wwPDB X-ray Structure Validation Summary Report (i)

Jan 27, 2024 – 04:12 PM EST

PDB ID	:	1ACM
Title	:	ARGININE 54 IN THE ACTIVE SITE OF ESCHERICHIA COLI ASPARTATE TRANSCARBAMOYLASE IS CRITICAL FOR CATALYSIS: A SITE-SPECIFIC MUTAGENESIS, NMR AND X-RAY CRYSTALLOGRAPHY STUDY
Authors	:	Stevens, R.C.; Kantrowitz, E.R.; Lipscomb, W.N.
Deposited on	:	1992-07-08
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 (i) 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 (1)) were used in the production of this report:

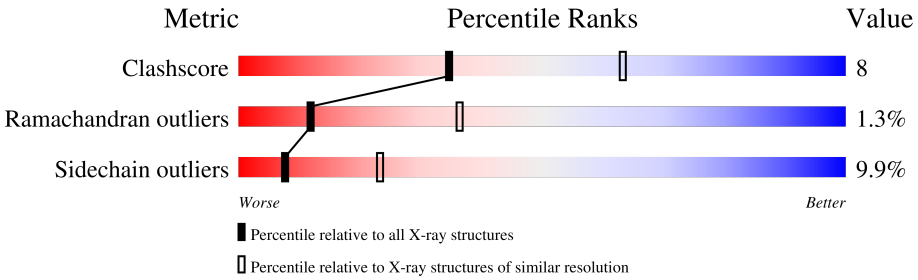
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	75% 21% • •
1	C	310	79% 17% •
2	B	153	51% 33% 10% • 5%
2	D	153	52% 35% 7% • 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7143 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 CARBAMOYLTRANSFERASE, CATALYTIC CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2409	1524	420	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2409	1524	420	456	9			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	ALA	ARG	conflict	UNP P0A786
A	60	GLN	GLU	conflict	UNP P0A786
A	147	GLN	GLU	conflict	UNP P0A786
A	149	GLU	GLN	conflict	UNP P0A786
A	196	GLU	GLN	conflict	UNP P0A786
C	54	ALA	ARG	conflict	UNP P0A786
C	60	GLN	GLU	conflict	UNP P0A786
C	147	GLN	GLU	conflict	UNP P0A786
C	149	GLU	GLN	conflict	UNP P0A786
C	196	GLU	GLN	conflict	UNP P0A786

- Molecule 2 is a protein called ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			
2	D	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	GLY	GLN	conflict	UNP P0A7F3

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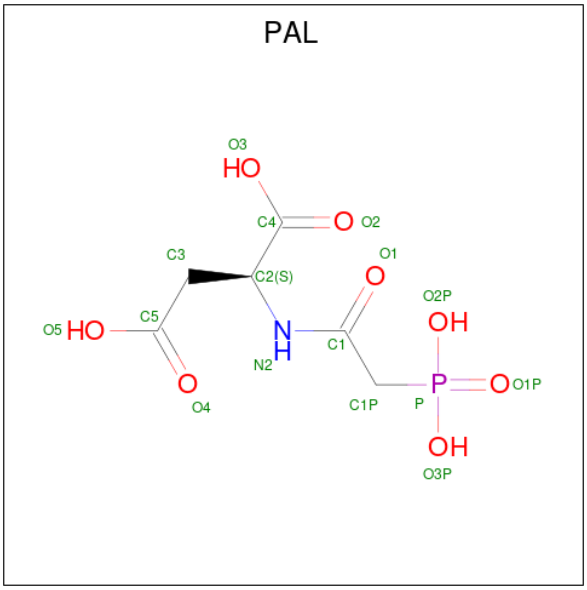
Chain	Residue	Modelled	Actual	Comment	Reference
D	8	GLY	GLN	conflict	UNP P0A7F3

- Molecule 3 is N-(PHOSPHONACETYL)-L-ASPARTIC ACID (three-letter code: PAL) (formula: $C_6H_{10}NO_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 16 6 1 8 1	0	0
3	C	1	Total C N O P 16 6 1 8 1	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	8	Total O 8 8	0	0
5	C	7	Total O 7 7	0	0

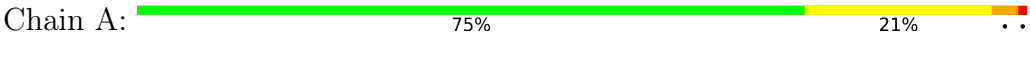
3 Residue-property plots (i)

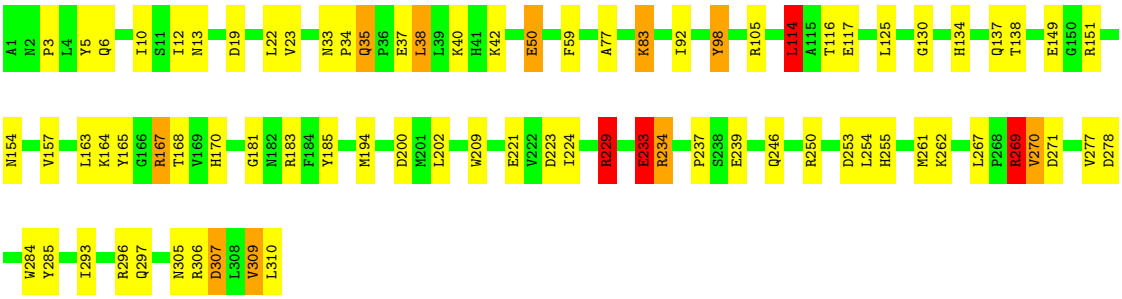
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 was not executed.

• Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE, CATALYTIC CHAIN

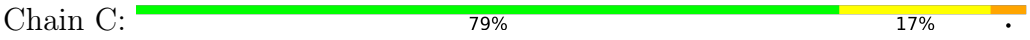
Chain A:

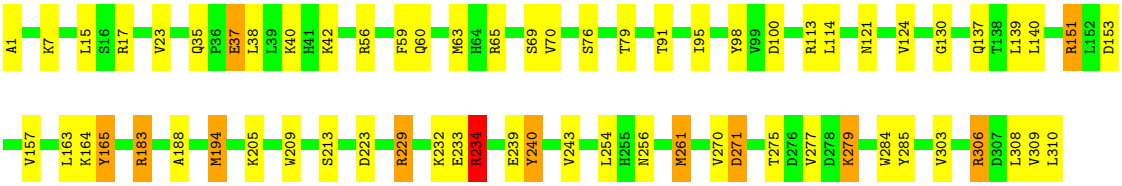




• Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE, CATALYTIC CHAIN

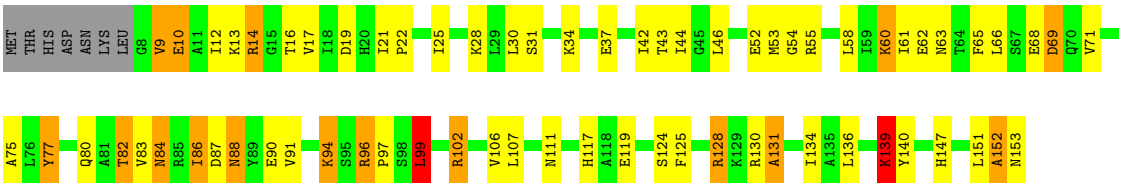
Chain C:





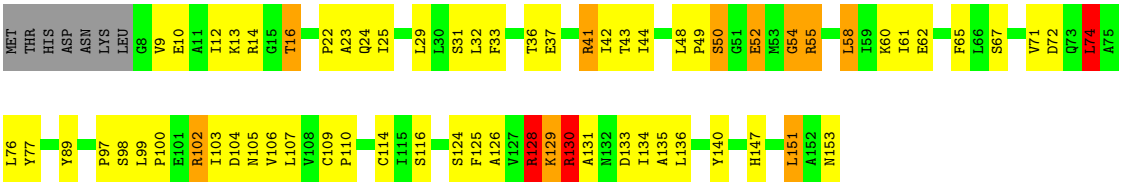
• Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN

Chain B:



• Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN

Chain D:


MET THR HIS ASP ASN LYS LEU G8 V9 E10 A11 I12 K13 R14 G15 T16 P22 A23 Q24 I25 L29 L30 S31 L32 F33 T36 E37 R41 I42 T43 I44 L48 P49 S50 G51 E52 M53 G54 R55 L58 I59 K60 I61 E62 F65 L66 S67 V71 D72 Q73 L74 A75
L76 Y77 Y89 P97 S98 L99 P100 E101 R102 I103 D104 N105 V106 L107 V108 C109 P110 C114 I115 S116 S124 F125 A126 V127 R128 K129 R130 A131 N132 D133 I134 A135 L136 Y140 H147 L151 A152 N153

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	122.20Å 122.20Å 156.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7143	wwPDB-VP
Average B, all atoms (Å^2)	32.0	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: PAL, ZN

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	0.82	0/2455	1.55	28/3332 (0.8%)
1	C	0.86	0/2455	1.53	36/3332 (1.1%)
2	B	0.71	0/1155	1.53	16/1561 (1.0%)
2	D	0.75	0/1155	1.52	13/1561 (0.8%)
All	All	0.81	0/7220	1.54	93/9786 (1.0%)

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	3
1	C	0	3
2	B	0	2
2	D	0	3
All	All	0	11

There are no bond length outliers.

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	229	ARG	NE-CZ-NH1	16.61	128.61	120.30
1	A	229	ARG	NE-CZ-NH2	-11.37	114.62	120.30
1	A	167	ARG	NE-CZ-NH1	10.65	125.62	120.30
1	C	234	ARG	NE-CZ-NH2	-10.59	115.01	120.30
1	A	233	GLU	CA-CB-CG	9.92	135.22	113.40

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	TYR	Sidechain
1	A	269	ARG	Sidechain
1	A	98	TYR	Sidechain
2	B	77	TYR	Sidechain
2	B	99	LEU	Peptide

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	2409	0	2414	26	0
1	C	2409	0	2414	19	0
2	B	1138	0	1154	38	0
2	D	1138	0	1154	39	0
3	A	16	0	6	0	0
3	C	16	0	6	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	8	0	0	0	0
5	C	7	0	0	0	0
All	All	7143	0	7148	118	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 8.

The worst 5 of 118 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)
2:B:22:PRO:HB2	2:B:25:ILE:HD12	1.60	0.84
2:D:102:ARG:NH2	2:D:124:SER:HB3	1.94	0.83
2:D:99:LEU:HD11	2:D:134:ILE:HD12	1.64	0.78
2:D:102:ARG:HH21	2:D:124:SER:HB3	1.47	0.78
2:D:22:PRO:HB2	2:D:25:ILE:HD12	1.70	0.72

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	308/310 (99%)	298 (97%)	7 (2%)	3 (1%)	15 44
1	C	308/310 (99%)	300 (97%)	7 (2%)	1 (0%)	41 72
2	B	144/153 (94%)	122 (85%)	16 (11%)	6 (4%)	3 9
2	D	144/153 (94%)	130 (90%)	12 (8%)	2 (1%)	11 34
All	All	904/926 (98%)	850 (94%)	42 (5%)	12 (1%)	12 36

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	VAL
2	B	10	GLU
2	B	152	ALA
2	B	131	ALA
2	D	131	ALA

5.3.2 Protein sidechains (i)

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	260/260 (100%)	232 (89%)	28 (11%)	6 19
1	C	260/260 (100%)	245 (94%)	15 (6%)	20 50
2	B	129/136 (95%)	112 (87%)	17 (13%)	4 12
2	D	129/136 (95%)	112 (87%)	17 (13%)	4 12
All	All	778/792 (98%)	701 (90%)	77 (10%)	8 23

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	271	ASP
2	D	98	SER
1	C	285	TYR
2	D	36	THR
2	D	151	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	70	GLN
1	C	291	ASN
2	B	84	ASN
2	D	20	HIS
1	C	60	GLN

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 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	PAL	C	311	-	15,15,15	1.23	3 (20%)	20,21,21	1.77	2 (10%)
3	PAL	A	311	-	15,15,15	1.46	4 (26%)	20,21,21	1.29	3 (15%)

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	PAL	C	311	-	-	2/17/17/17	-
3	PAL	A	311	-	-	0/17/17/17	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	311	PAL	P-O1P	3.04	1.56	1.50
3	A	311	PAL	P-C1P	2.88	1.84	1.79
3	C	311	PAL	P-O1P	2.40	1.55	1.50
3	A	311	PAL	O3-C4	-2.36	1.22	1.30
3	C	311	PAL	O3-C4	-2.27	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	311	PAL	C4-C2-N2	5.93	124.59	110.55
3	C	311	PAL	C3-C2-N2	-3.35	104.05	110.60
3	A	311	PAL	C4-C2-N2	2.40	116.24	110.55
3	A	311	PAL	O3P-P-O1P	-2.11	106.80	112.39
3	A	311	PAL	O3-C4-C2	2.00	120.05	113.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	311	PAL	C2-C3-C5-O5
3	C	311	PAL	C2-C3-C5-O4

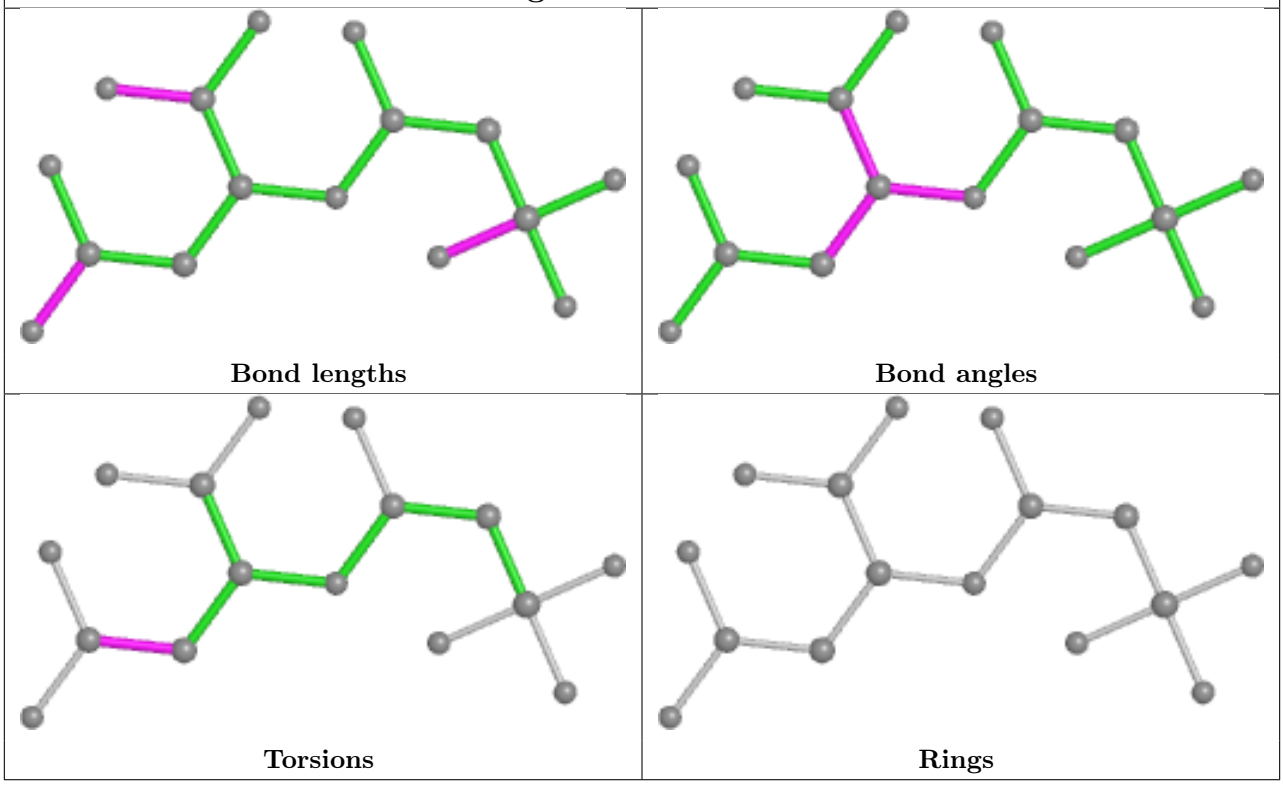
There are no ring outliers.

No monomer is involved in short contacts.

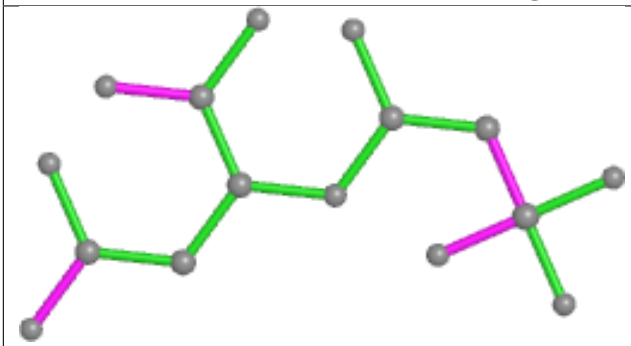
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 then 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.

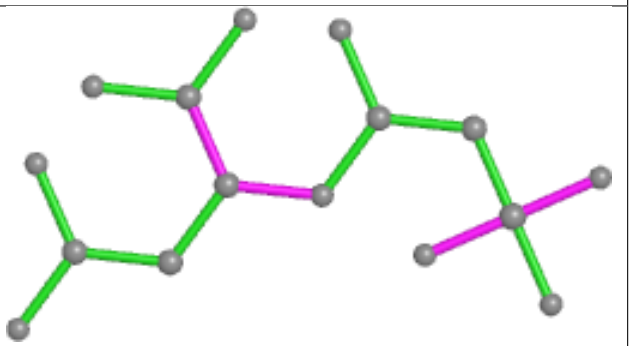
Ligand PAL C 311



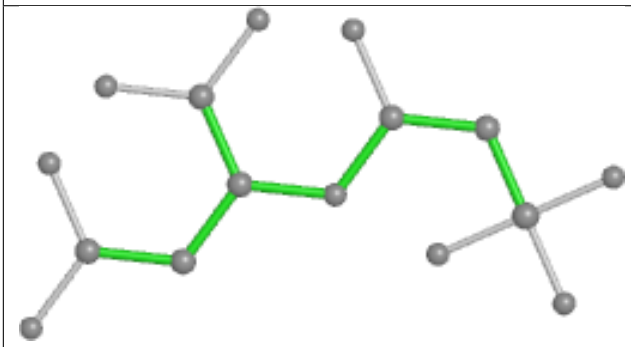
Ligand PAL A 311



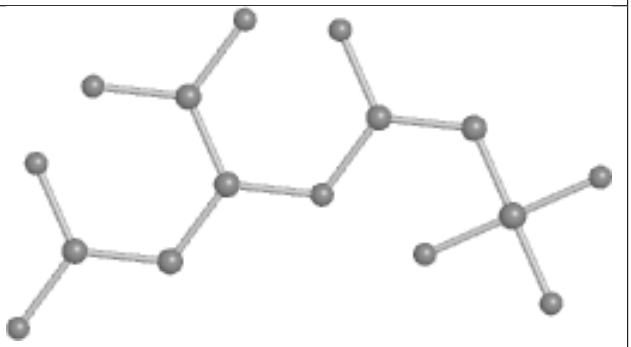
Bond lengths



Bond angles



Torsions



Rings

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.