



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 31, 2021 – 01:34 AM EDT

PDB ID : 1N3S
Title : Biosynthesis of pteridins. Reaction mechanism of GTP cyclohydrolase I
Authors : Rebelo, J.; Auerbach, G.; Bader, G.; Bracher, A.; Nar, H.; Hoesl, C.; Schramek, N.; Kaiser, J.; Bacher, A.; Huber, R.; Fischer, M.
Deposited on : 2002-10-29
Resolution : 2.55 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 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) : 2.23.2

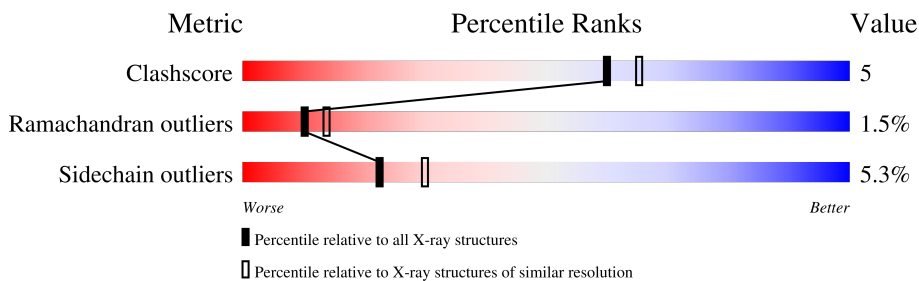
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)



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	221	
1	B	221	
1	C	221	
1	D	221	
1	E	221	
1	F	221	
1	G	221	
1	H	221	

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Mol	Chain	Length	Quality of chain
1	I	221	 88% 11% •
1	J	221	 82% 16% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17795 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 GTP cyclohydrolase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	221	1729	1085	307	328	9	0	0	0
1	B	221	1729	1085	307	328	9	0	0	0
1	C	221	1729	1085	307	328	9	0	0	0
1	D	221	1729	1085	307	328	9	0	0	0
1	E	221	1729	1085	307	328	9	0	0	0
1	F	221	1729	1085	307	328	9	0	0	0
1	G	221	1729	1085	307	328	9	0	0	0
1	H	221	1729	1085	307	328	9	0	0	0
1	I	221	1729	1085	307	328	9	0	0	0
1	J	221	1729	1085	307	328	9	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

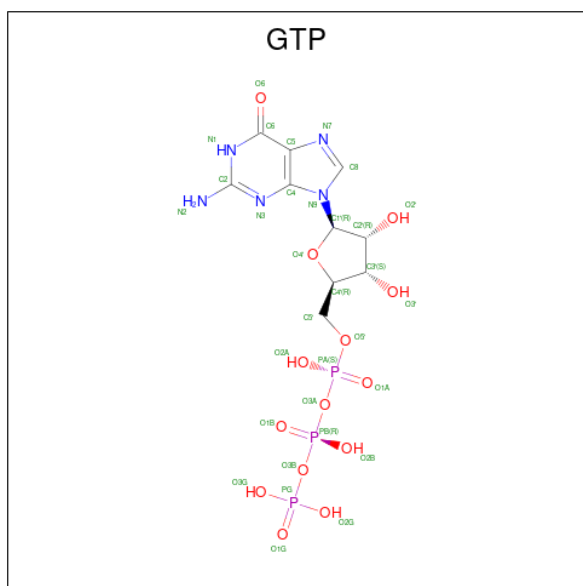
Chain	Residue	Modelled	Actual	Comment	Reference
A	113	SER	HIS	engineered mutation	UNP P0A6T5
B	113	SER	HIS	engineered mutation	UNP P0A6T5
C	113	SER	HIS	engineered mutation	UNP P0A6T5
D	113	SER	HIS	engineered mutation	UNP P0A6T5
E	113	SER	HIS	engineered mutation	UNP P0A6T5
F	113	SER	HIS	engineered mutation	UNP P0A6T5
G	113	SER	HIS	engineered mutation	UNP P0A6T5
H	113	SER	HIS	engineered mutation	UNP P0A6T5
I	113	SER	HIS	engineered mutation	UNP P0A6T5

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Chain	Residue	Modelled	Actual	Comment	Reference
J	113	SER	HIS	engineered mutation	UNP P0A6T5

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	G	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	H	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	I	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
2	J	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 3 is water.

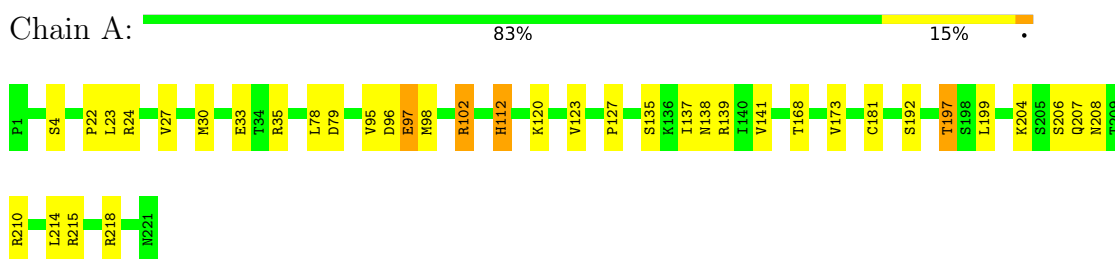
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	23	Total O 23 23	0	0
3	B	34	Total O 34 34	0	0
3	C	16	Total O 16 16	0	0
3	D	24	Total O 24 24	0	0
3	E	9	Total O 9 9	0	0
3	F	18	Total O 18 18	0	0
3	G	13	Total O 13 13	0	0
3	H	9	Total O 9 9	0	0
3	I	18	Total O 18 18	0	0
3	J	21	Total O 21 21	0	0

3 Residue-property plots [i](#)

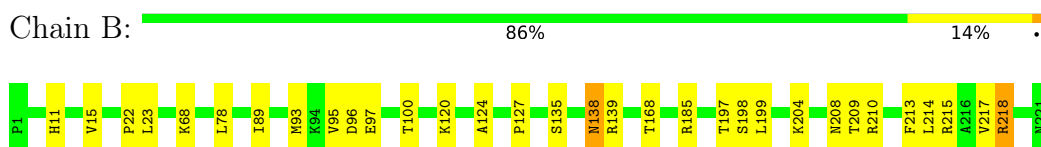
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

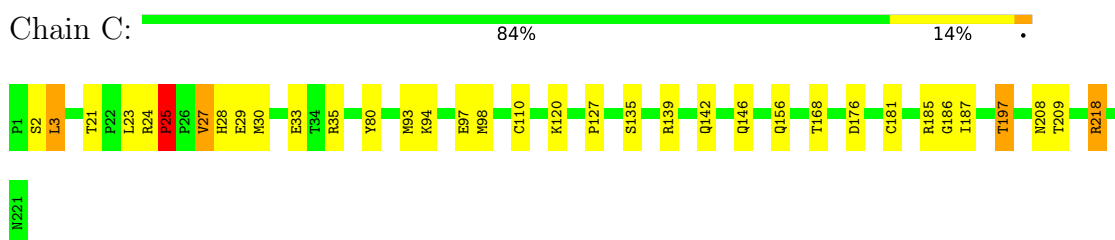
- Molecule 1: GTP cyclohydrolase I



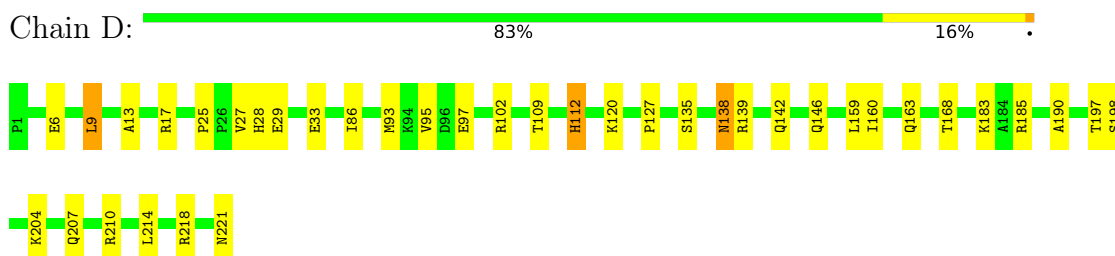
- Molecule 1: GTP cyclohydrolase I




- Molecule 1: GTP cyclohydrolase I

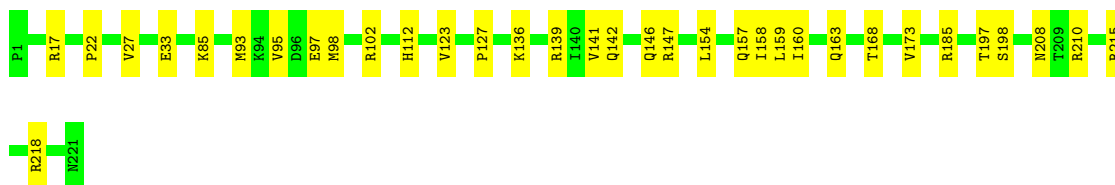


- Molecule 1: GTP cyclohydrolase I




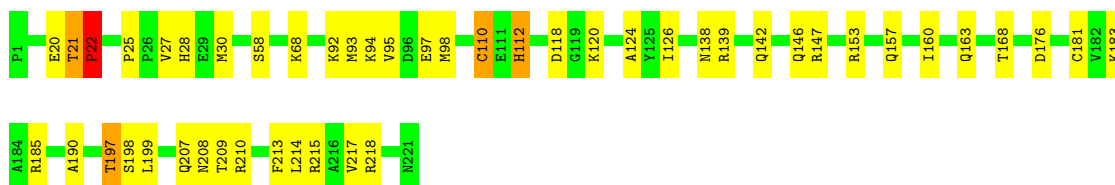
- Molecule 1: GTP cyclohydrolase I

Chain E:  85% 15%




• Molecule 1: GTP cyclohydrolase I

Chain F:  78% 19%



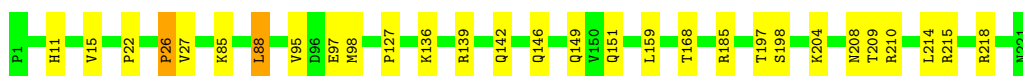
• Molecule 1: GTP cyclohydrolase I

Chain G:  85% 13%




• Molecule 1: GTP cyclohydrolase I

Chain H:  87% 12%




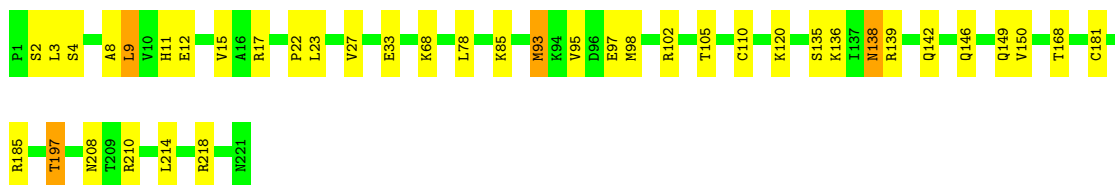
• Molecule 1: GTP cyclohydrolase I

Chain I:  88% 11%



• Molecule 1: GTP cyclohydrolase I

Chain J:  82% 16%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	124.30Å 124.30Å 389.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.55	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.55)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.262 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	17795	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP

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	0.61	0/1756	0.84	0/2377
1	B	0.59	0/1756	0.83	0/2377
1	C	0.67	0/1756	1.00	8/2377 (0.3%)
1	D	0.59	0/1756	0.86	1/2377 (0.0%)
1	E	0.60	0/1756	0.83	1/2377 (0.0%)
1	F	0.62	0/1756	1.01	5/2377 (0.2%)
1	G	0.61	0/1756	0.86	2/2377 (0.1%)
1	H	0.60	0/1756	0.83	3/2377 (0.1%)
1	I	0.57	0/1756	0.81	2/2377 (0.1%)
1	J	0.62	0/1756	0.88	6/2377 (0.3%)
All	All	0.61	0/17560	0.88	28/23770 (0.1%)

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	21	THR	C-N-CD	-19.65	77.36	120.60
1	C	24	ARG	C-N-CD	-18.21	80.55	120.60
1	F	21	THR	C-N-CA	12.01	172.42	122.00
1	C	24	ARG	C-N-CA	10.42	165.77	122.00
1	F	22	PRO	CA-N-CD	-8.33	99.84	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1729	0	1766	16	0
1	B	1729	0	1766	22	0
1	C	1729	0	1764	22	0
1	D	1729	0	1766	24	0
1	E	1729	0	1766	20	0
1	F	1729	0	1764	25	0
1	G	1729	0	1766	21	0
1	H	1729	0	1766	17	0
1	I	1729	0	1766	16	0
1	J	1729	0	1764	22	0
2	A	32	0	11	1	0
2	B	32	0	11	0	0
2	C	32	0	11	2	0
2	D	32	0	11	2	0
2	E	32	0	11	3	0
2	F	32	0	11	3	0
2	G	32	0	11	1	0
2	H	32	0	11	3	0
2	I	32	0	11	1	0
2	J	32	0	11	2	0
3	A	23	0	0	0	0
3	B	34	0	0	1	0
3	C	16	0	0	0	1
3	D	24	0	0	1	1
3	E	9	0	0	0	0
3	F	18	0	0	1	0
3	G	13	0	0	0	0
3	H	9	0	0	1	0
3	I	18	0	0	0	1
3	J	21	0	0	1	1
All	All	17795	0	17764	164	2

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 5.

The worst 5 of 164 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:210:ARG:HE	1:E:208:ASN:HD21	1.07	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ARG:HE	1:C:208:ASN:HD21	1.02	0.92
1:F:93:MET:HG2	1:J:17:ARG:O	1.72	0.89
1:D:210:ARG:NE	1:E:208:ASN:HD21	1.71	0.87
1:B:210:ARG:NE	1:C:208:ASN:HD21	1.75	0.83

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1423:HOH:O	3:J:8425:HOH:O[8_655]	2.04	0.16
3:D:2421:HOH:O	3:I:7429:HOH:O[8_655]	2.15	0.05

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	219/221 (99%)	204 (93%)	12 (6%)	3 (1%)	11	15
1	B	219/221 (99%)	203 (93%)	13 (6%)	3 (1%)	11	15
1	C	219/221 (99%)	199 (91%)	16 (7%)	4 (2%)	8	10
1	D	219/221 (99%)	199 (91%)	17 (8%)	3 (1%)	11	15
1	E	219/221 (99%)	201 (92%)	15 (7%)	3 (1%)	11	15
1	F	219/221 (99%)	194 (89%)	21 (10%)	4 (2%)	8	10
1	G	219/221 (99%)	203 (93%)	12 (6%)	4 (2%)	8	10
1	H	219/221 (99%)	201 (92%)	14 (6%)	4 (2%)	8	10
1	I	219/221 (99%)	203 (93%)	14 (6%)	2 (1%)	17	24
1	J	219/221 (99%)	201 (92%)	15 (7%)	3 (1%)	11	15
All	All	2190/2210 (99%)	2008 (92%)	149 (7%)	33 (2%)	10	14

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	C	23	LEU
1	C	25	PRO
1	C	27	VAL
1	C	29	GLU

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	194/194 (100%)	176 (91%)	18 (9%)	9 10
1	B	194/194 (100%)	185 (95%)	9 (5%)	27 36
1	C	194/194 (100%)	181 (93%)	13 (7%)	16 21
1	D	194/194 (100%)	184 (95%)	10 (5%)	23 30
1	E	194/194 (100%)	186 (96%)	8 (4%)	30 41
1	F	194/194 (100%)	184 (95%)	10 (5%)	23 30
1	G	194/194 (100%)	182 (94%)	12 (6%)	18 24
1	H	194/194 (100%)	188 (97%)	6 (3%)	40 54
1	I	194/194 (100%)	187 (96%)	7 (4%)	35 47
1	J	194/194 (100%)	185 (95%)	9 (5%)	27 36
All	All	1940/1940 (100%)	1838 (95%)	102 (5%)	22 30

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	218	ARG
1	G	68	LYS
1	J	168	THR
1	F	22	PRO
1	F	168	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	207	GLN
1	J	208	ASN
1	H	138	ASN
1	I	208	ASN
1	G	163	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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$
2	GTP	C	1411	-	26,34,34	4.08	10 (38%)	33,54,54	3.18	12 (36%)
2	GTP	B	411	-	26,34,34	4.09	11 (42%)	33,54,54	3.12	12 (36%)
2	GTP	E	3411	-	26,34,34	4.04	11 (42%)	33,54,54	3.05	12 (36%)
2	GTP	F	9411	-	26,34,34	4.16	11 (42%)	33,54,54	3.11	12 (36%)
2	GTP	A	4411	-	26,34,34	4.06	11 (42%)	33,54,54	3.08	12 (36%)
2	GTP	J	8411	-	26,34,34	4.04	10 (38%)	33,54,54	3.21	11 (33%)
2	GTP	G	5411	-	26,34,34	3.93	11 (42%)	33,54,54	3.13	12 (36%)
2	GTP	H	6411	-	26,34,34	4.16	10 (38%)	33,54,54	3.11	12 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GTP	D	2411	-	26,34,34	4.15	11 (42%)	33,54,54	3.14	12 (36%)
2	GTP	I	7411	-	26,34,34	4.16	10 (38%)	33,54,54	3.14	11 (33%)

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	GTP	C	1411	-	-	4/18/38/38	0/3/3/3
2	GTP	B	411	-	-	4/18/38/38	0/3/3/3
2	GTP	E	3411	-	-	4/18/38/38	0/3/3/3
2	GTP	F	9411	-	-	4/18/38/38	0/3/3/3
2	GTP	A	4411	-	-	4/18/38/38	0/3/3/3
2	GTP	J	8411	-	-	4/18/38/38	0/3/3/3
2	GTP	G	5411	-	-	5/18/38/38	0/3/3/3
2	GTP	H	6411	-	-	4/18/38/38	0/3/3/3
2	GTP	D	2411	-	-	3/18/38/38	0/3/3/3
2	GTP	I	7411	-	-	4/18/38/38	0/3/3/3

The worst 5 of 106 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	411	GTP	C6-N1	13.11	1.55	1.33
2	F	9411	GTP	C6-N1	12.81	1.55	1.33
2	H	6411	GTP	C6-N1	12.71	1.55	1.33
2	A	4411	GTP	C6-N1	12.59	1.55	1.33
2	I	7411	GTP	C6-N1	12.59	1.55	1.33

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1411	GTP	C5-C6-N1	-8.99	111.13	123.43
2	B	411	GTP	C5-C6-N1	-8.86	111.31	123.43
2	G	5411	GTP	C5-C6-N1	-8.84	111.35	123.43
2	D	2411	GTP	C5-C6-N1	-8.80	111.40	123.43
2	J	8411	GTP	C5-C6-N1	-8.75	111.47	123.43

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

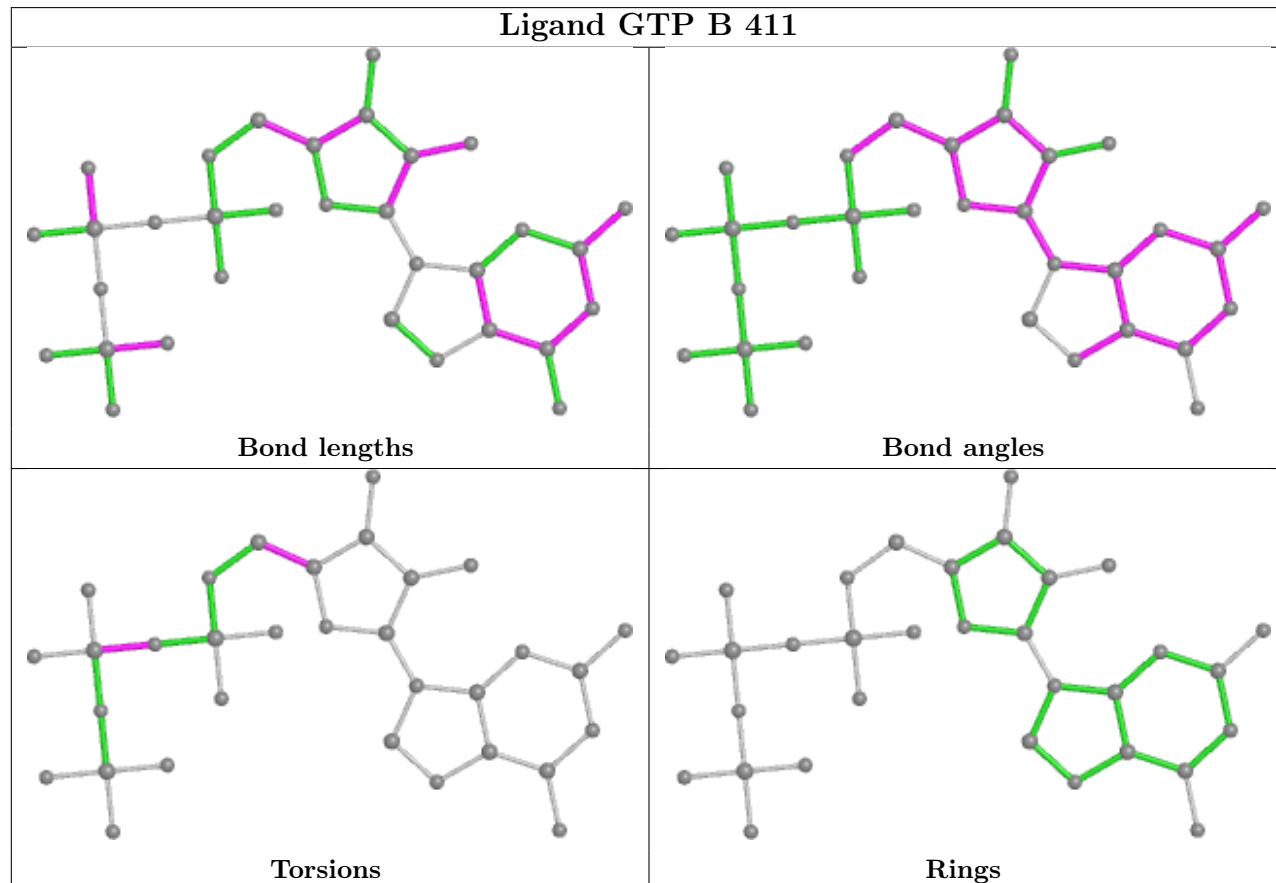
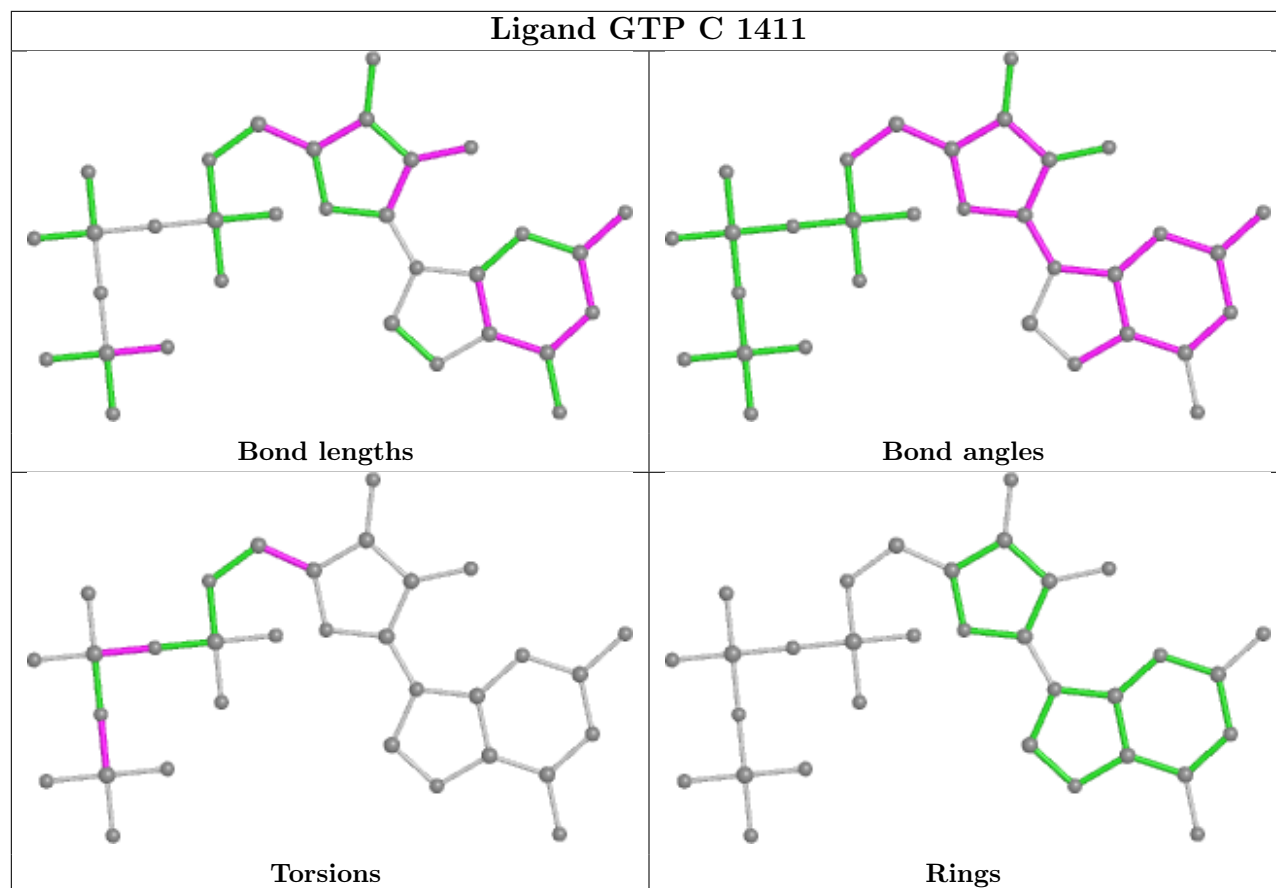
Mol	Chain	Res	Type	Atoms
2	C	1411	GTP	PB-O3B-PG-O3G
2	A	4411	GTP	O4'-C4'-C5'-O5'
2	A	4411	GTP	C3'-C4'-C5'-O5'
2	B	411	GTP	O4'-C4'-C5'-O5'
2	B	411	GTP	C3'-C4'-C5'-O5'

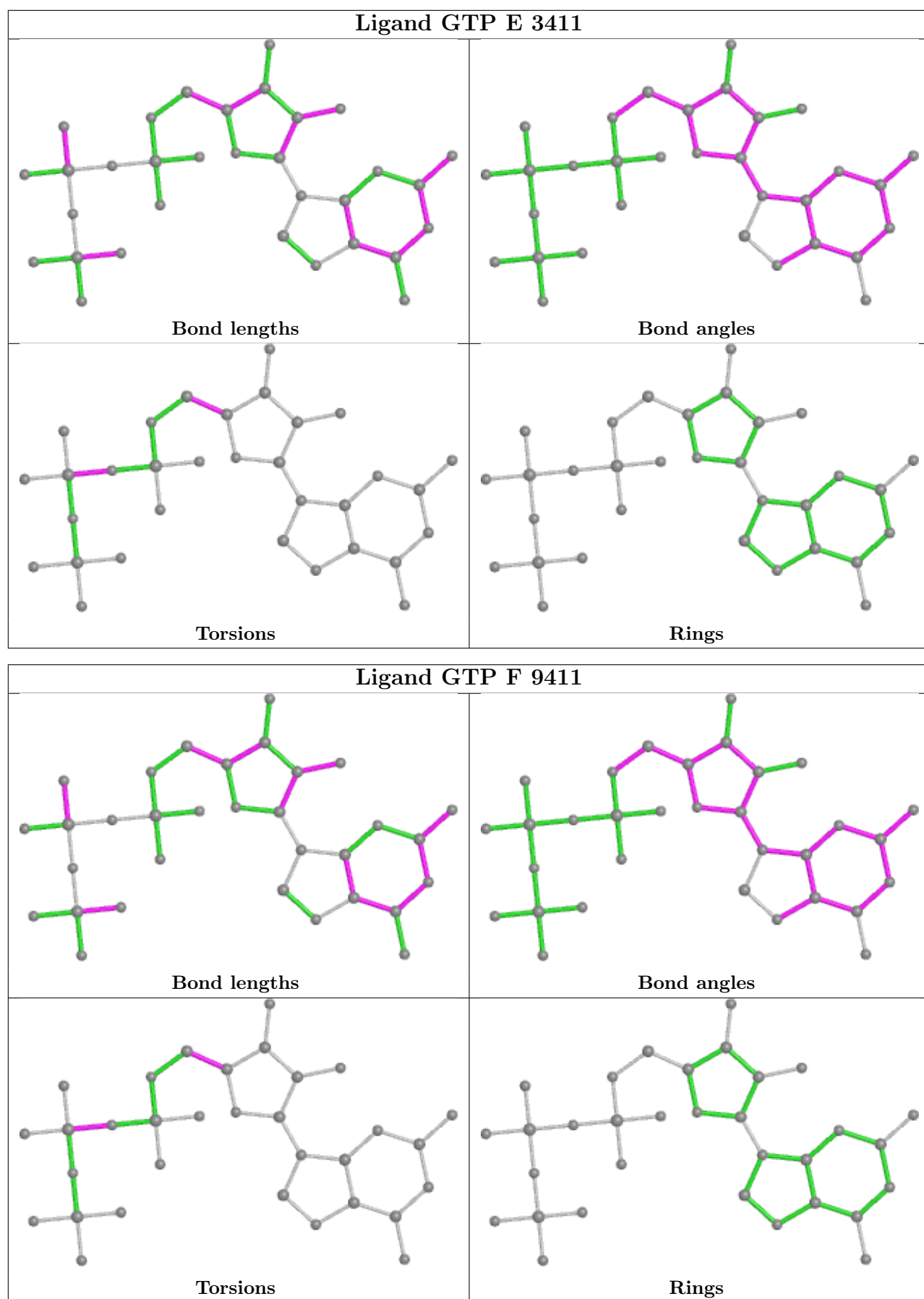
There are no ring outliers.

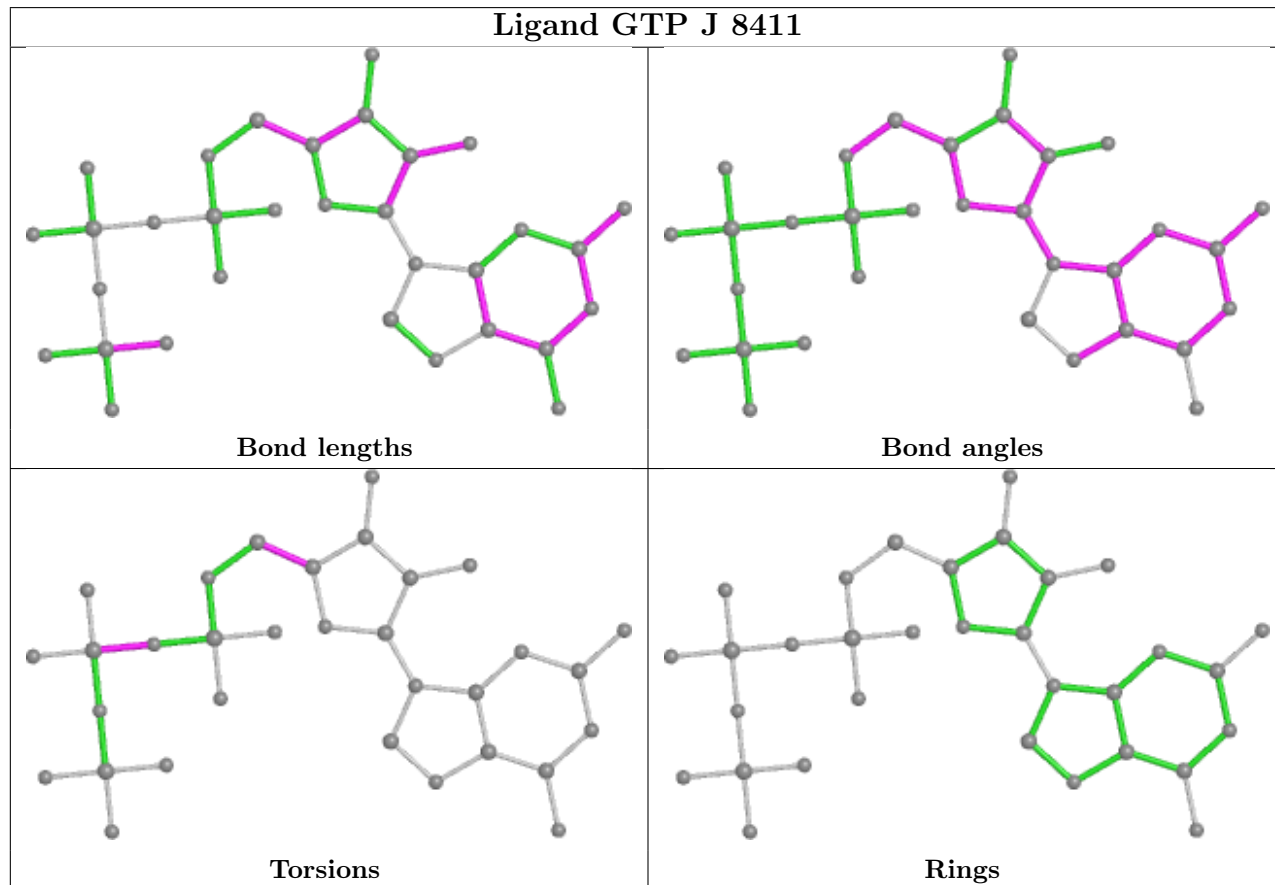
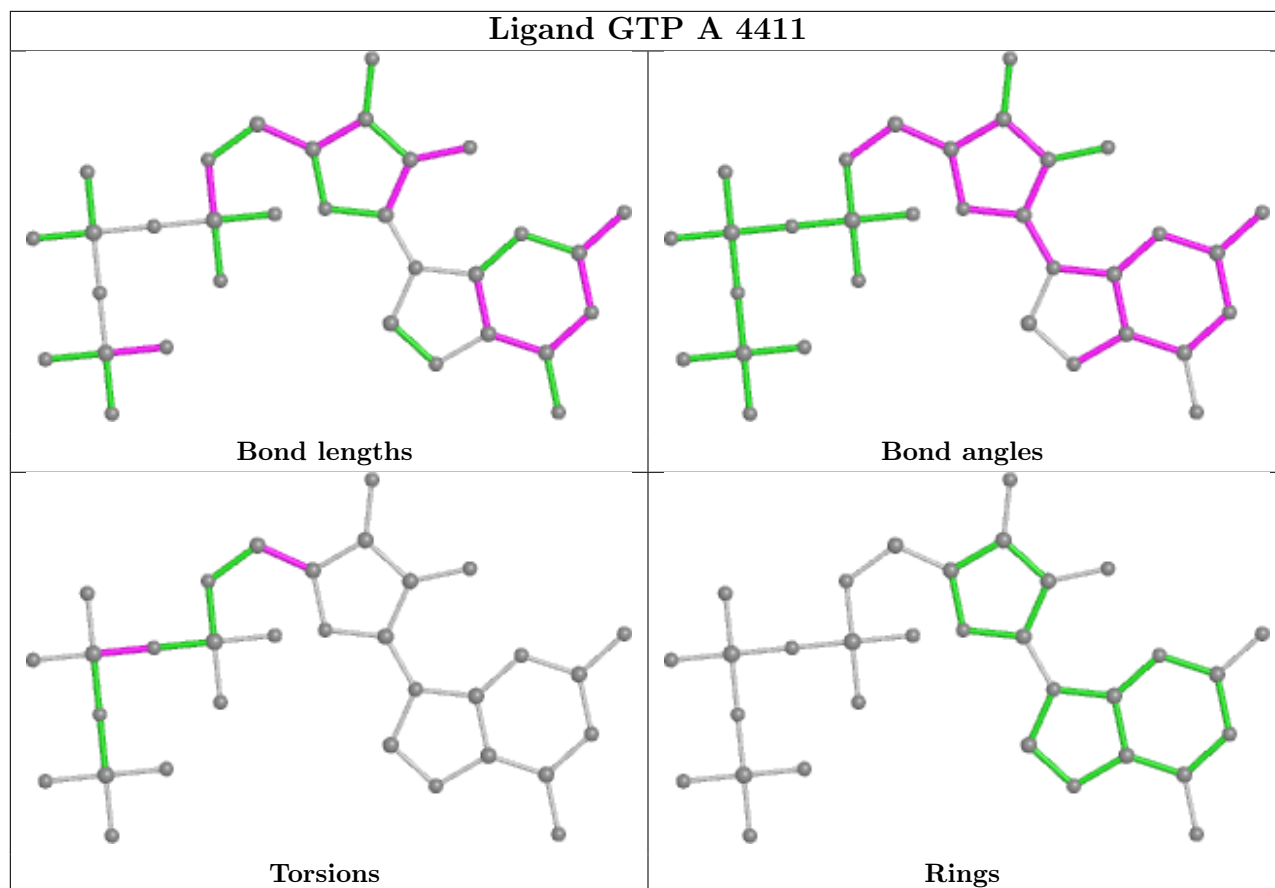
9 monomers are involved in 18 short contacts:

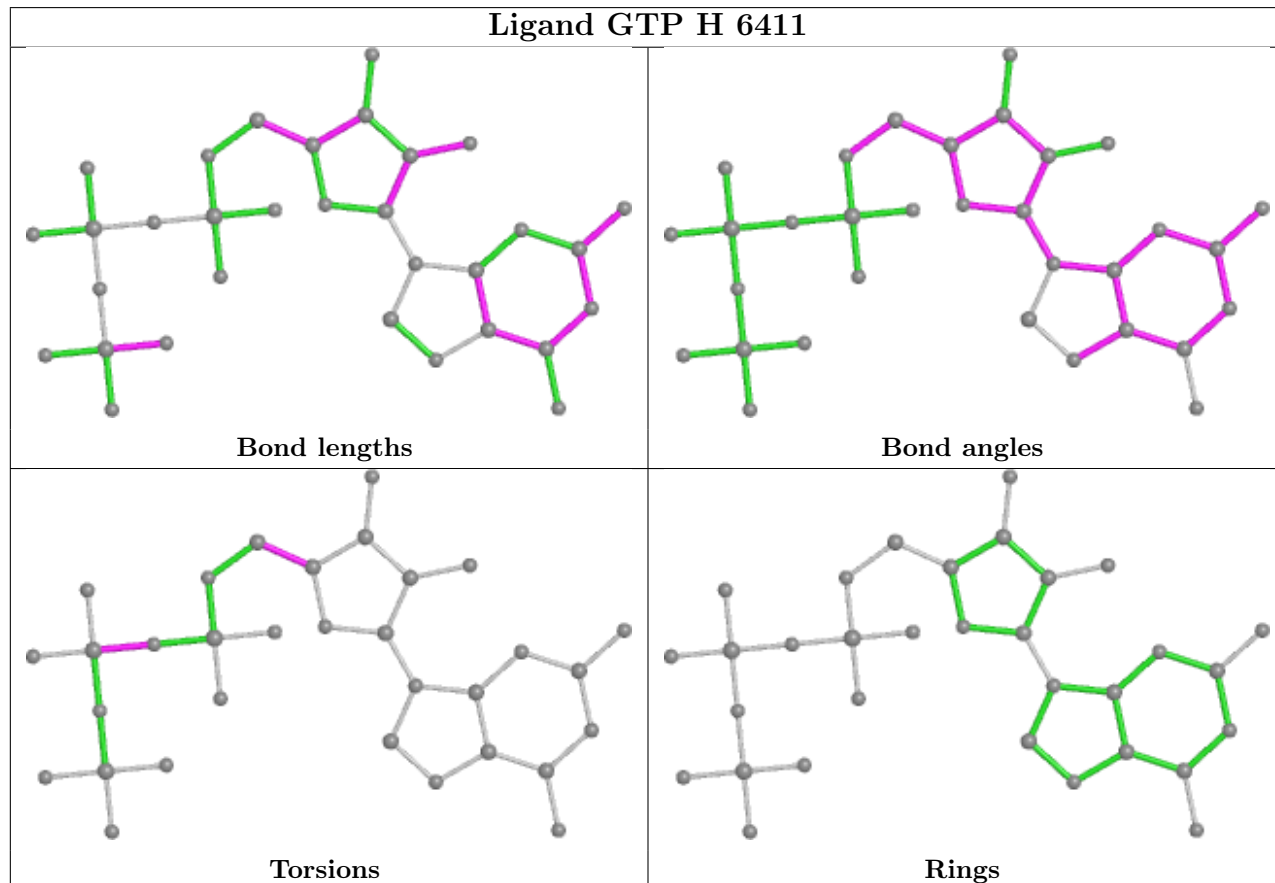
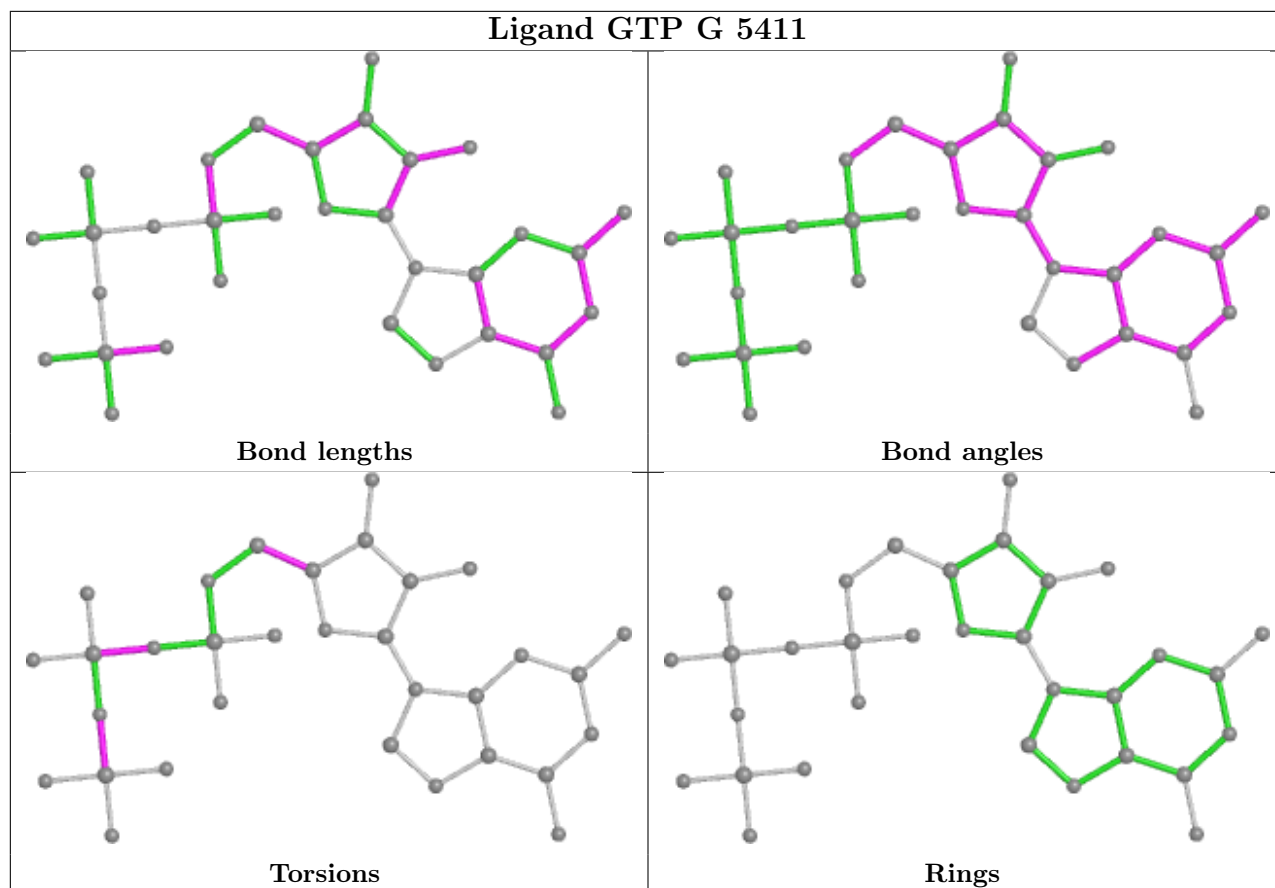
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1411	GTP	2	0
2	E	3411	GTP	3	0
2	F	9411	GTP	3	0
2	A	4411	GTP	1	0
2	J	8411	GTP	2	0
2	G	5411	GTP	1	0
2	H	6411	GTP	3	0
2	D	2411	GTP	2	0
2	I	7411	GTP	1	0

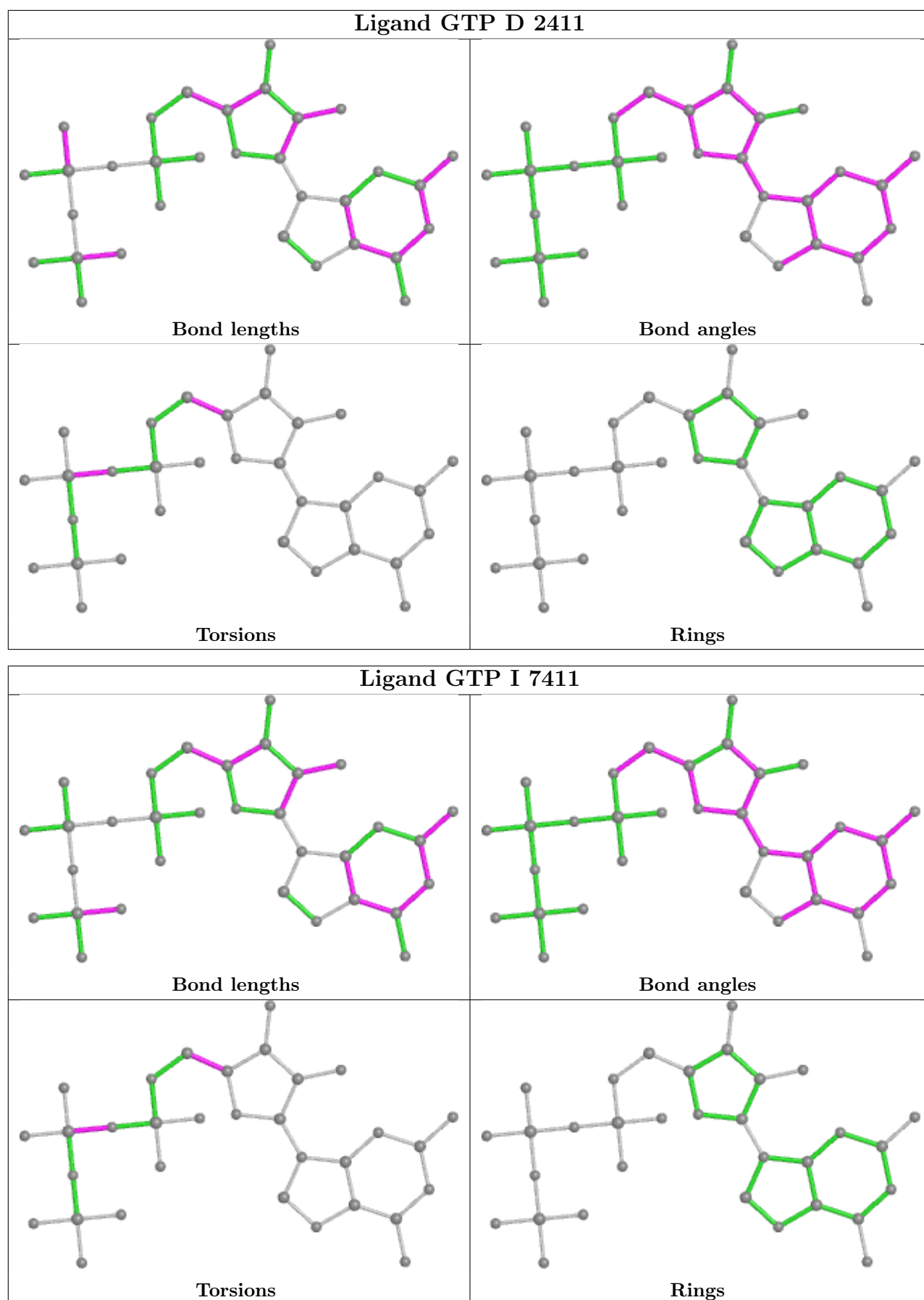
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.