



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 09:50 PM EDT

PDB ID : 1EIN
Title : THE STRUCTURAL ORIGINS OF INTERFACIAL ACTIVATION IN THERMOMYCES (HUMICOLA) LANUGINOSA LIPASE
Authors : Brozozowski, A.M.; Savage, H.
Deposited on : 2000-02-26
Resolution : 3.00 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

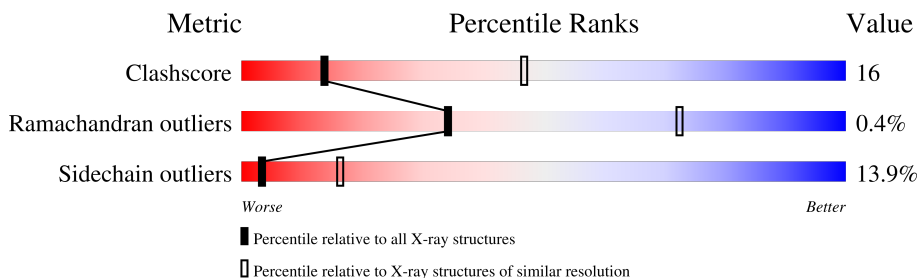
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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	269	<div> <div style="width: 62%; background-color: green;"></div> <div style="width: 30%; background-color: yellow;"></div> <div style="width: 6%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> </div> <div>62% 30% 6% •</div>
1	B	269	<div> <div style="width: 60%; background-color: green;"></div> <div style="width: 33%; background-color: yellow;"></div> <div style="width: 5%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> </div> <div>60% 33% 5% •</div>
1	C	269	<div> <div style="width: 58%; background-color: green;"></div> <div style="width: 34%; background-color: yellow;"></div> <div style="width: 6%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> </div> <div>58% 34% 6% •</div>

2 Entry composition [i](#)

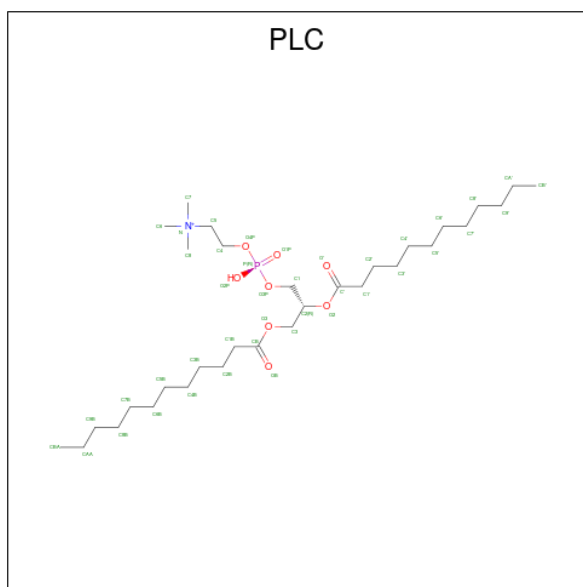
There are 3 unique types of molecules in this entry. The entry contains 6499 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LIPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2063	1301	356	400	6			
1	B	269	Total	C	N	O	S	0	0	0
			2063	1301	356	400	6			
1	C	269	Total	C	N	O	S	0	0	0
			2063	1301	356	400	6			

- Molecule 2 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: $C_{32}H_{65}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			42	32	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			42	32	1	8	1		
2	C	1	Total	C	N	O	P	0	0
			42	32	1	8	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total 68	O 68	0	0
3	B	57	Total 57	O 57	0	0
3	C	59	Total 59	O 59	0	0

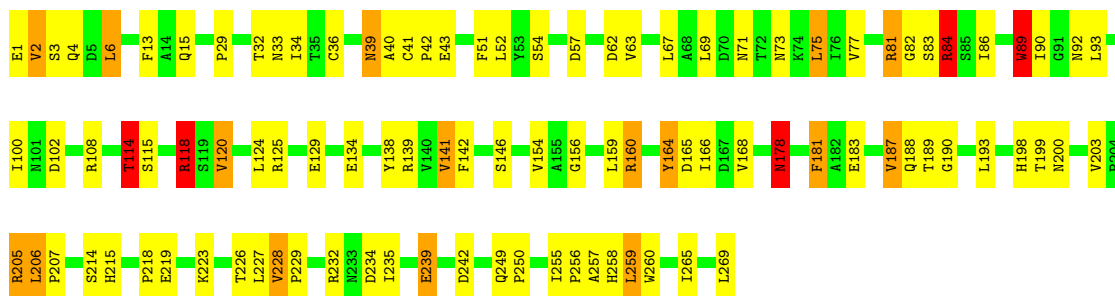
3 Residue-property plots

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.

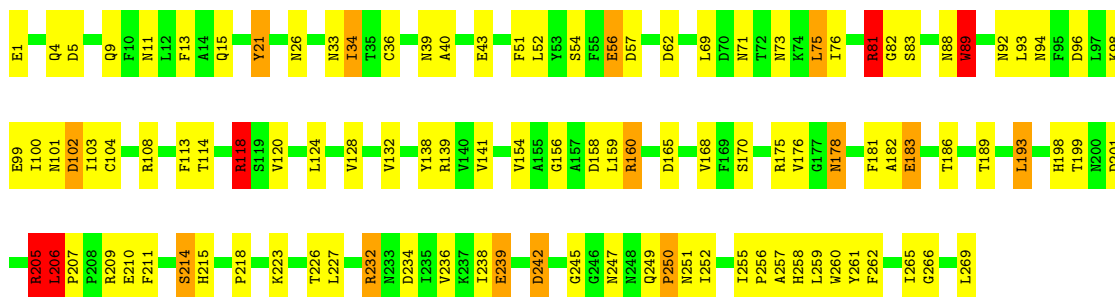
• Molecule 1: LIPASE

Chain A: 



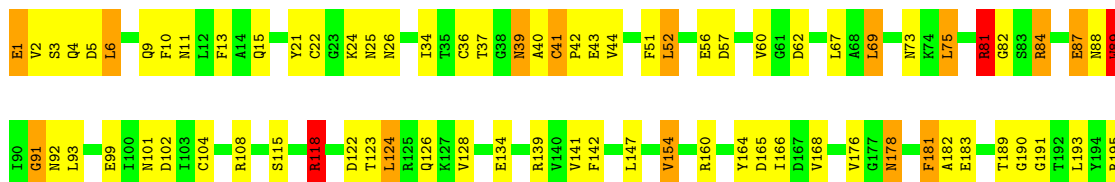
• Molecule 1: LIPASE

Chain B: 



• Molecule 1: LIPASE

Chain C: 



H198	T199	I202	V203	P204	R205	L206	R209	S214	E219	Y220	K223	S224	G225	T226	L227	V228	R232	N233	D234	I235	V236	K237	I238	E239	G240	I241	P250	N251	I252	P253	D254	I255	P256	A257	R258	L259	Y261	F262	I265	L269
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	135.95Å 135.95Å 149.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.40 – 3.00	Depositor
% Data completeness (in resolution range)	99.8 (27.40-3.00)	Depositor
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.210 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6499	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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: PLC

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	0.43	0/2113	1.21	12/2878 (0.4%)
1	B	0.43	0/2113	1.30	18/2878 (0.6%)
1	C	0.42	0/2113	1.27	14/2878 (0.5%)
All	All	0.43	0/6339	1.26	44/8634 (0.5%)

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	11
1	B	0	7
1	C	0	10
All	All	0	28

There are no bond length outliers.

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	ARG	NE-CZ-NH1	11.11	125.85	120.30
1	C	81	ARG	CD-NE-CZ	10.95	138.93	123.60
1	B	160	ARG	NE-CZ-NH1	-10.88	114.86	120.30
1	C	205	ARG	NE-CZ-NH2	10.60	125.60	120.30
1	C	209	ARG	NE-CZ-NH2	-10.57	115.01	120.30

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	GLU	Mainchain
1	A	134	GLU	Mainchain
1	A	3	SER	Mainchain
1	A	41	CYS	Mainchain
1	A	92	ASN	Mainchain

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	2063	0	1956	50	0
1	B	2063	0	1956	62	0
1	C	2063	0	1956	64	0
2	A	42	0	64	15	0
2	B	42	0	64	12	0
2	C	42	0	64	16	0
3	A	68	0	0	1	0
3	B	57	0	0	1	0
3	C	59	0	0	0	0
All	All	6499	0	6060	197	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 16.

The worst 5 of 197 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:B:15:GLN:HE22	1:B:43:GLU:H	1.09	0.97
1:A:15:GLN:HE22	1:A:43:GLU:H	1.18	0.91
2:A:601:PLC:H5'2	1:C:89:TRP:HZ3	1.39	0.87
1:B:81:ARG:HG2	1:B:81:ARG:HH21	1.39	0.87
1:C:36:CYS:HB3	1:C:40:ALA:HB3	1.56	0.86

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	267/269 (99%)	246 (92%)	20 (8%)	1 (0%)	34	72
1	B	267/269 (99%)	250 (94%)	16 (6%)	1 (0%)	34	72
1	C	267/269 (99%)	246 (92%)	20 (8%)	1 (0%)	34	72
All	All	801/807 (99%)	742 (93%)	56 (7%)	3 (0%)	34	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	THR
1	C	199	THR
1	B	199	THR

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	218/220 (99%)	184 (84%)	34 (16%)	2	13
1	B	218/220 (99%)	190 (87%)	28 (13%)	4	19
1	C	218/220 (99%)	189 (87%)	29 (13%)	4	17
All	All	654/660 (99%)	563 (86%)	91 (14%)	3	16

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	214	SER
1	C	84	ARG
1	B	239	GLU
1	C	11	ASN
1	C	124	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	71	ASN
1	C	178	ASN
1	B	178	ASN
1	C	247	ASN
1	C	71	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](#)

3 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	PLC	C	801	-	41,41,41	0.70	0	47,49,49	1.03	3 (6%)
2	PLC	B	701	-	41,41,41	0.72	0	47,49,49	1.19	6 (12%)
2	PLC	A	601	-	41,41,41	0.73	0	47,49,49	1.16	6 (12%)

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	PLC	C	801	-	-	26/45/45/45	-
2	PLC	B	701	-	-	21/45/45/45	-
2	PLC	A	601	-	-	23/45/45/45	-

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	PLC	C4-C5-N	-3.52	104.03	115.78
2	A	601	PLC	C2-O2-C'	-2.99	110.42	117.79
2	A	601	PLC	O2P-P-O4P	-2.71	95.15	107.75
2	C	801	PLC	C2B-C1B-CB	-2.61	104.14	113.62
2	A	601	PLC	C7-N-C6	2.53	115.48	108.97

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	PLC	O4P-C4-C5-N
2	A	601	PLC	C1B-CB-O3-C3
2	A	601	PLC	C1-O3P-P-O4P
2	B	701	PLC	C1B-CB-O3-C3
2	B	701	PLC	OB-CB-O3-C3

There are no ring outliers.

3 monomers are involved in 31 short contacts:

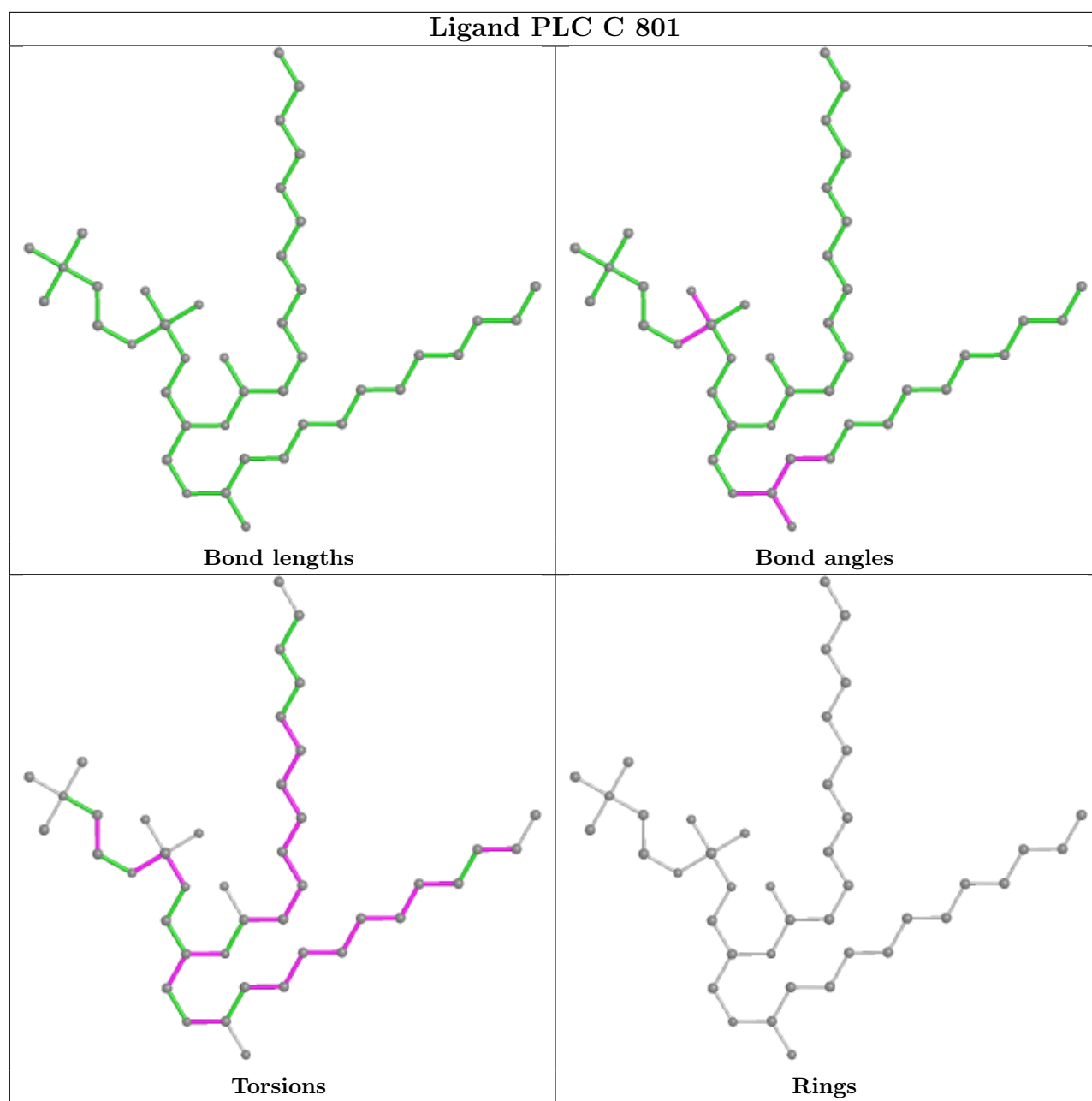
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	PLC	16	0

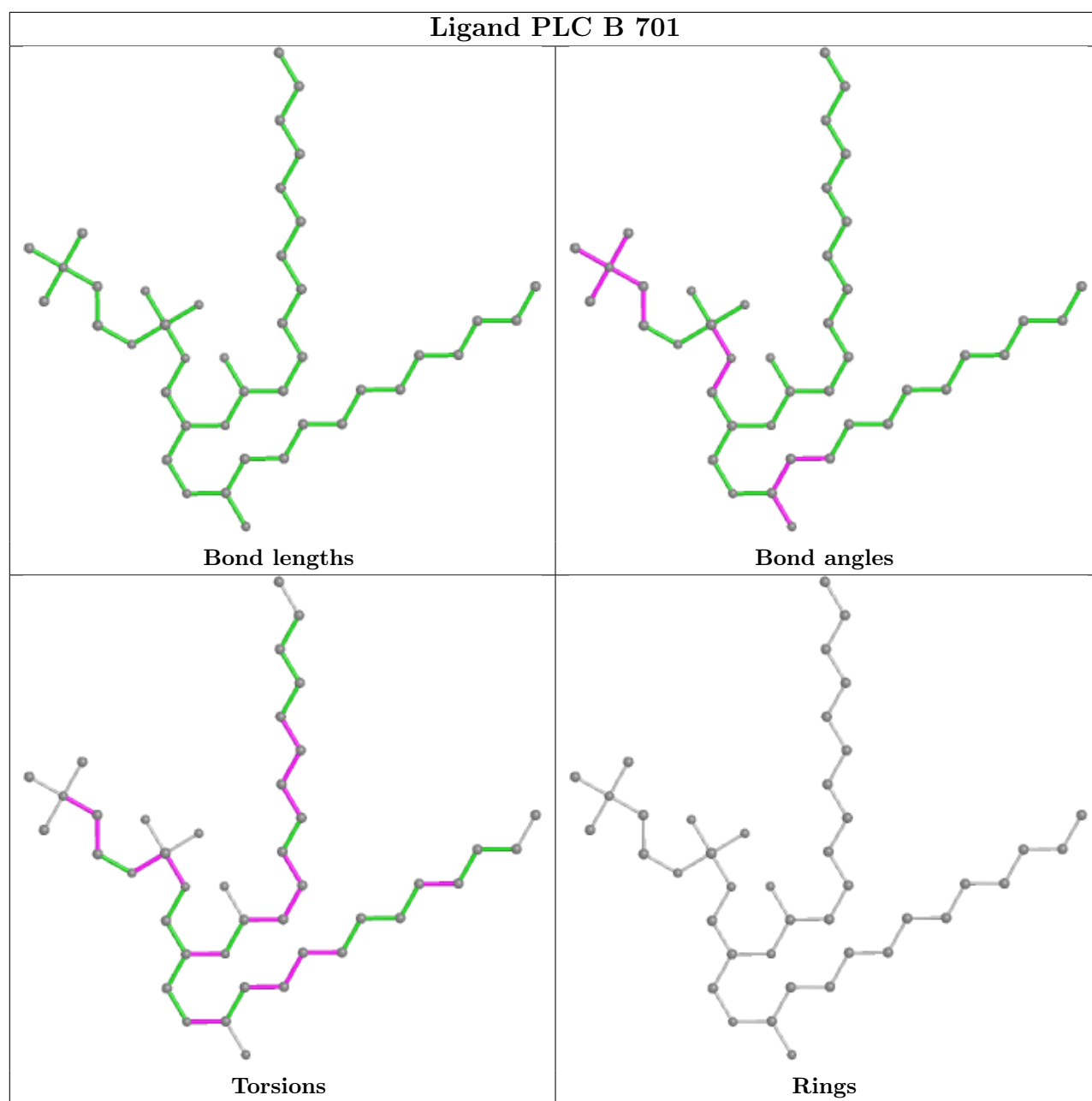
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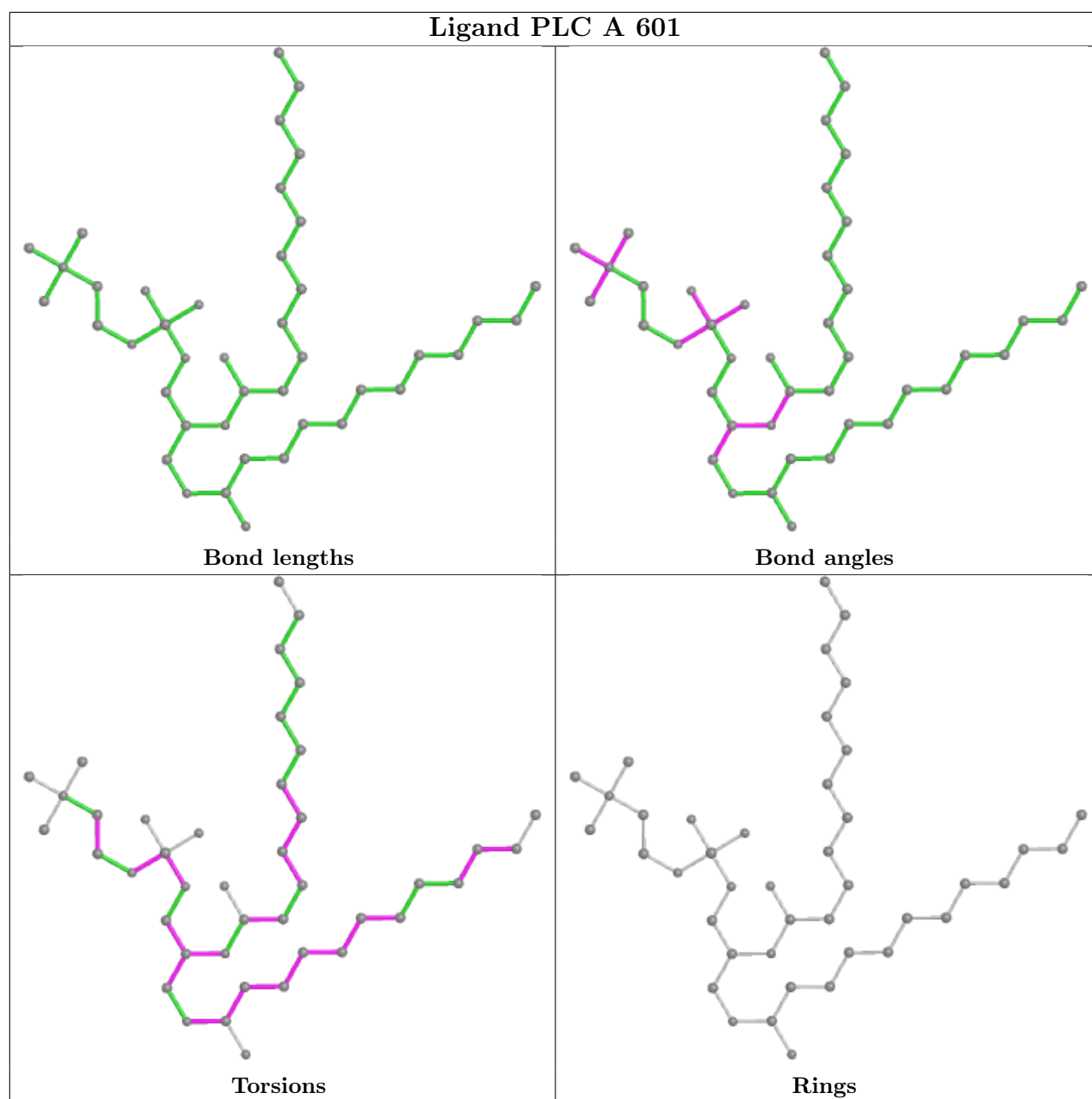
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	PLC	12	0
2	A	601	PLC	15	0

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.