



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 07:03 pm BST

PDB ID : 1ECB
Title : ESCHERICHIA COLI GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE (PRPP) AMIDOTRANSFERASE COMPLEXED WITH 2 GMP, 1 MG PER SUBUNIT
Authors : Krahn, J.M.; Smith, J.L.
Deposited on : 1997-07-15
Resolution : 2.70 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)
Xtriage (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)	:	2.11

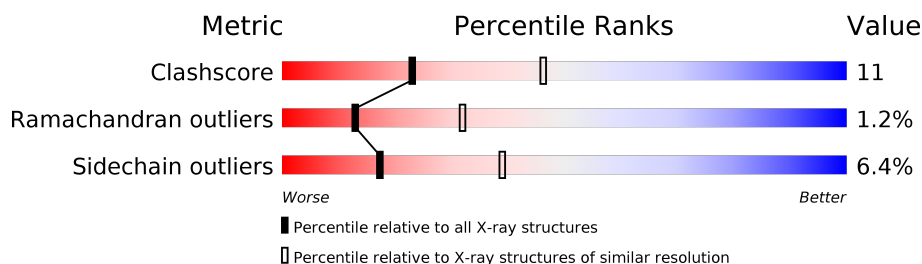
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 on 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	504	
1	B	504	
1	C	504	
1	D	504	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15139 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.

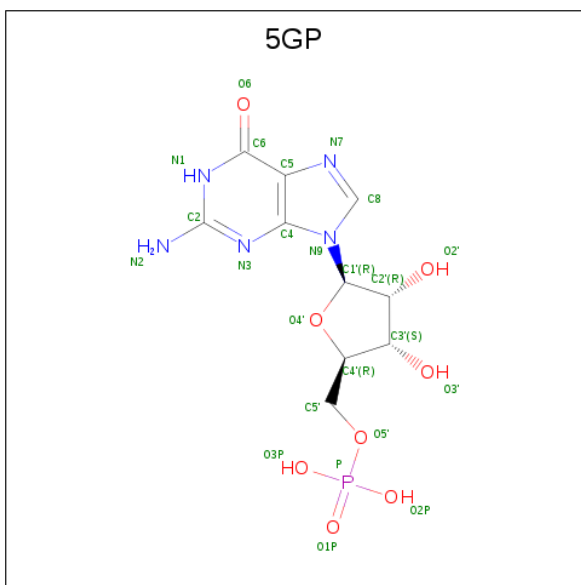
- Molecule 1 is a protein called GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3724	2345	657	705	17			
1	B	470	Total	C	N	O	S	0	0	0
			3685	2320	651	697	17			
1	C	482	Total	C	N	O	S	0	0	0
			3787	2381	675	714	17			
1	D	473	Total	C	N	O	S	0	0	0
			3708	2334	654	703	17			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: C₁₀H₁₄N₅O₈P).



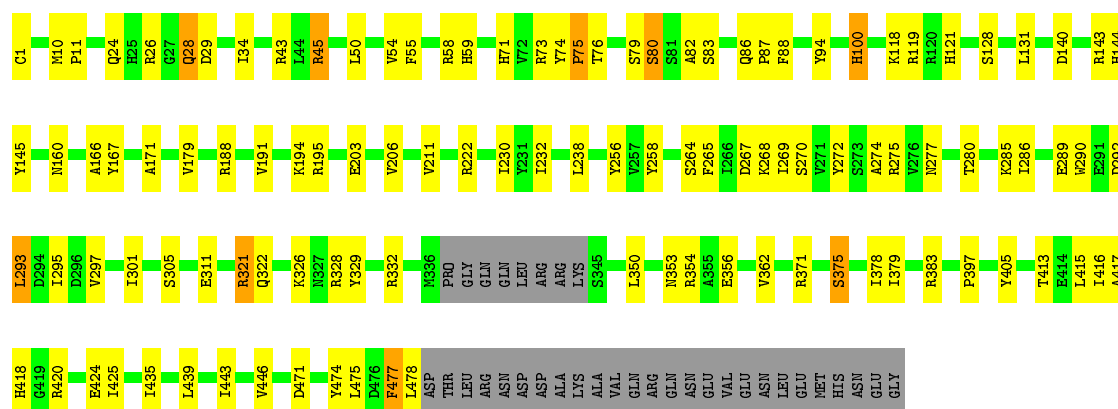
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	C	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	C	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	D	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
3	D	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	8	Total	O	0	0
			8	8		
4	C	13	Total	O	0	0
			13	13		
4	D	11	Total	O	0	0
			11	11		

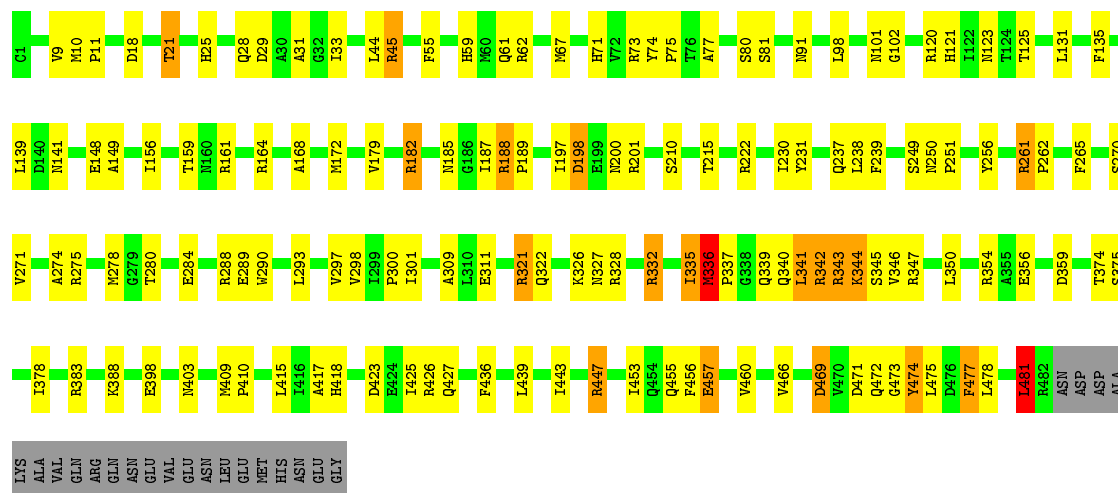
Note EDS was not executed.

- Chain A:  68% 25% 6%



• Molecule 1: GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE

Chain C:  67% 24%



4 Data and refinement statistics

Xtriage (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	95.80 Å 113.20 Å 199.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70	Depositor
% Data completeness (in resolution range)	97.7 (15.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.208 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15139	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: MG, 5GP

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	0.62	0/3791	0.82	1/5133 (0.0%)
1	B	0.65	0/3751	0.82	0/5078
1	C	0.66	0/3855	0.85	2/5218 (0.0%)
1	D	0.65	1/3774 (0.0%)	0.84	3/5110 (0.1%)
All	All	0.65	1/15171 (0.0%)	0.83	6/20539 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	329	TYR	CE1-CZ	-5.12	1.31	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	293	LEU	CA-CB-CG	5.98	129.05	115.30
1	D	26	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	C	168	ALA	N-CA-C	-5.76	95.46	111.00
1	D	275	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	168	ALA	N-CA-C	-5.24	96.86	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	145	TYR	Sidechain

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	3724	0	3687	89	0
1	B	3685	0	3645	82	0
1	C	3787	0	3757	96	0
1	D	3708	0	3667	85	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	48	0	22	6	0
3	B	48	0	22	2	0
3	C	48	0	21	2	0
3	D	48	0	22	3	0
4	A	7	0	0	0	0
4	B	8	0	0	0	0
4	C	13	0	0	1	0
4	D	11	0	0	0	0
All	All	15139	0	14843	342	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 11.

The worst 5 of 342 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:C:336:MET:HB2	1:C:337:PRO:HD3	1.39	1.02
1:C:164:ARG:HD2	1:C:469:ASP:HB3	1.47	0.94
1:A:80:SER:HB2	1:A:83:SER:HB2	1.52	0.90
1:C:342:ARG:HA	1:C:342:ARG:NE	1.85	0.89
1:B:80:SER:HB2	1:B:83:SER:HB2	1.52	0.88

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	471/504 (94%)	427 (91%)	38 (8%)	6 (1%)	12	30
1	B	466/504 (92%)	427 (92%)	36 (8%)	3 (1%)	25	50
1	C	480/504 (95%)	431 (90%)	39 (8%)	10 (2%)	7	18
1	D	469/504 (93%)	431 (92%)	35 (8%)	3 (1%)	25	50
All	All	1886/2016 (94%)	1716 (91%)	148 (8%)	22 (1%)	13	32

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	GLU
1	C	80	SER
1	C	339	GLN
1	C	343	ARG
1	D	80	SER

5.3.2 Protein sidechains

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	397/422 (94%)	373 (94%)	24 (6%)	19	42
1	B	392/422 (93%)	374 (95%)	18 (5%)	27	54
1	C	403/422 (96%)	370 (92%)	33 (8%)	11	26
1	D	395/422 (94%)	368 (93%)	27 (7%)	16	36
All	All	1587/1688 (94%)	1485 (94%)	102 (6%)	17	39

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

Mol	Chain	Res	Type
1	C	98	LEU
1	C	261	ARG
1	D	261	ARG
1	C	101	ASN
1	C	182	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	185	ASN
1	B	322	GLN
1	D	101	ASN
1	B	160	ASN
1	D	121	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
3	5GP	B	505	2	22,26,26	2.00	6 (27%)	27,40,40	2.59	10 (37%)
3	5GP	D	505	2	22,26,26	1.90	4 (18%)	27,40,40	2.66	11 (40%)
3	5GP	C	505	2	22,26,26	2.00	4 (18%)	27,40,40	2.50	9 (33%)
3	5GP	A	505	2	22,26,26	2.22	6 (27%)	27,40,40	2.65	9 (33%)
3	5GP	C	506	-	22,26,26	1.97	5 (22%)	27,40,40	3.29	12 (44%)
3	5GP	A	506	-	22,26,26	1.83	5 (22%)	27,40,40	2.93	10 (37%)
3	5GP	D	506	-	22,26,26	1.82	5 (22%)	27,40,40	2.91	7 (25%)
3	5GP	B	506	-	22,26,26	1.92	7 (31%)	27,40,40	3.17	9 (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
3	5GP	B	505	2	-	0/6/26/26	0/3/3/3
3	5GP	D	505	2	-	0/6/26/26	0/3/3/3
3	5GP	C	505	2	-	0/6/26/26	0/3/3/3
3	5GP	A	505	2	-	0/6/26/26	0/3/3/3
3	5GP	C	506	-	-	6/6/26/26	0/3/3/3
3	5GP	A	506	-	-	5/6/26/26	0/3/3/3
3	5GP	D	506	-	-	6/6/26/26	0/3/3/3
3	5GP	B	506	-	-	6/6/26/26	0/3/3/3

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	505	5GP	C6-N1	6.63	1.44	1.33
3	D	505	5GP	C6-N1	6.38	1.44	1.33
3	C	505	5GP	C6-N1	6.30	1.44	1.33
3	B	505	5GP	C6-N1	6.02	1.43	1.33
3	C	506	5GP	C6-N1	5.49	1.42	1.33

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	506	5GP	C5-C6-N1	-11.32	107.95	123.43
3	B	506	5GP	C5-C6-N1	-10.55	109.00	123.43
3	D	506	5GP	C5-C6-N1	-10.43	109.17	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	506	5GP	C5-C6-N1	-9.53	110.40	123.43
3	A	506	5GP	C2-N3-C4	-7.36	106.95	115.36

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	506	5GP	C5'-O5'-P-O1P
3	D	506	5GP	C5'-O5'-P-O2P
3	D	506	5GP	C5'-O5'-P-O3P
3	C	506	5GP	C5'-O5'-P-O1P
3	C	506	5GP	C5'-O5'-P-O2P

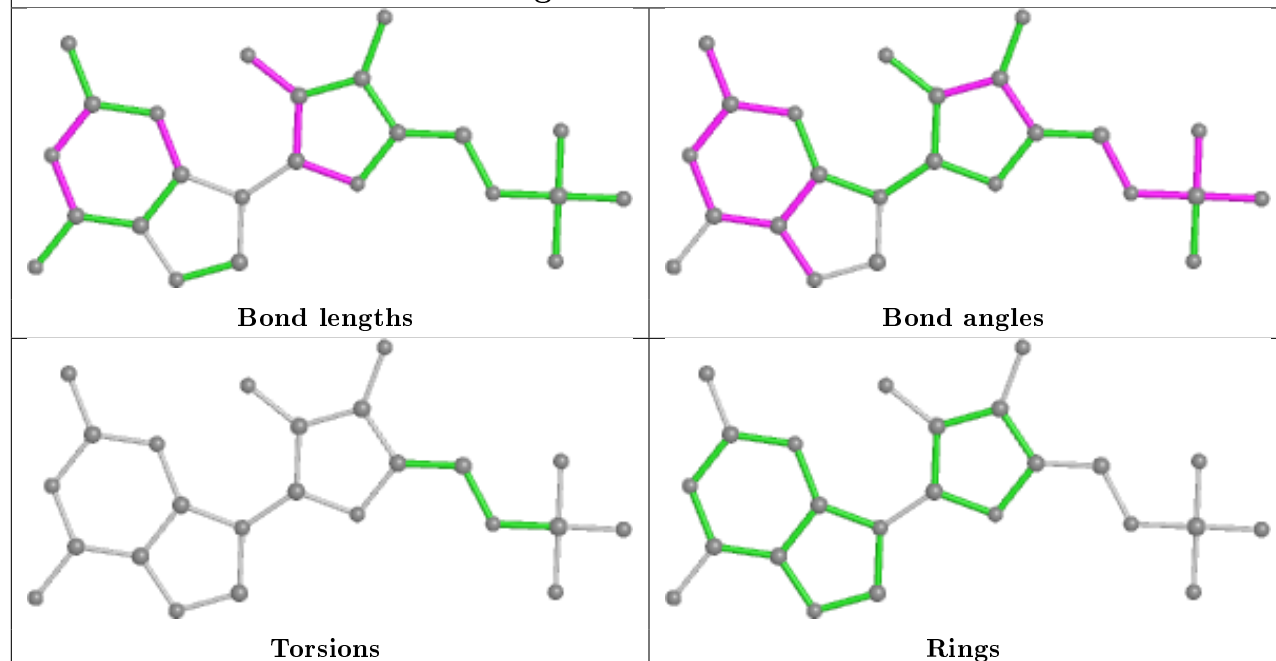
There are no ring outliers.

8 monomers are involved in 13 short contacts:

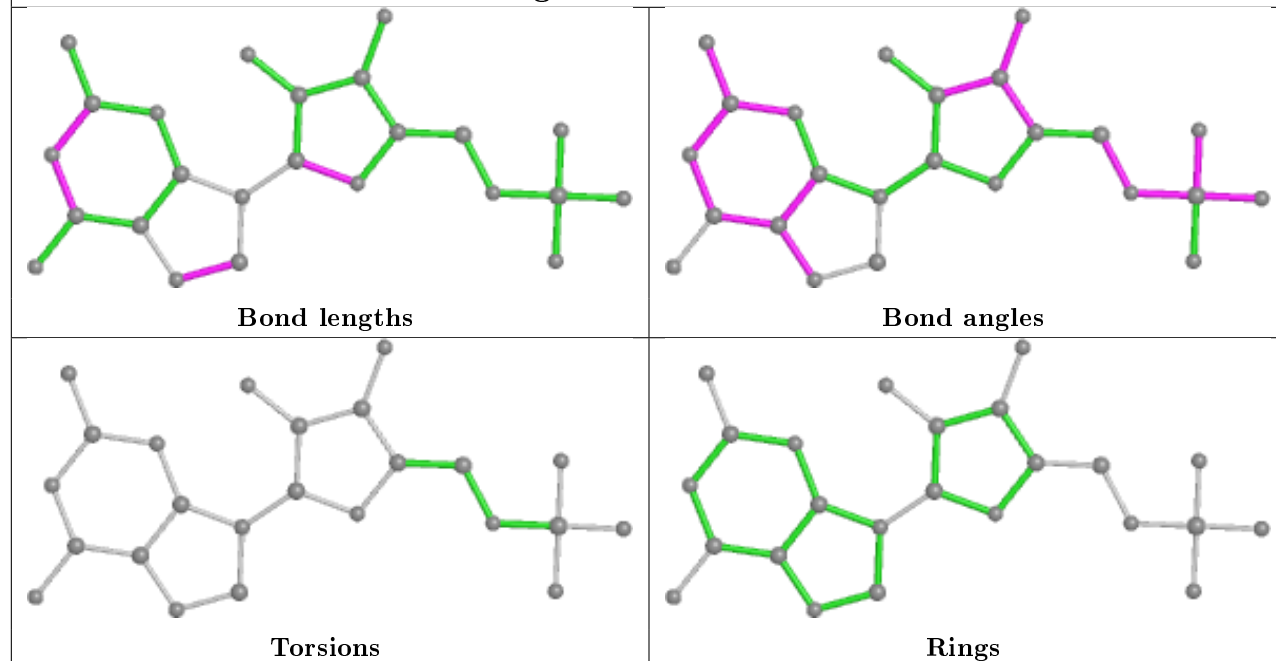
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	505	5GP	1	0
3	D	505	5GP	2	0
3	C	505	5GP	1	0
3	A	505	5GP	4	0
3	C	506	5GP	1	0
3	A	506	5GP	2	0
3	D	506	5GP	1	0
3	B	506	5GP	1	0

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.

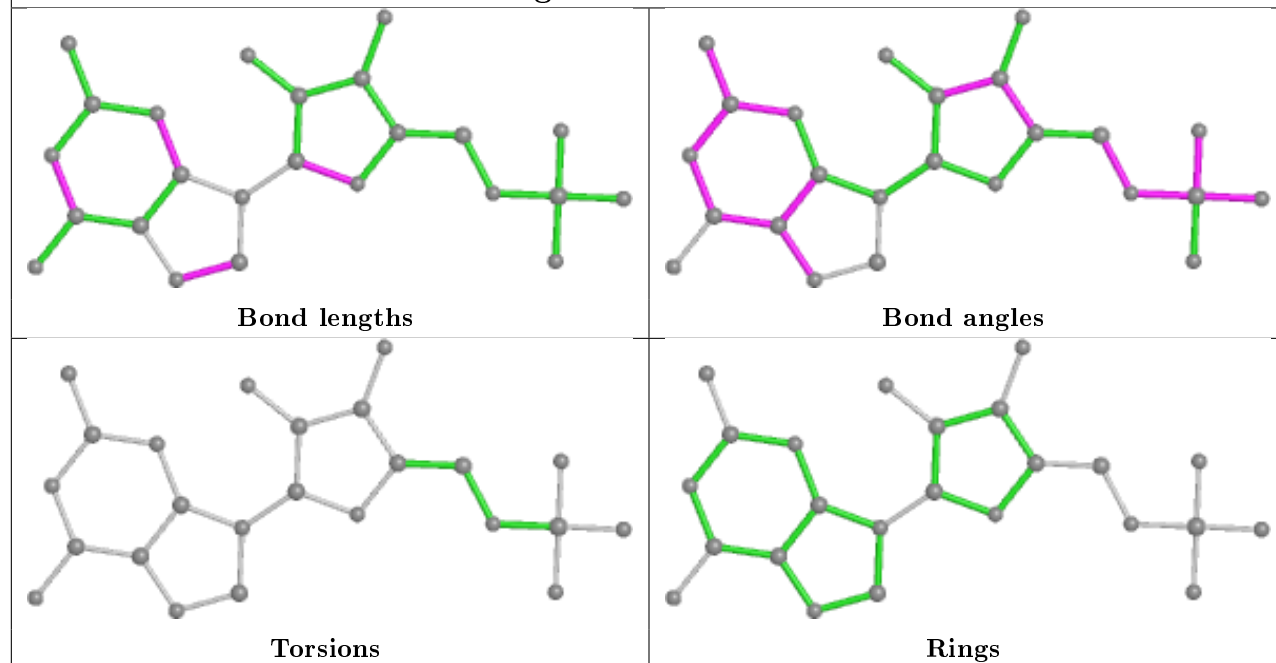
Ligand 5GP B 505



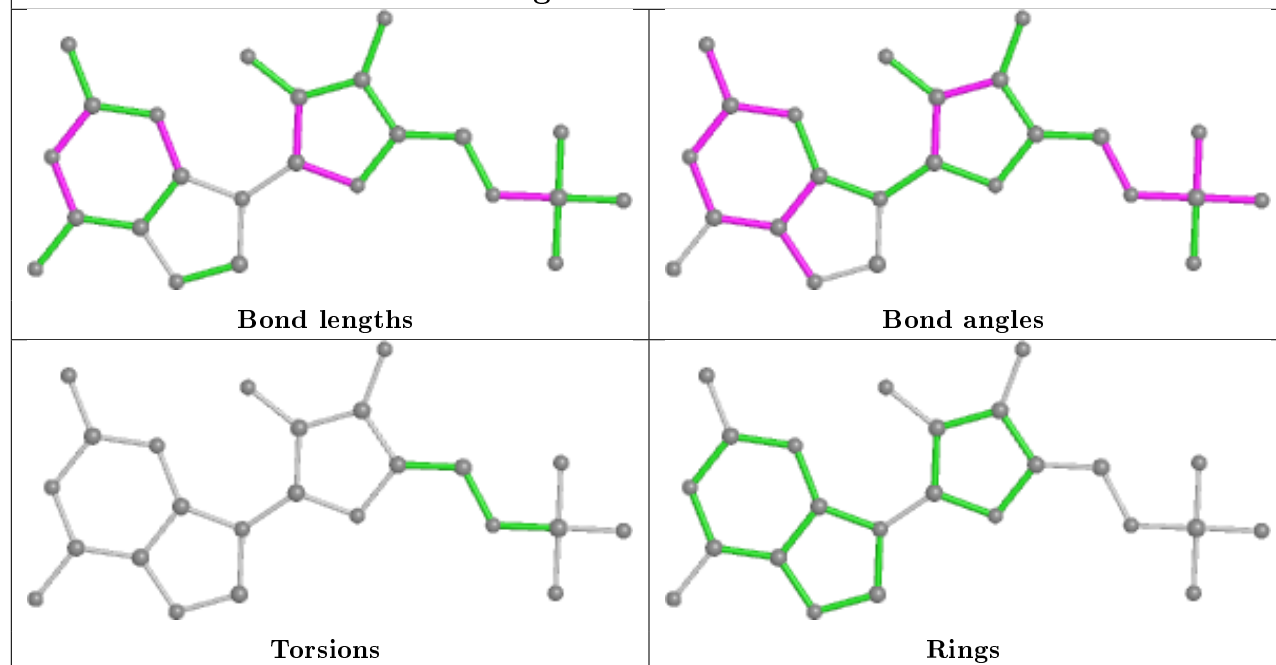
Ligand 5GP D 505



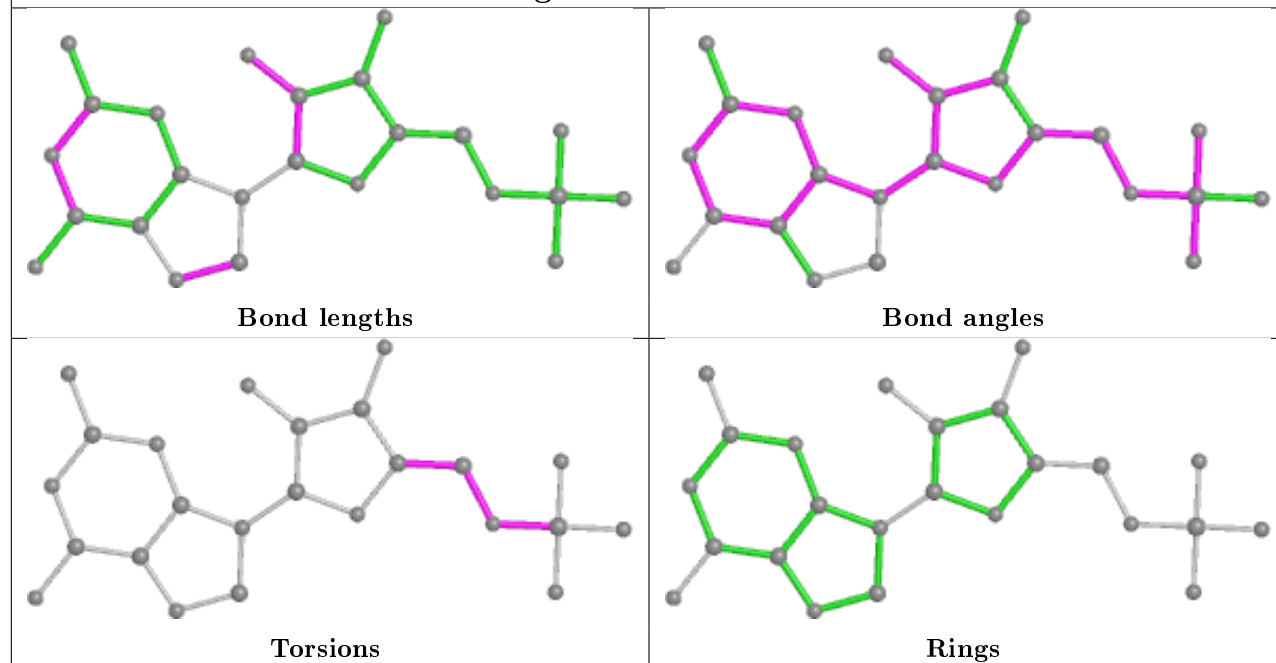
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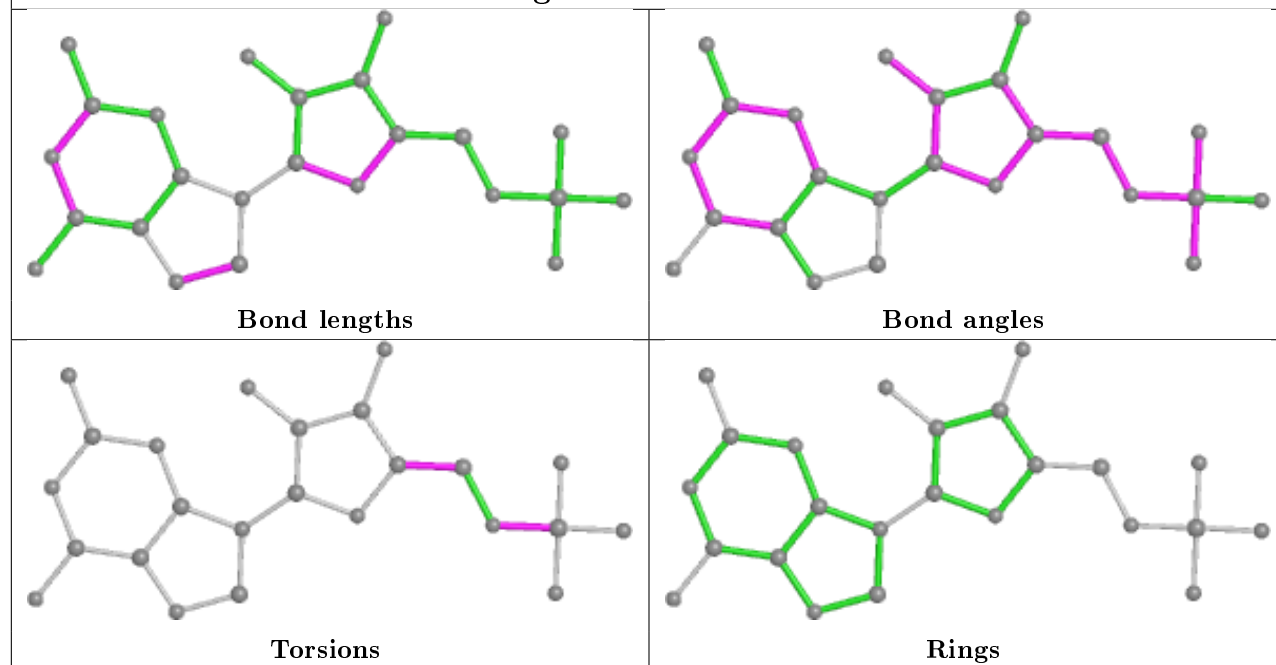
Ligand 5GP A 505

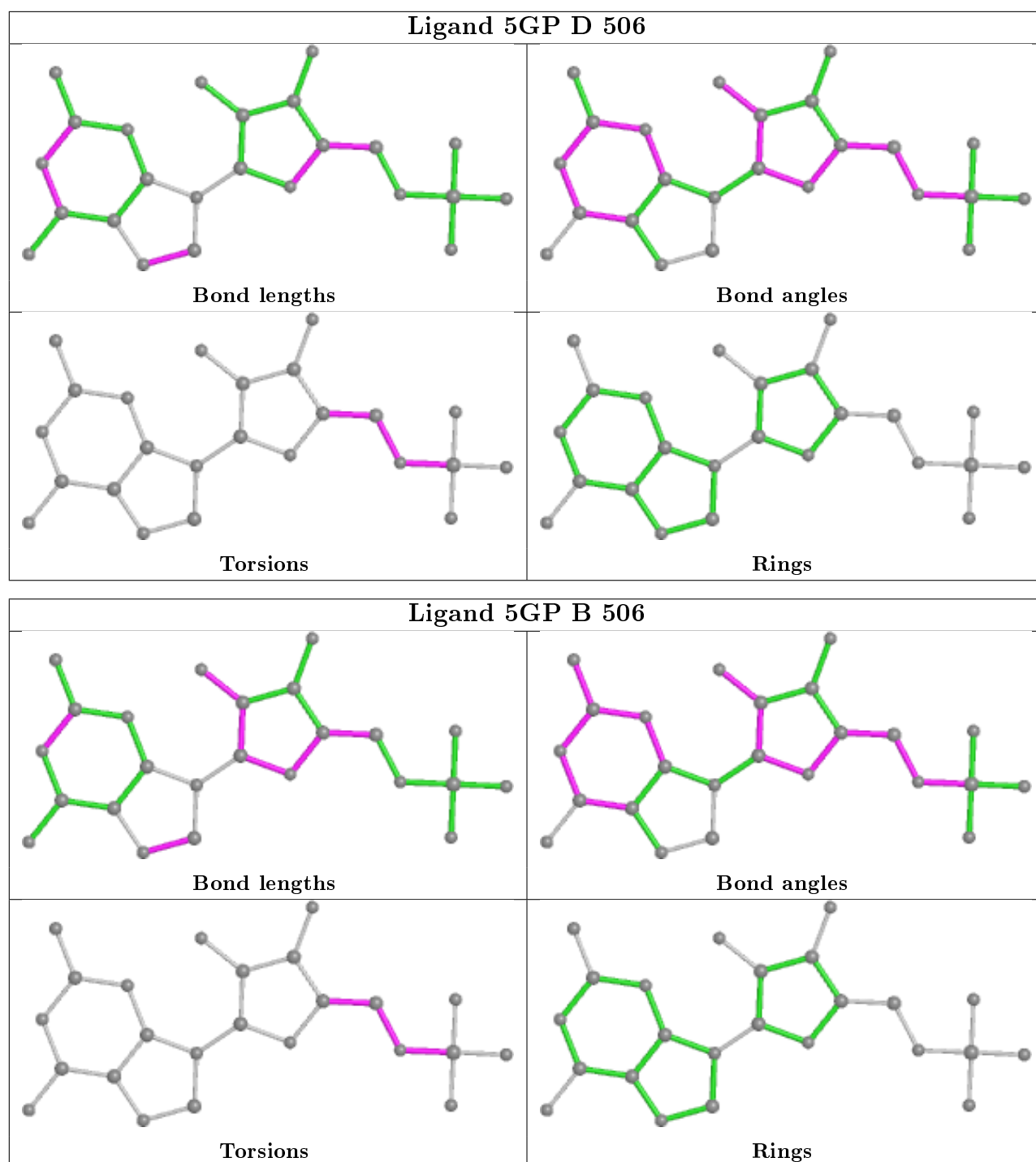


Ligand 5GP C 506



Ligand 5GP A 506





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.