



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 02:08 PM BST

PDB ID : 4AYX
Title : STRUCTURE OF THE HUMAN MITOCHONDRIAL ABC TRANSPORTER, ABCB10 (ROD FORM B)
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Deposited on : 2012-06-22
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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) : 1.13
EDS : **FAILED**
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) : 2.14.4.dev1

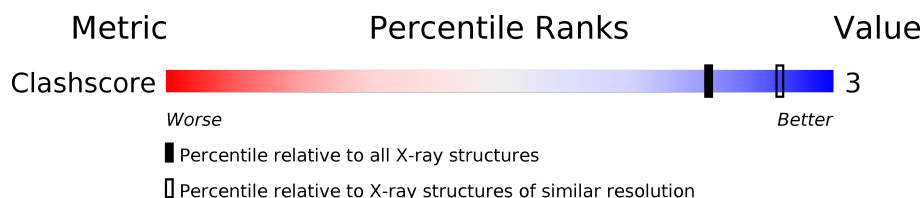
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2172 (2.90-2.90)

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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	595	 90% 6% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CDL	A	1721	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4428 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.

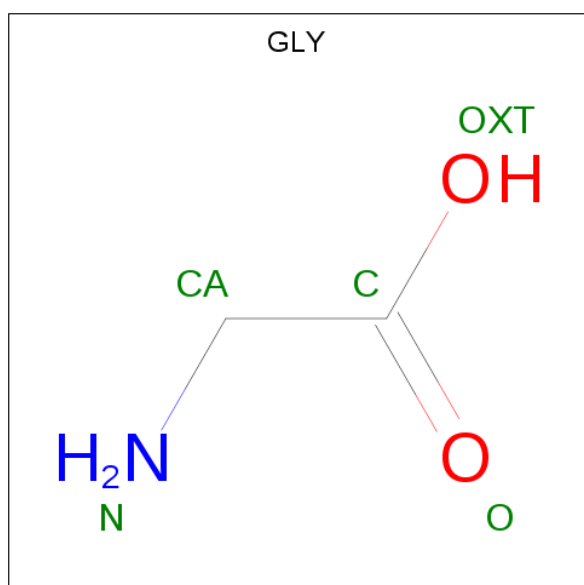
- Molecule 1 is a protein called ATP-BINDING CASSETTE SUB-FAMILY B MEMBER 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	571	4200	2687	726	771	16	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	MET	-	expression tag	UNP Q9NRK6
A	739	ALA	-	expression tag	UNP Q9NRK6
A	740	GLU	-	expression tag	UNP Q9NRK6
A	741	ASN	-	expression tag	UNP Q9NRK6
A	742	LEU	-	expression tag	UNP Q9NRK6
A	743	TYR	-	expression tag	UNP Q9NRK6
A	744	PHE	-	expression tag	UNP Q9NRK6
A	745	GLN	-	expression tag	UNP Q9NRK6

- Molecule 2 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).

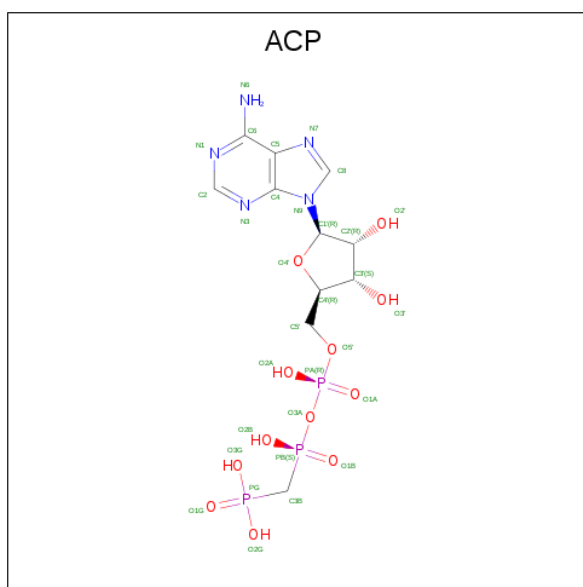


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

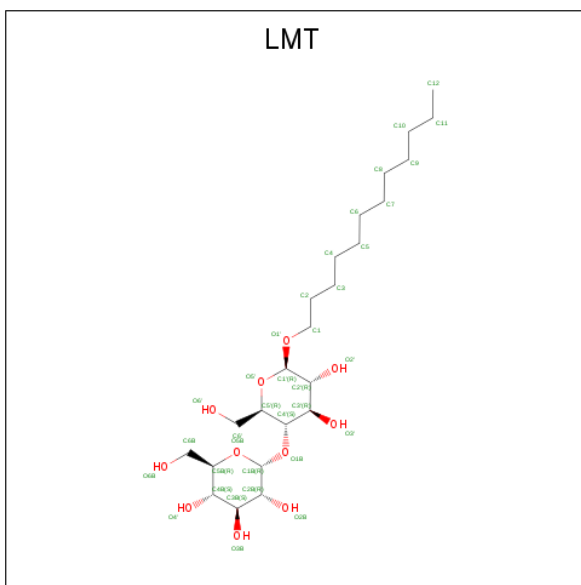
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



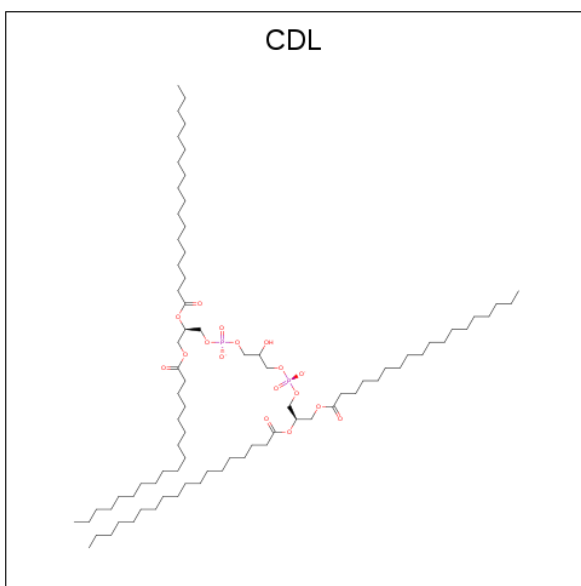
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 5 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 35	C 24	O 11	0	0
5	A	1	Total 35	C 24	O 11	0	0

- Molecule 6 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O P 74 55 17 2	0	0
6	A	1	Total C O 14 12 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	33	Total 33	O 33	0	0

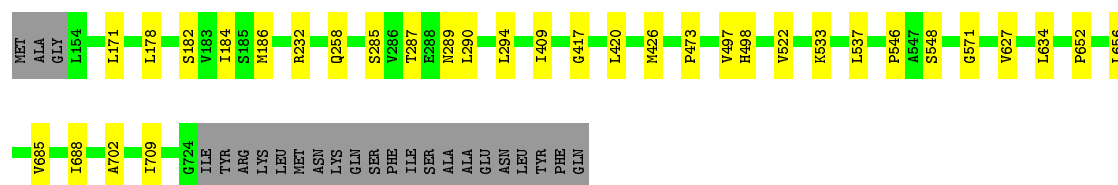
3 Residue-property plots [i](#)

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 failed to run properly.

- Molecule 1: ATP-BINDING CASSETTE SUB-FAMILY B MEMBER 10

Chain A: 



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	180.14Å 180.14Å 50.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.00 – 2.90	Depositor
% Data completeness (in resolution range)	99.6 (39.00-2.90)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.90Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.223 , 0.267	Depositor
Wilson B-factor (Å ²)	79.9	Xtriage
Anisotropy	0.501	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,l	Xtriage
Total number of atoms	4428	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, MG, ACP, LMT

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	0.45	0/4276	0.59	0/5811

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4200	0	4192	19	0
2	A	5	0	2	0	0
3	A	1	0	0	0	0
4	A	31	0	14	0	0
5	A	70	0	92	2	0
6	A	88	0	116	4	0
7	A	33	0	0	0	0
All	All	4428	0	4416	23	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 3.

All (23) 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)
6:A:1721:CDL:HA4	6:A:1721:CDL:OA9	1.68	0.91
6:A:1721:CDL:CA4	6:A:1721:CDL:OA9	2.28	0.79
1:A:537:LEU:HD22	1:A:656:LEU:HB3	1.76	0.68
6:A:1721:CDL:HA31	6:A:1721:CDL:OA7	1.96	0.64
1:A:171:LEU:HD21	1:A:287:THR:HG22	1.84	0.59
1:A:182:SER:O	1:A:186:MET:HG2	2.05	0.57
1:A:178:LEU:HB2	1:A:232:ARG:HD2	1.88	0.55
1:A:258:GLN:HA	1:A:473:PRO:HB3	1.89	0.55
1:A:498:HIS:HB2	1:A:548:SER:HB3	1.90	0.54
1:A:571:GLY:HA3	1:A:652:PRO:HG3	1.92	0.50
1:A:702:ALA:HB1	1:A:709:ILE:HD12	1.96	0.47
1:A:497:VAL:HG13	1:A:546:PRO:HB3	1.96	0.47
1:A:522:VAL:HG22	1:A:685:VAL:HB	1.99	0.45
1:A:420:LEU:HB2	1:A:426:MET:HE2	2.00	0.44
1:A:533:LYS:HB3	1:A:688:ILE:HG12	1.98	0.44
1:A:409:ILE:HG13	5:A:1724:LMT:H122	2.00	0.43
1:A:417:GLY:HA2	1:A:426:MET:HE1	2.01	0.42
1:A:627:VAL:HG11	1:A:634:LEU:HD11	2.00	0.42
5:A:1724:LMT:H5B	5:A:1724:LMT:H6D	2.02	0.41
1:A:184:ILE:HB	6:A:1726:CDL:H381	2.03	0.41
1:A:285:SER:HA	1:A:289:ASN:HB3	2.03	0.40
1:A:290:LEU:O	1:A:294:LEU:HB2	2.21	0.40
1:A:294:LEU:HA	1:A:294:LEU:HD12	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	$\# Z > 2$
4	ACP	A	900	3	27,33,33	0.65	0	32,52,52	1.13	4 (12%)
5	LMT	A	1724	-	36,36,36	0.23	0	47,47,47	0.38	0
5	LMT	A	1720	-	36,36,36	0.19	0	47,47,47	0.41	0
6	CDL	A	1726	-	13,13,99	0.80	1 (7%)	13,13,111	0.65	0
6	CDL	A	1721	-	73,73,99	0.66	2 (2%)	79,85,111	0.62	4 (5%)
2	GLY	A	1717	-	1,4,4	0.01	0	0,4,4	0.00	-

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
4	ACP	A	900	3	-	3/15/38/38	0/3/3/3
5	LMT	A	1724	-	-	4/21/61/61	0/2/2/2
5	LMT	A	1720	-	-	4/21/61/61	0/2/2/2
6	CDL	A	1726	-	-	3/12/12/110	-
6	CDL	A	1721	-	1/1/9/9	29/84/84/110	-
2	GLY	A	1717	-	-	0/0/2/2	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1721	CDL	C79-C78	-3.40	1.32	1.51
6	A	1721	CDL	C39-C38	-3.38	1.32	1.51
6	A	1726	CDL	C39-C38	-2.70	1.32	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	900	ACP	O1B-PB-C3B	3.12	117.31	109.07
4	A	900	ACP	O2A-PA-O5'	-3.11	93.32	107.75
6	A	1721	CDL	C39-C38-C37	2.45	126.86	114.42
6	A	1721	CDL	C79-C78-C77	2.33	126.27	114.42
6	A	1721	CDL	C80-C79-C78	2.31	126.13	114.42
4	A	900	ACP	O2B-PB-O1B	2.22	117.50	110.07
4	A	900	ACP	C5-C6-N6	2.18	123.67	120.35
6	A	1721	CDL	C40-C39-C38	2.18	125.50	114.42

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1721	CDL	CA4

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	900	ACP	C5'-O5'-PA-O3A
6	A	1721	CDL	CA2-C1-CB2-OB2
6	A	1721	CDL	CA3-OA5-PA1-OA2
6	A	1721	CDL	CA3-OA5-PA1-OA3
6	A	1721	CDL	CA3-OA5-PA1-OA4
6	A	1721	CDL	CB2-OB2-PB2-OB3
6	A	1721	CDL	CB2-OB2-PB2-OB4
6	A	1721	CDL	CB2-OB2-PB2-OB5
6	A	1721	CDL	CA4-CA6-OA8-CA7
6	A	1721	CDL	O1-C1-CB2-OB2
5	A	1720	LMT	O1'-C1-C2-C3
5	A	1720	LMT	C1-C2-C3-C4
5	A	1724	LMT	C7-C8-C9-C10
5	A	1724	LMT	C11-C10-C9-C8
6	A	1726	CDL	C31-C32-C33-C34
6	A	1721	CDL	OA5-CA3-CA4-CA6
6	A	1721	CDL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
6	A	1721	CDL	OB5-CB3-CB4-CB6
6	A	1721	CDL	CA7-C31-C32-C33
6	A	1721	CDL	C79-C80-C81-C82
6	A	1721	CDL	CB3-OB5-PB2-OB2
5	A	1720	LMT	C3-C4-C5-C6
4	A	900	ACP	C5'-O5'-PA-O1A
4	A	900	ACP	C5'-O5'-PA-O2A
6	A	1721	CDL	OA5-CA3-CA4-OA6
6	A	1721	CDL	OB5-CB3-CB4-OB6
6	A	1721	CDL	CA5-C11-C12-C13
5	A	1724	LMT	O1'-C1-C2-C3
6	A	1721	CDL	CB6-CB4-OB6-CB5
6	A	1721	CDL	CB4-CB3-OB5-PB2
6	A	1721	CDL	OB6-CB4-CB6-OB8
5	A	1724	LMT	C4-C5-C6-C7
6	A	1721	CDL	CA3-CA4-OA6-CA5
6	A	1721	CDL	C42-C43-C44-C45
6	A	1721	CDL	C11-CA5-OA6-CA4
5	A	1720	LMT	C2-C3-C4-C5
6	A	1721	CDL	C12-C11-CA5-OA6
6	A	1721	CDL	C80-C81-C82-C83
6	A	1721	CDL	CB3-OB5-PB2-OB3
6	A	1721	CDL	C12-C11-CA5-OA7
6	A	1721	CDL	CA6-CA4-OA6-CA5
6	A	1726	CDL	C32-C31-CA7-OA8
6	A	1726	CDL	C32-C31-CA7-OA9

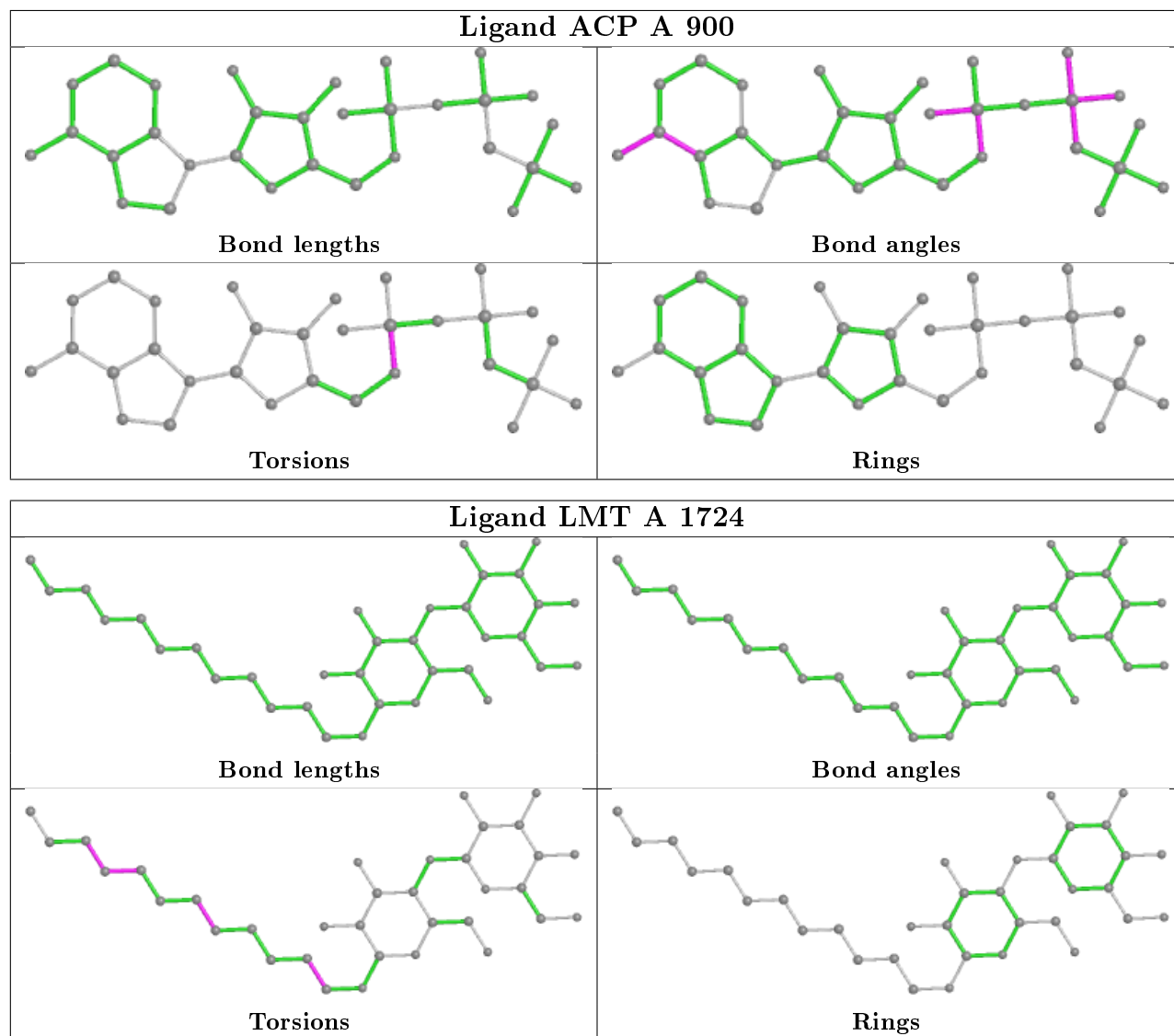
There are no ring outliers.

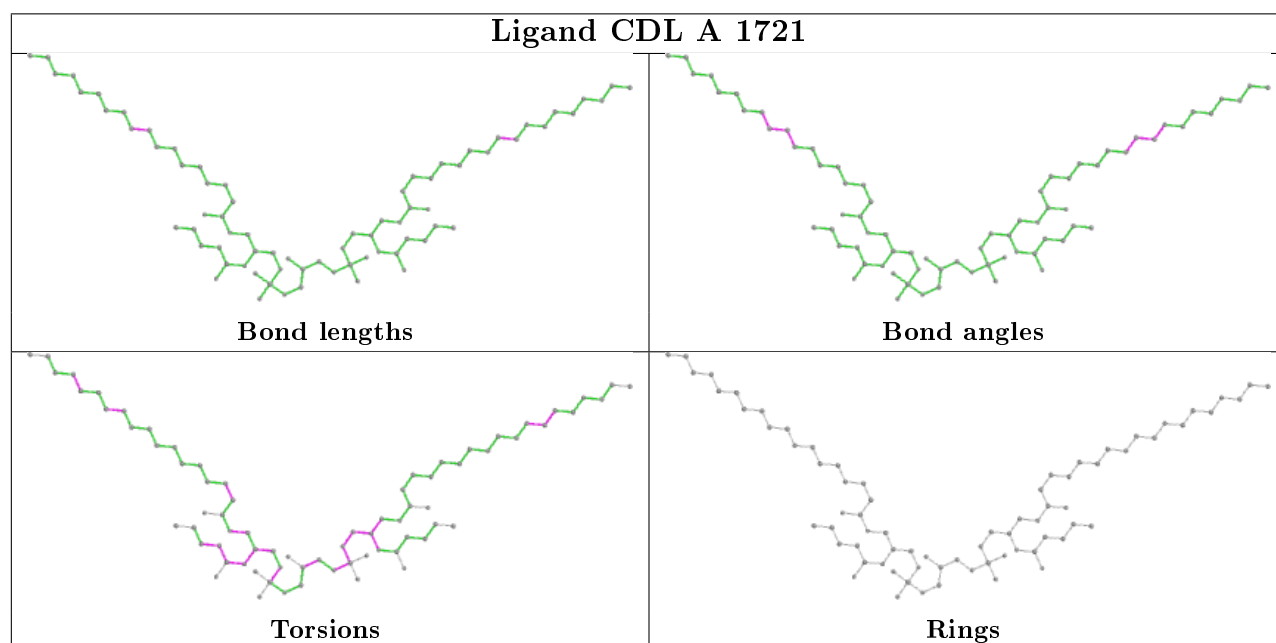
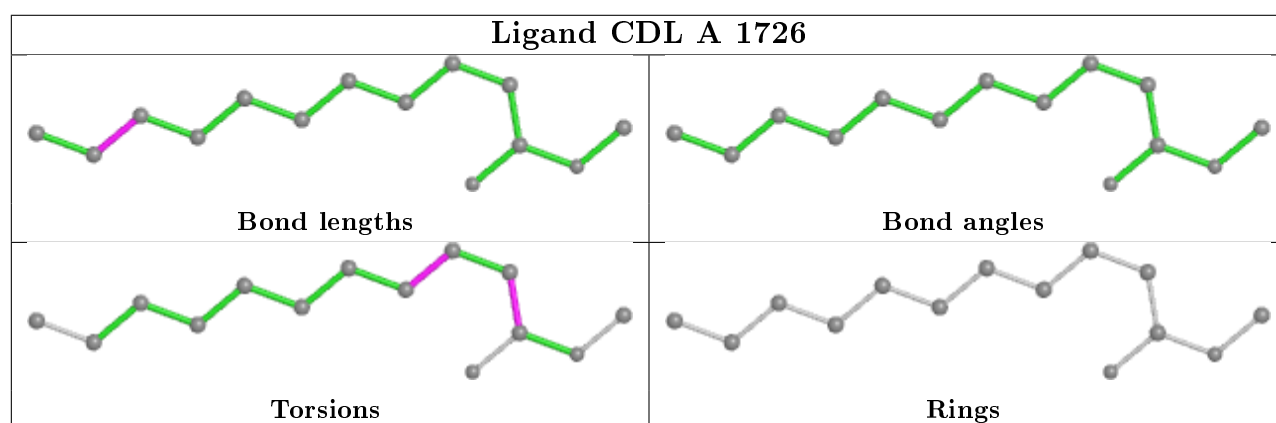
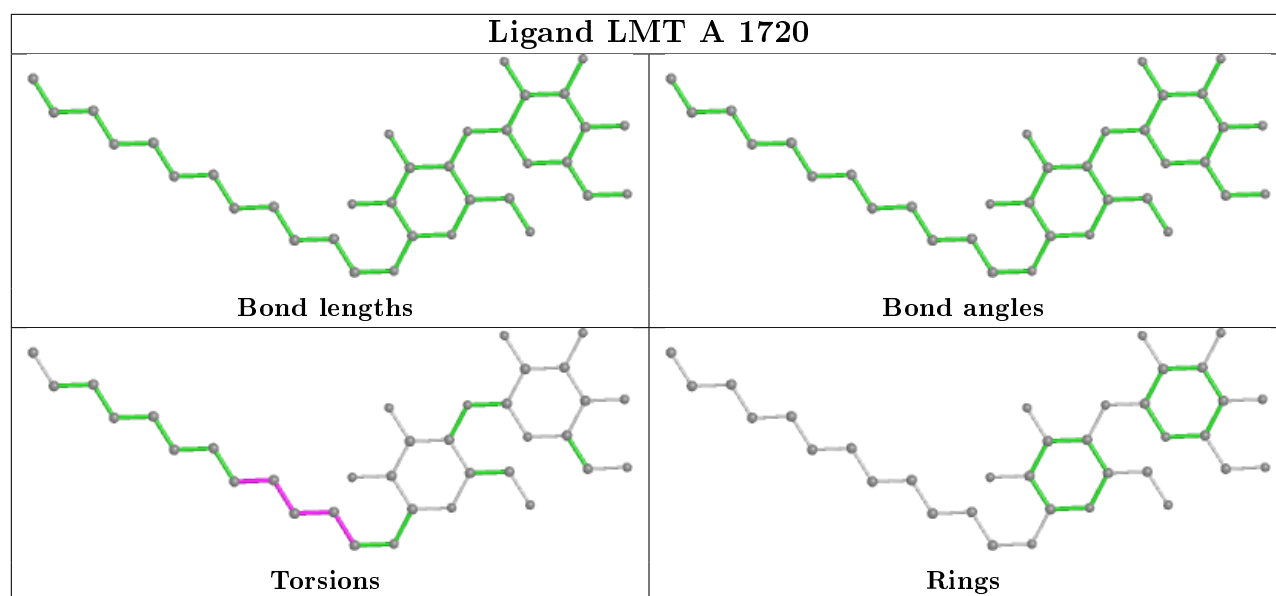
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1724	LMT	2	0
6	A	1726	CDL	1	0
6	A	1721	CDL	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.