



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:06 PM UTC

PDB ID : 1TAS / pdb_00001tas
Title : CRYSTALLINE MITOCHONDRIAL ASPARTATE AMINOTRANSFERASE EXISTS IN ONLY TWO CONFORMATIONS
Authors : Hohenester, E.; Jansonius, J.N.
Deposited on : 1993-10-04
Resolution : 2.80 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

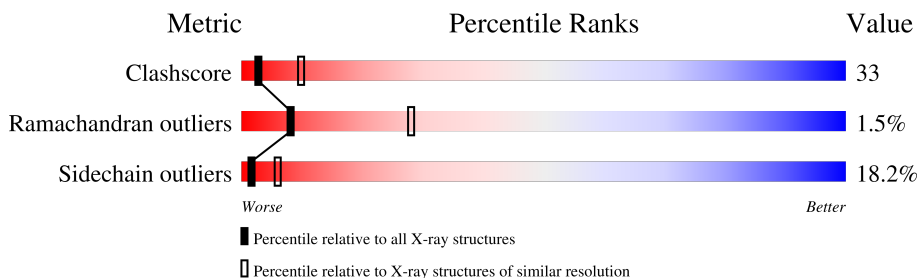
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	401	
1	B	401	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6372 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.

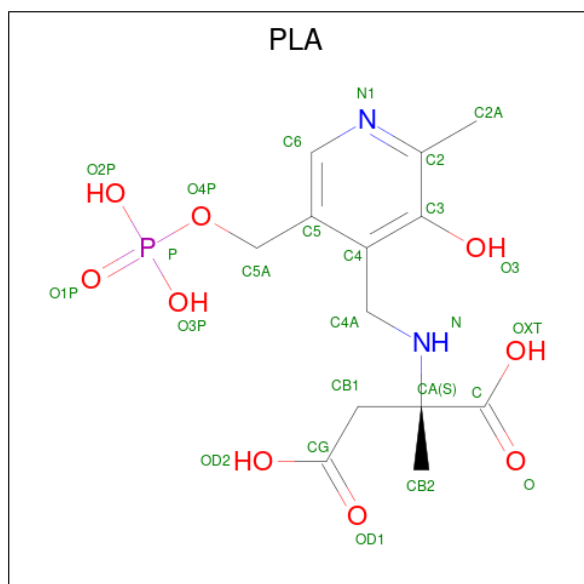
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	124	0	0
			3161	2004	558	581	18			
1	B	401	Total	C	N	O	S	139	0	0
			3161	2004	558	581	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	PRO	SER	conflict	UNP P00508
B	47	PRO	SER	conflict	UNP P00508

- Molecule 2 is 2-[(3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDI N-4-YLMETHYL)-AMINO]-2-METHYL-SUCCINIC ACID (CCD ID: PLA) (formula: C₁₃H₁₉N₂O₉P).



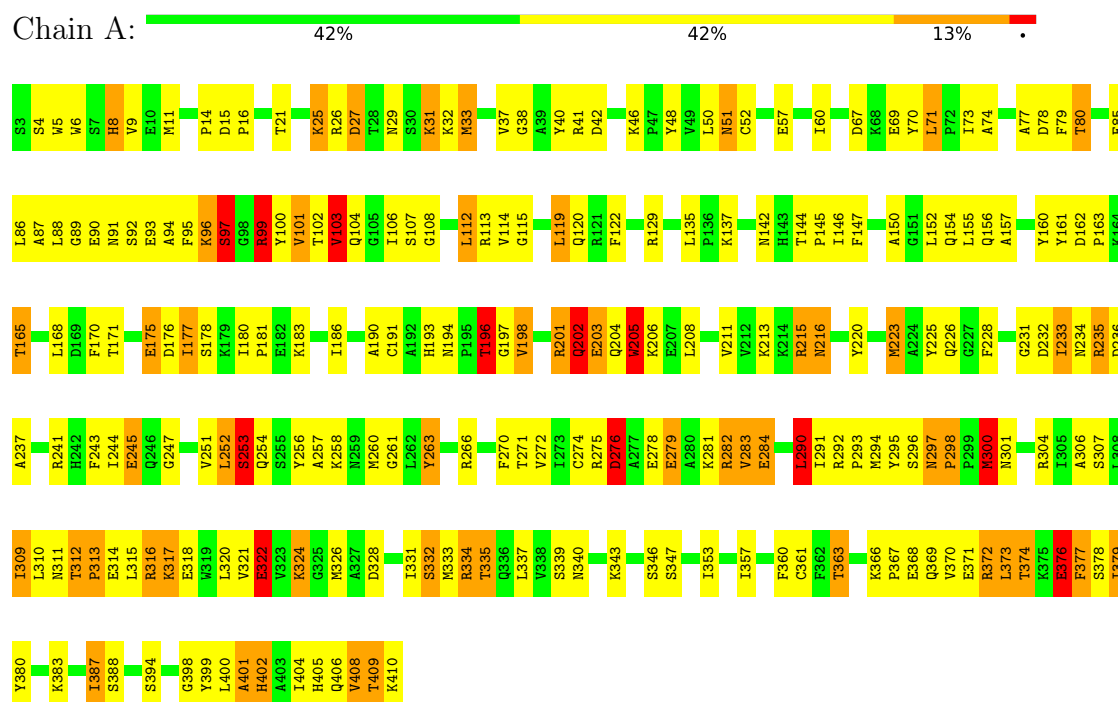
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
2	B	1	Total	C	N	O	P	0	0
			25	13	2	9	1		

3 Residue-property plots

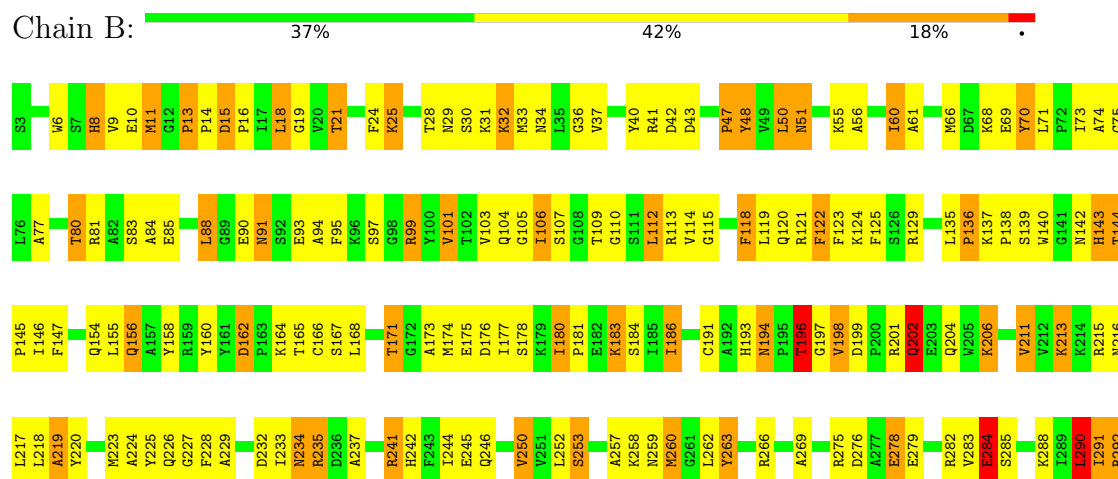
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: ASPARTATE AMINOTRANSFERASE



P283	M294	Y295	S296	N297	P298	P299	M300	N301		R304	I305	A306	S307	L308	I309	L310	N311	T312	P313		R316	K317	E318	M319	L320	V321	E322		M326	A327	D328	R329	I330	I331	S332	M333	R334	I335	Q336	L337	V338	S339	N340	L341	K342	K343	E344		S347		W350		I353	T354	D355	Q356	I357	G358	M359
F360	C361	F362	T363		K366	P367	E368	Q369	V370	E371	R372	L373	T374	K375	E376	F377	S378	I379	Y380	M381		R386	I387	S388	V389	A390	G391	V392	A393	S394		V397	Q398	Y399	L400	A401	H402	A403	I404	H405	Q406	V408	T409	K410															

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	57.40Å 52.40Å 136.90Å 90.00° 101.50° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6372	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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: PLA

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	1.58	20/3231 (0.6%)	1.95	79/4360 (1.8%)
1	B	1.52	15/3231 (0.5%)	1.99	94/4360 (2.2%)
All	All	1.55	35/6462 (0.5%)	1.97	173/8720 (2.0%)

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	GLU	CD-OE2	8.44	1.41	1.25
1	A	119	LEU	C-O	-8.03	1.14	1.24
1	B	180	ILE	CA-C	-6.59	1.47	1.53
1	A	60	ILE	CA-CB	-6.53	1.46	1.54
1	A	40	TYR	N-CA	-6.45	1.37	1.46

The worst 5 of 173 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	PHE	N-CA-C	11.94	125.67	111.82
1	B	125	PHE	N-CA-C	11.54	125.29	111.33
1	B	176	ASP	CA-CB-CG	-10.77	101.83	112.60
1	A	176	ASP	CA-CB-CG	-10.51	102.09	112.60
1	A	175	GLU	N-CA-CB	10.16	125.27	109.82

There are no chirality outliers.

There are no planarity outliers.

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	3161	0	3154	178	0
1	B	3161	0	3154	234	0
2	A	25	0	14	6	0
2	B	25	0	14	6	0
All	All	6372	0	6336	398	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 33.

The worst 5 of 398 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:260:MET:HE2	1:B:309:ILE:HD12	1.43	0.97
1:B:327:ALA:HA	1:B:330:ILE:HD12	1.49	0.94
1:B:196:THR:HG23	1:B:198:VAL:HG23	1.49	0.92
1:B:174:MET:HE1	1:B:211:VAL:HG21	1.51	0.92
1:B:366:LYS:H	1:B:369:GLN:NE2	1.69	0.90

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	399/401 (100%)	354 (89%)	41 (10%)	4 (1%)	12	38
1	B	399/401 (100%)	358 (90%)	33 (8%)	8 (2%)	6	21
All	All	798/802 (100%)	712 (89%)	74 (9%)	12 (2%)	8	28

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	77	ALA
1	A	313	PRO
1	B	50	LEU
1	B	202	GLN
1	A	183	LYS

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	335/335 (100%)	276 (82%)	59 (18%)	2	7
1	B	335/335 (100%)	272 (81%)	63 (19%)	1	5
All	All	670/670 (100%)	548 (82%)	122 (18%)	2	6

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	409	THR
1	B	353	ILE
1	B	83	SER
1	B	343	LYS
1	B	387	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	117	ASN
1	B	216	ASN
1	B	369	GLN
1	B	156	GLN
1	B	234	ASN

5.3.3 RNA ⓘ

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](#)

2 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	PLA	A	411	-	25,25,25	1.77	7 (28%)	34,37,37	2.64	13 (38%)
2	PLA	B	411	-	25,25,25	1.97	5 (20%)	34,37,37	2.94	14 (41%)

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	PLA	A	411	-	-	13/23/23/23	0/1/1/1
2	PLA	B	411	-	-	10/23/23/23	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	411	PLA	C5-C4	5.93	1.48	1.40
2	A	411	PLA	C4A-C4	-4.94	1.44	1.52
2	B	411	PLA	CA-N	4.41	1.53	1.47
2	B	411	PLA	C3-C4	-3.32	1.35	1.40
2	A	411	PLA	C4A-N	-2.96	1.29	1.45

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	411	PLA	C2A-C2-C3	7.15	129.16	120.80
2	A	411	PLA	O4P-C5A-C5	7.05	122.56	109.36
2	B	411	PLA	C4A-C4-C5	7.02	127.39	119.75
2	A	411	PLA	C2A-C2-C3	5.53	127.27	120.80
2	B	411	PLA	O4P-C5A-C5	5.23	119.17	109.36

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

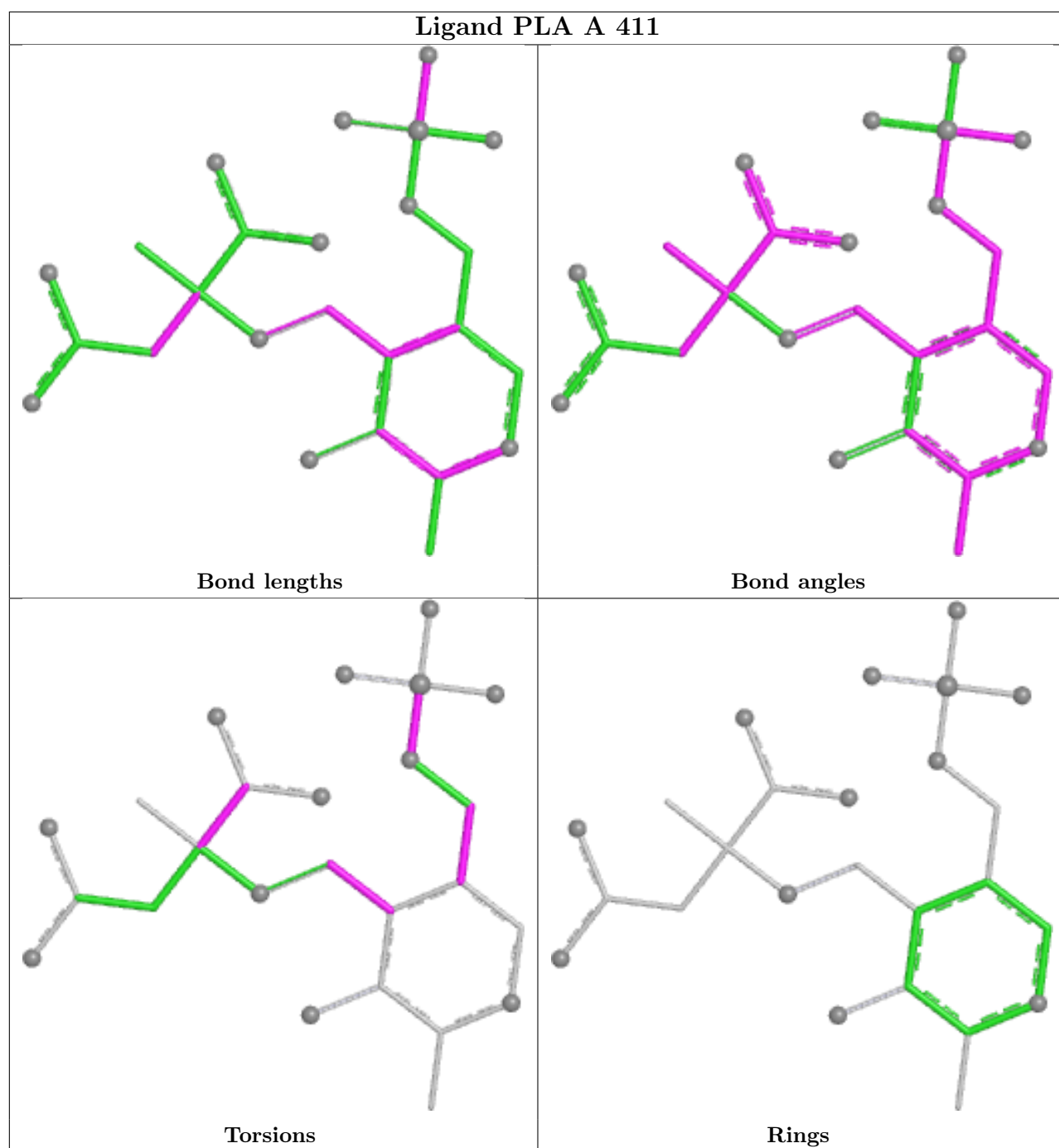
Mol	Chain	Res	Type	Atoms
2	A	411	PLA	C5-C4-C4A-N
2	A	411	PLA	C4-C5-C5A-O4P
2	A	411	PLA	C6-C5-C5A-O4P
2	A	411	PLA	C5A-O4P-P-O1P
2	A	411	PLA	C5A-O4P-P-O2P

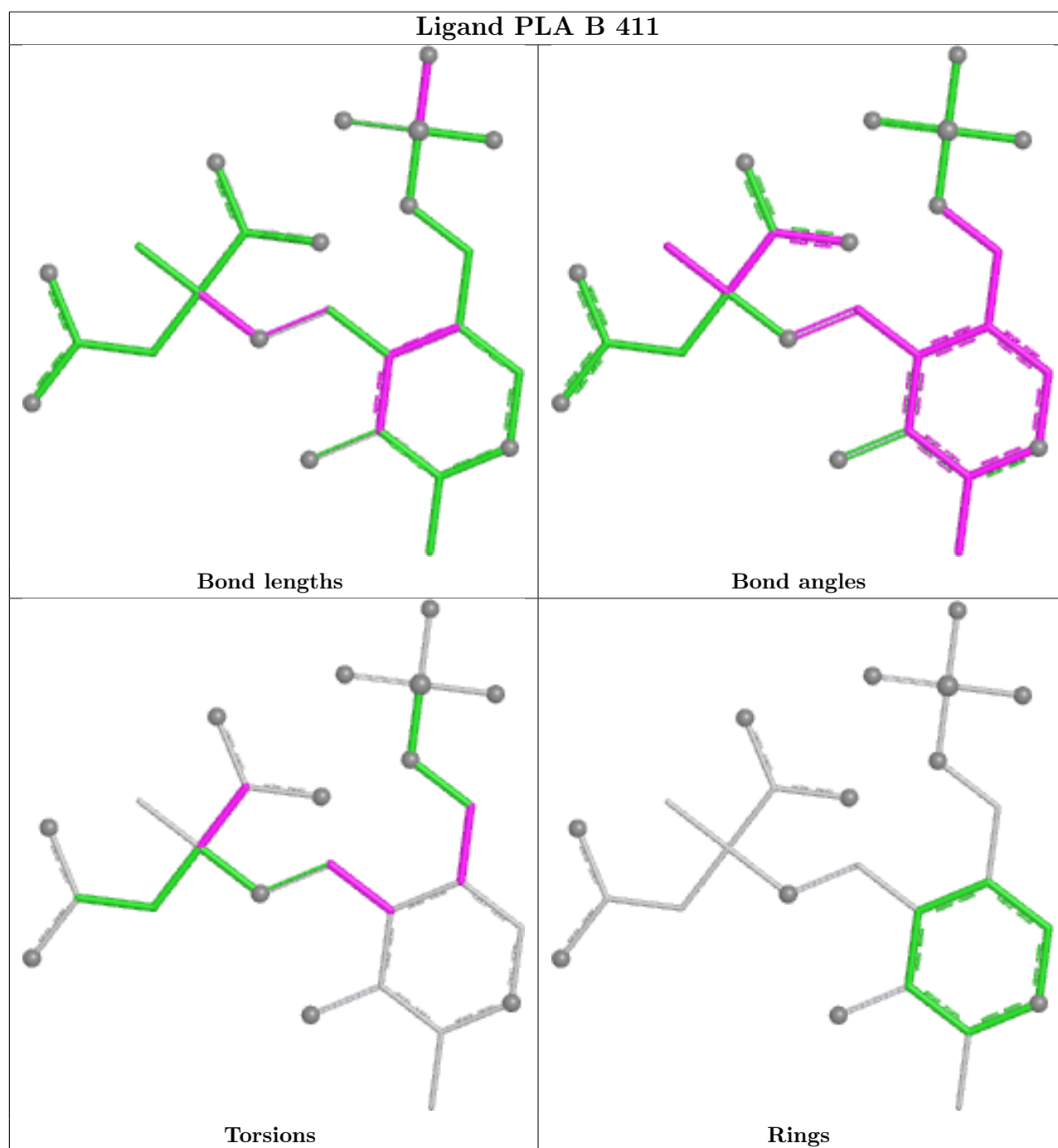
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	411	PLA	6	0
2	B	411	PLA	6	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.