



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 3, 2024 – 06:50 PM EST

PDB ID : 1LRT
Title : CRYSTAL STRUCTURE OF TERNARY COMPLEX OF TRITRICHOMONAS FOETUS INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE: STRUCTURAL CHARACTERIZATION OF NAD⁺ SITE IN MICROBIAL ENZYME
Authors : Gan, L.; Petsko, G.A.; Hedstrom, L.
Deposited on : 2002-05-15
Resolution : 2.20 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 : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

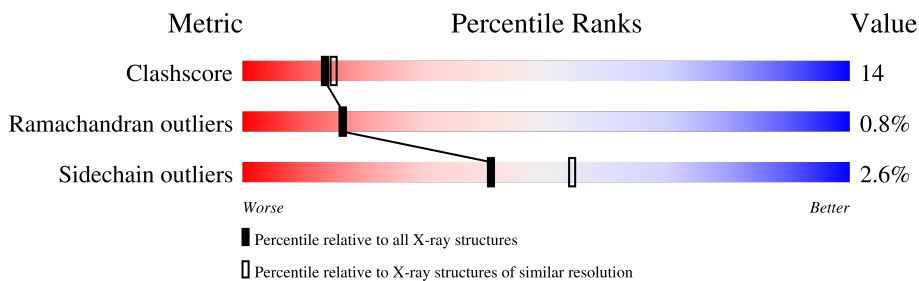
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)

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	376	69% 19% • 10%
1	B	376	63% 24% • 11%
1	C	376	67% 20% • 11%
1	D	376	64% 23% • 10%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11238 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 INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	338	2583	1638	437	493	15	0	0	0
1	B	334	2554	1621	433	485	15	0	0	0
1	C	334	2554	1621	433	485	15	0	0	0
1	D	340	2600	1649	442	494	15	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	ASP	GLU	SEE REMARK 999	UNP P50097
B	279	ASP	GLU	SEE REMARK 999	UNP P50097
C	279	ASP	GLU	SEE REMARK 999	UNP P50097
D	279	ASP	GLU	SEE REMARK 999	UNP P50097

- Molecule 2 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C₁₄H₂₈O₆).

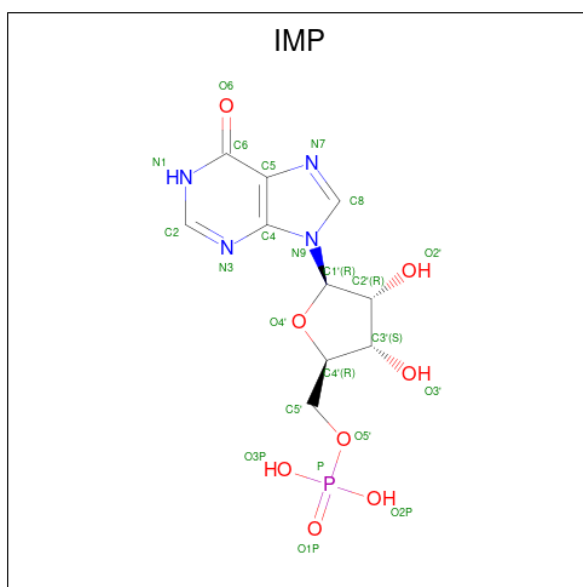


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C O	0	0
			20	14 6		
2	A	1	Total	C O	0	0
			20	14 6		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

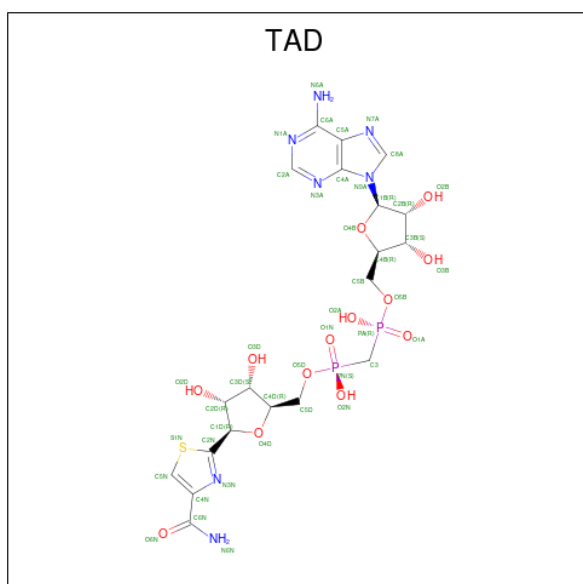
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		
3	B	1	Total	K	0	0
			1	1		
3	C	1	Total	K	0	0
			1	1		
3	D	1	Total	K	0	0
			1	1		

- Molecule 4 is INOSINIC ACID (three-letter code: IMP) (formula: C₁₀H₁₃N₄O₈P).



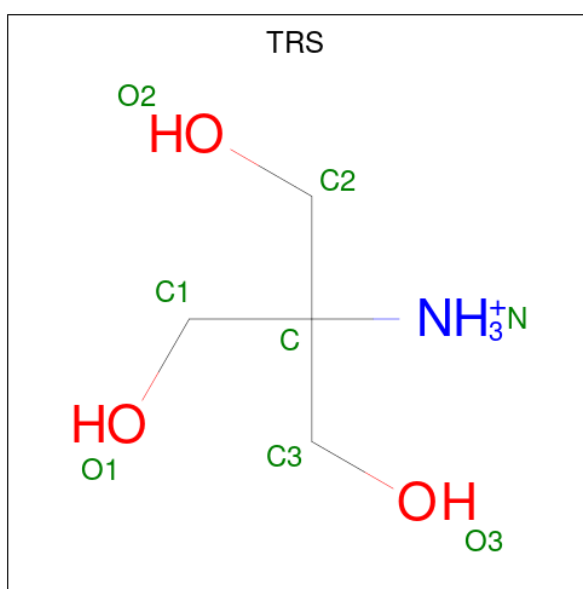
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
4	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 5 is BETA-METHYLENE-THIAZOLE-4-CARBOXYAMIDE-ADENINE DINUCLEOTIDE (three-letter code: TAD) (formula: $C_{20}H_{27}N_7O_{13}P_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	N	O	P	S	0	0
			43	20	7	13	2	1		
5	B	1	Total	C	N	O	P	S	0	0
			43	20	7	13	2	1		
5	C	1	Total	C	N	O	P	S	0	0
			43	20	7	13	2	1		
5	D	1	Total	C	N	O	P	S	0	0
			43	20	7	13	2	1		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			8	4	1	3		
6	A	1	Total	C	N	O	0	0
			8	4	1	3		
6	A	1	Total	C	N	O	0	0
			8	4	1	3		
6	A	1	Total	C	N	O	0	0
			8	4	1	3		
6	B	1	Total	C	N	O	0	0
			8	4	1	3		
6	B	1	Total	C	N	O	0	0
			8	4	1	3		
6	B	1	Total	C	N	O	0	0
			8	4	1	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			8	4	1	3		
6	C	1	Total	C	N	O	0	0
			8	4	1	3		
6	D	1	Total	C	N	O	0	0
			8	4	1	3		
6	D	1	Total	C	N	O	0	0
			8	4	1	3		
6	D	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	160	Total	O	0	0
			160	160		
7	B	128	Total	O	0	0
			128	128		
7	C	122	Total	O	0	0
			122	122		
7	D	133	Total	O	0	0
			133	133		

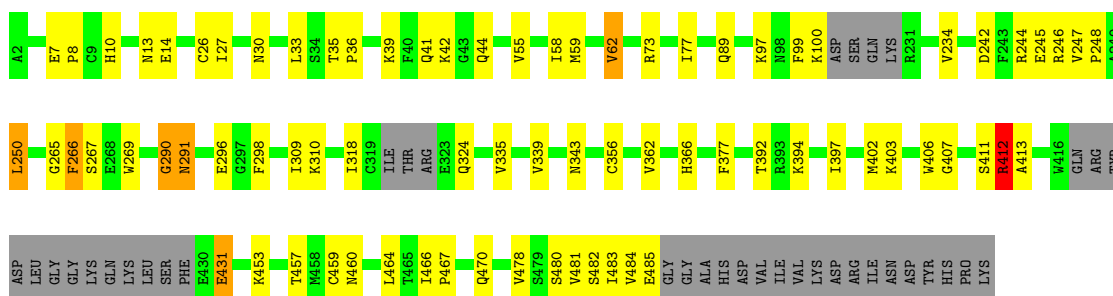
3 Residue-property plots [i](#)

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.

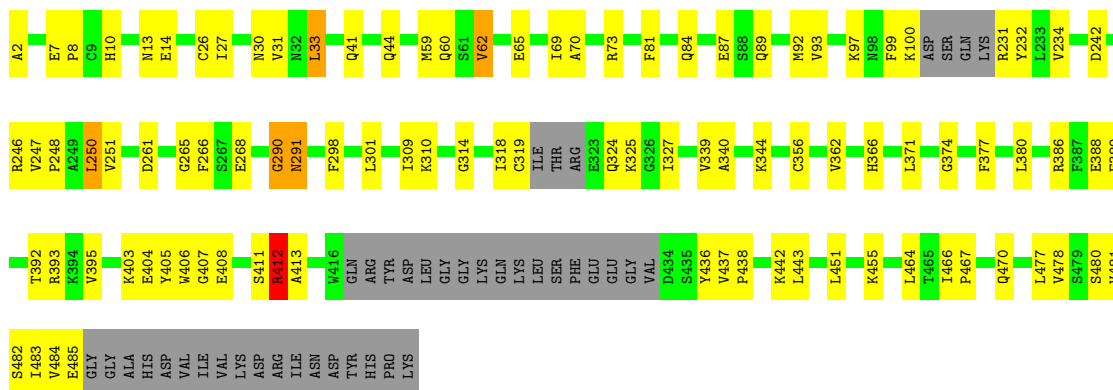
• Molecule 1: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE

Chain A: 



• Molecule 1: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE

Chain B: 



• Molecule 1: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE

Chain C: 





PRO
LYS

• Molecule 1: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE

Chain D: 64% 23% 10%



ILE
VAL
LYS
ASP
ARG
ILE
ASN
ASP
TYR
HIS
PRO
LYS

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.14Å 112.37Å 162.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 2.20	Depositor
% Data completeness (in resolution range)	91.4 (29.86-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.212 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	11238	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: IMP, K, TAD, TRS, BOG

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	0.34	0/2627	0.61	1/3541 (0.0%)
1	B	0.32	0/2598	0.59	1/3502 (0.0%)
1	C	0.33	0/2598	0.60	1/3502 (0.0%)
1	D	0.33	0/2645	0.60	1/3567 (0.0%)
All	All	0.33	0/10468	0.60	4/14112 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	GLY	N-CA-C	6.85	130.22	113.10
1	C	290	GLY	N-CA-C	6.83	130.18	113.10
1	D	290	GLY	N-CA-C	6.76	129.99	113.10
1	B	290	GLY	N-CA-C	6.16	128.50	113.10

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	2583	0	2572	65	0
1	B	2554	0	2548	82	0
1	C	2554	0	2548	71	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2600	0	2598	100	0
2	A	40	0	56	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	23	0	11	0	0
4	B	23	0	11	0	0
4	C	23	0	11	0	0
4	D	23	0	11	2	0
5	A	43	0	24	0	0
5	B	43	0	24	1	0
5	C	43	0	24	0	0
5	D	43	0	24	3	0
6	A	32	0	48	5	0
6	B	24	0	36	2	0
6	C	16	0	24	4	0
6	D	24	0	36	7	0
7	A	160	0	0	3	0
7	B	128	0	0	0	0
7	C	122	0	0	2	0
7	D	133	0	0	1	0
All	All	11238	0	10606	307	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 14.

The worst 5 of 307 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:D:322:ARG:HH22	5:D:904:TAD:H5N	1.25	1.02
1:D:322:ARG:HB3	1:D:326:GLY:H	1.35	0.89
1:D:322:ARG:HG2	1:D:327:ILE:H	1.36	0.89
1:C:7:GLU:HG3	1:C:8:PRO:HD2	1.60	0.83
1:C:343:ASN:ND2	6:C:605:TRS:H11	1.93	0.83

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	330/376 (88%)	316 (96%)	12 (4%)	2 (1%)	22	23
1	B	326/376 (87%)	308 (94%)	16 (5%)	2 (1%)	22	23
1	C	326/376 (87%)	306 (94%)	18 (6%)	2 (1%)	22	23
1	D	334/376 (89%)	313 (94%)	17 (5%)	4 (1%)	11	9
All	All	1316/1504 (88%)	1243 (94%)	63 (5%)	10 (1%)	16	16

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	ASN
1	B	291	ASN
1	B	412	ARG
1	C	291	ASN
1	D	291	ASN

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	275/308 (89%)	269 (98%)	6 (2%)	47	61
1	B	272/308 (88%)	266 (98%)	6 (2%)	47	61
1	C	272/308 (88%)	265 (97%)	7 (3%)	41	54
1	D	277/308 (90%)	268 (97%)	9 (3%)	34	45
All	All	1096/1232 (89%)	1068 (97%)	28 (3%)	41	54

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	250	LEU
1	D	412	ARG
1	C	412	ARG
1	D	266	PHE
1	C	365	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	366	HIS
1	C	44	GLN
1	D	366	HIS
1	C	13	ASN
1	C	331	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 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
6	TRS	D	609	-	7,7,7	0.92	0	9,9,9	1.99	2 (22%)
4	IMP	B	802	-	21,25,25	2.37	8 (38%)	22,38,38	2.42	8 (36%)
4	IMP	A	801	-	21,25,25	2.31	8 (38%)	22,38,38	2.52	8 (36%)
6	TRS	C	605	-	7,7,7	0.98	0	9,9,9	1.74	2 (22%)
5	TAD	B	902	-	36,47,47	1.49	7 (19%)	39,72,72	2.50	15 (38%)
6	TRS	D	606	-	7,7,7	0.87	0	9,9,9	1.94	2 (22%)
2	BOG	A	752	-	20,20,20	1.39	2 (10%)	25,25,25	0.63	0
6	TRS	D	604	-	7,7,7	0.94	0	9,9,9	1.88	2 (22%)
6	TRS	A	601	-	7,7,7	0.98	0	9,9,9	1.94	1 (11%)
6	TRS	B	603	-	7,7,7	0.98	0	9,9,9	1.86	2 (22%)
6	TRS	A	610	-	7,7,7	0.86	0	9,9,9	1.93	2 (22%)
5	TAD	A	901	-	36,47,47	1.47	7 (19%)	39,72,72	2.45	13 (33%)
5	TAD	D	904	-	36,47,47	1.53	7 (19%)	39,72,72	3.30	15 (38%)
6	TRS	B	608	-	7,7,7	0.90	0	9,9,9	1.93	1 (11%)
2	BOG	A	751	-	20,20,20	1.34	1 (5%)	25,25,25	0.61	0
6	TRS	A	607	-	7,7,7	1.04	1 (14%)	9,9,9	1.68	2 (22%)
4	IMP	D	804	-	21,25,25	2.25	7 (33%)	22,38,38	2.45	8 (36%)
6	TRS	A	600	3	7,7,7	1.00	0	9,9,9	1.91	2 (22%)
6	TRS	C	602	-	7,7,7	0.97	0	9,9,9	1.81	2 (22%)
5	TAD	C	903	-	36,47,47	1.47	6 (16%)	39,72,72	2.46	13 (33%)
6	TRS	B	611	-	7,7,7	0.92	0	9,9,9	1.84	2 (22%)
4	IMP	C	803	-	21,25,25	2.34	7 (33%)	22,38,38	2.39	7 (31%)

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
6	TRS	D	609	-	-	5/9/9/9	-
4	IMP	B	802	-	-	4/6/26/26	0/3/3/3
4	IMP	A	801	-	-	1/6/26/26	0/3/3/3
6	TRS	C	605	-	-	3/9/9/9	-
5	TAD	B	902	-	-	4/18/62/62	0/5/5/5
6	TRS	D	606	-	-	3/9/9/9	-
2	BOG	A	752	-	-	2/11/31/31	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TRS	D	604	-	-	2/9/9/9	-
6	TRS	A	601	-	-	3/9/9/9	-
6	TRS	B	603	-	-	4/9/9/9	-
6	TRS	A	610	-	-	4/9/9/9	-
5	TAD	A	901	-	-	1/18/62/62	0/5/5/5
5	TAD	D	904	-	-	3/18/62/62	0/5/5/5
6	TRS	B	608	-	-	4/9/9/9	-
2	BOG	A	751	-	-	1/11/31/31	0/1/1/1
6	TRS	A	607	-	-	4/9/9/9	-
4	IMP	D	804	-	-	5/6/26/26	0/3/3/3
6	TRS	A	600	3	-	6/9/9/9	-
6	TRS	C	602	-	-	1/9/9/9	-
5	TAD	C	903	-	-	1/18/62/62	0/5/5/5
6	TRS	B	611	-	-	3/9/9/9	-
4	IMP	C	803	-	-	4/6/26/26	0/3/3/3

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	IMP	C8-N7	5.68	1.43	1.34
4	B	802	IMP	C8-N7	5.53	1.43	1.34
4	C	803	IMP	C8-N7	5.43	1.43	1.34
4	D	804	IMP	C8-N7	5.36	1.43	1.34
4	C	803	IMP	C2-N1	5.18	1.44	1.35

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	904	TAD	O6N-C6N-C4N	11.84	129.57	119.65
5	D	904	TAD	C4N-C6N-N6N	-8.87	107.49	116.22
4	A	801	IMP	O4'-C1'-N9	8.60	120.16	108.75
4	D	804	IMP	O4'-C1'-N9	8.11	119.49	108.75
4	B	802	IMP	O4'-C1'-N9	7.99	119.34	108.75

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	802	IMP	C5'-O5'-P-O2P

Continued on next page...

Continued from previous page...

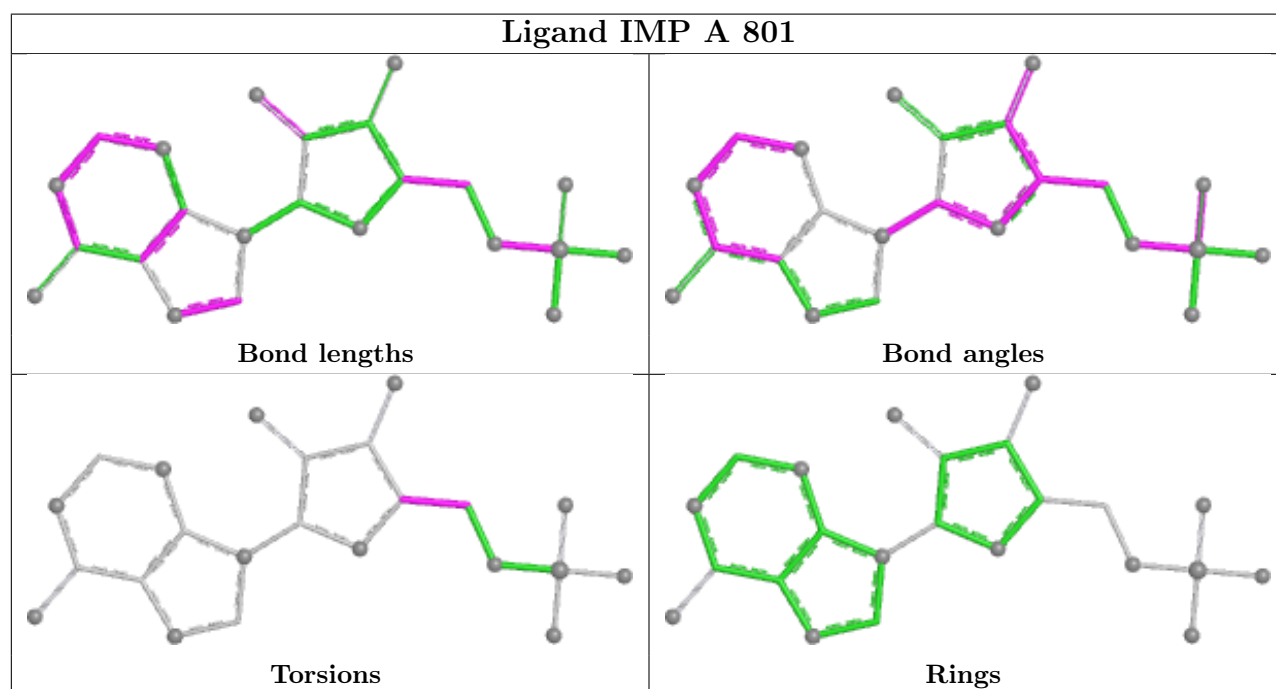
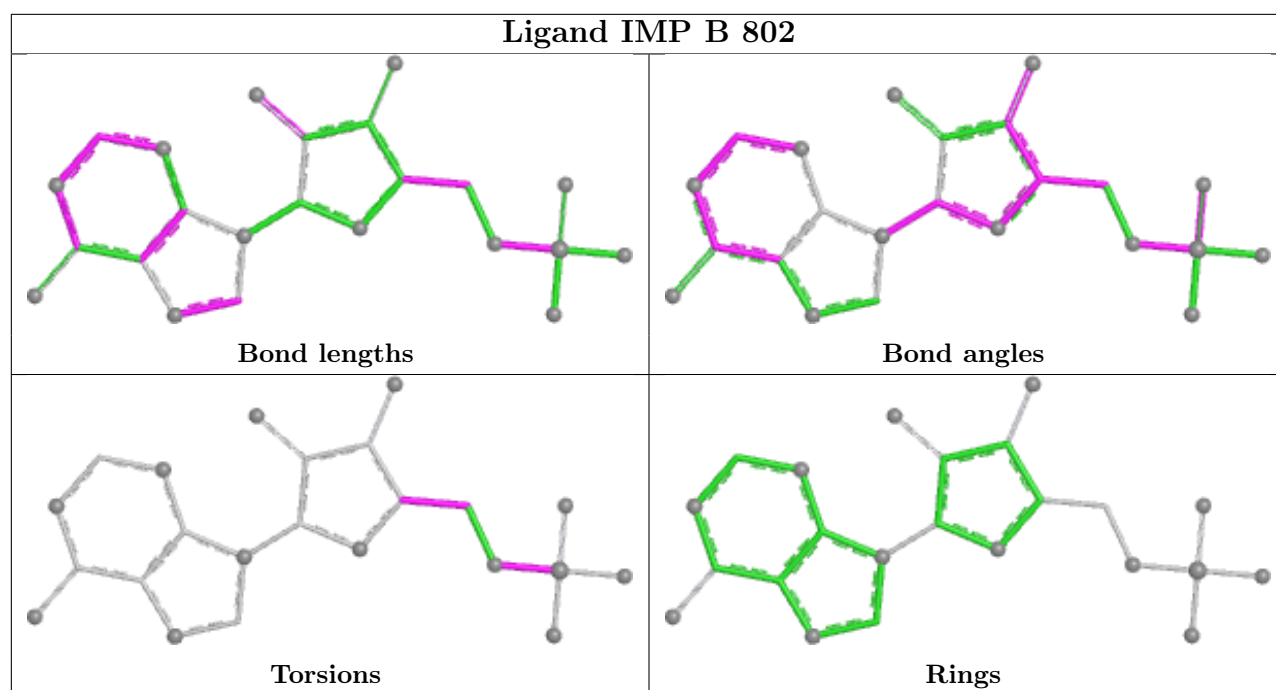
Mol	Chain	Res	Type	Atoms
4	C	803	IMP	C5'-O5'-P-O2P
4	D	804	IMP	C5'-O5'-P-O2P
4	D	804	IMP	C5'-O5'-P-O3P
5	B	902	TAD	PA-C3-PN-O5D

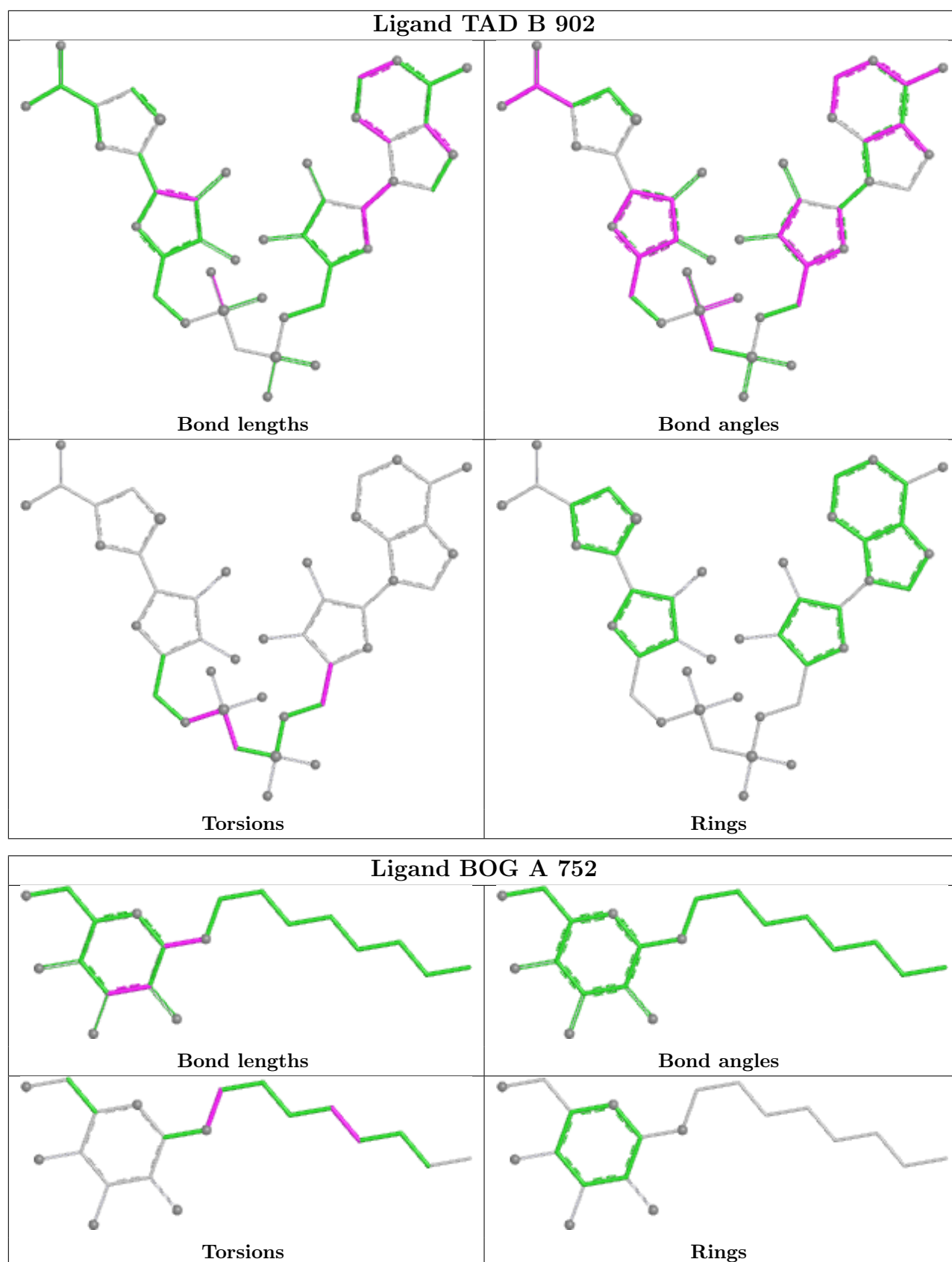
There are no ring outliers.

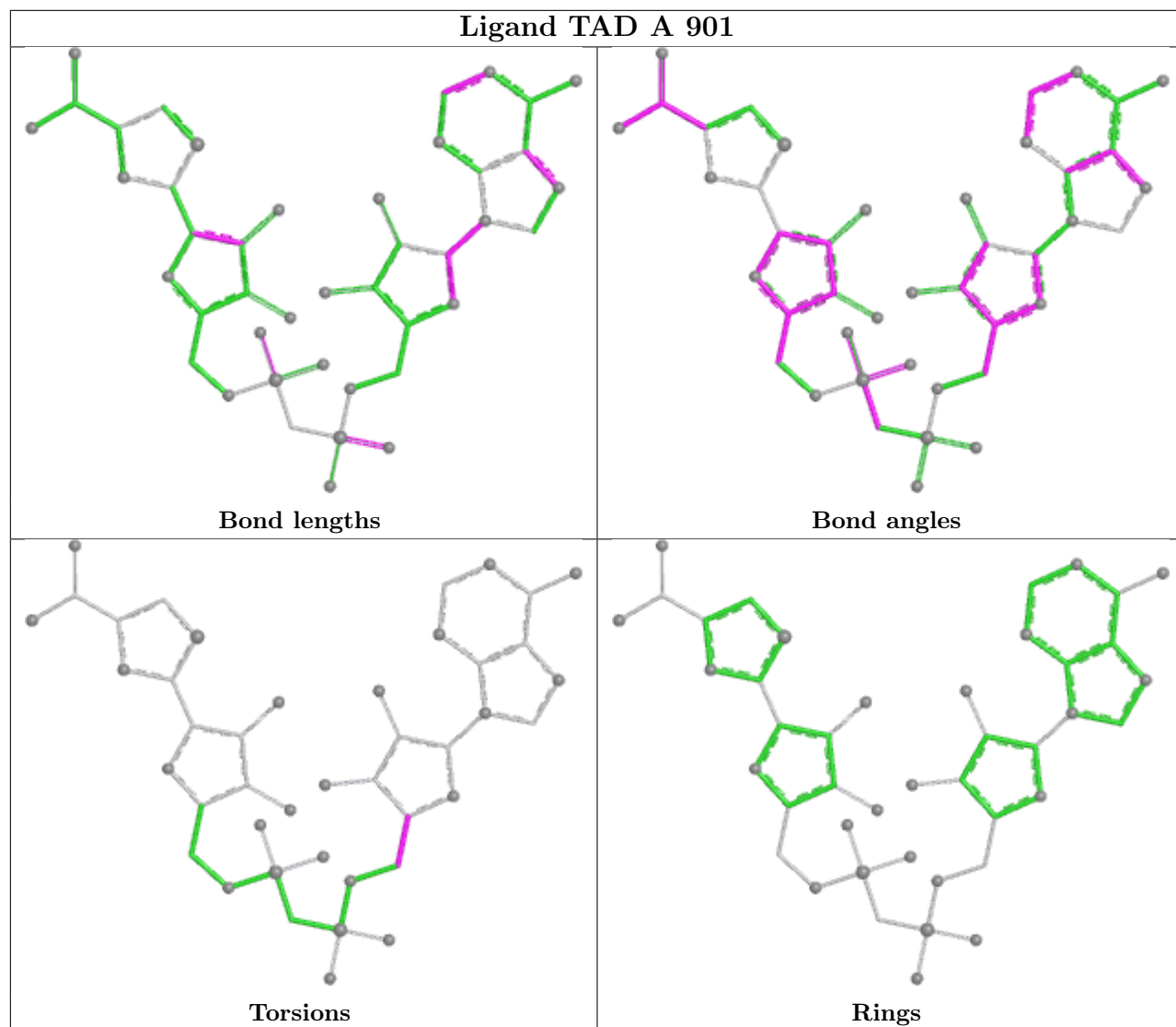
15 monomers are involved in 26 short contacts:

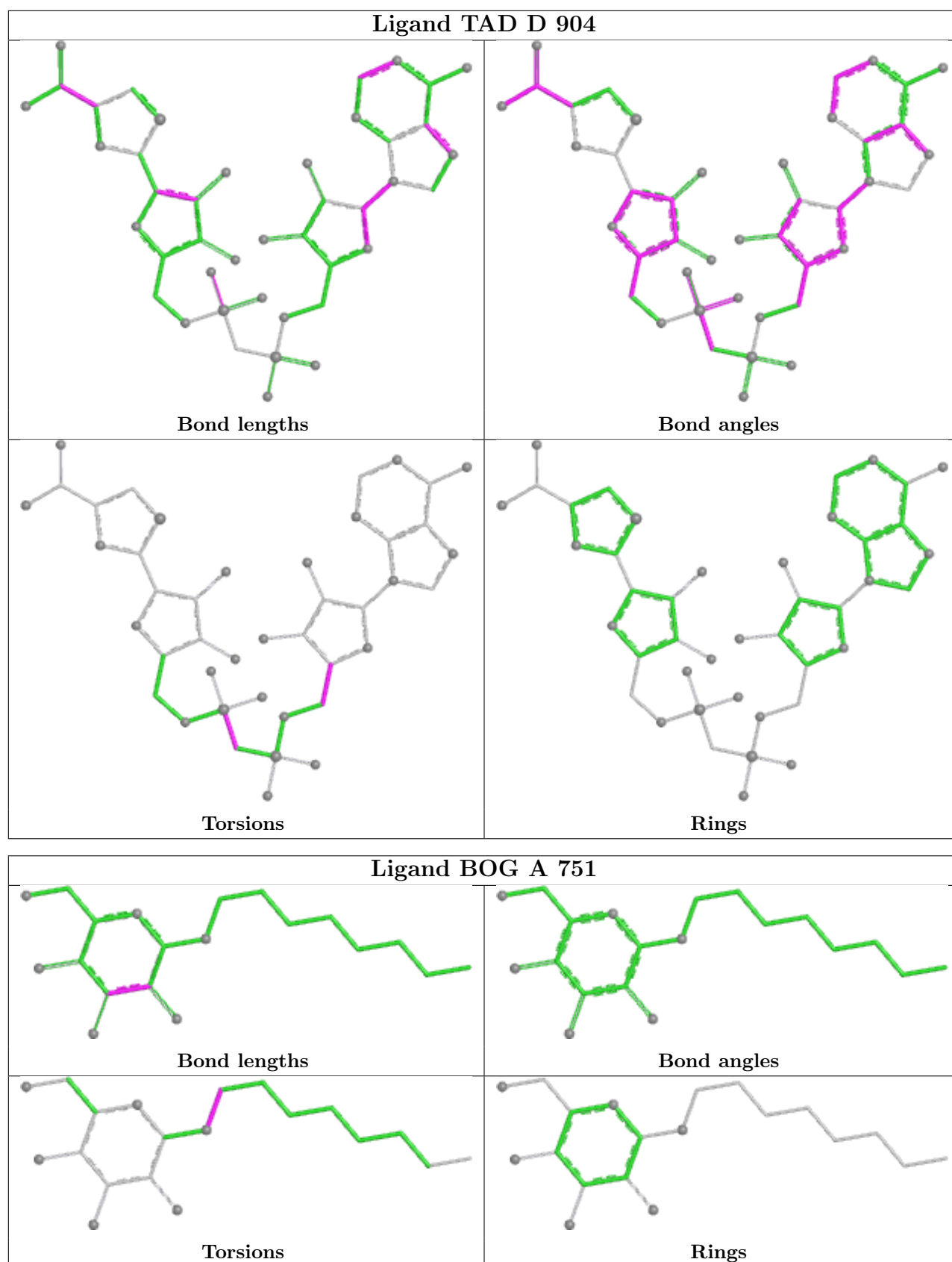
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	609	TRS	3	0
6	C	605	TRS	4	0
5	B	902	TAD	1	0
6	D	606	TRS	2	0
2	A	752	BOG	2	0
6	D	604	TRS	2	0
6	A	601	TRS	1	0
6	B	603	TRS	1	0
6	A	610	TRS	1	0
5	D	904	TAD	3	0
6	B	608	TRS	1	0
2	A	751	BOG	1	0
6	A	607	TRS	2	0
4	D	804	IMP	2	0
6	A	600	TRS	1	0

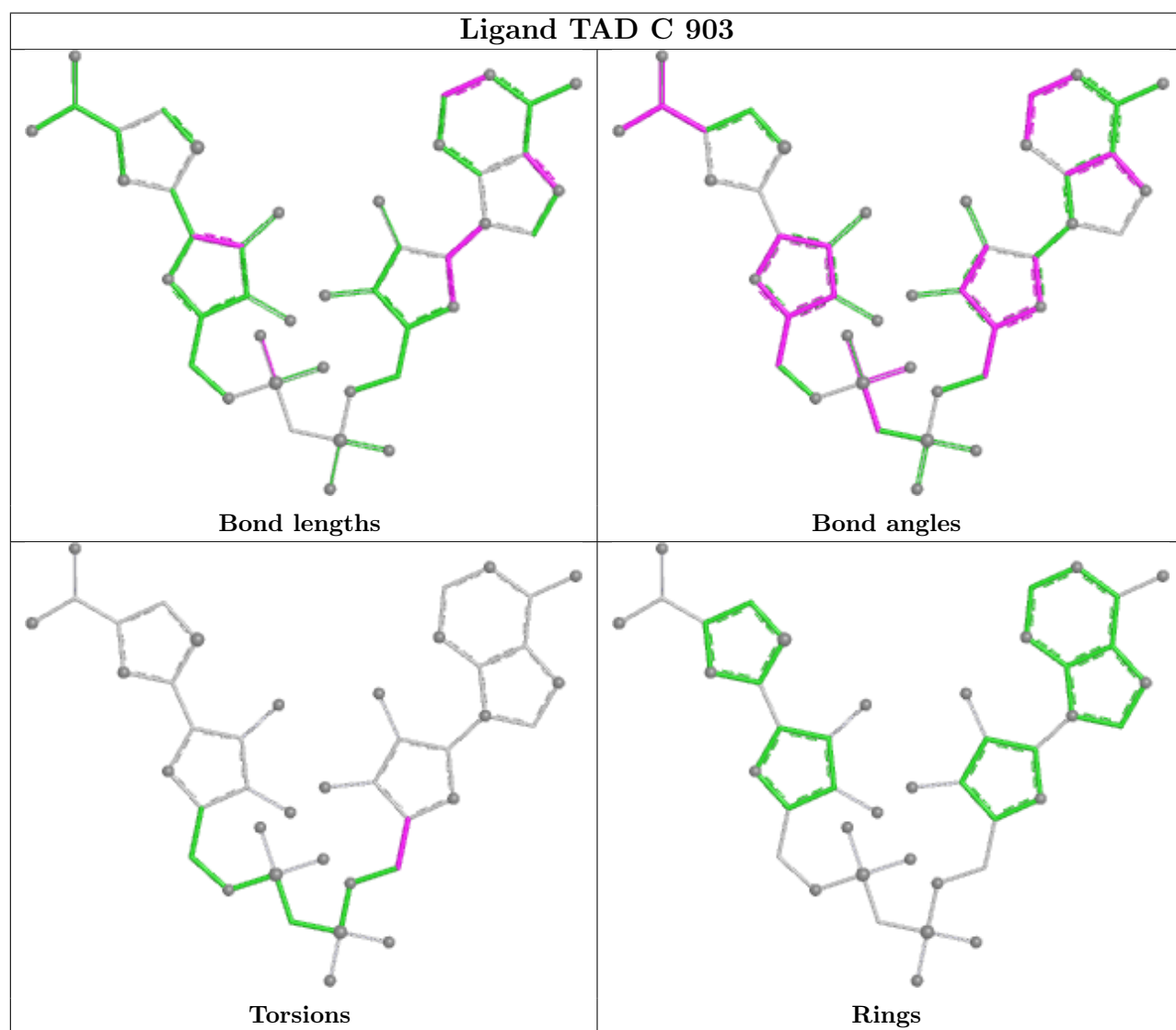
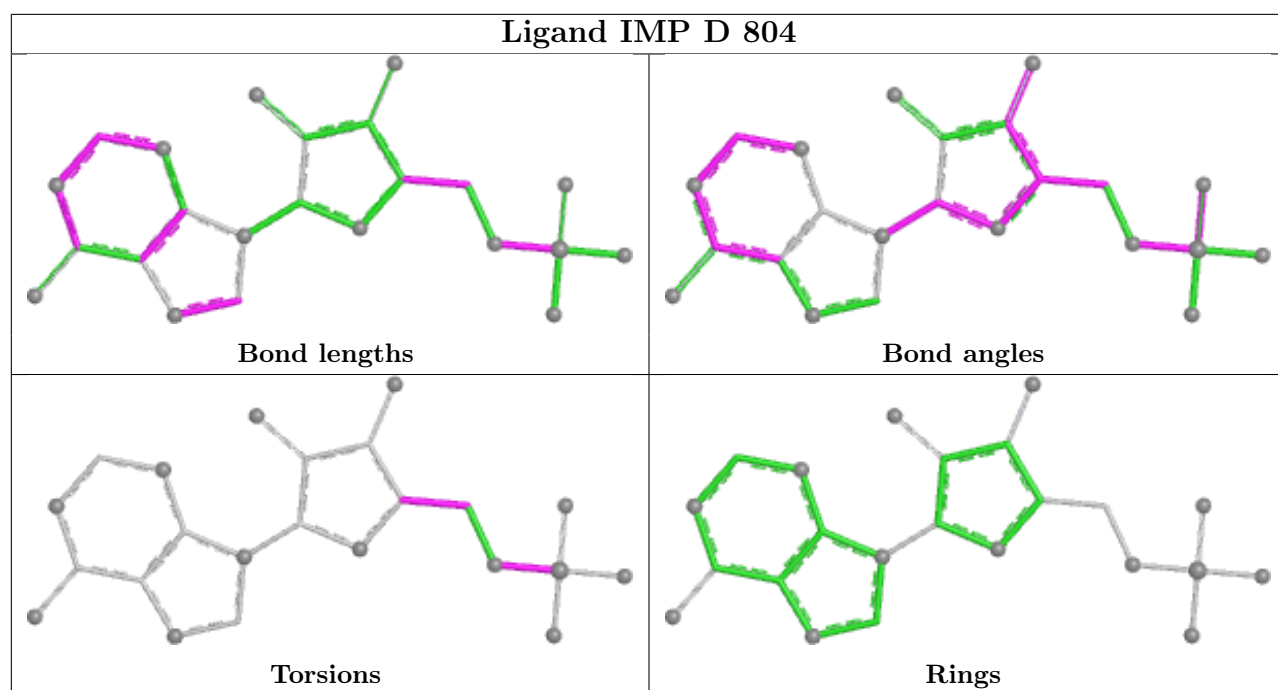
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

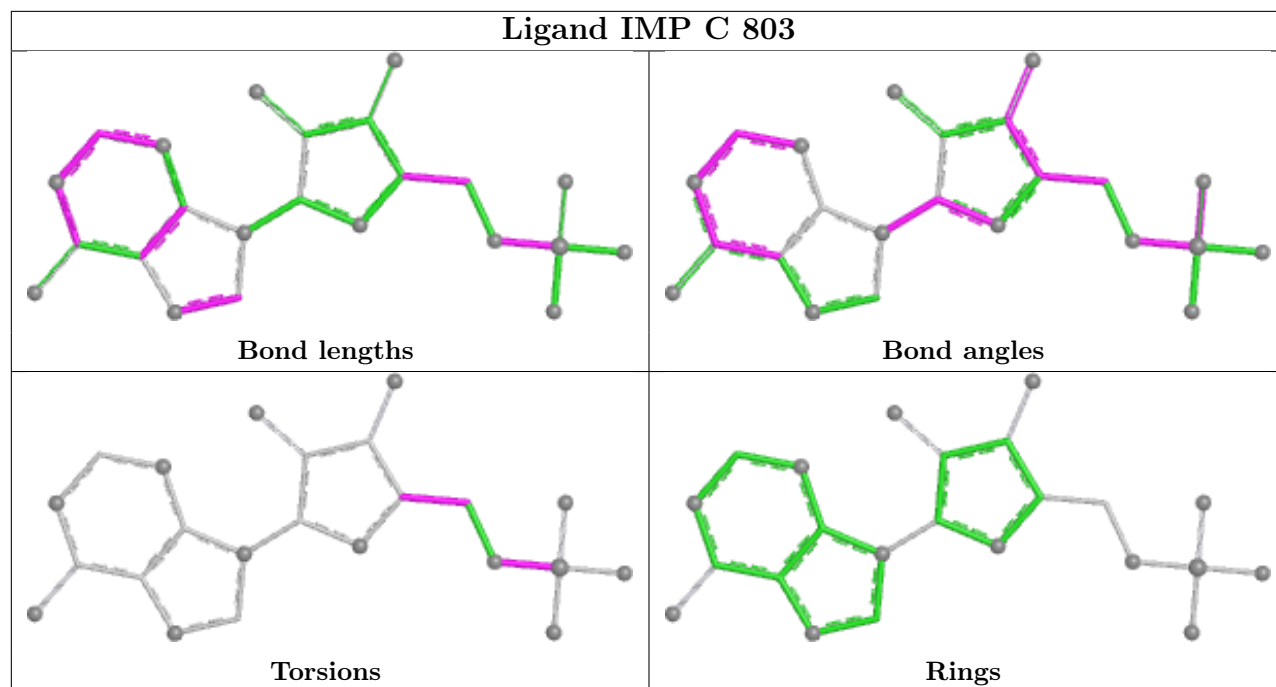












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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.