6/6
3	936	D	702	-	-	3/7/27/27	0/3/3/3

The worst 5 of 114 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	702	936	O36-N34	10.95	1.41	1.22
3	B	704	936	O36-N34	10.59	1.40	1.22
3	C	701	936	O36-N34	10.24	1.40	1.22
3	A	703	936	O36-N34	9.77	1.39	1.22
3	C	701	936	C3-C2	-8.62	1.35	1.50

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	702	936	O44-C6-C5	8.16	118.42	111.47
3	B	704	936	O44-C6-C5	7.39	117.77	111.47
3	C	701	936	O44-C6-C5	7.04	117.47	111.47
3	A	703	936	O44-C6-C5	7.00	117.43	111.47
3	A	703	936	C12-N7-C3	5.19	130.18	124.49

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	936	C26-C27-N34-O36
3	A	703	936	C28-C27-N34-O36
3	C	701	936	C28-C27-N34-O36
3	D	702	936	C26-C27-N34-O36
3	D	702	936	C28-C27-N34-O36

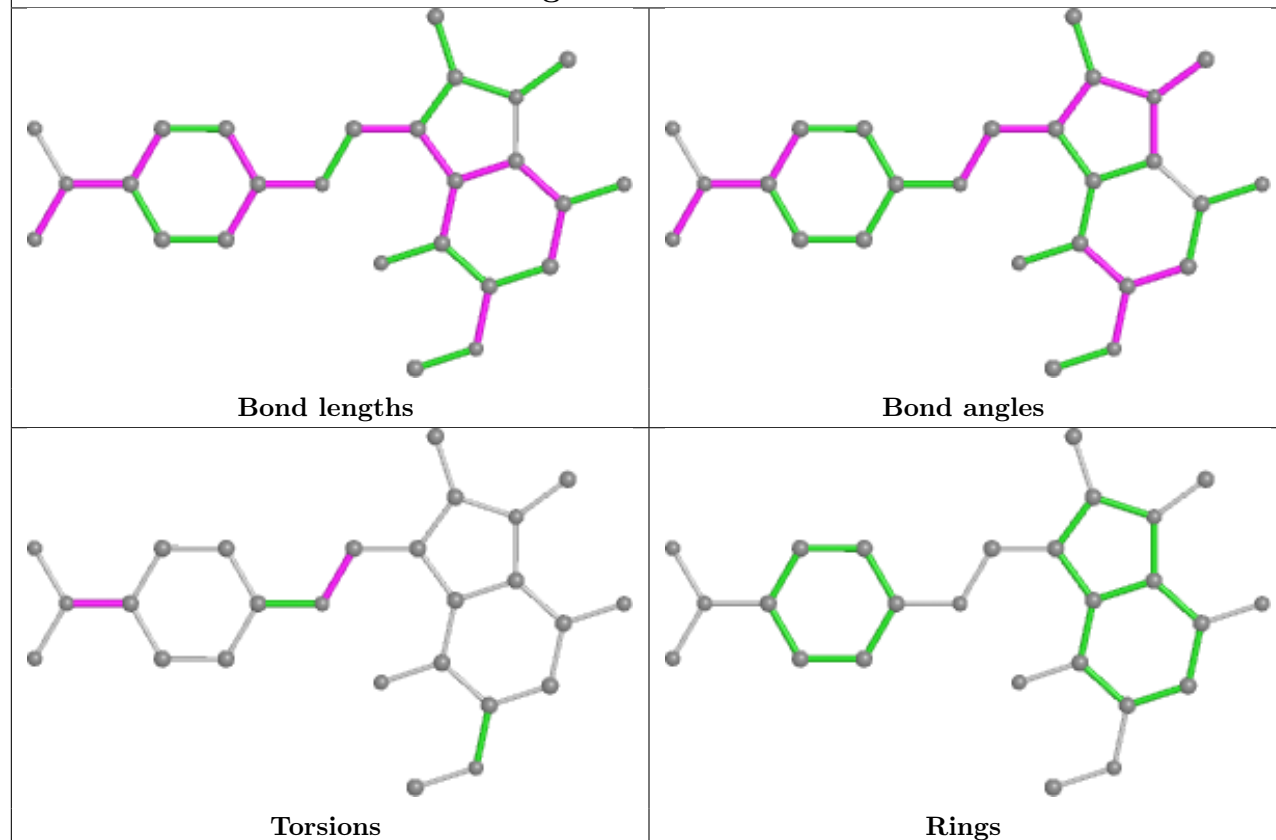
There are no ring outliers.

8 monomers are involved in 23 short contacts:

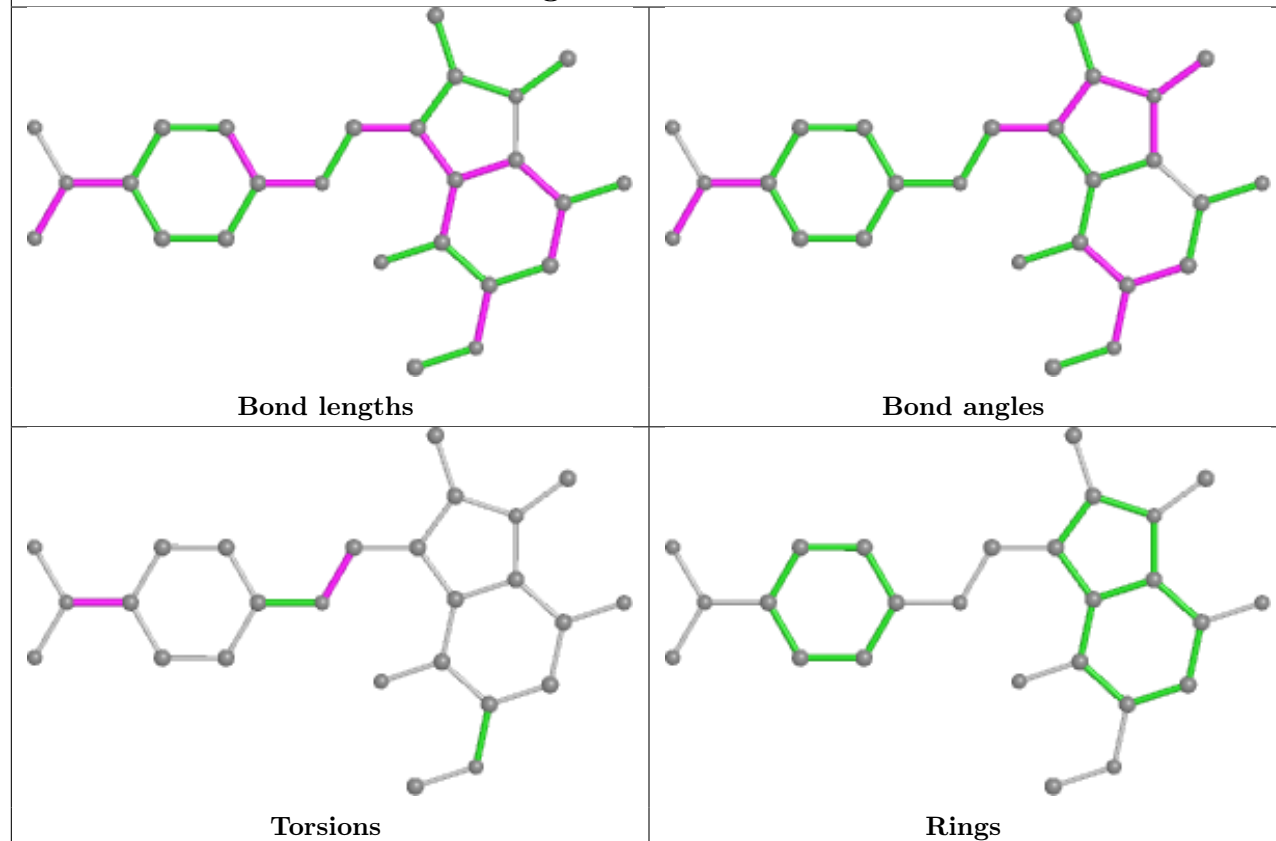
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	704	936	2	0
3	A	703	936	1	0
2	B	602	FAD	3	0
2	C	603	FAD	3	0
2	D	604	FAD	3	0
3	C	701	936	2	0
2	A	601	FAD	6	0
3	D	702	936	3	0

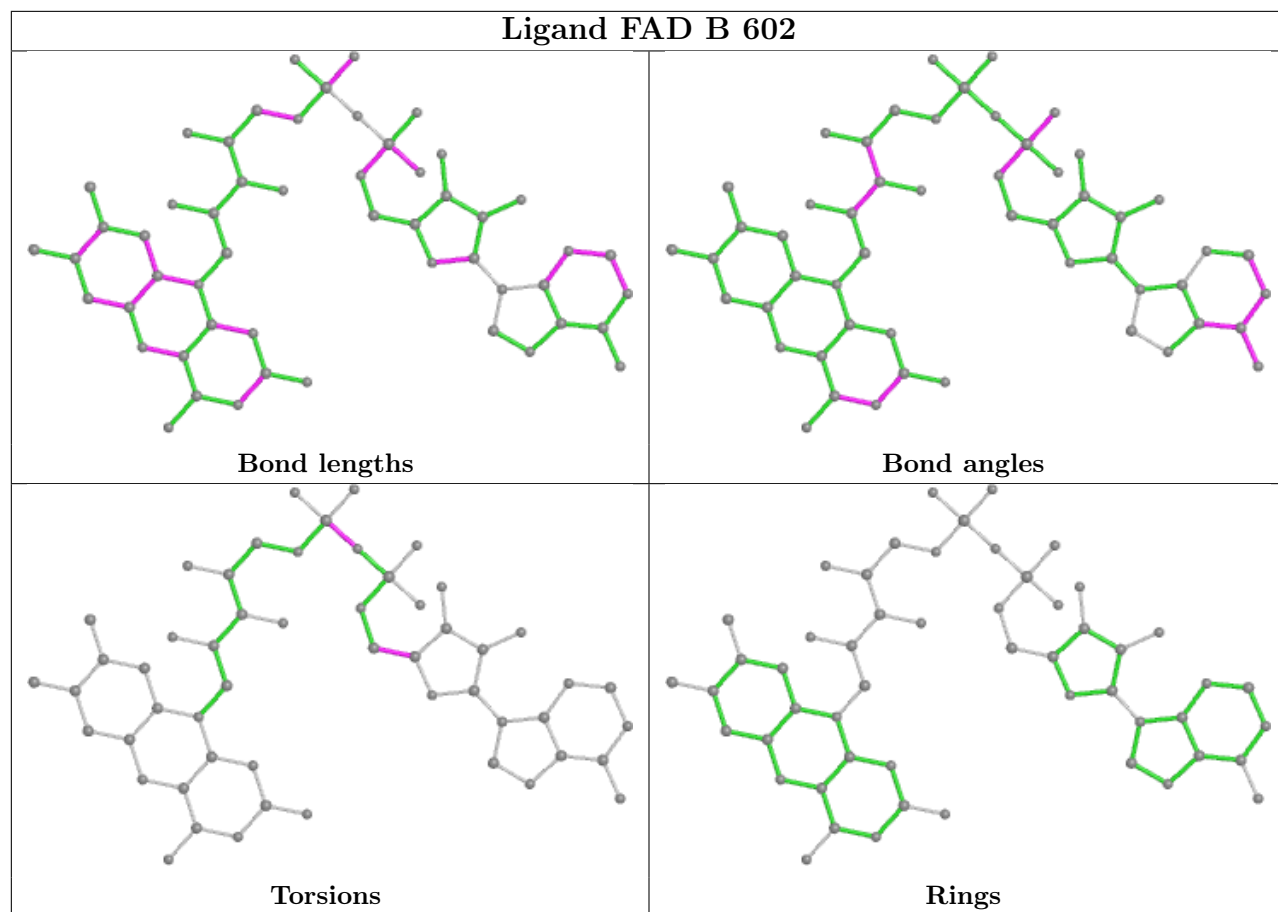
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

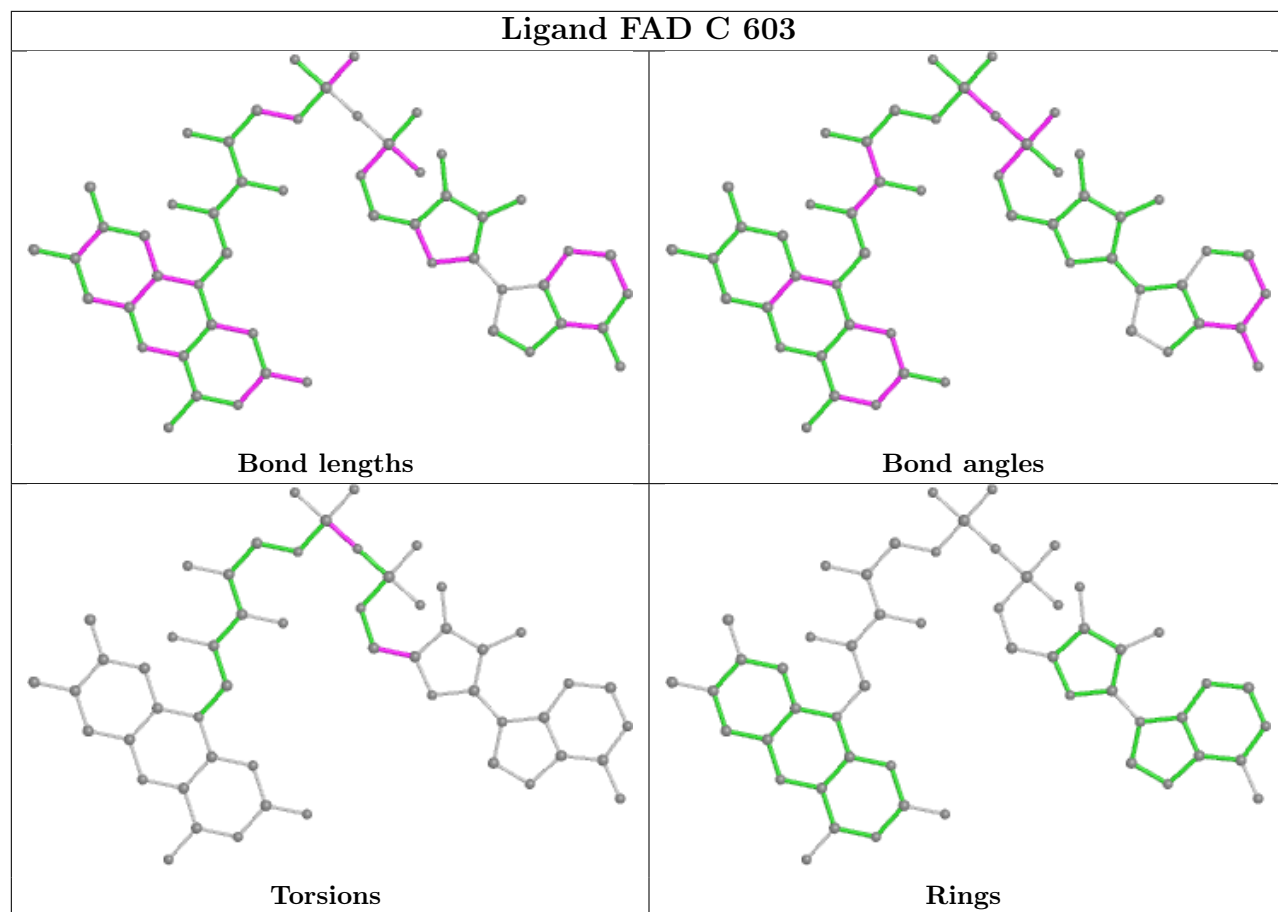
Ligand 936 B 704

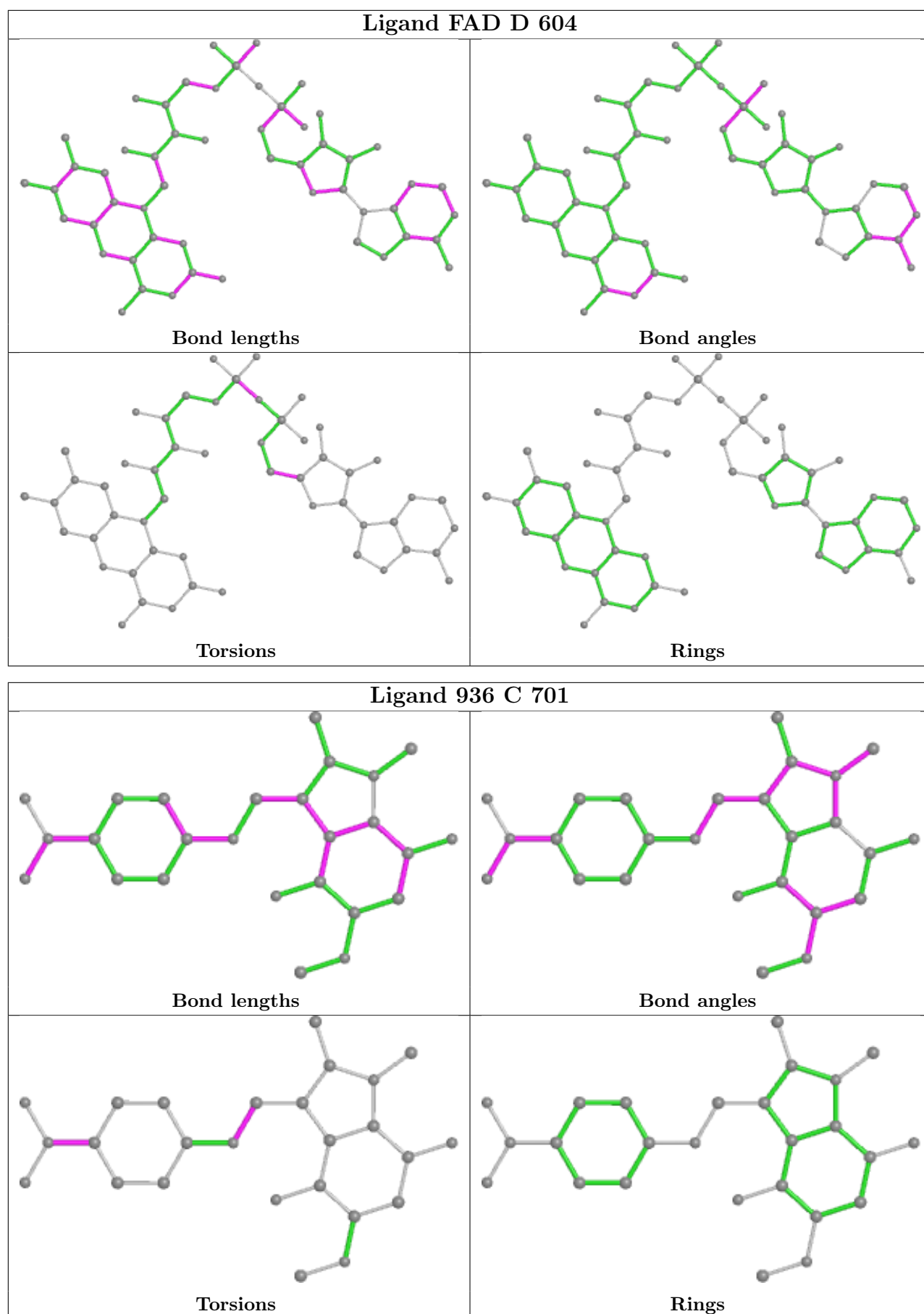


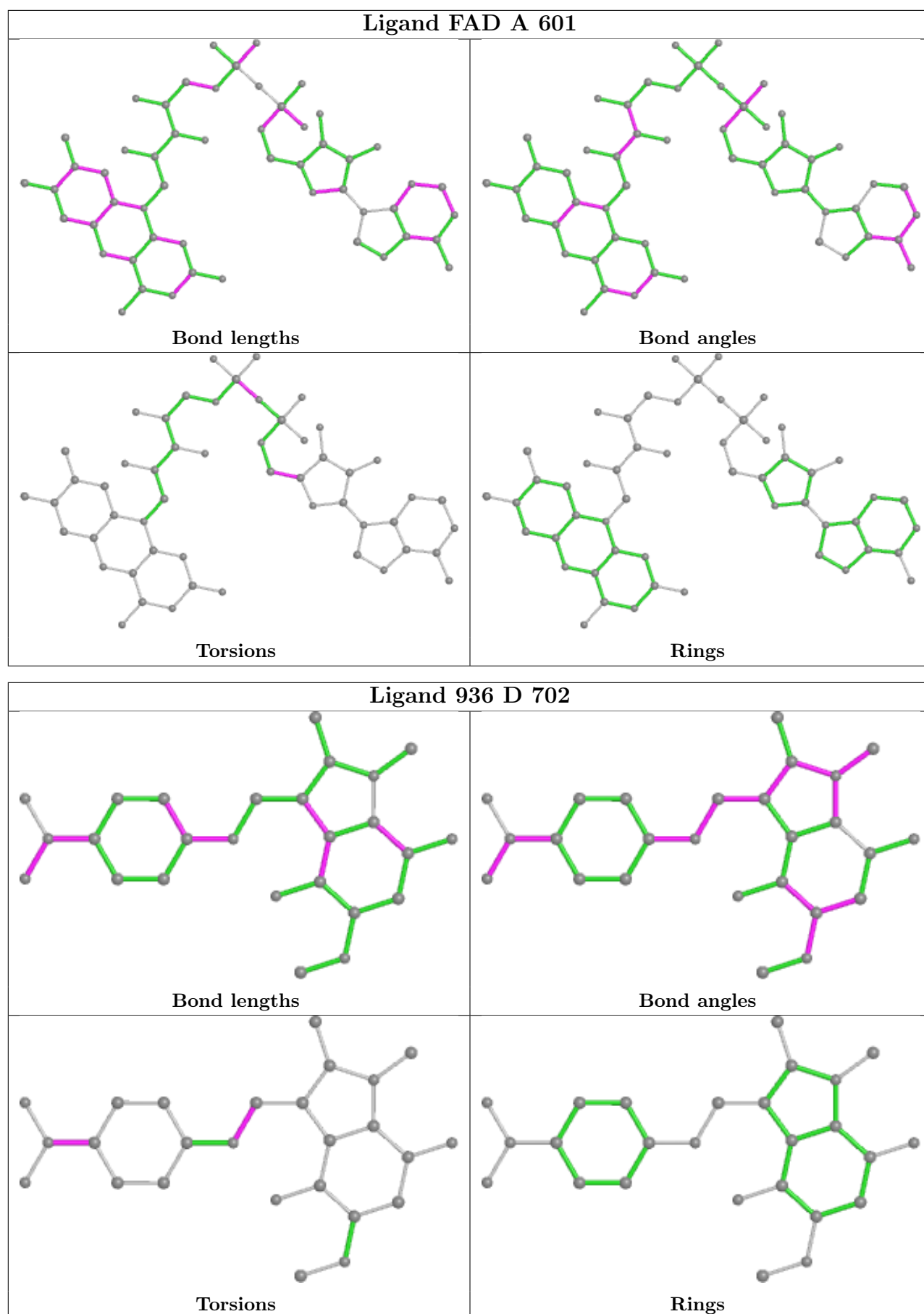
Ligand 936 A 703











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.