



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2024 – 05:34 PM EDT

PDB ID : 1PYG
Title : STRUCTURAL BASIS FOR THE ACTIVATION OF GLYCOGEN PHOSPHORYLASE B BY ADENOSINE MONOPHOSPHATE
Authors : Sprang, S.
Deposited on : 1992-07-07
Resolution : 2.87 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)
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)	:	2.36.2

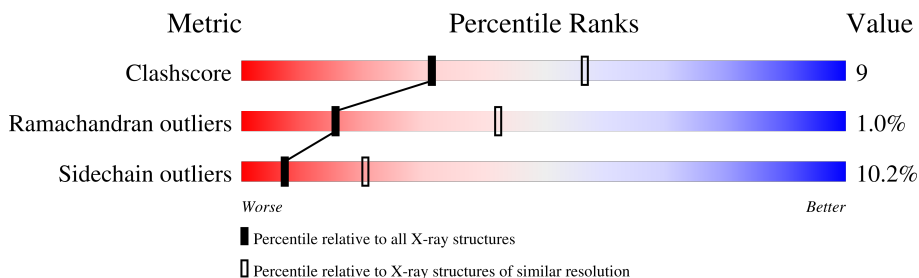
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)

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	842	
1	B	842	
1	C	842	
1	D	842	

2 Entry composition [i](#)

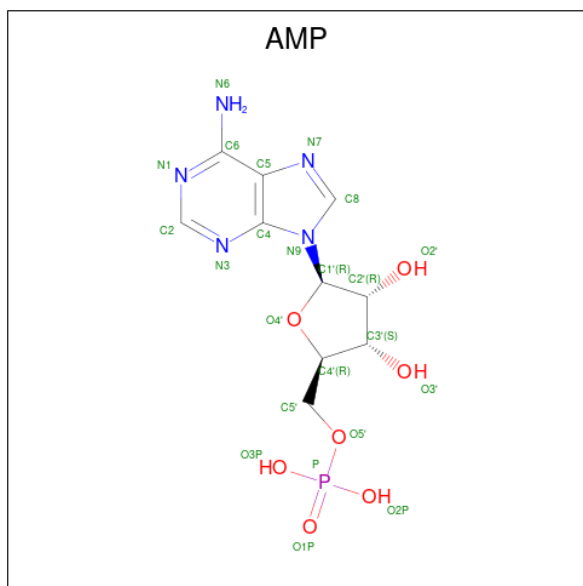
There are 3 unique types of molecules in this entry. The entry contains 26214 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLYCOGEN PHOSPHORYLASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	801	Total	C	N	O	S	0	0	0
			6512	4147	1155	1180	30			
1	B	791	Total	C	N	O	S	0	0	0
			6434	4099	1137	1168	30			
1	C	801	Total	C	N	O	S	0	0	0
			6512	4147	1155	1180	30			
1	D	801	Total	C	N	O	S	0	0	0
			6512	4147	1155	1180	30			

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



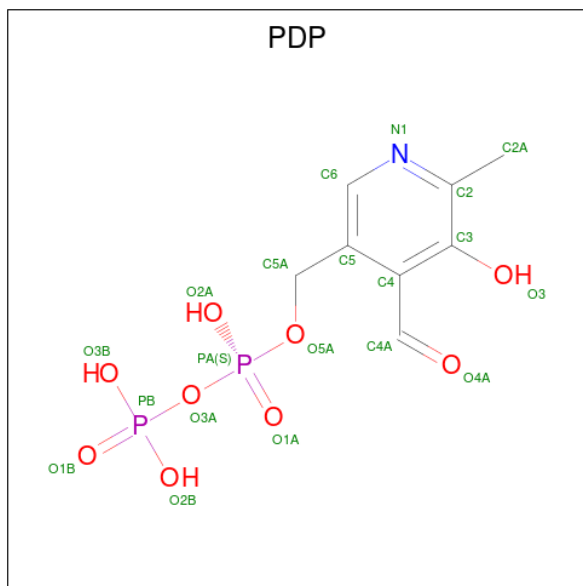
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is PYRIDOXAL-5'-DIPHOSPHATE (three-letter code: PDP) (formula: $C_8H_{11}NO_9P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			38	16	2	16	4		
3	B	1	Total	C	N	O	P	0	1
			38	16	2	16	4		
3	C	1	Total	C	N	O	P	0	1
			38	16	2	16	4		
3	D	1	Total	C	N	O	P	0	1
			38	16	2	16	4		

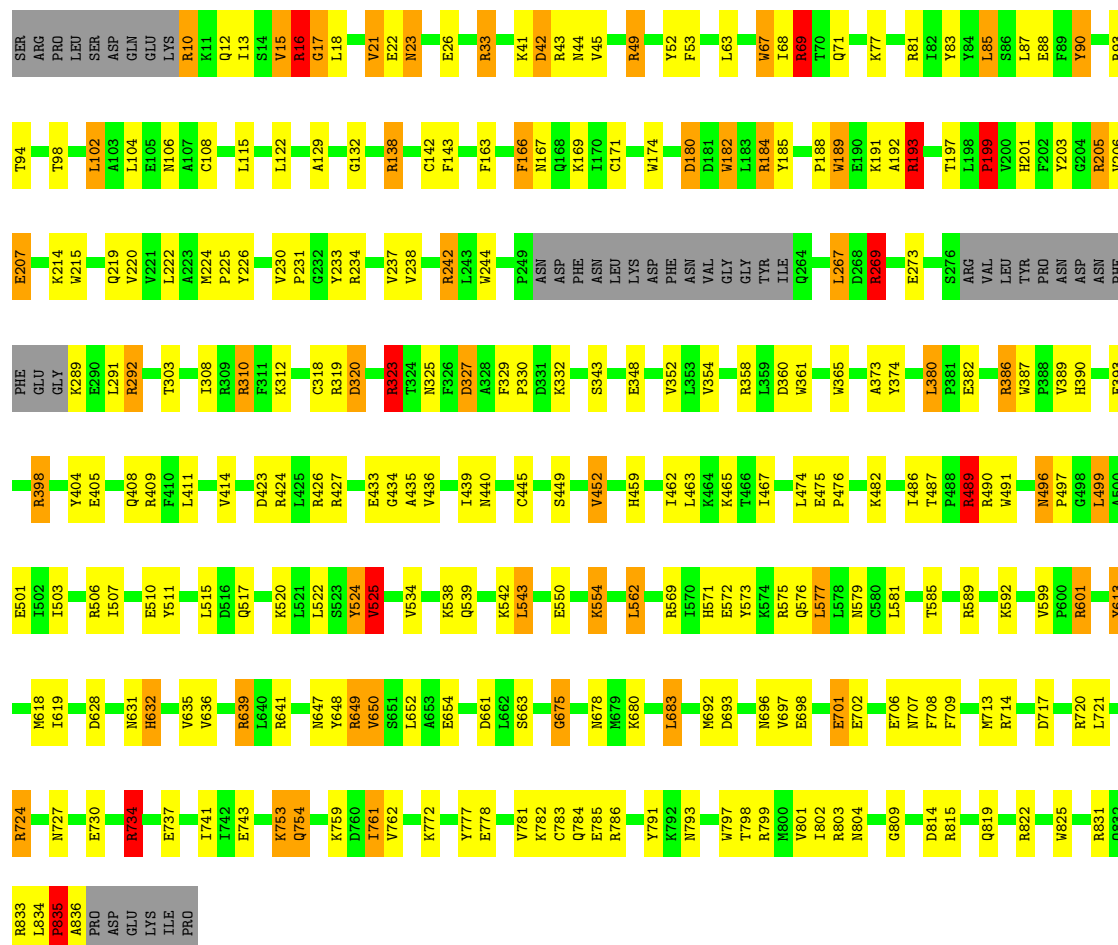


SER	R724	V603	R506	H390	ASN	P194	R893	ARG	PRO
	G725	M604	R506	L391	PHE	H201	L104	LEU	LEU
	Y726	G606	E510	L392	GLU	G205	A111	SER	ASP
	E730	Y613	Y511	R398	GLY	K214	T112	GLN	GLN
	Y731	Y613	L521	M407	K289	W215	Y113	LYS	LYS
	Y732	A616	L522	Q408	E290	D216	L115	R10	K11
	R734	K617	R292	R409	R292	V217	L122	V15	R16
	I735	M618	W525	F410	L293	D217	L122	V21	E22
	R736	I619	L411	L411	K294	V220	L122	K11	N23
	E737	L622	T531	M412	Q295	V220	L122	K11	V24
	R739	I623	R532	R413	R310	M224	I125	V15	E22
	F750	I623	Q539	V414	R310	P225	E127	R16	N23
	F750	V629	Q539	V414	R319	Y226	D128	V21	E22
	K753	V630	L543	V422	R319	Y226	D128	V21	N23
	K753	M631	L543	D423	R323	R234	L131	V21	N23
	D756	H632	A546	R424	R323	N235	G132	N23	V24
	D756	D633	A547	L425	K332	N236	G132	N23	V24
	K759	P634	Y548	R426	K332	V237	L136	K28	L27
	K759	V635	L549	R427	L337	R242	G137	K28	L27
	D760	V636	E550	R427	N338	L243	R138	K28	L27
I761	V636	R551	V436	D339	R242	R138	K28	L27	
M766	R639	E552	R437	S343	L243	R138	K28	L27	
M766	L640	Y553	R438	L344	P249	F143	N32	R33	
R770	R641	K554	A442	A345	ASN	F144	N32	R33	
R770	V642	V555	A442	A345	ASP	F144	N32	R33	
I643	V643	H556	C445	P347	PHE	M147	K41	D42	
E646	E646	L557	C445	E348	ASN	M147	K41	D42	
R775	M647	S561	L446	L349	ASN	Y155	R43	R43	
R776	Y648	L562	S449	L349	LEU	G156	R43	R43	
Y777	R649	R562	S449	L349	LYS	Y157	V45	V45	
E778	R649	R562	S449	L349	LYS	G158	V45	V45	
E779	L652	Q566	V455	L353	ASP	I159	P48	P48	
Y780	L652	V567	V456	L359	PHE	R160	P48	P48	
C783	S674	K568	R457	D560	ASN	R160	P48	P48	
C783	S674	R569	R457	V361	VAL	Y161	Y52	Y52	
Y791	G677	K574	L462	V365	GLY	F163	Y59	V59	
Y791	G677	R575	L463	V365	TYR	F163	V59	V59	
K792	K680	Q576	L464	V365	ILE	F166	R60	R60	
N793	K680	L577	L467	T368	ILE	F166	R60	R60	
R795	L683	L578	L467	T368	ILE	F166	R60	R60	
Y796	L683	L578	L467	T368	ILE	F166	R60	R60	
Y797	G690	N579	Y472	C372	V266	Q168	R66	R66	
Y797	G690	C580	E473	C372	V266	Q168	R66	R66	
Y798	G690	L581	L474	A373	D268	I170	R69	R69	
R799	E705	H582	L474	A373	D268	I170	R69	R69	
R799	E705	H582	L474	A373	D268	I170	R69	R69	
E706	E706	V583	L486	N376	R269	C171	K77	K77	
N707	E706	V583	L486	N376	R269	C171	K77	K77	
R803	N707	V583	L486	N376	R269	C171	K77	K77	
R803	N707	V583	L486	N376	R269	C171	K77	K77	
A806	F708	L586	L487	H377	N270	W174	D78	D78	
A806	F709	L586	L487	H377	N270	W174	D78	D78	
I710	I710	R589	R490	V379	L271	Q175	R81	R81	
I710	I710	R589	R490	V379	L271	Q175	R81	R81	
R714	R714	P594	W491	E382	N274	M176	R81	R81	
R815	R714								



• Molecule 1: GLYCOGEN PHOSPHORYLASE B

Chain D: 63% 25% 6% • 5%



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 2	Depositor
Cell constants a, b, c, α , β , γ	169.90Å 209.90Å 123.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.87	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.87)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26214	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: AMP, PDP

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	0.85	0/6655	1.66	128/9001 (1.4%)
1	B	0.86	0/6577	1.63	129/8898 (1.4%)
1	C	0.82	0/6655	1.63	124/9001 (1.4%)
1	D	0.86	0/6655	1.65	132/9001 (1.5%)
All	All	0.85	0/26542	1.64	513/35901 (1.4%)

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	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

The worst 5 of 513 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	310	ARG	NE-CZ-NH2	-14.56	113.02	120.30
1	D	601	ARG	NE-CZ-NH1	14.01	127.31	120.30
1	A	639	ARG	NE-CZ-NH2	-12.78	113.91	120.30
1	B	489	ARG	NE-CZ-NH1	12.58	126.59	120.30
1	D	138	ARG	NE-CZ-NH2	-12.42	114.09	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	297	TYR	Sidechain
1	A	52	TYR	Sidechain
1	B	52	TYR	Sidechain
1	B	834	LEU	Peptide
1	C	52	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	6512	0	6484	115	0
1	B	6434	0	6393	121	0
1	C	6512	0	6484	131	0
1	D	6512	0	6484	113	0
2	A	23	0	12	0	0
2	B	23	0	12	1	0
2	C	23	0	12	0	0
2	D	23	0	12	0	0
3	A	38	0	14	0	0
3	B	38	0	14	1	0
3	C	38	0	13	0	0
3	D	38	0	14	0	0
All	All	26214	0	25948	468	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 9.

The worst 5 of 468 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:193:ARG:HB2	1:D:225:PRO:HG2	1.63	0.81
1:C:225:PRO:HB2	1:C:242:ARG:HD2	1.61	0.79
1:C:549:LEU:HD12	1:C:557:ILE:HD13	1.65	0.79
1:B:325:ASN:HD21	1:B:327:ASP:HB2	1.52	0.75
1:C:88:GLU:HB2	1:C:132:GLY:HA2	1.68	0.75

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	795/842 (94%)	733 (92%)	51 (6%)	11 (1%)	11	34
1	B	785/842 (93%)	725 (92%)	52 (7%)	8 (1%)	15	42
1	C	795/842 (94%)	727 (91%)	61 (8%)	7 (1%)	17	45
1	D	795/842 (94%)	746 (94%)	42 (5%)	7 (1%)	17	45
All	All	3170/3368 (94%)	2931 (92%)	206 (6%)	33 (1%)	15	42

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	166	PHE
1	A	322	VAL
1	B	166	PHE
1	B	321	PRO

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	693/731 (95%)	631 (91%)	62 (9%)	9	27
1	B	685/731 (94%)	614 (90%)	71 (10%)	7	19
1	C	693/731 (95%)	614 (89%)	79 (11%)	5	16
1	D	693/731 (95%)	622 (90%)	71 (10%)	7	20
All	All	2764/2924 (94%)	2481 (90%)	283 (10%)	7	20

5 of 283 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	205	ARG
1	D	292	ARG
1	D	562	LEU
1	B	489	ARG
1	B	452	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	632	HIS
1	D	541	ASN
1	C	744	GLN
1	D	274	ASN
1	D	579	ASN

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](#)

12 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	AMP	A	843	-	22,25,25	0.99	1 (4%)	25,38,38	1.05	1 (4%)
3	PDP	C	860[B]	1	17,19,20	2.48	5 (29%)	24,29,30	1.69	7 (29%)
3	PDP	A	860[A]	1	17,19,20	2.10	5 (29%)	24,29,30	1.82	5 (20%)
2	AMP	B	843	-	22,25,25	1.13	1 (4%)	25,38,38	1.07	1 (4%)
2	AMP	D	843	-	22,25,25	1.12	2 (9%)	25,38,38	1.54	3 (12%)
3	PDP	D	860[A]	1	17,19,20	2.33	5 (29%)	24,29,30	1.88	8 (33%)
3	PDP	B	860[A]	1	17,19,20	2.29	5 (29%)	24,29,30	1.66	6 (25%)
3	PDP	C	860[A]	1	17,19,20	2.63	6 (35%)	24,29,30	1.74	6 (25%)
2	AMP	C	843	-	22,25,25	1.22	2 (9%)	25,38,38	1.39	2 (8%)
3	PDP	A	860[B]	1	17,19,20	2.42	6 (35%)	24,29,30	1.80	8 (33%)
3	PDP	D	860[B]	1	17,19,20	2.32	5 (29%)	24,29,30	1.96	7 (29%)
3	PDP	B	860[B]	1	17,19,20	2.19	5 (29%)	24,29,30	2.53	7 (29%)

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	AMP	A	843	-	-	2/6/26/26	0/3/3/3
3	PDP	C	860[B]	1	-	4/12/12/14	0/1/1/1
3	PDP	A	860[A]	1	-	2/12/12/14	0/1/1/1
2	AMP	B	843	-	-	0/6/26/26	0/3/3/3
2	AMP	D	843	-	-	1/6/26/26	0/3/3/3
3	PDP	D	860[A]	1	-	1/12/12/14	0/1/1/1
3	PDP	B	860[A]	1	-	4/12/12/14	0/1/1/1
3	PDP	C	860[A]	1	-	1/12/12/14	0/1/1/1
2	AMP	C	843	-	-	0/6/26/26	0/3/3/3
3	PDP	A	860[B]	1	-	2/12/12/14	0/1/1/1
3	PDP	D	860[B]	1	-	3/12/12/14	0/1/1/1
3	PDP	B	860[B]	1	-	1/12/12/14	0/1/1/1

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	860[B]	PDP	C4A-C4	-6.64	1.37	1.51
3	D	860[B]	PDP	C4A-C4	-6.05	1.39	1.51
3	D	860[A]	PDP	C4A-C4	-6.04	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	860[A]	PDP	C4A-C4	-5.96	1.39	1.51
3	C	860[A]	PDP	C4A-C4	-5.88	1.39	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	860[B]	PDP	O5A-C5A-C5	7.51	123.67	109.35
3	B	860[B]	PDP	PA-O3A-PB	-5.36	114.44	132.83
3	C	860[A]	PDP	PA-O3A-PB	-4.45	117.56	132.83
3	A	860[A]	PDP	PA-O3A-PB	-4.35	117.88	132.83
3	D	860[B]	PDP	PA-O3A-PB	-4.34	117.93	132.83

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

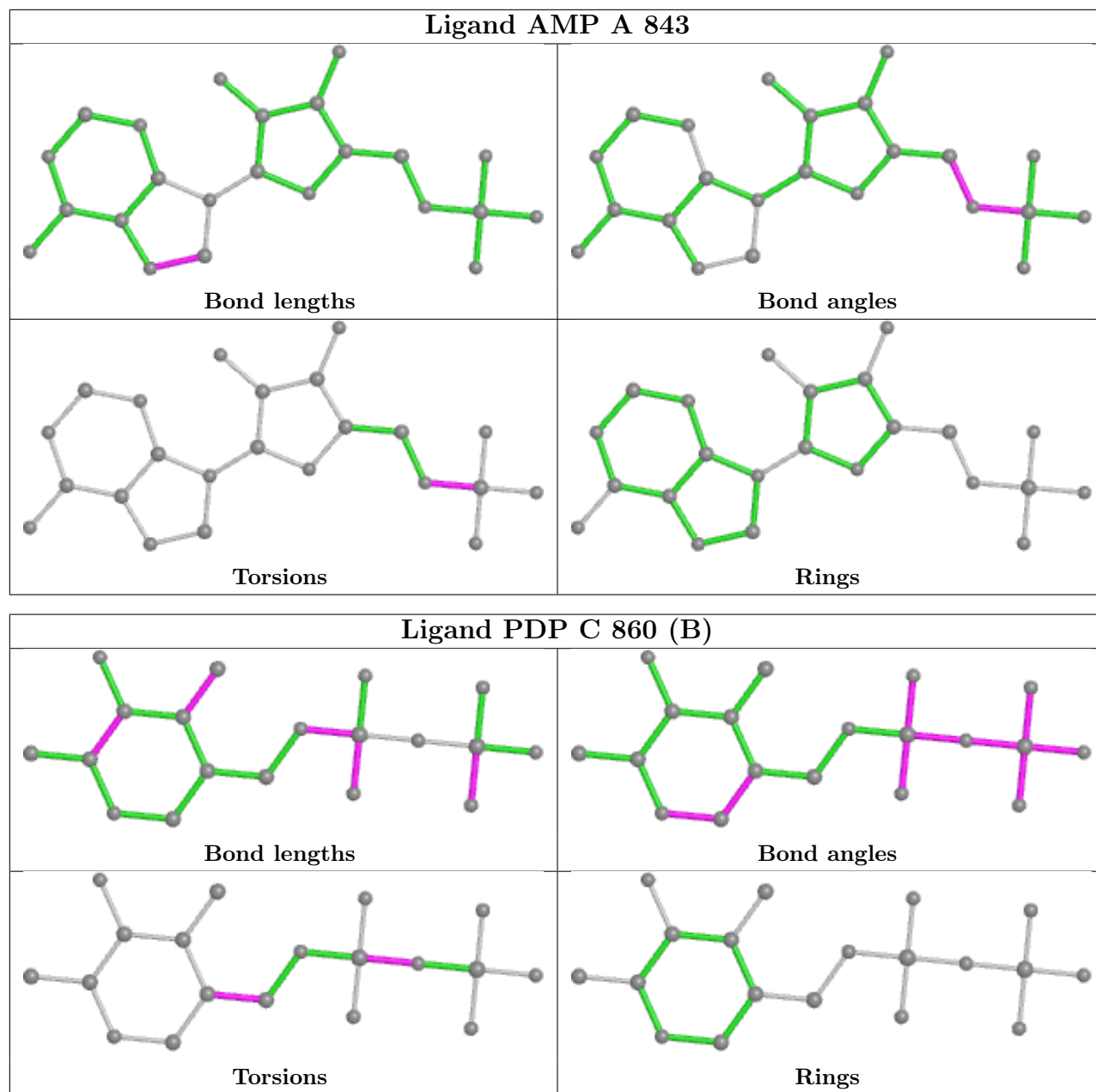
Mol	Chain	Res	Type	Atoms
2	A	843	AMP	C5'-O5'-P-O2P
2	A	843	AMP	C5'-O5'-P-O3P
3	B	860[A]	PDP	C5A-O5A-PA-O1A
3	B	860[A]	PDP	C5A-O5A-PA-O3A
3	D	860[A]	PDP	C5A-O5A-PA-O1A

There are no ring outliers.

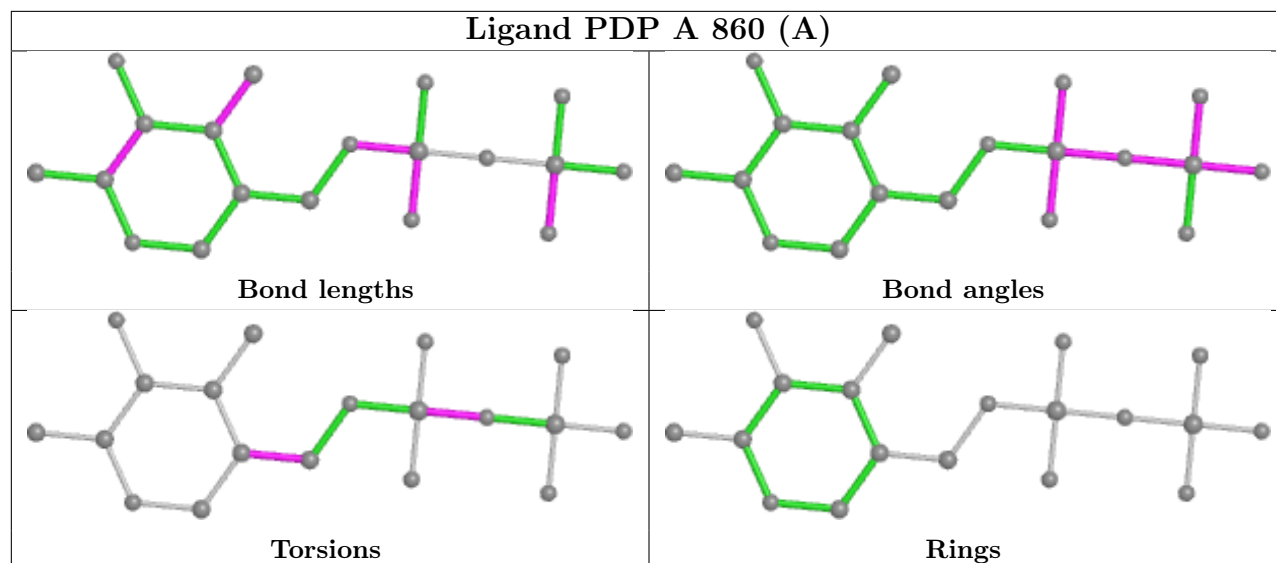
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	843	AMP	1	0
3	B	860[B]	PDP	1	0

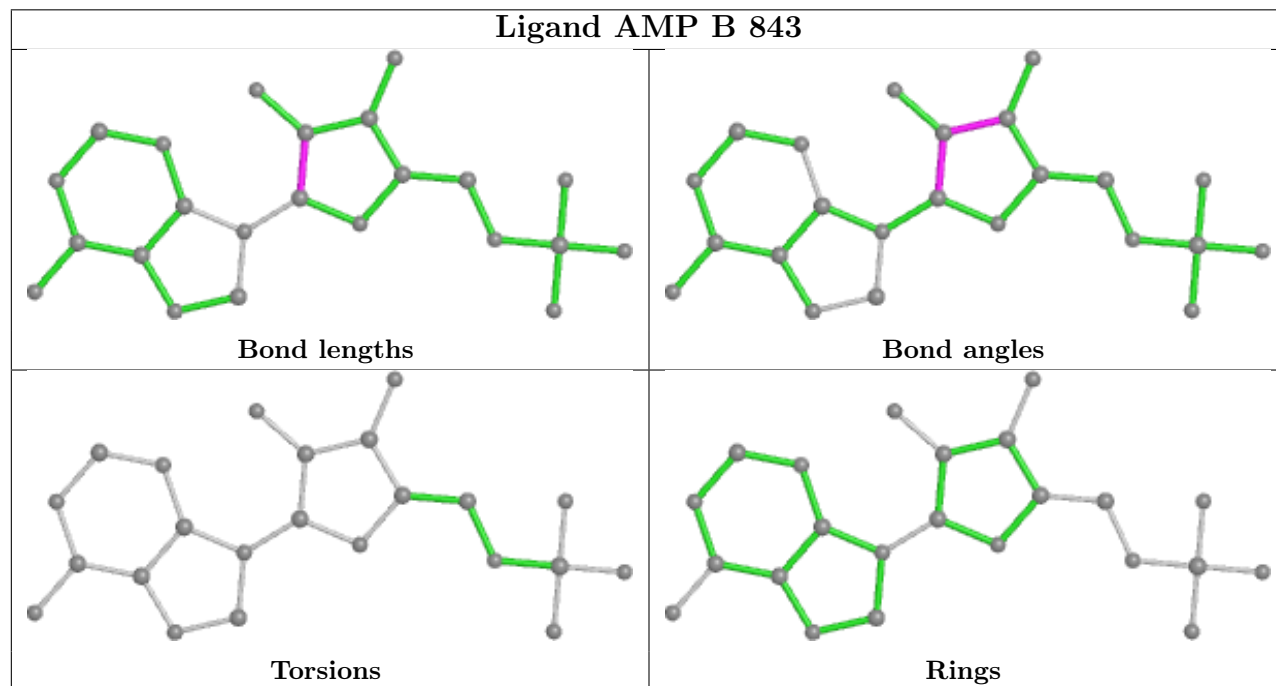
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



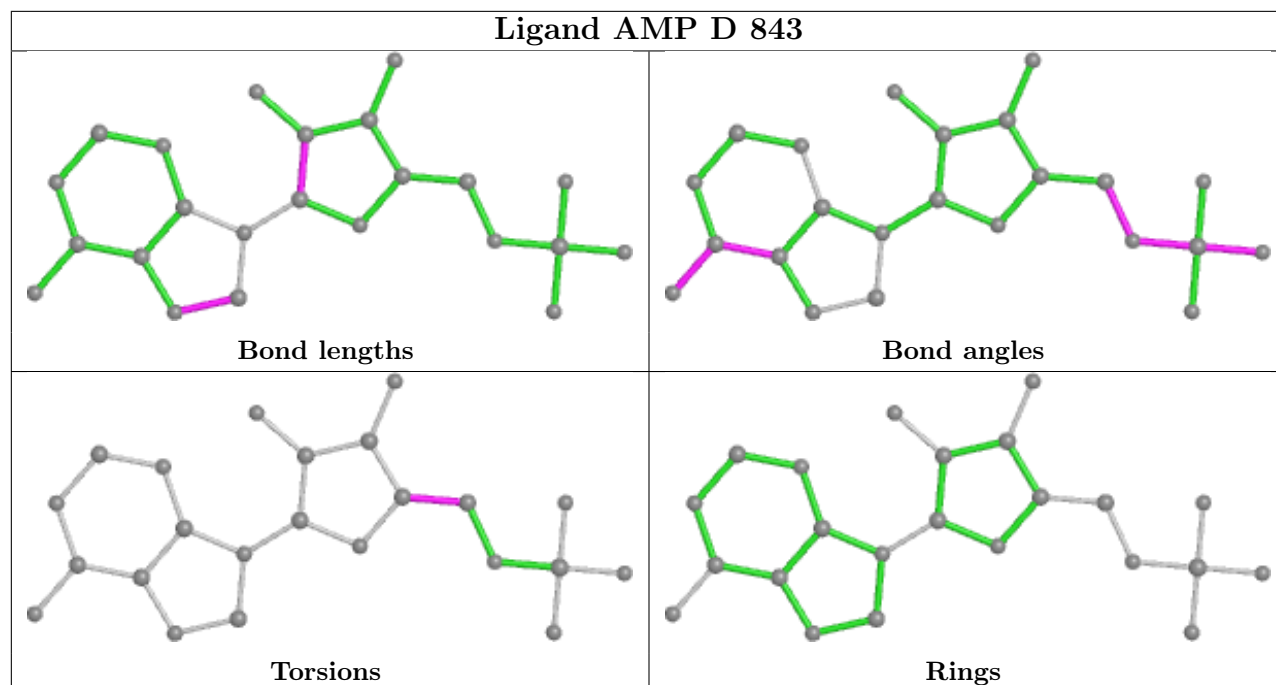
Ligand PDP A 860 (A)



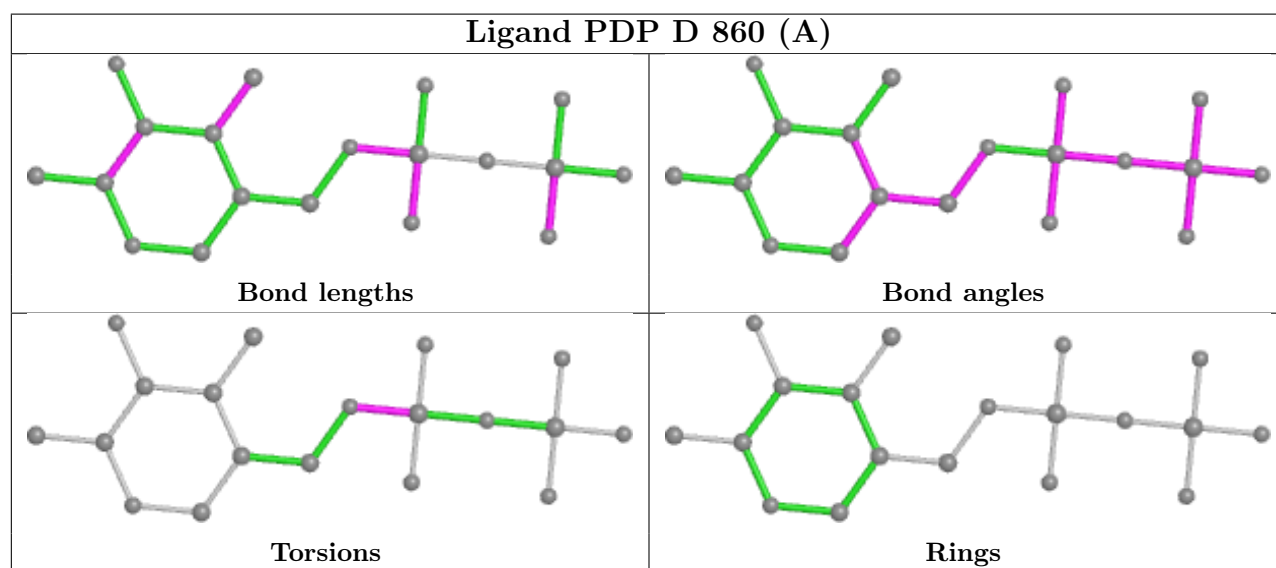
Ligand AMP B 843



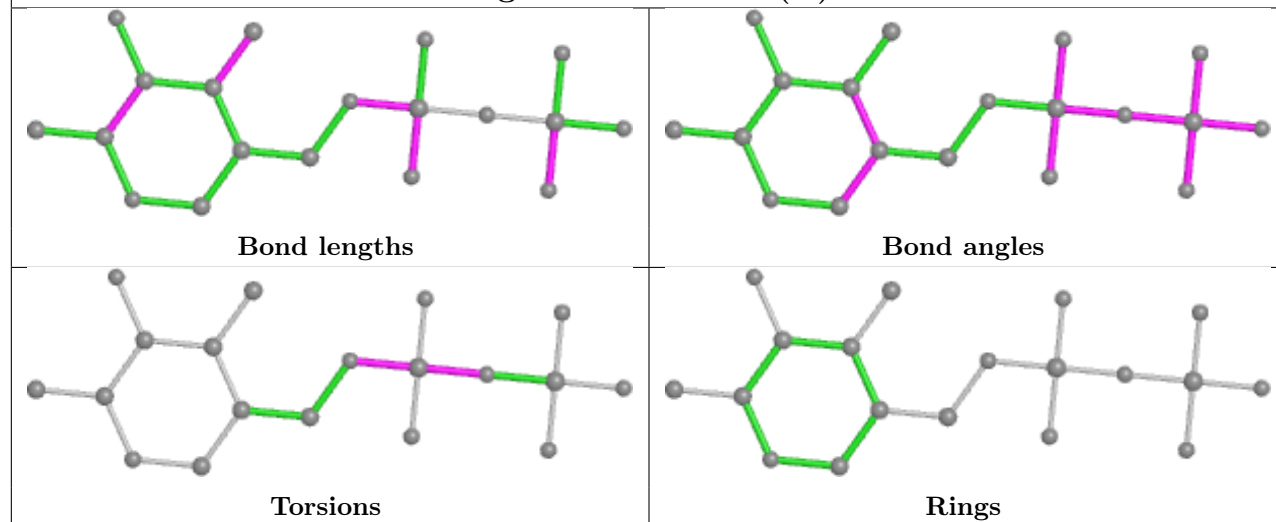
Ligand AMP D 843



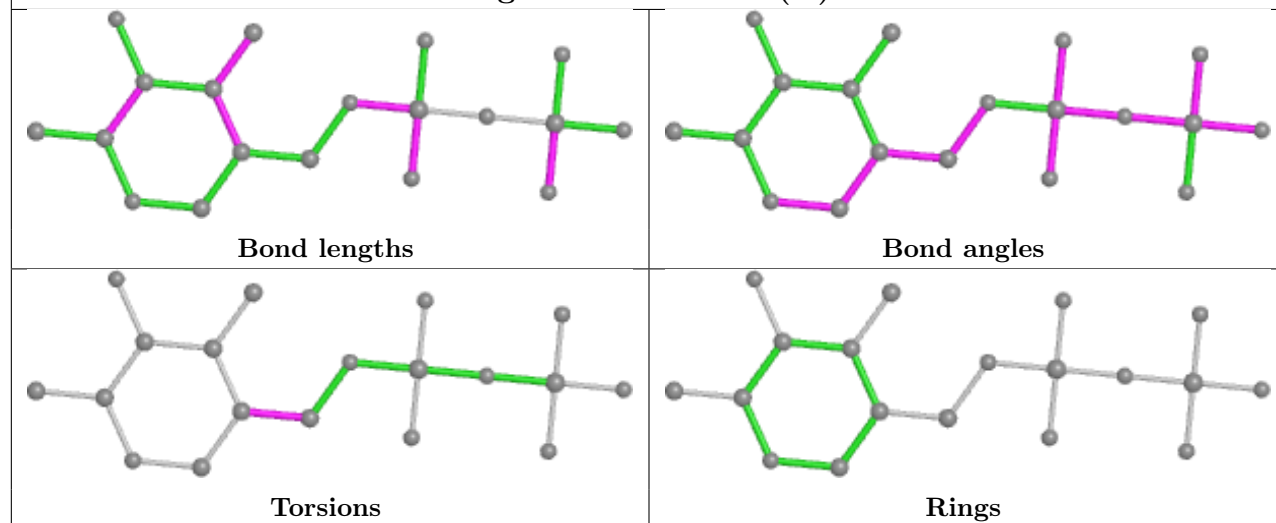
Ligand PDP D 860 (A)

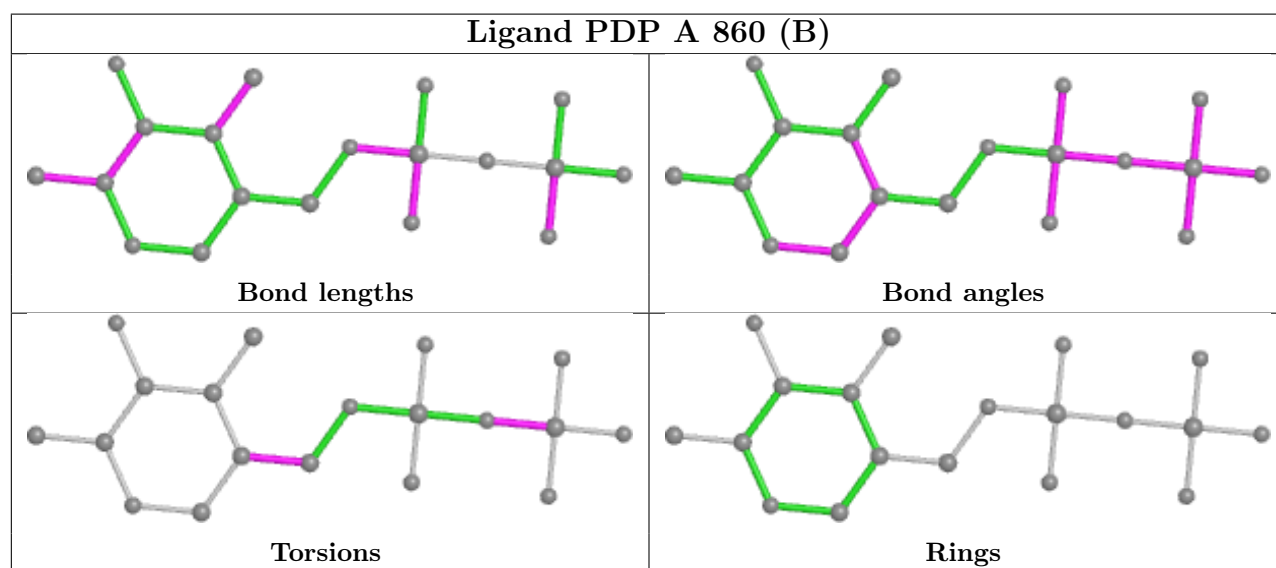
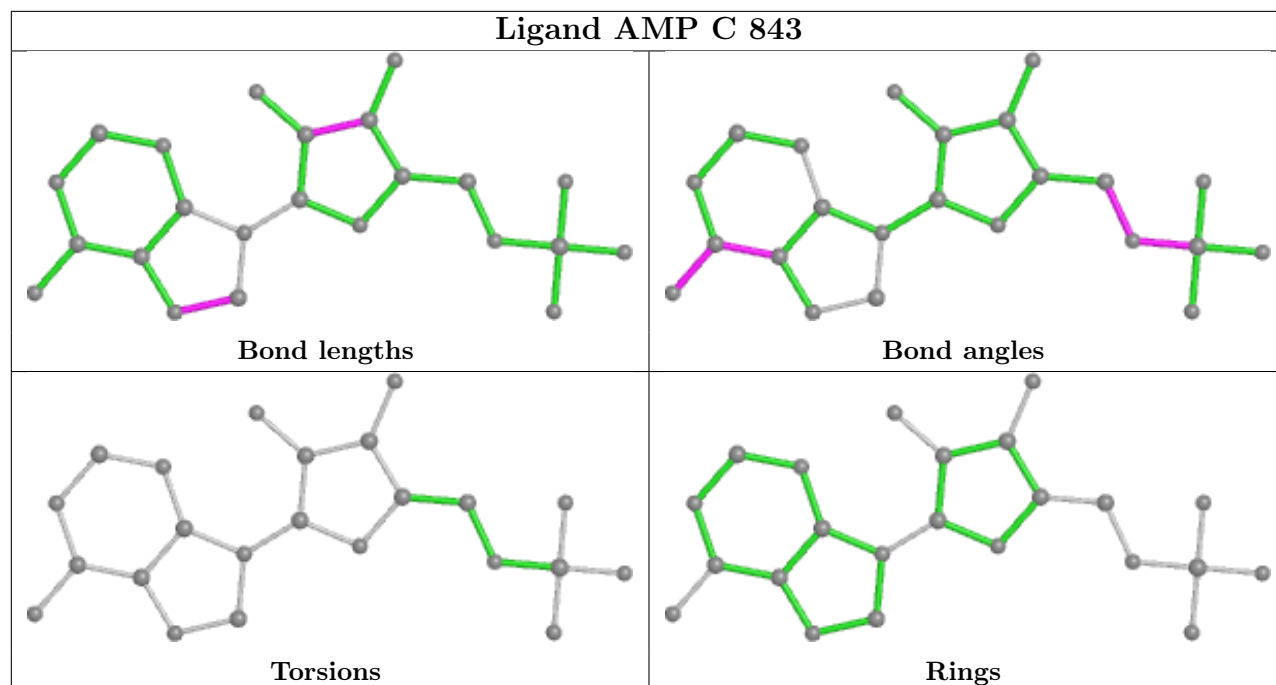


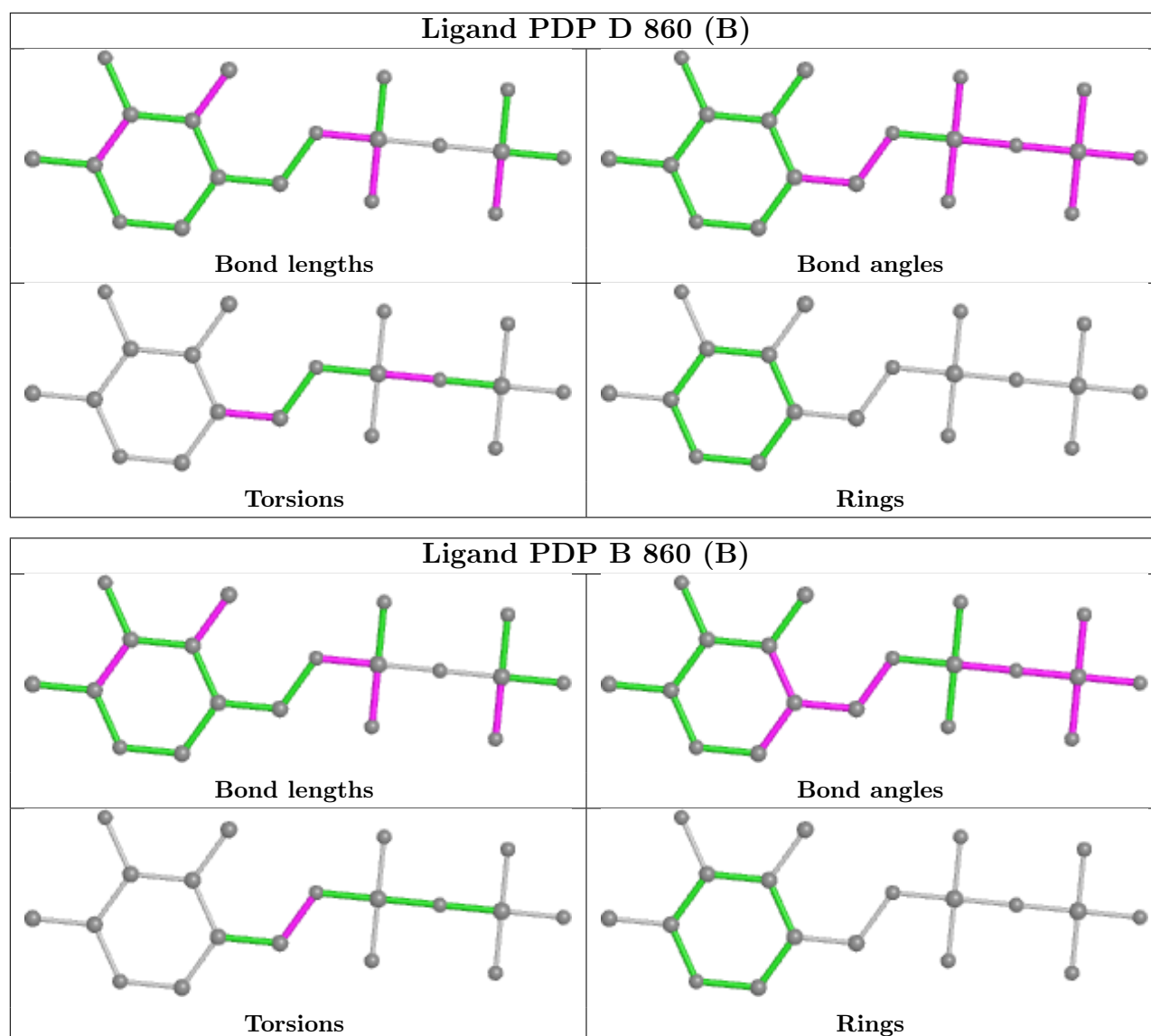
Ligand PDP B 860 (A)



Ligand PDP C 860 (A)







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.