



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2026 – 06:14 PM UTC

PDB ID : 6SJY / pdb_00006sjy
Title : Diaminobutyrate acetyltransferase EctA from *Paenibacillus lautus* in complex with its product ADABA
Authors : Richter, A.A.; Kobus, S.; Czech, L.; Hoepfner, A.; Bremer, E.; Smits, S.H.J.
Deposited on : 2019-08-14
Resolution : 2.20 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)	:	2.0
EDS	:	FAILED
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

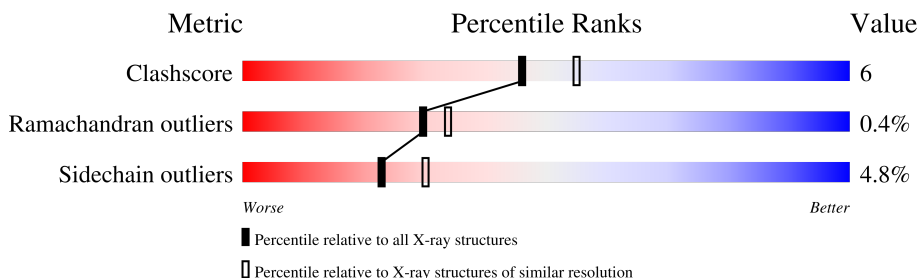
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	181	
1	B	181	
1	C	181	

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
4	TRS	B	203	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4233 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 L-2,4-diaminobutyric acid acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	0	1	0
			1312	829	223	251	9			
1	C	162	Total	C	N	O	S	0	2	0
			1280	811	219	241	9			
1	B	175	Total	C	N	O	S	0	1	0
			1362	863	230	260	9			

There are 33 discrepancies between the modelled and reference sequences:

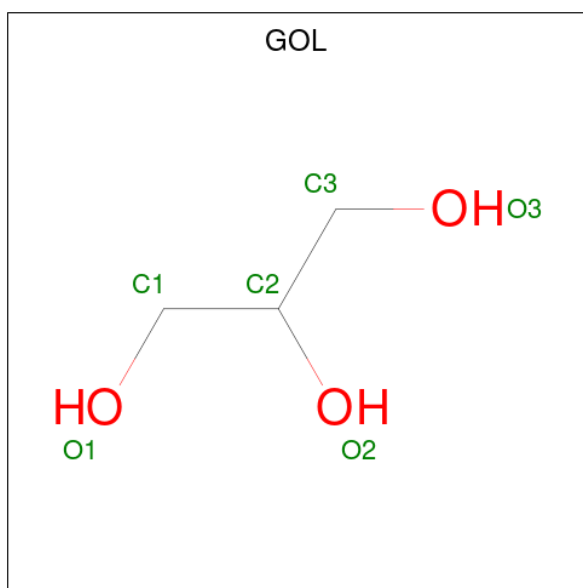
Chain	Residue	Modelled	Actual	Comment	Reference
A	171	GLY	-	expression tag	UNP D3EKC1
A	172	SER	-	expression tag	UNP D3EKC1
A	173	ALA	-	expression tag	UNP D3EKC1
A	174	TRP	-	expression tag	UNP D3EKC1
A	175	SER	-	expression tag	UNP D3EKC1
A	176	HIS	-	expression tag	UNP D3EKC1
A	177	PRO	-	expression tag	UNP D3EKC1
A	178	GLN	-	expression tag	UNP D3EKC1
A	179	PHE	-	expression tag	UNP D3EKC1
A	180	GLU	-	expression tag	UNP D3EKC1
A	181	LYS	-	expression tag	UNP D3EKC1
C	171	GLY	-	expression tag	UNP D3EKC1
C	172	SER	-	expression tag	UNP D3EKC1
C	173	ALA	-	expression tag	UNP D3EKC1
C	174	TRP	-	expression tag	UNP D3EKC1
C	175	SER	-	expression tag	UNP D3EKC1
C	176	HIS	-	expression tag	UNP D3EKC1
C	177	PRO	-	expression tag	UNP D3EKC1
C	178	GLN	-	expression tag	UNP D3EKC1
C	179	PHE	-	expression tag	UNP D3EKC1
C	180	GLU	-	expression tag	UNP D3EKC1
C	181	LYS	-	expression tag	UNP D3EKC1
B	171	GLY	-	expression tag	UNP D3EKC1

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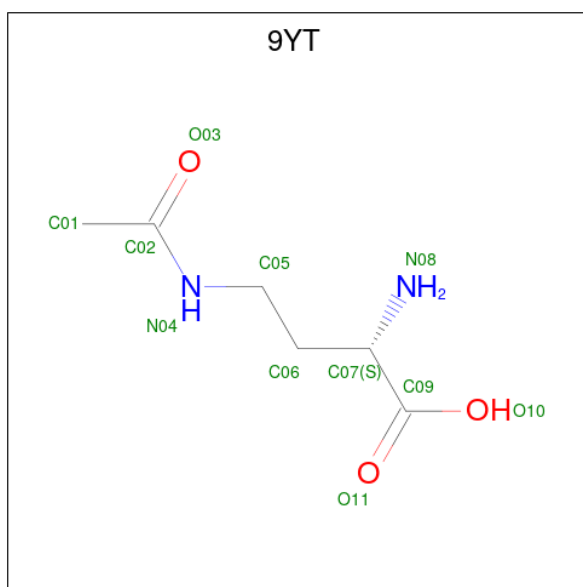
Chain	Residue	Modelled	Actual	Comment	Reference
B	172	SER	-	expression tag	UNP D3EKC1
B	173	ALA	-	expression tag	UNP D3EKC1
B	174	TRP	-	expression tag	UNP D3EKC1
B	175	SER	-	expression tag	UNP D3EKC1
B	176	HIS	-	expression tag	UNP D3EKC1
B	177	PRO	-	expression tag	UNP D3EKC1
B	178	GLN	-	expression tag	UNP D3EKC1
B	179	PHE	-	expression tag	UNP D3EKC1
B	180	GLU	-	expression tag	UNP D3EKC1
B	181	LYS	-	expression tag	UNP D3EKC1

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



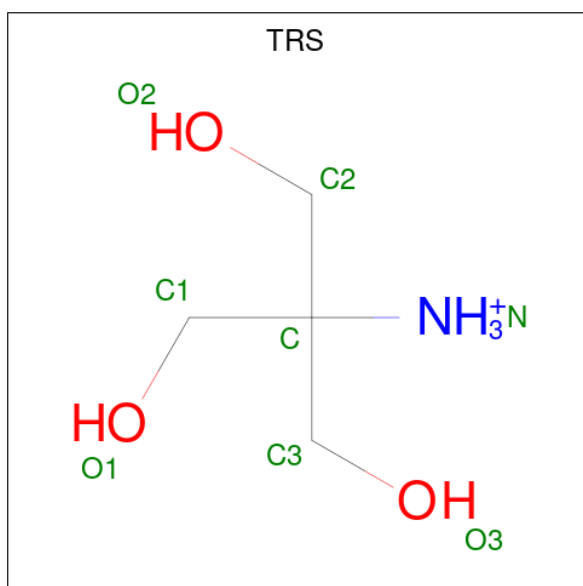
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0

- Molecule 3 is (2 {S})-4-acetamido-2-azanyl-butanoic acid (CCD ID: 9YT) (formula: $C_6H_{12}N_2O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	6	2	3		
3	C	1	Total	C	N	O	0	0
			11	6	2	3		
3	B	1	Total	C	N	O	0	0
			11	6	2	3		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is water.

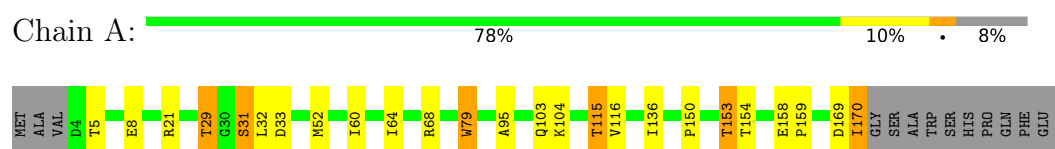
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	60	Total	O	0	0
			60	60		
5	C	83	Total	O	0	0
			83	83		
5	B	77	Total	O	0	0
			77	77		

3 Residue-property plots [i](#)

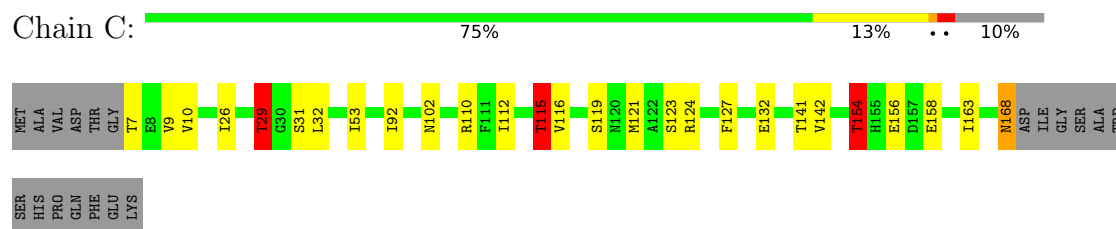
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

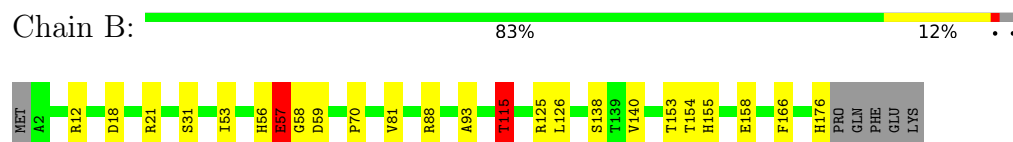
- Molecule 1: L-2,4-diaminobutyric acid acetyltransferase



- Molecule 1: L-2,4-diaminobutyric acid acetyltransferase



- Molecule 1: L-2,4-diaminobutyric acid acetyltransferase



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	174.21Å 174.21Å 60.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	123.19 – 2.20	Depositor
% Data completeness (in resolution range)	100.0 (123.19-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.167 , 0.207	Depositor
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.078	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4233	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: TRS, 9YT, GOL

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	1.36	6/1347 (0.4%)	1.18	1/1830 (0.1%)
1	B	1.36	5/1400 (0.4%)	1.18	7/1903 (0.4%)
1	C	1.28	4/1318 (0.3%)	1.22	4/1790 (0.2%)
All	All	1.33	15/4065 (0.4%)	1.19	12/5523 (0.2%)

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	TRP	C-O	-7.88	1.17	1.23
1	B	115	THR	CB-CG2	-6.02	1.32	1.52
1	C	29	THR	CB-CG2	-5.78	1.33	1.52
1	B	166	PHE	C-O	-5.69	1.16	1.24
1	A	5	THR	CA-C	5.66	1.60	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	SER	N-CA-C	7.55	121.75	112.54
1	C	29	THR	N-CA-CB	-6.96	98.84	110.39
1	B	57	GLU	N-CA-C	-6.24	97.52	110.80
1	A	31	SER	N-CA-C	6.22	120.33	112.87
1	C	154	THR	CB-CA-C	5.81	120.99	111.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	ASP	Peptide

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	1312	0	1256	15	0
1	B	1362	0	1290	14	0
1	C	1280	0	1230	15	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
3	A	11	0	0	3	0
3	B	11	0	0	0	0
3	C	11	0	0	1	0
4	B	8	0	11	3	0
5	A	60	0	0	3	0
5	B	77	0	0	4	0
5	C	83	0	0	0	0
All	All	4233	0	3811	45	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 6.

The worst 5 of 45 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:33:ASP:HA	5:A:345:HOH:O	1.58	1.03
1:B:57:GLU:CB	1:B:58:GLY:HA3	1.99	0.93
1:A:115:THR:HG23	1:A:158:GLU:OE1	1.72	0.88
1:C:29:THR:HG22	1:C:31:SER:H	1.41	0.85
1:B:57:GLU:HB2	1:B:58:GLY:HA3	1.58	0.84

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	166/181 (92%)	162 (98%)	3 (2%)	1 (1%)	21	23
1	B	174/181 (96%)	170 (98%)	3 (2%)	1 (1%)	21	23
1	C	162/181 (90%)	160 (99%)	2 (1%)	0	100	100
All	All	502/543 (92%)	492 (98%)	8 (2%)	2 (0%)	30	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	57	GLU
1	A	153	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	142/153 (93%)	137 (96%)	5 (4%)	32	43
1	B	145/153 (95%)	141 (97%)	4 (3%)	38	52
1	C	138/153 (90%)	127 (92%)	11 (8%)	11	13
All	All	425/459 (93%)	405 (95%)	20 (5%)	23	31

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	154	THR

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Mol	Chain	Res	Type
1	B	115	THR
1	B	176	HIS
1	B	138	SER
1	C	10	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	B	35	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 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	$\# Z > 2$
3	9YT	A	202	-	9,10,10	2.45	2 (22%)	8,12,12	3.79	5 (62%)
2	GOL	B	201	-	5,5,5	0.80	0	5,5,5	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	TRS	B	203	-	7,7,7	2.12	3 (42%)	9,9,9	2.48	5 (55%)
2	GOL	C	201	-	5,5,5	1.11	0	5,5,5	2.56	1 (20%)
2	GOL	A	201	-	5,5,5	0.79	0	5,5,5	0.89	0
3	9YT	B	202	-	9,10,10	2.20	1 (11%)	8,12,12	2.67	4 (50%)
3	9YT	C	202	-	9,10,10	2.07	2 (22%)	8,12,12	3.23	4 (50%)

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	9YT	A	202	-	-	4/10/10/10	-
2	GOL	B	201	-	-	0/4/4/4	-
4	TRS	B	203	-	-	6/9/9/9	-
2	GOL	C	201	-	-	4/4/4/4	-
2	GOL	A	201	-	-	0/4/4/4	-
3	9YT	B	202	-	-	3/10/10/10	-
3	9YT	C	202	-	-	2/10/10/10	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202	9YT	C02-N04	6.16	1.50	1.34
3	B	202	9YT	C02-N04	5.45	1.48	1.34
3	C	202	9YT	C02-N04	5.05	1.47	1.34
4	B	203	TRS	C2-C	-3.81	1.42	1.53
4	B	203	TRS	C1-C	-3.18	1.44	1.53

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202	9YT	O03-C02-N04	6.16	137.94	121.78
3	A	202	9YT	C01-C02-N04	-5.86	106.12	116.12
3	C	202	9YT	C01-C02-N04	5.84	126.08	116.12
3	B	202	9YT	C01-C02-N04	5.66	125.78	116.12
3	C	202	9YT	C05-N04-C02	5.25	130.31	122.56

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

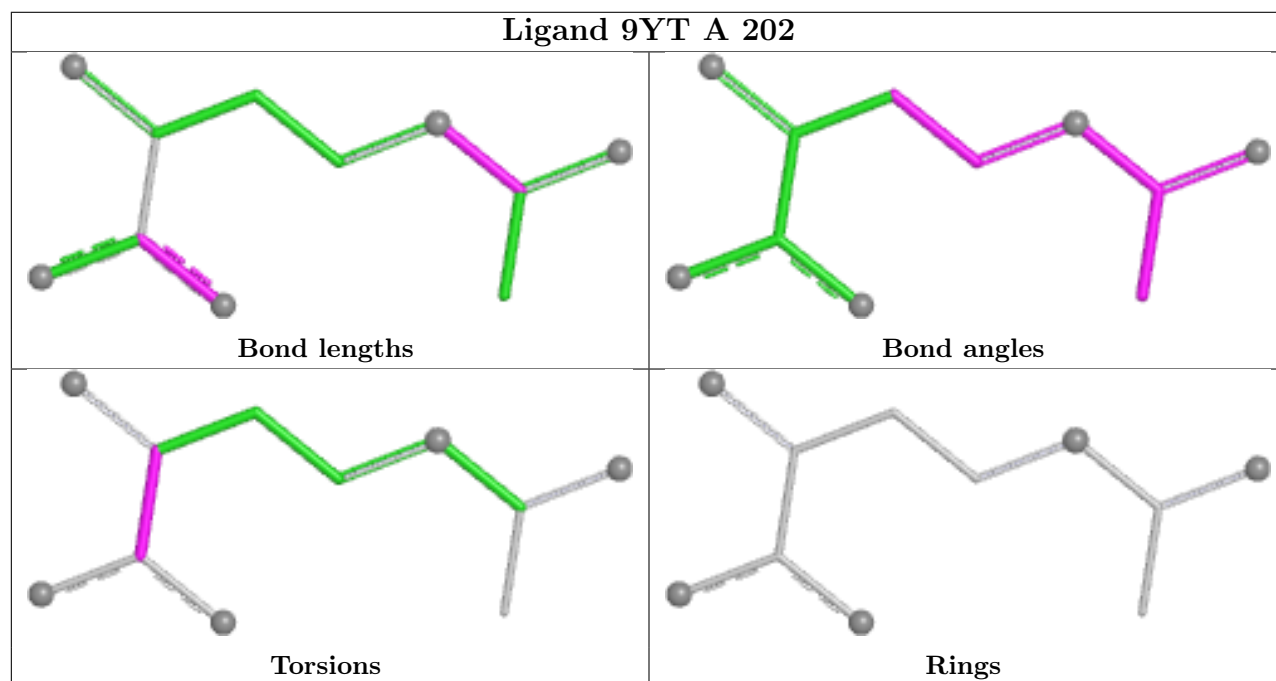
Mol	Chain	Res	Type	Atoms
2	C	201	GOL	O1-C1-C2-C3
2	C	201	GOL	C1-C2-C3-O3
3	A	202	9YT	N08-C07-C09-O11
4	B	203	TRS	C2-C-C3-O3
4	B	203	TRS	N-C-C3-O3

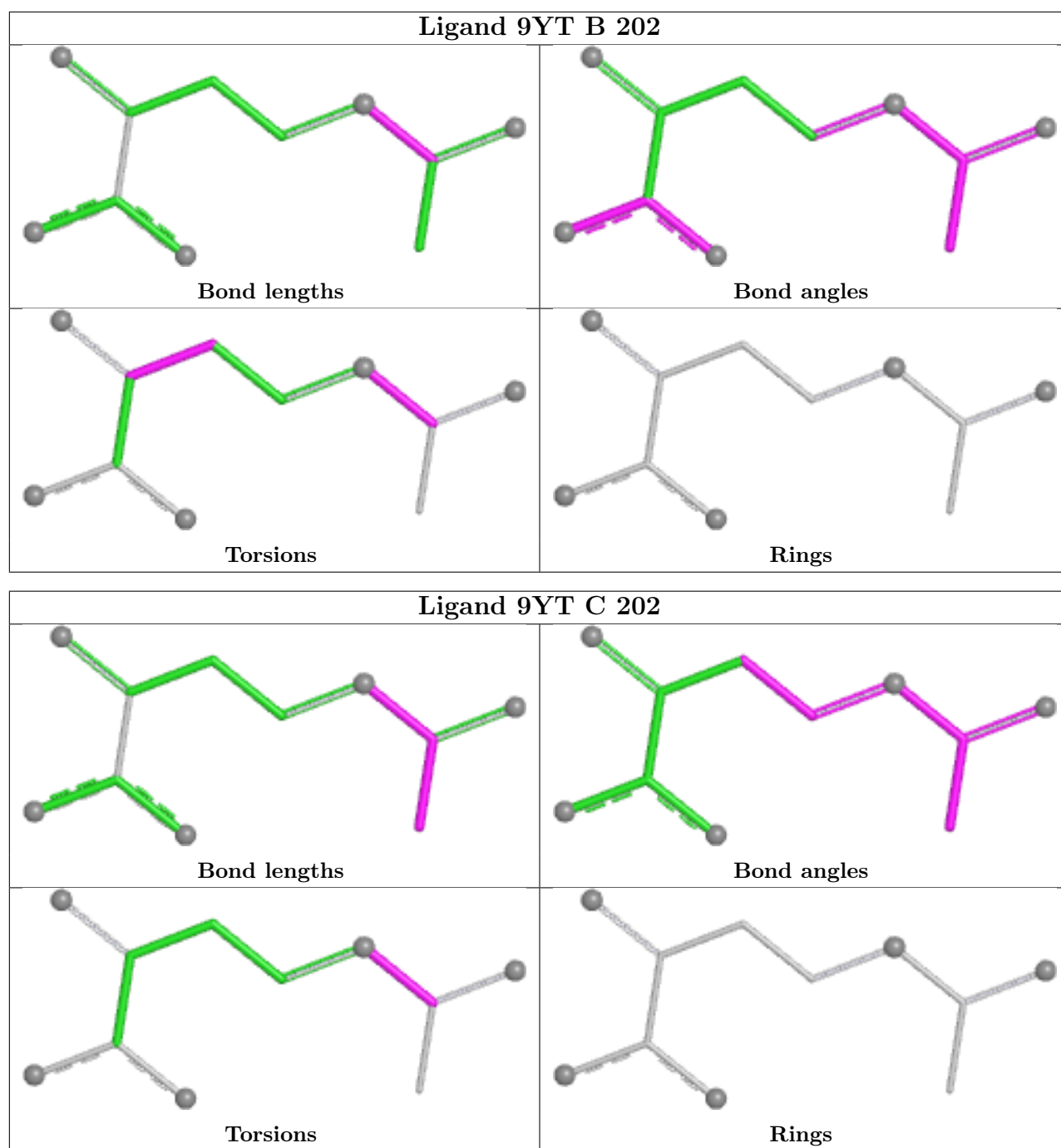
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	202	9YT	3	0
4	B	203	TRS	3	0
3	C	202	9YT	1	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 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.