



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 10:20 AM UTC

PDB ID : 1L8A / pdb_00001l8a
Title : E. COLI PYRUVATE DEHYDROGENASE
Authors : Furey, W.; Arjunan, P.
Deposited on : 2002-03-19
Resolution : 1.85 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

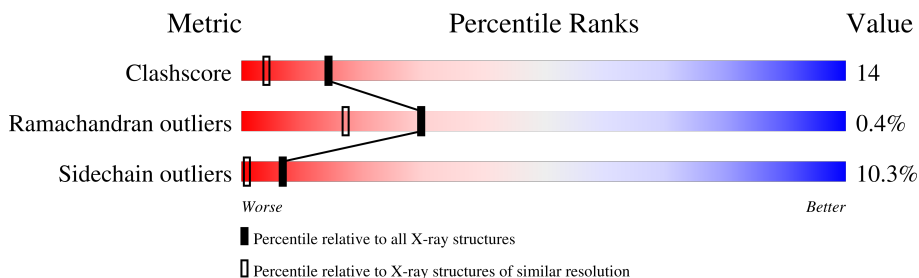
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)

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	886	
1	B	886	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13418 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.

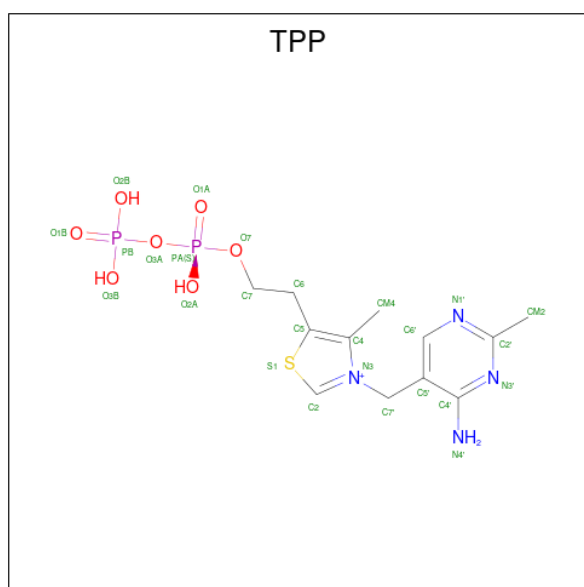
- Molecule 1 is a protein called Pyruvate dehydrogenase E1 component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	801	Total	C	N	O	S	0	0	0
			6341	4018	1093	1204	26			
1	B	801	Total	C	N	O	S	0	0	0
			6341	4018	1093	1204	26			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 4 is water.

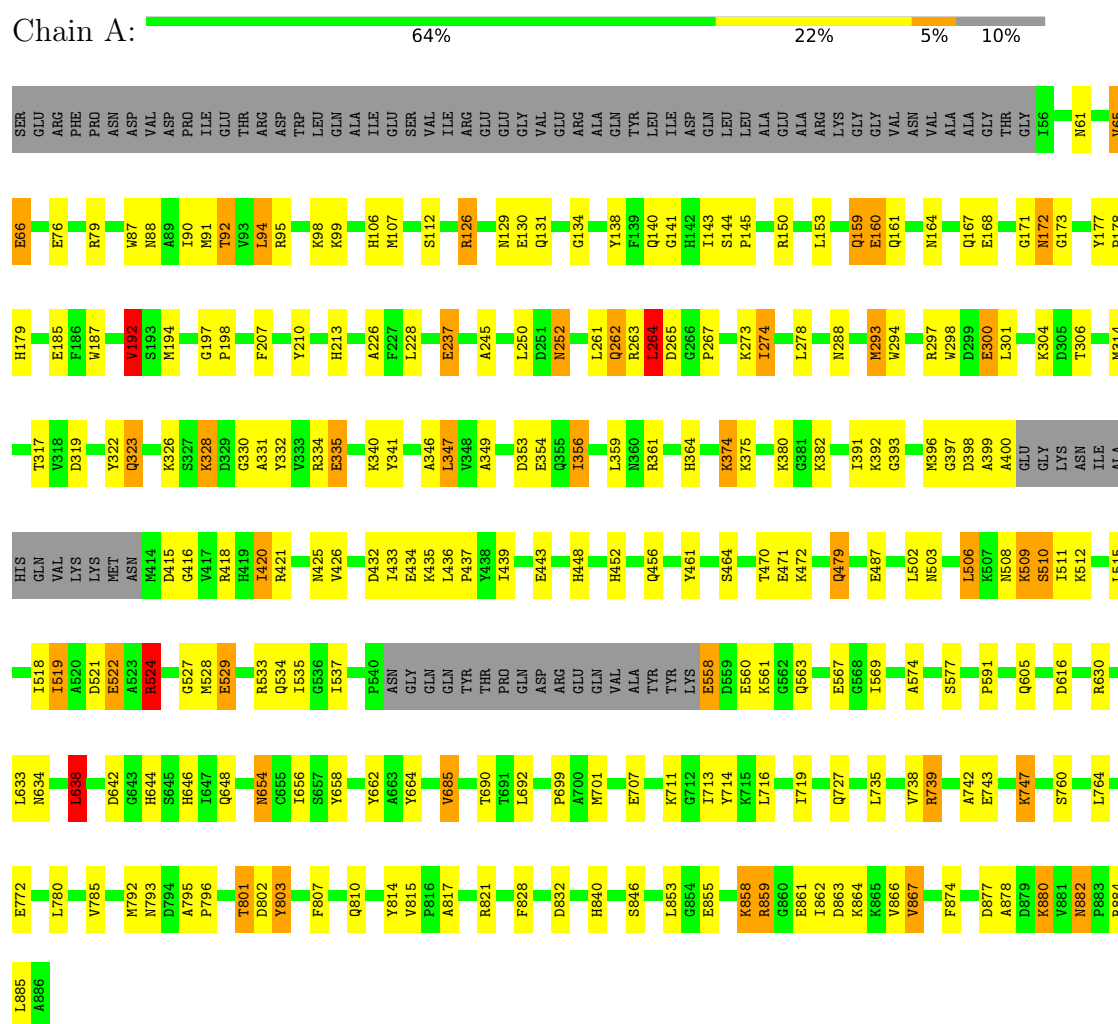
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	330	Total	O	0	0
			330	330		
4	B	352	Total	O	0	0
			352	352		

3 Residue-property plots

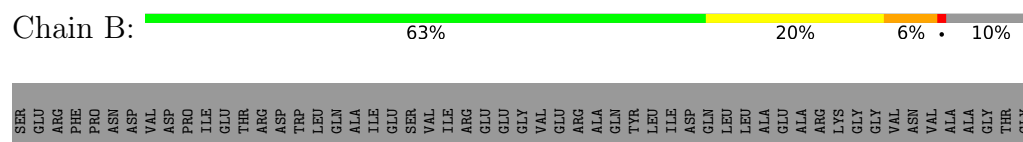
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Pyruvate dehydrogenase E1 component



• Molecule 1: Pyruvate dehydrogenase E1 component



L764	G635	D415	K326	V65	E66
D770	E636	G416	S327	H213	E67
M776	G637	V417	K328	K221	Q68
L777	L638	R418			P69
H778	Q639	H419	Y332	D234	E70
P779	A523	I420	V333		
L780	R524	R421	R334		
E781	E529	D422		E237	N74
M792	D642	R423	Y341	L244	E76
N793	G643	F424	P342	A245	L77
S800	S645	N425	E343	T246	E78
Y803	H646	V426	T344	R247	R79
M804	N654	P427	T352		R80
R812	Y658	S429	Q355	L250	
D818	Y662	D430	N252	D251	W87
D819	A663	A431			I90
Y820	Y664	D432	N360	N260	M91
R821	R676	I433	R361	L261	
D828		E434	G362	Q262	L94
		K435	G363	R263	R95
		L436	H364	L264	
		P437		D265	
		Y438	K368	G266	K98
		I439	G374	P267	K99
		T440	K375		H106
		F441	A376	I274	
		P442	Q377		S112
				L278	H123
				E279	F124
				E283	
					Q140
				G286	T143
				W287	
				N288	L153
				V289	
				G393	Q159
				Y394	
				G395	Q167
				M396	E168
				G397	V169
				D398	H170
				A399	G171
				A400	N172
				GLU	G173
				LYS	
				GLY	
				R303	
				K304	
				ASN	
				ILE	
				K309	
				ALA	
				HIS	
				N315	
				GLN	
				VAL	
				LVS	
				G320	
				LVS	
				LVS	
				MET	
				T324	
				F198	
				T325	
				M414	
				</	

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.69Å 141.60Å 82.46Å 90.00° 102.40° 90.00°	Depositor
Resolution (Å)	8.00 – 1.85	Depositor
% Data completeness (in resolution range)	85.4 (8.00-1.85)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.189 , 0.236	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13418	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: TPP, MG

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	0.42	0/6484	0.94	18/8766 (0.2%)
1	B	0.44	1/6484 (0.0%)	0.99	28/8766 (0.3%)
All	All	0.43	1/12968 (0.0%)	0.96	46/17532 (0.3%)

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	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	264	LEU	N-CA	7.09	1.55	1.46

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	394	TYR	O-C-N	-16.68	100.41	122.59
1	A	634	ASN	N-CA-C	10.63	124.19	111.33
1	B	264	LEU	N-CA-C	9.90	131.89	110.80
1	B	634	ASN	N-CA-C	9.32	122.61	111.33
1	B	633	LEU	N-CA-C	-9.09	99.20	110.65

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	803	TYR	Sidechain
1	B	803	TYR	Sidechain

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	6341	0	6179	181	0
1	B	6341	0	6179	186	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	26	0	16	3	0
3	B	26	0	16	3	0
4	A	330	0	0	11	0
4	B	352	0	0	9	0
All	All	13418	0	12390	354	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 354 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:A:801:THR:HG22	1:A:803:TYR:H	1.13	1.08
1:A:61:ASN:HD21	1:A:294:TRP:H	1.06	0.92
1:A:364:HIS:HE1	1:A:391:ILE:H	1.16	0.88
1:B:620:ARG:HH12	1:B:682:GLN:HE21	1.18	0.88
1:B:644:HIS:HB3	1:B:804:MET:HE3	1.55	0.85

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	795/886 (90%)	756 (95%)	38 (5%)	1 (0%)	48	35
1	B	795/886 (90%)	754 (95%)	36 (4%)	5 (1%)	21	10
All	All	1590/1772 (90%)	1510 (95%)	74 (5%)	6 (0%)	30	17

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	172	ASN
1	B	397	GLY
1	A	397	GLY
1	B	394	TYR
1	B	521	ASP

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	665/735 (90%)	600 (90%)	65 (10%)	7	1
1	B	665/735 (90%)	593 (89%)	72 (11%)	6	1
All	All	1330/1470 (90%)	1193 (90%)	137 (10%)	7	1

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	522	GLU
1	B	560	GLU
1	B	776	MET
1	A	558	GLU
1	A	533	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	793	ASN
1	B	123	HIS
1	B	727	GLN
1	A	810	GLN
1	B	58	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	TPP	A	887	2	26,27,27	1.44	4 (15%)	38,40,40	0.93	1 (2%)
3	TPP	B	887	2	26,27,27	1.47	4 (15%)	38,40,40	0.90	1 (2%)

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	TPP	A	887	2	-	1/17/17/17	0/2/2/2
3	TPP	B	887	2	-	3/17/17/17	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	887	TPP	C4'-N3'	3.87	1.40	1.35
3	A	887	TPP	C5'-C4'	3.74	1.49	1.42
3	B	887	TPP	C5'-C4'	3.43	1.48	1.42
3	A	887	TPP	C4'-N3'	3.30	1.39	1.35
3	A	887	TPP	C2'-N1'	2.70	1.38	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	887	TPP	C6'-N1'-C2'	2.56	120.28	116.07
3	B	887	TPP	C6'-N1'-C2'	2.51	120.20	116.07

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	887	TPP	PB-O3A-PA-O7
3	B	887	TPP	C5-C6-C7-O7
3	A	887	TPP	PA-O3A-PB-O2B
3	B	887	TPP	PA-O3A-PB-O2B

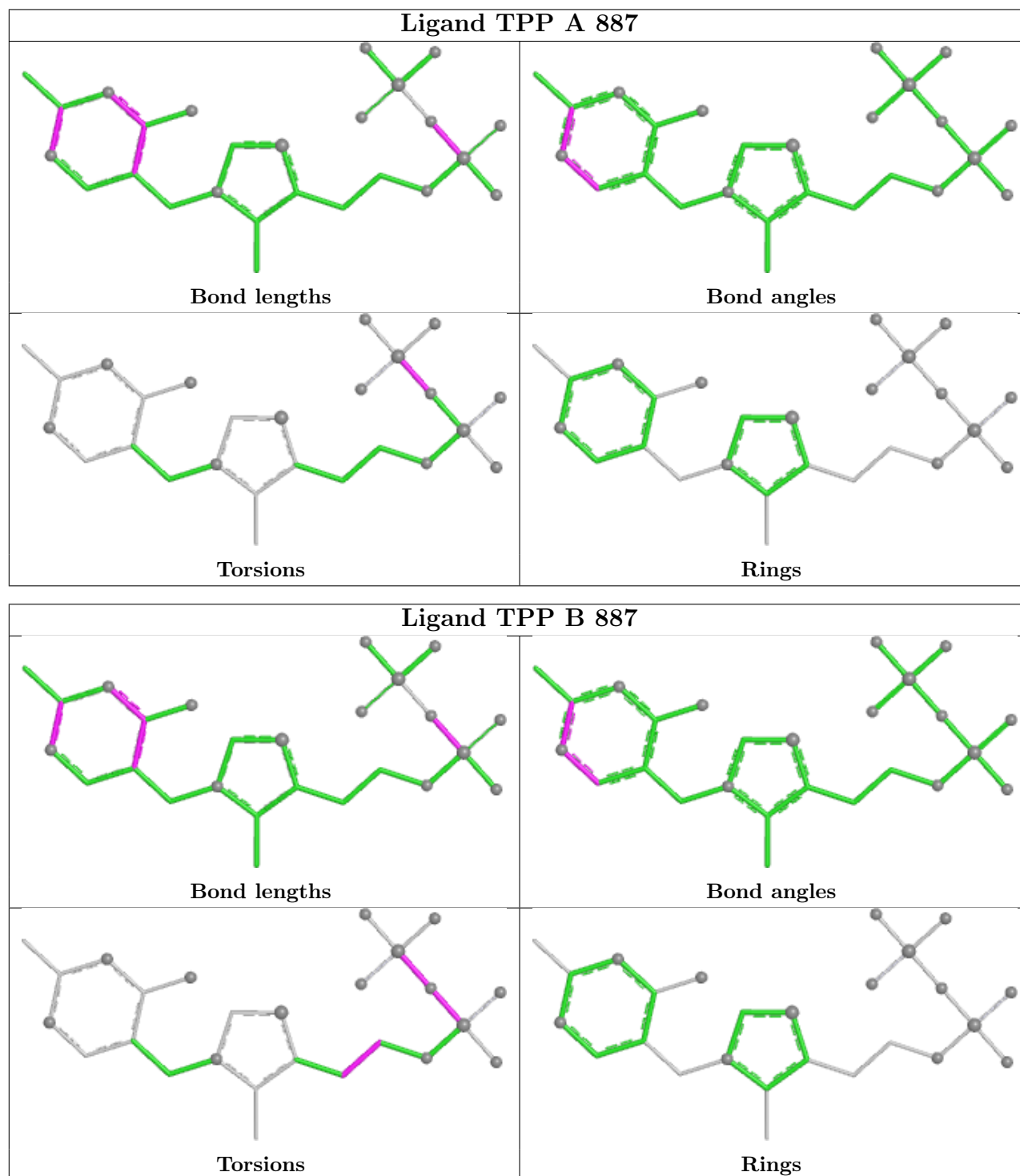
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	887	TPP	3	0
3	B	887	TPP	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.



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.