



# wwPDB EM Model Validation Summary Report ⓘ

May 28, 2020 – 01:17 PM EDT

PDB ID : 6TBU  
EMDB ID : EMD-10452  
Title : Structure of Drosophila melanogaster Dispatched  
Authors : Korkhov, V.M.; Cannac, F.  
Deposited on : 2019-11-04  
Resolution : 3.16 Å(reported)

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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)  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.10.1

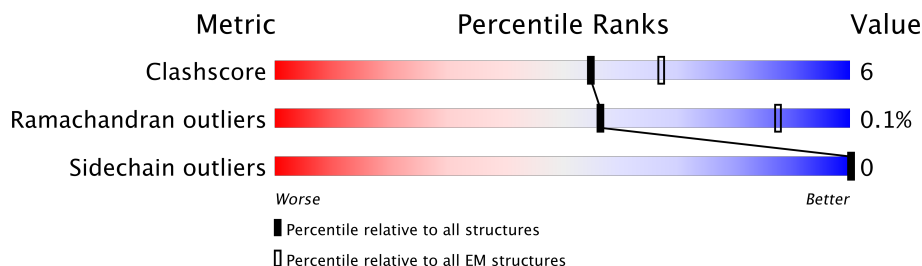
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.16 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	1218	

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
3	NAG	A	1512	X	-	-	-



In the tables below, 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.

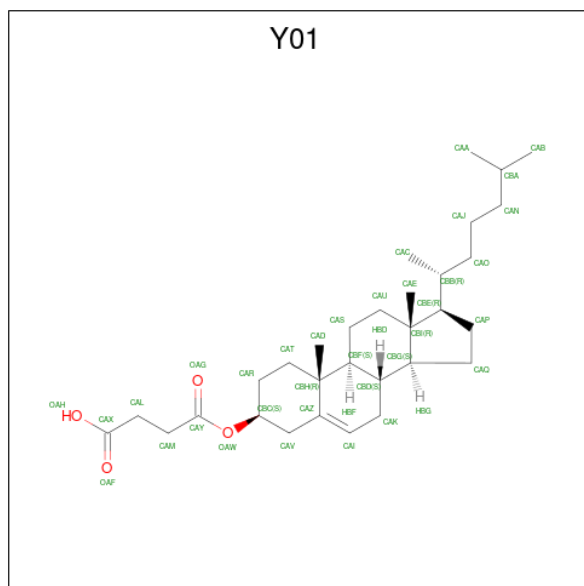
- Molecule 1 is a protein called Protein dispatched.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	842	Total	C	H	N	O	S	0	0
			13376	4440	6645	1055	1186	50		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	731	TYR	GLU	conflict	UNP Q9VNIJ5

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula:  $C_{31}H_{50}O_4$ ).



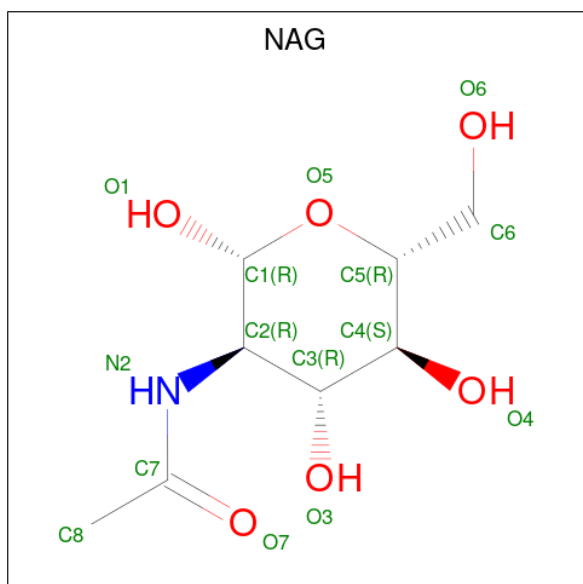
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total 756	C 279	H 441	O 36	0
2	A	1	Total 756	C 279	H 441	O 36	0
2	A	1	Total 756	C 279	H 441	O 36	0

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Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	H	O	0
			756	279	441	36	
2	A	1	Total	C	H	O	0
			756	279	441	36	
2	A	1	Total	C	H	O	0
			756	279	441	36	
2	A	1	Total	C	H	O	0
			756	279	441	36	
2	A	1	Total	C	H	O	0
			756	279	441	36	

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	N	O	0
			80	24	38	3	15	
3	A	1	Total	C	H	N	O	0
			80	24	38	3	15	
3	A	1	Total	C	H	N	O	0
			80	24	38	3	15	



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	286136	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y01, NAG

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	0.35	0/6915	0.57	15/9413 (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	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	1048	LEU	CB-CG-CD2	6.77	122.50	111.00
1	A	983	VAL	CG1-CB-CG2	6.56	121.39	110.90
1	A	1009	LEU	CB-CG-CD2	6.45	121.97	111.00
1	A	337	LEU	CB-CG-CD1	6.05	121.29	111.00
1	A	483	LEU	CB-CG-CD2	5.93	121.09	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	369	LEU	Peptide
1	A	422	ILE	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	6731	6645	6637	71	0
2	A	315	441	439	18	0
3	A	42	38	38	0	0
All	All	7088	7124	7114	83	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 83 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:1017:GLU:OE2	1:A:1086:GLN:NE2	2.21	0.74
1:A:17:ALA:O	1:A:627:ARG:NH2	2.21	0.74
1:A:698:GLU:O	1:A:914:THR:OG1	2.06	0.71
1:A:576:VAL:HG12	1:A:1033:LEU:HD13	1.74	0.70
1:A:842:TYR:O	1:A:846:GLN:NE2	2.26	0.69

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 PDB entries followed by that with respect to all EM entries.

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	820/1218 (67%)	778 (95%)	41 (5%)	1 (0%)	53 86

All (1) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	370	ASN

### 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 PDB entries followed by that with respect to all EM entries.

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	736/1087 (68%)	736 (100%)	0	100	100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	954	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 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	Y01	A	1506	-	35,38,38	1.92	8 (22%)	54,57,57	3.04	26 (48%)
2	Y01	A	1501	1	35,38,38	2.27	12 (34%)	54,57,57	3.77	28 (51%)
2	Y01	A	1502	-	35,38,38	1.85	6 (17%)	54,57,57	3.22	28 (51%)
3	NAG	A	1510	1	14,14,15	0.18	0	17,19,21	0.51	0
2	Y01	A	1507	-	35,38,38	1.81	7 (20%)	54,57,57	3.21	27 (50%)
2	Y01	A	1509	-	35,38,38	1.82	8 (22%)	54,57,57	3.17	29 (53%)
2	Y01	A	1503	-	35,38,38	1.83	7 (20%)	54,57,57	3.12	25 (46%)
2	Y01	A	1504	-	35,38,38	1.90	6 (17%)	54,57,57	3.25	28 (51%)
3	NAG	A	1512	3	14,14,15	0.30	0	17,19,21	1.02	2 (11%)
2	Y01	A	1508	-	35,38,38	1.96	9 (25%)	54,57,57	3.13	24 (44%)
2	Y01	A	1505	-	35,38,38	1.83	7 (20%)	54,57,57	3.24	26 (48%)
3	NAG	A	1511	1,3	14,14,15	0.23	0	17,19,21	0.48	0

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	Y01	A	1506	-	-	10/17/77/77	0/4/4/4
2	Y01	A	1501	1	-	8/17/77/77	0/4/4/4
2	Y01	A	1502	-	-	7/17/77/77	0/4/4/4
3	NAG	A	1510	1	-	0/6/23/26	0/1/1/1
2	Y01	A	1507	-	-	9/17/77/77	0/4/4/4
2	Y01	A	1509	-	-	5/17/77/77	0/4/4/4
2	Y01	A	1503	-	-	6/17/77/77	0/4/4/4
2	Y01	A	1504	-	-	11/17/77/77	0/4/4/4
3	NAG	A	1512	3	1/1/6/7	3/6/23/26	0/1/1/1
2	Y01	A	1508	-	-	3/17/77/77	0/4/4/4
2	Y01	A	1505	-	-	6/17/77/77	0/4/4/4
3	NAG	A	1511	1,3	-	2/6/23/26	0/1/1/1

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1504	Y01	CAE-CBI	6.27	1.65	1.54
2	A	1501	Y01	CAE-CBI	5.95	1.64	1.54
2	A	1506	Y01	CAE-CBI	5.82	1.64	1.54
2	A	1502	Y01	CAE-CBI	5.78	1.64	1.54
2	A	1505	Y01	CAE-CBI	5.70	1.64	1.54

The worst 5 of 243 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1501	Y01	CBD-CAK-CAI	-12.43	94.88	112.73
2	A	1501	Y01	CBC-CAV-CAZ	8.02	123.97	111.52
2	A	1502	Y01	CBG-CBI-CBE	-8.01	90.58	100.07
2	A	1501	Y01	CAD-CBH-CAZ	-7.83	95.67	108.34
2	A	1504	Y01	CBG-CBI-CBE	-7.80	90.83	100.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1512	NAG	C1

5 of 70 torsion outliers are listed below:

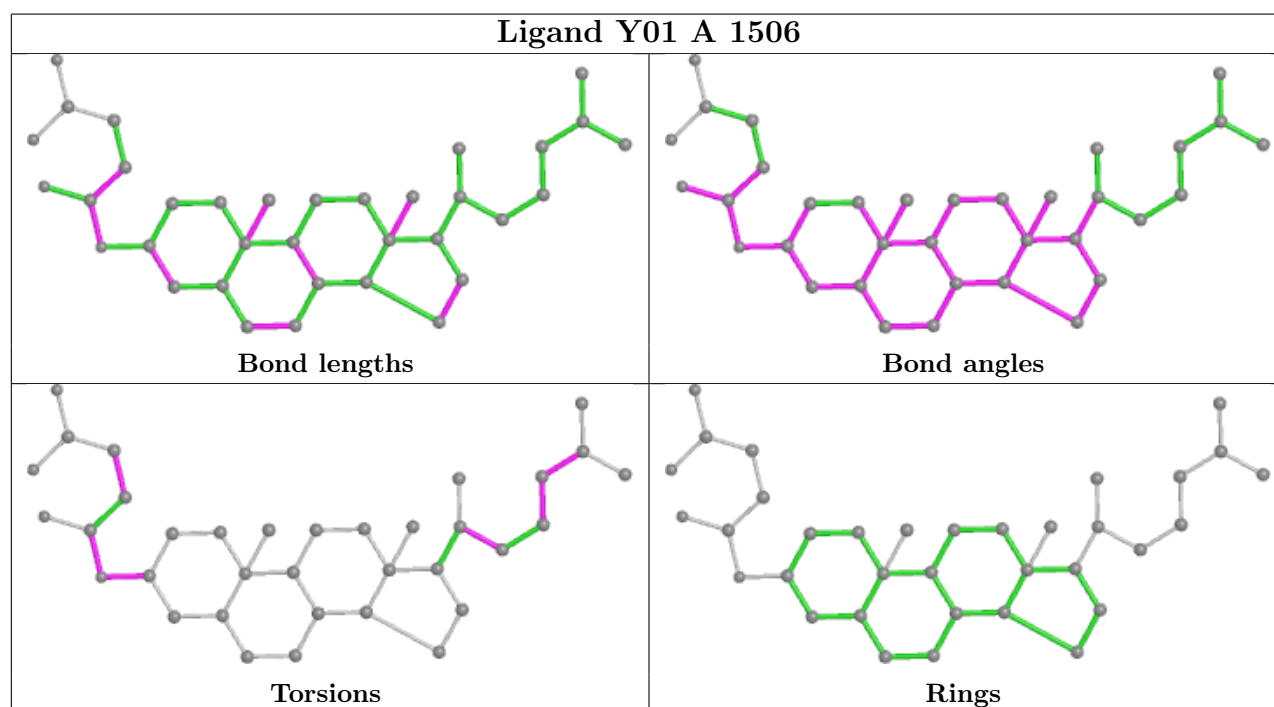
Mol	Chain	Res	Type	Atoms
2	A	1506	Y01	OAG-CAY-OAW-CBC
2	A	1506	Y01	CAM-CAY-OAW-CBC
2	A	1501	Y01	OAG-CAY-OAW-CBC
2	A	1501	Y01	CAM-CAY-OAW-CBC
2	A	1502	Y01	OAG-CAY-OAW-CBC

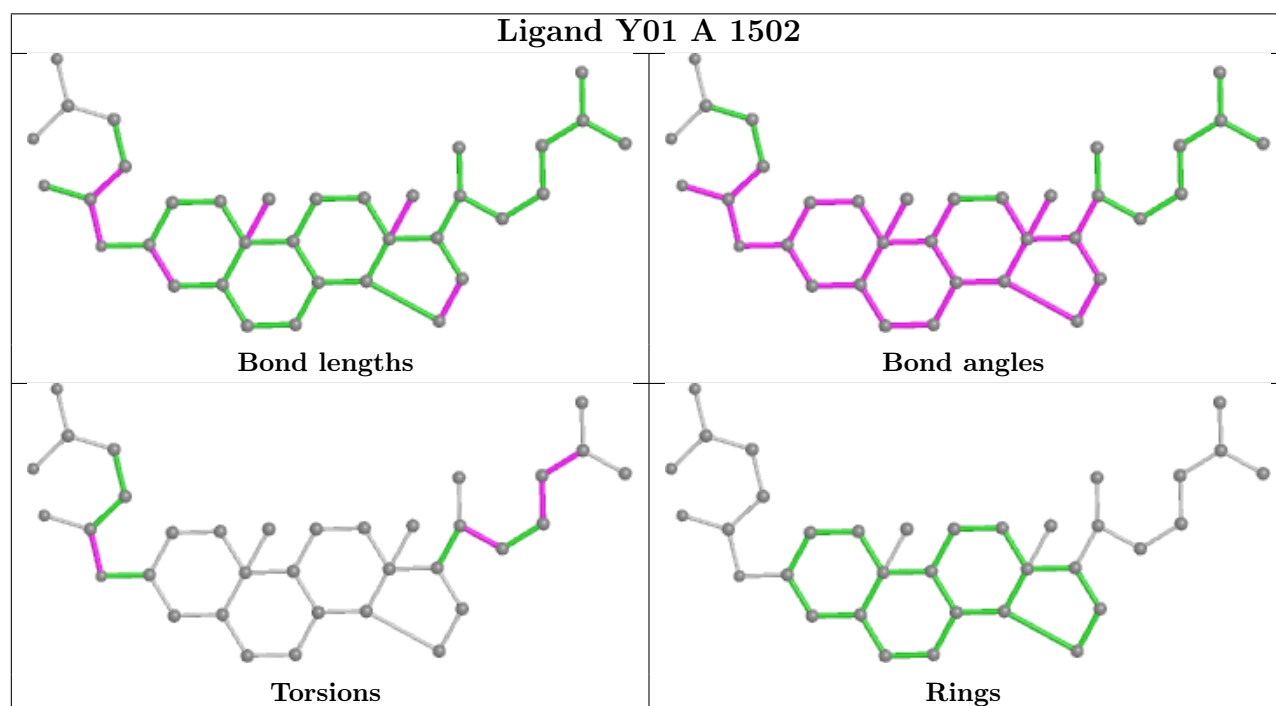
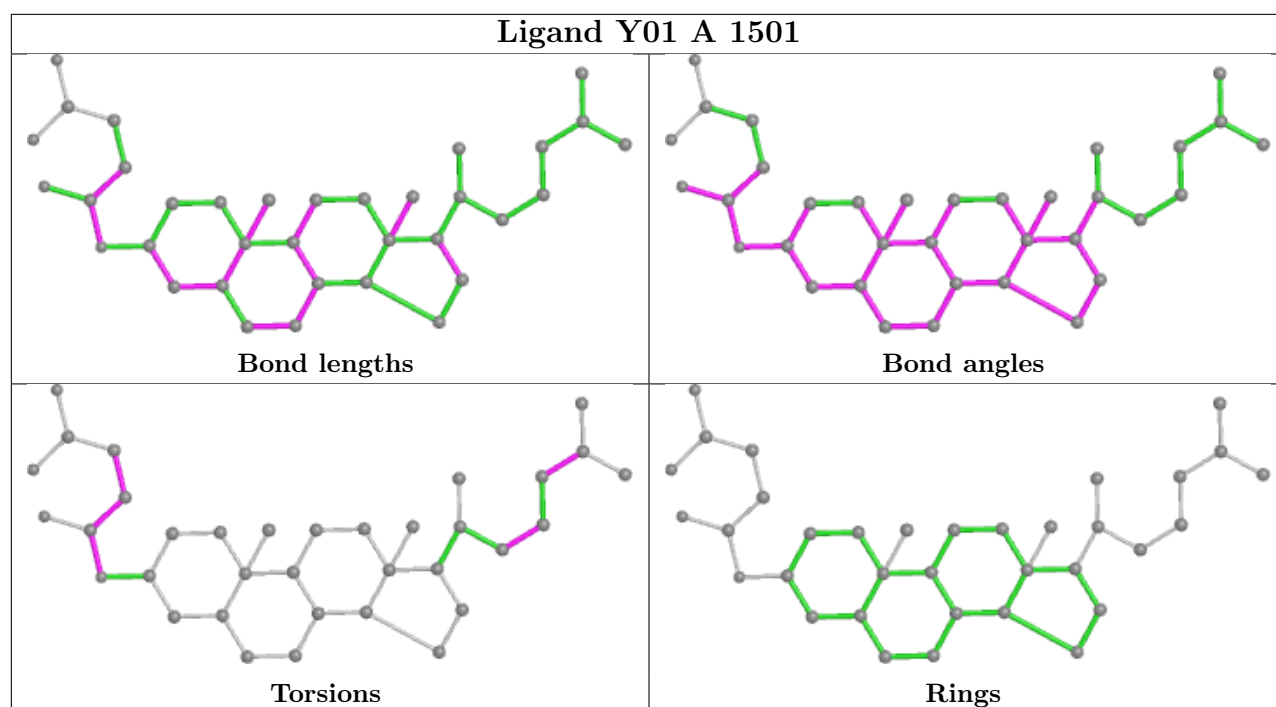
There are no ring outliers.

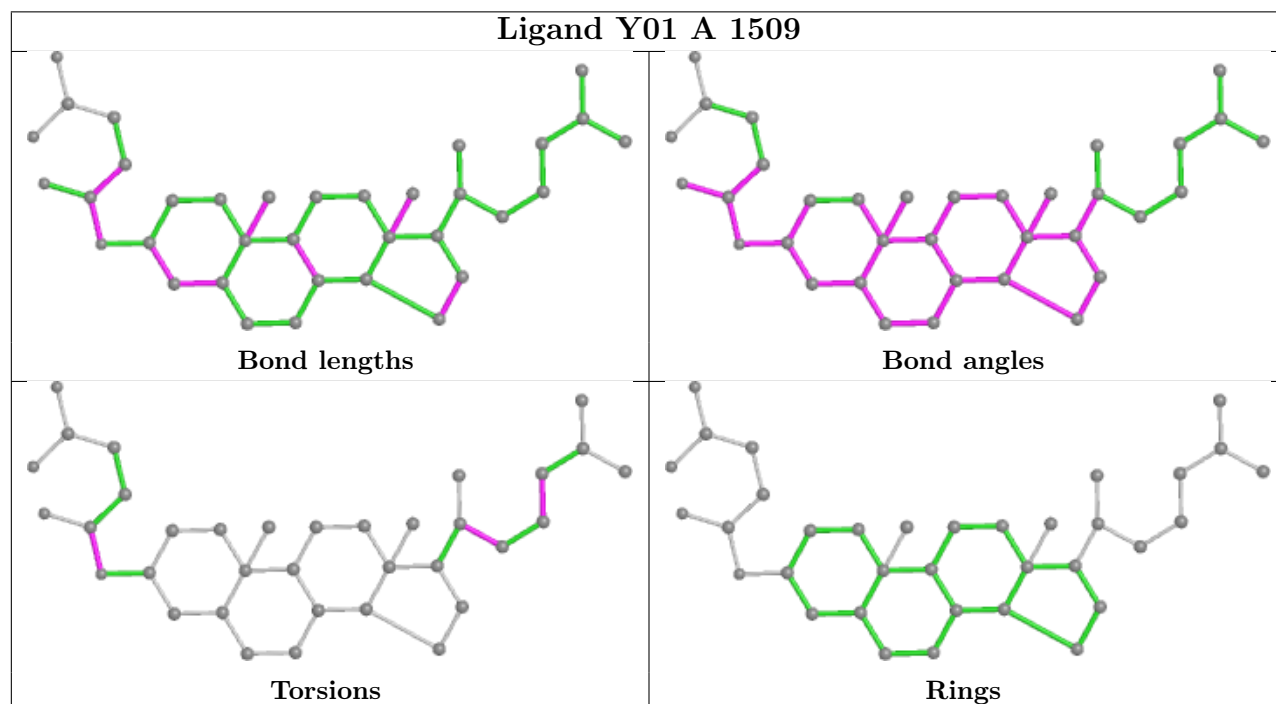
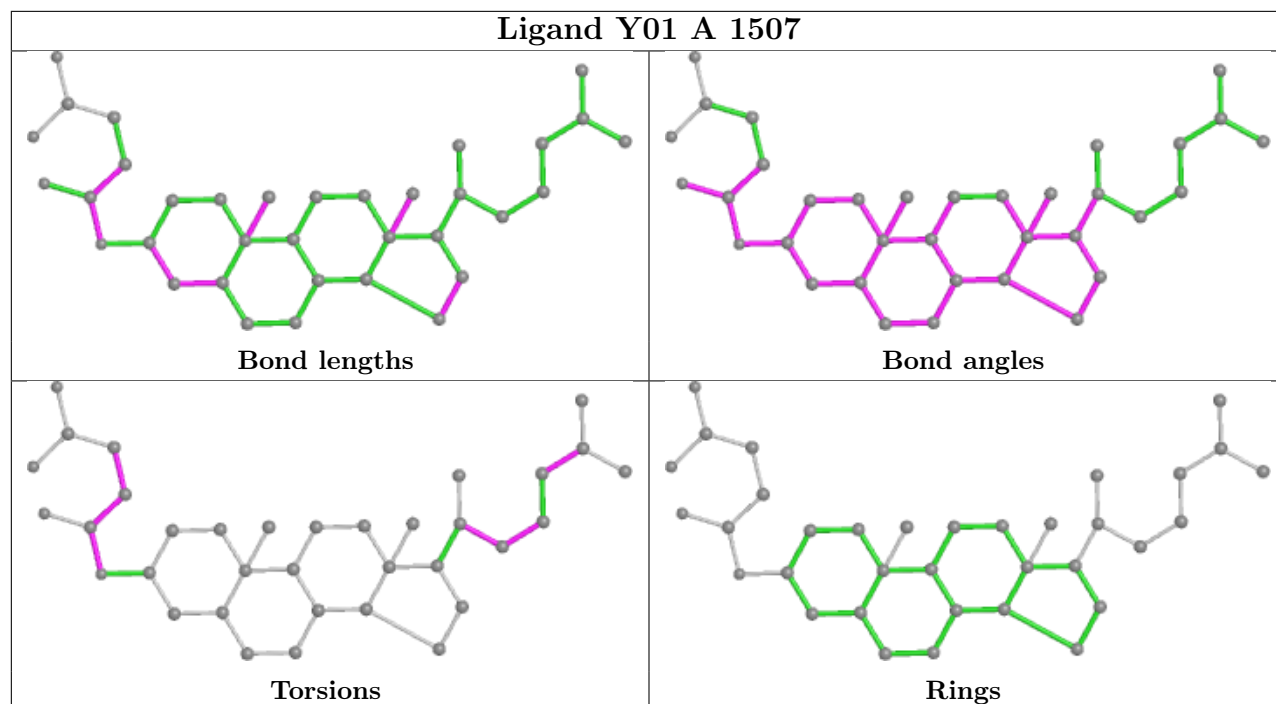
9 monomers are involved in 18 short contacts:

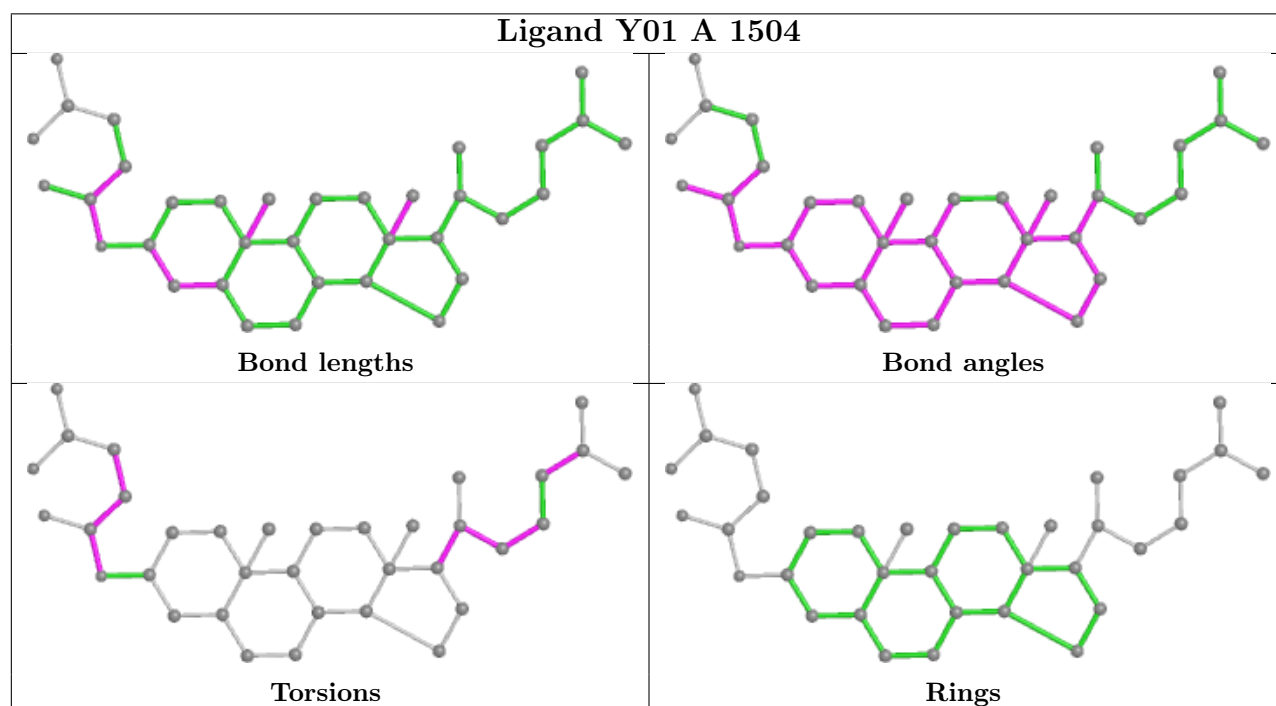
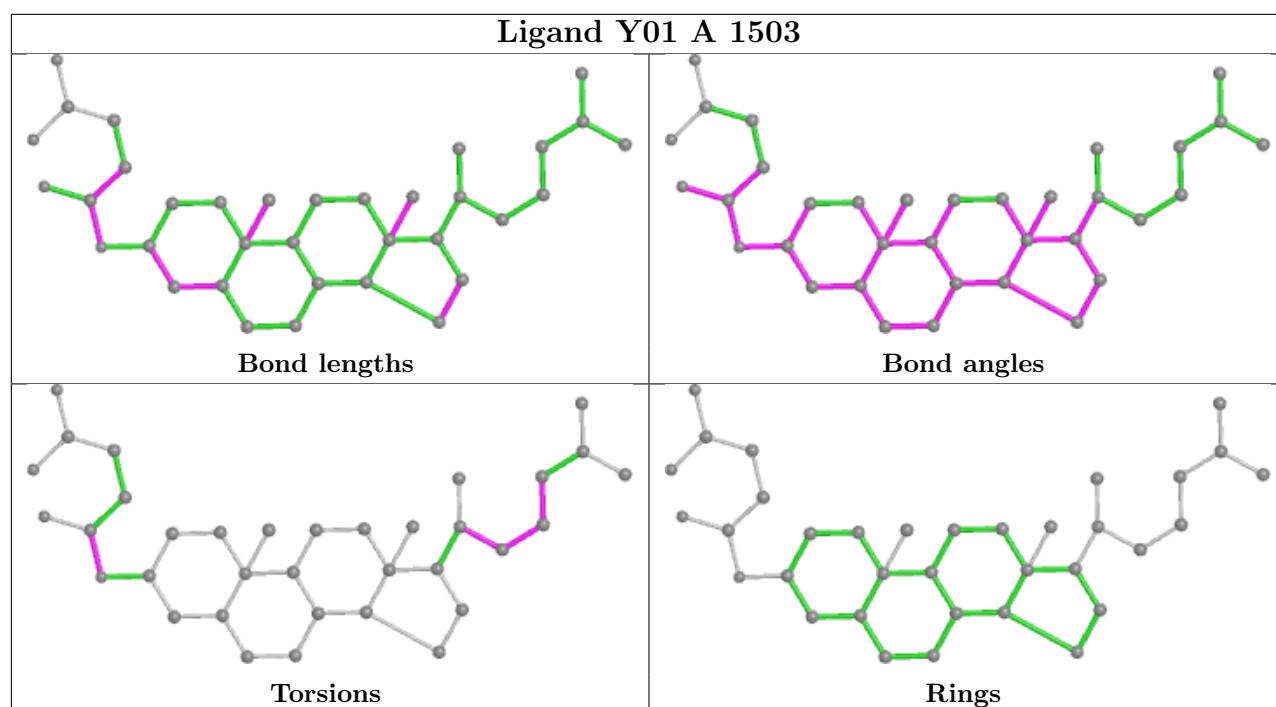
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1506	Y01	5	0
2	A	1501	Y01	2	0
2	A	1502	Y01	2	0
2	A	1507	Y01	2	0
2	A	1509	Y01	1	0
2	A	1503	Y01	1	0
2	A	1504	Y01	1	0
2	A	1508	Y01	1	0
2	A	1505	Y01	3	0

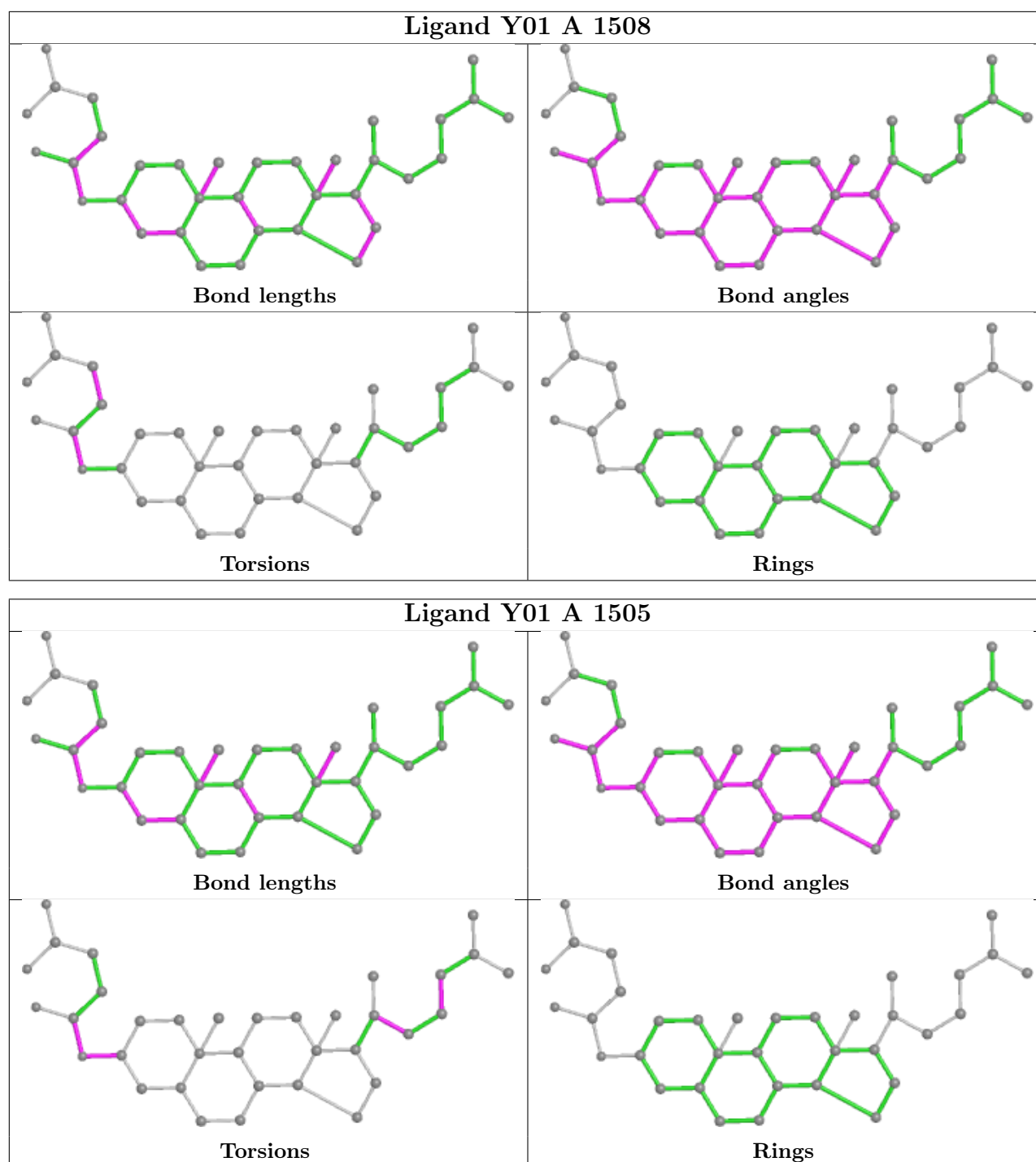
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.