



Full wwPDB EM Model Validation 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 Full wwPDB EM Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at 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.

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

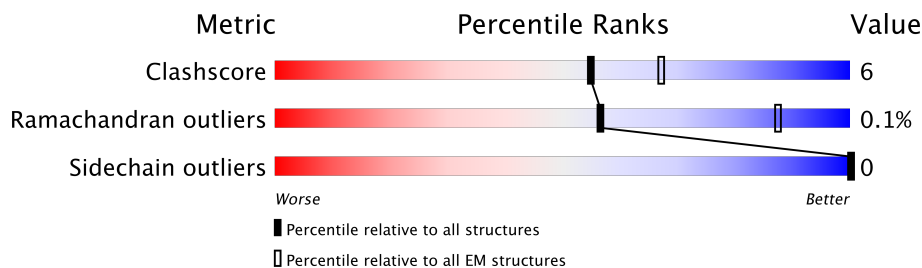
1 Overall quality at a glance

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 ≥ 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	-	-	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 14212 atoms, of which 7124 are hydrogens and 0 are deuteriums.

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.

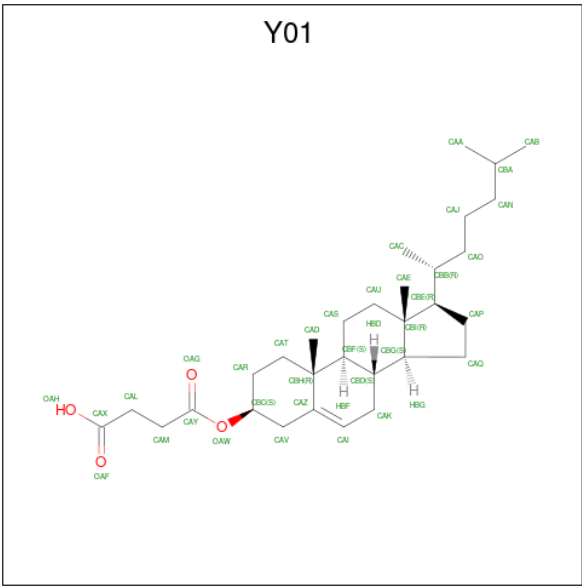
- Molecule 1 is a protein called Protein dispatched.

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 Q9VNJ5

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C₃₁H₅₀O₄).



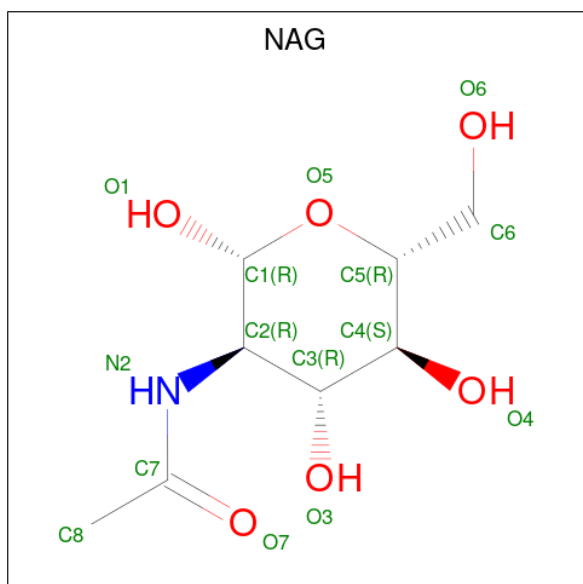
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	H	O	0
			756	279	441	36	
2	A	1	Total	C	H	O	0
			756	279	441	36	
2	A	1	Total	C	H	O	0
			756	279	441	36	

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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: $C_8H_{15}NO_6$).

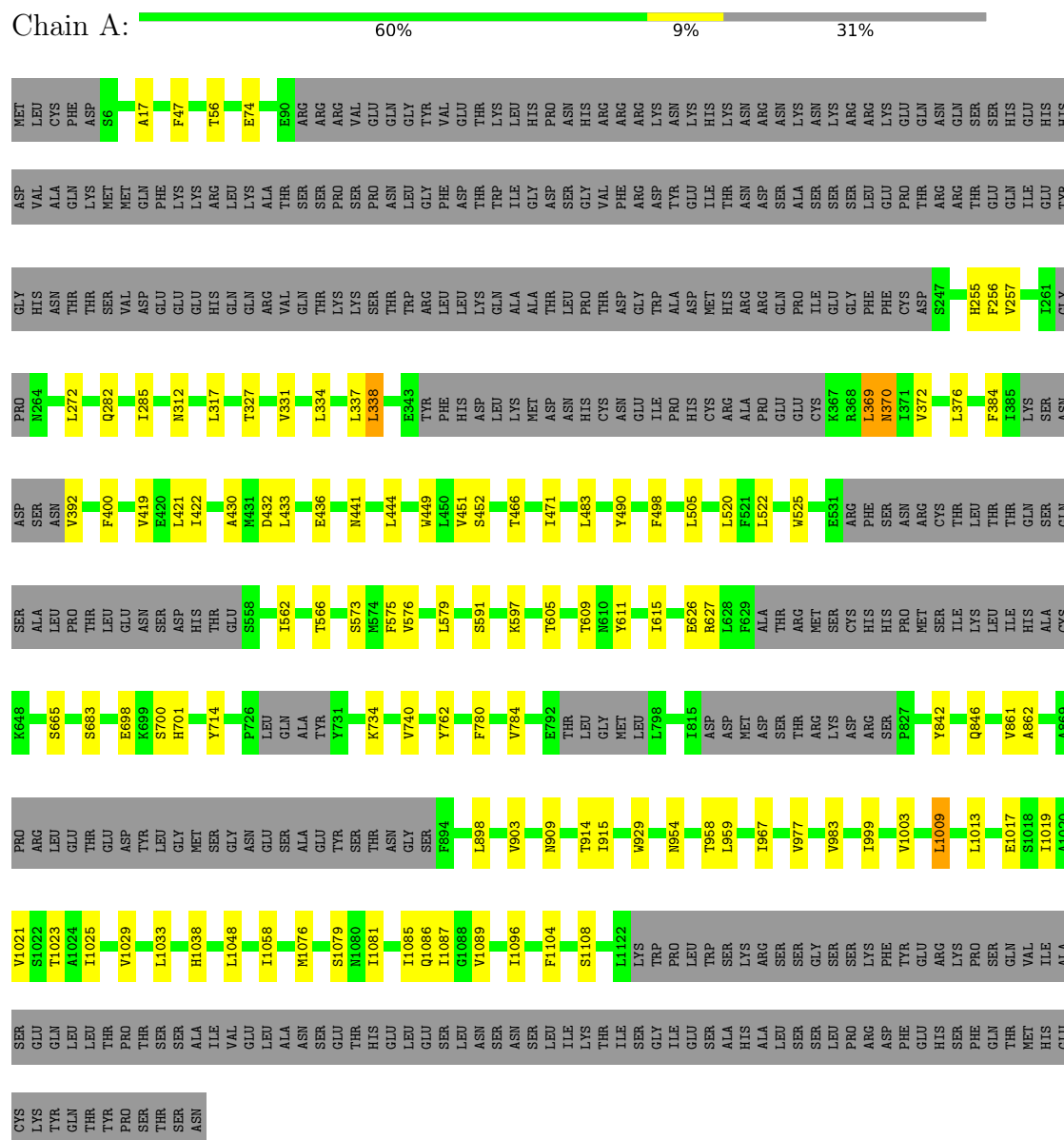


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	H	N	O	0
			80	24	38	3	15	
3	A	1	Total	C	H	N	O	0
			80	24	38	3	15	
3	A	1	Total	C	H	N	O	0
			80	24	38	3	15	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

- Molecule 1: Protein dispatched



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.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	A	421	LEU	CB-CG-CD1	5.90	121.03	111.00
1	A	338	LEU	CB-CG-CD1	5.89	121.01	111.00
1	A	898	LEU	CB-CG-CD2	5.78	120.82	111.00
1	A	334	LEU	CB-CG-CD1	5.58	120.49	111.00
1	A	334	LEU	CB-CG-CD2	5.50	120.36	111.00
1	A	338	LEU	CB-CG-CD2	5.30	120.01	111.00
1	A	421	LEU	CB-CG-CD2	5.28	119.98	111.00
1	A	898	LEU	CB-CG-CD1	5.26	119.95	111.00
1	A	483	LEU	CB-CG-CD1	5.20	119.85	111.00
1	A	337	LEU	CB-CG-CD2	5.17	119.79	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

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.

All (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
1:A:1025:ILE:O	1:A:1029:VAL:HG23	1.94	0.67
1:A:591:SER:O	1:A:597:LYS:NZ	2.28	0.67
1:A:384:PHE:O	1:A:392:VAL:N	2.28	0.67
1:A:611:TYR:CZ	1:A:615:ILE:HD11	2.30	0.67
1:A:861:VAL:HG12	1:A:903:VAL:HG21	1.81	0.63
1:A:520:LEU:HD21	1:A:573:SER:OG	1.99	0.62
1:A:444:LEU:HD12	1:A:1081:ILE:HD13	1.81	0.61
1:A:780:PHE:O	1:A:784:VAL:HG23	2.00	0.61
1:A:734:LYS:NZ	1:A:909:ASN:O	2.23	0.60
1:A:525:TRP:NE1	1:A:626:GLU:OE2	2.35	0.59
1:A:525:TRP:HE3	1:A:566:THR:HG21	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1079:SER:O	1:A:1085:ILE:HD11	2.04	0.58
2:A:1506:Y01:HAC1	2:A:1506:Y01:HAU2	1.87	0.57
1:A:505:LEU:HD22	1:A:1087:ILE:CD1	2.34	0.57
1:A:327:THR:O	1:A:331:VAL:N	2.39	0.55
1:A:784:VAL:HG22	1:A:929:TRP:HH2	1.71	0.55
1:A:1104:PHE:O	1:A:1108:SER:OG	2.16	0.55
1:A:575:PHE:CZ	1:A:579:LEU:HD12	2.42	0.55
1:A:520:LEU:HD13	1:A:1058:ILE:HD11	1.90	0.54
1:A:576:VAL:CG1	1:A:1033:LEU:HD13	2.38	0.53
1:A:272:LEU:HD13	1:A:327:THR:CB	2.39	0.52
2:A:1509:Y01:HAC1	2:A:1509:Y01:HAU2	1.91	0.52
1:A:784:VAL:HG22	1:A:929:TRP:CH2	2.45	0.52
1:A:576:VAL:HG13	1:A:977:VAL:HG11	1.93	0.51
2:A:1503:Y01:HAC1	2:A:1503:Y01:HAU2	1.93	0.51
1:A:525:TRP:CE3	1:A:566:THR:HG21	2.44	0.51
1:A:999:ILE:O	1:A:1003:VAL:HG23	2.10	0.51
1:A:1017:GLU:N	1:A:1017:GLU:OE1	2.44	0.51
1:A:432:ASP:O	1:A:433:LEU:HD23	2.10	0.50
1:A:700:SER:OG	1:A:701:HIS:N	2.45	0.50
2:A:1501:Y01:HAC1	2:A:1501:Y01:HAU2	1.94	0.50
1:A:1019:ILE:O	1:A:1023:THR:HG23	2.12	0.50
1:A:451:VAL:HG22	1:A:1076:MET:SD	2.52	0.50
1:A:505:LEU:HD13	1:A:1087:ILE:HD11	1.94	0.49
1:A:562:ILE:O	1:A:566:THR:HG22	2.12	0.49
1:A:56:THR:OG1	1:A:954:ASN:ND2	2.46	0.49
2:A:1501:Y01:HAC1	2:A:1501:Y01:CAU	2.43	0.49
2:A:1507:Y01:HAC1	2:A:1507:Y01:HAU2	1.93	0.48
1:A:282:GLN:NE2	1:A:312:ASN:OD1	2.46	0.48
1:A:449:TRP:O	1:A:452:SER:OG	2.15	0.48
1:A:430:ALA:HB1	1:A:714:TYR:HB2	1.95	0.48
1:A:257:VAL:HB	1:A:430:ALA:HB3	1.94	0.47
1:A:436:GLU:OE1	1:A:436:GLU:N	2.47	0.47
1:A:698:GLU:HB3	1:A:915:ILE:HG22	1.96	0.47
1:A:56:THR:HG21	1:A:958:THR:OG1	2.14	0.47
1:A:490:TYR:OH	1:A:498:PHE:O	2.29	0.47
2:A:1508:Y01:HAU2	2:A:1508:Y01:HAC1	1.95	0.47
1:A:967:ILE:HD11	1:A:1021:VAL:HG12	1.97	0.47
1:A:1096:ILE:HD11	2:A:1505:Y01:HAA2	1.97	0.47
1:A:740:VAL:HG22	1:A:903:VAL:HG12	1.98	0.46
1:A:471:ILE:HD13	1:A:522:LEU:HD11	1.98	0.46
1:A:317:LEU:HD11	1:A:372:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LEU:HD21	1:A:376:LEU:HD22	1.98	0.45
1:A:959:LEU:HD21	1:A:1013:LEU:HD22	1.98	0.45
1:A:256:PHE:CE2	1:A:285:ILE:HD13	2.52	0.45
1:A:1009:LEU:HD21	2:A:1506:Y01:HAK1	1.99	0.44
1:A:1009:LEU:HD11	2:A:1506:Y01:HAK2	1.99	0.44
2:A:1505:Y01:HAC1	2:A:1505:Y01:HAU2	1.99	0.44
1:A:683:SER:OG	2:A:1507:Y01:HAB2	2.18	0.44
1:A:505:LEU:HD22	1:A:1087:ILE:HD11	2.00	0.44
1:A:466:THR:HG22	1:A:522:LEU:HD13	2.00	0.43
1:A:74:GLU:OE2	1:A:762:TYR:OH	2.36	0.43
1:A:1038:HIS:CE1	1:A:1058:ILE:HD13	2.54	0.43
2:A:1502:Y01:HAC1	2:A:1502:Y01:HAU2	2.00	0.43
2:A:1506:Y01:HAS2	2:A:1506:Y01:HAD2	1.91	0.43
1:A:1009:LEU:HD11	2:A:1506:Y01:CAK	2.49	0.42
1:A:862:ALA:HA	1:A:903:VAL:HG23	2.02	0.42
1:A:665:SER:HB3	2:A:1504:Y01:HAE1	2.01	0.42
1:A:255:HIS:HB3	1:A:400:PHE:CD1	2.55	0.42
2:A:1505:Y01:CAU	2:A:1505:Y01:HAC1	2.50	0.41
1:A:369:LEU:HD23	1:A:370:ASN:H	1.84	0.41
1:A:1009:LEU:HD13	1:A:1089:VAL:HG11	2.02	0.41
1:A:419:VAL:O	1:A:419:VAL:HG23	2.20	0.41
2:A:1502:Y01:CAU	2:A:1502:Y01:HAC1	2.51	0.41
1:A:47:PHE:O	1:A:441:ASN:ND2	2.53	0.41
1:A:605:THR:O	1:A:609:THR:HG23	2.20	0.40
1:A:576:VAL:HG13	1:A:977:VAL:CG1	2.51	0.40
1:A:444:LEU:HD12	1:A:1081:ILE:CD1	2.48	0.40

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
2	A	1507	Y01	CAE-CBI	5.69	1.64	1.54
2	A	1508	Y01	CAE-CBI	5.53	1.64	1.54
2	A	1503	Y01	CAE-CBI	5.51	1.64	1.54
2	A	1509	Y01	CAE-CBI	5.00	1.63	1.54
2	A	1501	Y01	CAK-CBD	4.96	1.61	1.53
2	A	1506	Y01	CAD-CBH	4.49	1.62	1.54
2	A	1508	Y01	CAD-CBH	4.19	1.61	1.54
2	A	1501	Y01	CAV-CBC	4.07	1.61	1.52
2	A	1509	Y01	CAV-CBC	4.07	1.61	1.52
2	A	1501	Y01	CBD-CBF	3.98	1.61	1.53
2	A	1508	Y01	CAV-CBC	3.94	1.61	1.52
2	A	1501	Y01	CAD-CBH	3.80	1.61	1.54
2	A	1504	Y01	CAV-CBC	3.72	1.61	1.52
2	A	1505	Y01	CAV-CBC	3.63	1.60	1.52
2	A	1503	Y01	CAD-CBH	3.60	1.60	1.54
2	A	1502	Y01	CAD-CBH	3.57	1.60	1.54
2	A	1503	Y01	CAV-CBC	3.56	1.60	1.52
2	A	1506	Y01	CAM-CAY	3.51	1.61	1.50
2	A	1507	Y01	CAD-CBH	3.44	1.60	1.54
2	A	1501	Y01	CAV-CAZ	3.38	1.59	1.51
2	A	1502	Y01	CAM-CAY	3.33	1.60	1.50
2	A	1508	Y01	CAV-CAZ	3.30	1.58	1.51
2	A	1507	Y01	CAV-CBC	3.26	1.59	1.52
2	A	1507	Y01	CAM-CAY	3.24	1.60	1.50
2	A	1504	Y01	CAD-CBH	3.17	1.60	1.54
2	A	1502	Y01	CAV-CBC	3.16	1.59	1.52
2	A	1505	Y01	CAM-CAY	3.14	1.59	1.50
2	A	1508	Y01	CAM-CAY	3.09	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1509	Y01	CAD-CBH	3.07	1.59	1.54
2	A	1509	Y01	CAM-CAY	3.05	1.59	1.50
2	A	1504	Y01	CAM-CAY	3.04	1.59	1.50
2	A	1509	Y01	CAV-CAZ	3.03	1.58	1.51
2	A	1503	Y01	CAM-CAY	2.99	1.59	1.50
2	A	1506	Y01	CAQ-CAP	-2.95	1.45	1.54
2	A	1501	Y01	CAM-CAY	2.93	1.59	1.50
2	A	1504	Y01	CAV-CAZ	2.88	1.57	1.51
2	A	1502	Y01	OAW-CAY	2.82	1.42	1.34
2	A	1505	Y01	CAD-CBH	2.80	1.59	1.54
2	A	1506	Y01	CAV-CBC	2.77	1.58	1.52
2	A	1506	Y01	OAW-CAY	2.77	1.42	1.34
2	A	1505	Y01	CAV-CAZ	2.75	1.57	1.51
2	A	1505	Y01	OAW-CAY	2.70	1.41	1.34
2	A	1501	Y01	OAW-CAY	2.69	1.41	1.34
2	A	1507	Y01	OAW-CAY	2.67	1.41	1.34
2	A	1504	Y01	OAW-CAY	2.65	1.41	1.34
2	A	1509	Y01	OAW-CAY	2.65	1.41	1.34
2	A	1506	Y01	CAK-CAI	-2.65	1.44	1.50
2	A	1508	Y01	CAP-CBE	2.58	1.59	1.54
2	A	1501	Y01	CAK-CAI	2.48	1.55	1.50
2	A	1503	Y01	CAV-CAZ	2.47	1.57	1.51
2	A	1508	Y01	OAW-CAY	2.46	1.41	1.34
2	A	1503	Y01	OAW-CAY	2.46	1.41	1.34
2	A	1509	Y01	CAQ-CAP	-2.37	1.47	1.54
2	A	1503	Y01	CAQ-CAP	-2.36	1.47	1.54
2	A	1507	Y01	CAV-CAZ	2.35	1.56	1.51
2	A	1505	Y01	CBD-CBF	2.33	1.58	1.53
2	A	1508	Y01	CAQ-CAP	-2.19	1.48	1.54
2	A	1507	Y01	CAQ-CAP	-2.15	1.48	1.54
2	A	1501	Y01	CBH-CAZ	-2.11	1.48	1.52
2	A	1509	Y01	CBD-CBF	2.09	1.57	1.53
2	A	1508	Y01	CBD-CBF	2.06	1.57	1.53
2	A	1506	Y01	CBD-CBF	2.02	1.57	1.53
2	A	1502	Y01	CAQ-CAP	-2.02	1.48	1.54
2	A	1501	Y01	CAP-CBE	2.02	1.58	1.54
2	A	1501	Y01	CAS-CBF	-2.00	1.50	1.53

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
2	A	1505	Y01	CBG-CBI-CBE	-7.68	90.98	100.07
2	A	1508	Y01	CBC-CAV-CAZ	7.65	123.40	111.52
2	A	1501	Y01	CBG-CBI-CBE	-7.47	91.22	100.07
2	A	1507	Y01	CBG-CBI-CBE	-7.44	91.26	100.07
2	A	1507	Y01	OAW-CAY-CAM	7.41	127.48	111.50
2	A	1502	Y01	OAW-CAY-CAM	7.36	127.37	111.50
2	A	1509	Y01	OAW-CAY-CAM	7.33	127.30	111.50
2	A	1501	Y01	OAW-CAY-CAM	7.31	127.25	111.50
2	A	1504	Y01	OAW-CAY-CAM	7.29	127.20	111.50
2	A	1505	Y01	OAW-CAY-CAM	7.22	127.07	111.50
2	A	1503	Y01	OAW-CAY-CAM	7.16	126.93	111.50
2	A	1508	Y01	OAW-CAY-CAM	7.13	126.86	111.50
2	A	1506	Y01	OAW-CAY-CAM	7.12	126.85	111.50
2	A	1509	Y01	CBC-CAV-CAZ	7.02	122.42	111.52
2	A	1503	Y01	CBG-CBI-CBE	-6.98	91.81	100.07
2	A	1508	Y01	CBG-CBI-CBE	-6.97	91.82	100.07
2	A	1504	Y01	CBC-CAV-CAZ	6.87	122.18	111.52
2	A	1504	Y01	CAD-CBH-CAZ	-6.86	97.24	108.34
2	A	1503	Y01	CBC-CAV-CAZ	6.80	122.08	111.52
2	A	1505	Y01	CAV-CAZ-CAI	6.77	130.36	120.61
2	A	1509	Y01	CBG-CBI-CBE	-6.72	92.12	100.07
2	A	1505	Y01	CBC-CAV-CAZ	6.70	121.93	111.52
2	A	1509	Y01	CAV-CAZ-CAI	6.64	130.18	120.61
2	A	1506	Y01	CBG-CBI-CBE	-6.59	92.27	100.07
2	A	1503	Y01	CAD-CBH-CAZ	-6.58	97.70	108.34
2	A	1504	Y01	CAV-CAZ-CAI	6.57	130.07	120.61
2	A	1505	Y01	CAD-CBH-CAZ	-6.56	97.73	108.34
2	A	1502	Y01	CAD-CBH-CAZ	-6.54	97.76	108.34
2	A	1507	Y01	CAV-CAZ-CAI	6.53	130.01	120.61
2	A	1503	Y01	CAV-CAZ-CAI	6.49	129.96	120.61
2	A	1501	Y01	CAV-CAZ-CAI	6.46	129.91	120.61
2	A	1507	Y01	CAD-CBH-CAZ	-6.44	97.92	108.34
2	A	1509	Y01	CAD-CBH-CAZ	-6.43	97.93	108.34
2	A	1508	Y01	CAV-CAZ-CAI	6.34	129.74	120.61
2	A	1508	Y01	CAD-CBH-CAZ	-6.24	98.25	108.34
2	A	1506	Y01	CBD-CAK-CAI	-6.21	103.81	112.73
2	A	1502	Y01	CAV-CAZ-CAI	6.14	129.46	120.61
2	A	1507	Y01	CBC-CAV-CAZ	6.12	121.03	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1501	Y01	CAK-CBD-CBF	6.10	117.10	109.71
2	A	1506	Y01	CBC-CAV-CAZ	6.09	120.97	111.52
2	A	1502	Y01	CBC-CAV-CAZ	5.53	120.11	111.52
2	A	1506	Y01	CAD-CBH-CAZ	-5.51	99.42	108.34
2	A	1507	Y01	CAV-CAZ-CBH	-5.49	109.12	116.42
2	A	1509	Y01	CBD-CAK-CAI	-5.46	104.88	112.73
2	A	1509	Y01	CAV-CAZ-CBH	-5.43	109.21	116.42
2	A	1502	Y01	CAV-CAZ-CBH	-5.43	109.21	116.42
2	A	1505	Y01	CAV-CAZ-CBH	-5.39	109.26	116.42
2	A	1503	Y01	CAP-CAQ-CBG	-5.32	94.59	105.13
2	A	1504	Y01	CAV-CAZ-CBH	-5.31	109.37	116.42
2	A	1508	Y01	CAP-CAQ-CBG	-5.30	94.63	105.13
2	A	1501	Y01	CBH-CAZ-CAI	-5.21	114.93	122.90
2	A	1503	Y01	CAV-CAZ-CBH	-5.09	109.65	116.42
2	A	1506	Y01	CAE-CBI-CBG	5.05	121.13	111.71
2	A	1506	Y01	CAV-CAZ-CBH	-5.00	109.77	116.42
2	A	1505	Y01	CBD-CAK-CAI	-4.99	105.56	112.73
2	A	1501	Y01	CAP-CBE-CBI	-4.95	97.88	103.84
2	A	1502	Y01	CAP-CAQ-CBG	-4.95	95.33	105.13
2	A	1507	Y01	OAW-CBC-CAV	4.95	118.24	108.12
2	A	1504	Y01	CAP-CBE-CBI	-4.93	97.90	103.84
2	A	1508	Y01	CBD-CAK-CAI	-4.93	105.65	112.73
2	A	1502	Y01	CAR-CBC-CAV	-4.81	103.81	110.99
2	A	1508	Y01	CAV-CAZ-CBH	-4.79	110.05	116.42
2	A	1509	Y01	CAE-CBI-CBG	4.78	120.64	111.71
2	A	1507	Y01	CAP-CAQ-CBG	-4.75	95.71	105.13
2	A	1502	Y01	OAW-CBC-CAV	4.71	117.77	108.12
2	A	1505	Y01	CAP-CBE-CBI	-4.71	98.17	103.84
2	A	1504	Y01	CAP-CAQ-CBG	-4.67	95.88	105.13
2	A	1504	Y01	OAW-CBC-CAV	4.67	117.67	108.12
2	A	1509	Y01	OAW-CBC-CAV	4.64	117.61	108.12
2	A	1503	Y01	CBD-CAK-CAI	-4.62	106.09	112.73
2	A	1501	Y01	CAV-CAZ-CBH	-4.60	110.30	116.42
2	A	1507	Y01	CAR-CBC-CAV	-4.59	104.14	110.99
2	A	1508	Y01	OAW-CBC-CAV	4.58	117.50	108.12
2	A	1507	Y01	CBD-CAK-CAI	-4.56	106.18	112.73
2	A	1501	Y01	CAP-CAQ-CBG	-4.56	96.09	105.13
2	A	1505	Y01	OAW-CBC-CAV	4.52	117.38	108.12
2	A	1502	Y01	CBD-CAK-CAI	-4.49	106.27	112.73
2	A	1505	Y01	CAE-CBI-CBG	4.49	120.09	111.71
2	A	1507	Y01	CAE-CBI-CBG	4.48	120.07	111.71
2	A	1503	Y01	OAW-CBC-CAV	4.42	117.16	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1506	Y01	OAW-CBC-CAV	4.39	117.10	108.12
2	A	1506	Y01	CAR-CBC-CAV	-4.38	104.45	110.99
2	A	1501	Y01	OAW-CBC-CAV	4.37	117.07	108.12
2	A	1504	Y01	CBD-CAK-CAI	-4.35	106.49	112.73
2	A	1508	Y01	CAE-CBI-CBG	4.28	119.69	111.71
2	A	1506	Y01	CAQ-CBG-CBD	-4.26	112.07	119.08
2	A	1506	Y01	CAE-CBI-CAU	-4.24	103.89	110.59
2	A	1503	Y01	CAE-CBI-CBG	4.24	119.61	111.71
2	A	1505	Y01	CAP-CAQ-CBG	-4.21	96.78	105.13
2	A	1509	Y01	CAP-CAQ-CBG	-4.17	96.86	105.13
2	A	1501	Y01	CAS-CBF-CBH	-4.17	107.59	113.08
2	A	1502	Y01	CAT-CBH-CAZ	4.15	116.36	108.75
2	A	1507	Y01	OAW-CAY-OAG	-4.11	113.78	123.70
2	A	1502	Y01	OAW-CAY-OAG	-4.08	113.83	123.70
2	A	1509	Y01	OAW-CAY-OAG	-4.04	113.93	123.70
2	A	1502	Y01	CAS-CBF-CBH	-4.04	107.76	113.08
2	A	1503	Y01	OAW-CAY-OAG	-4.02	113.98	123.70
2	A	1508	Y01	OAW-CAY-OAG	-4.02	114.00	123.70
2	A	1505	Y01	OAW-CAY-OAG	-4.01	114.00	123.70
2	A	1504	Y01	OAW-CAY-OAG	-4.01	114.01	123.70
2	A	1501	Y01	OAW-CAY-OAG	-4.01	114.02	123.70
2	A	1505	Y01	CAR-CBC-CAV	-4.00	105.02	110.99
2	A	1506	Y01	CAP-CAQ-CBG	-3.99	97.23	105.13
2	A	1506	Y01	OAW-CAY-OAG	-3.97	114.11	123.70
2	A	1501	Y01	CAP-CBE-CBB	3.96	118.27	112.15
2	A	1504	Y01	CAR-CBC-CAV	-3.95	105.09	110.99
2	A	1507	Y01	CAS-CBF-CBH	-3.94	107.88	113.08
2	A	1502	Y01	CAE-CBI-CBG	3.93	119.05	111.71
2	A	1502	Y01	CAP-CBE-CBI	-3.89	99.15	103.84
2	A	1509	Y01	CAE-CBI-CAU	-3.85	104.50	110.59
2	A	1501	Y01	CAE-CBI-CBG	3.85	118.89	111.71
2	A	1509	Y01	CAQ-CBG-CBD	-3.84	112.76	119.08
2	A	1508	Y01	CAQ-CBG-CBD	-3.75	112.90	119.08
2	A	1503	Y01	CAE-CBI-CAU	-3.75	104.66	110.59
2	A	1504	Y01	CAE-CBI-CBG	3.72	118.66	111.71
2	A	1505	Y01	CAE-CBI-CAU	-3.72	104.72	110.59
2	A	1503	Y01	CAR-CBC-CAV	-3.69	105.48	110.99
2	A	1507	Y01	CAT-CBH-CAZ	3.68	115.49	108.75
2	A	1502	Y01	CAE-CBI-CAU	-3.67	104.79	110.59
2	A	1506	Y01	CAV-CAZ-CAI	3.67	125.90	120.61
2	A	1507	Y01	CAE-CBI-CAU	-3.67	104.80	110.59
2	A	1503	Y01	CAS-CBF-CBH	-3.67	108.25	113.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1505	Y01	CAQ-CBG-CBD	-3.66	113.06	119.08
2	A	1506	Y01	CAT-CBH-CAZ	3.64	115.42	108.75
2	A	1505	Y01	CAS-CBF-CBH	-3.64	108.28	113.08
2	A	1509	Y01	CAS-CBF-CBH	-3.64	108.28	113.08
2	A	1503	Y01	CAQ-CBG-CBD	-3.61	113.14	119.08
2	A	1504	Y01	CAQ-CBG-CBD	-3.59	113.17	119.08
2	A	1501	Y01	CAE-CBI-CAU	-3.59	104.92	110.59
2	A	1507	Y01	CAQ-CBG-CBD	-3.56	113.22	119.08
2	A	1504	Y01	CAT-CBH-CAZ	3.55	115.25	108.75
2	A	1508	Y01	CAS-CBF-CBH	-3.53	108.43	113.08
2	A	1502	Y01	CAQ-CBG-CBD	-3.50	113.31	119.08
2	A	1509	Y01	CAR-CBC-CAV	-3.50	105.77	110.99
2	A	1504	Y01	CAK-CAI-CAZ	3.49	131.50	125.06
2	A	1505	Y01	CAT-CBH-CAZ	3.48	115.12	108.75
2	A	1502	Y01	CAK-CBD-CBF	3.47	113.92	109.71
2	A	1501	Y01	CAQ-CBG-CBD	-3.46	113.38	119.08
2	A	1508	Y01	CAR-CBC-CAV	-3.46	105.83	110.99
2	A	1509	Y01	CBI-CBG-CBD	-3.45	109.27	114.38
2	A	1502	Y01	CAK-CAI-CAZ	3.44	131.41	125.06
2	A	1507	Y01	CAP-CBE-CBI	-3.43	99.71	103.84
2	A	1506	Y01	CBH-CAZ-CAI	-3.43	117.66	122.90
2	A	1504	Y01	CAS-CBF-CBH	-3.41	108.59	113.08
2	A	1503	Y01	CAT-CBH-CAZ	3.37	114.92	108.75
2	A	1505	Y01	CBI-CBG-CBD	-3.37	109.39	114.38
2	A	1504	Y01	CAP-CBE-CBB	3.32	117.29	112.15
2	A	1507	Y01	CAK-CAI-CAZ	3.32	131.18	125.06
2	A	1507	Y01	CBI-CBG-CBD	-3.29	109.51	114.38
2	A	1509	Y01	CAT-CBH-CAZ	3.23	114.67	108.75
2	A	1504	Y01	CAK-CBD-CBF	3.23	113.63	109.71
2	A	1506	Y01	CBH-CBF-CBD	-3.20	107.94	112.73
2	A	1506	Y01	CBI-CBG-CBD	-3.19	109.66	114.38
2	A	1501	Y01	CAD-CBH-CAT	3.18	114.44	109.43
2	A	1504	Y01	CBI-CBG-CBD	-3.17	109.69	114.38
2	A	1508	Y01	CAT-CBH-CAZ	3.12	114.47	108.75
2	A	1505	Y01	CAP-CBE-CBB	3.10	116.95	112.15
2	A	1503	Y01	CBI-CBG-CBD	-3.08	109.81	114.38
2	A	1508	Y01	CAE-CBI-CAU	-3.07	105.73	110.59
2	A	1506	Y01	CAQ-CAP-CBE	3.06	111.21	105.13
2	A	1507	Y01	CAK-CBD-CBF	3.05	113.41	109.71
2	A	1506	Y01	CAP-CBE-CBI	-3.04	100.17	103.84
2	A	1502	Y01	CBI-CBG-CBD	-3.04	109.88	114.38
3	A	1512	NAG	C1-O5-C5	3.01	116.28	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1501	Y01	CAR-CBC-CAV	-3.01	106.50	110.99
2	A	1508	Y01	CAK-CBD-CBF	3.01	113.36	109.71
2	A	1501	Y01	CBI-CBG-CBD	-3.01	109.93	114.38
2	A	1501	Y01	CAT-CBH-CAZ	3.00	114.24	108.75
2	A	1505	Y01	CAK-CAI-CAZ	2.97	130.54	125.06
2	A	1505	Y01	CAK-CBD-CBF	2.96	113.30	109.71
2	A	1508	Y01	CAK-CAI-CAZ	2.93	130.46	125.06
2	A	1501	Y01	CBI-CBE-CBB	-2.92	114.91	119.49
2	A	1503	Y01	CAK-CAI-CAZ	2.92	130.44	125.06
2	A	1508	Y01	CAP-CBE-CBI	-2.90	100.35	103.84
2	A	1508	Y01	CBI-CBG-CBD	-2.90	110.09	114.38
2	A	1503	Y01	CBI-CBE-CBB	-2.87	115.00	119.49
2	A	1502	Y01	CAR-CAT-CBH	2.79	118.79	112.74
2	A	1503	Y01	CAK-CBD-CBF	2.79	113.09	109.71
2	A	1504	Y01	CBI-CBE-CBB	-2.78	115.13	119.49
2	A	1508	Y01	CAQ-CAP-CBE	2.76	110.61	105.13
2	A	1506	Y01	CAS-CBF-CBH	-2.76	109.45	113.08
2	A	1501	Y01	CBH-CBF-CBD	-2.74	108.62	112.73
2	A	1507	Y01	CAQ-CAP-CBE	2.73	110.55	105.13
2	A	1503	Y01	CAQ-CAP-CBE	2.73	110.54	105.13
2	A	1509	Y01	CAK-CAI-CAZ	2.73	130.09	125.06
2	A	1506	Y01	CBI-CBE-CBB	-2.72	115.23	119.49
2	A	1502	Y01	CAP-CBE-CBB	2.68	116.30	112.15
2	A	1509	Y01	CBH-CBF-CBD	-2.66	108.74	112.73
2	A	1506	Y01	CAQ-CBG-CBI	2.66	107.05	103.84
2	A	1509	Y01	CAP-CBE-CBI	-2.65	100.65	103.84
2	A	1505	Y01	CBI-CBE-CBB	-2.63	115.36	119.49
2	A	1502	Y01	CAS-CBF-CBD	-2.61	107.99	111.75
2	A	1509	Y01	CAQ-CAP-CBE	2.61	110.30	105.13
2	A	1508	Y01	CAS-CBF-CBD	-2.59	108.02	111.75
2	A	1508	Y01	CBI-CBE-CBB	-2.58	115.45	119.49
2	A	1502	Y01	CAQ-CAP-CBE	2.56	110.20	105.13
2	A	1501	Y01	CAU-CBI-CBG	2.53	111.20	107.27
2	A	1502	Y01	CBI-CBE-CBB	-2.50	115.58	119.49
2	A	1509	Y01	CBI-CBE-CBB	-2.48	115.60	119.49
2	A	1507	Y01	CAR-CAT-CBH	2.46	118.08	112.74
2	A	1502	Y01	CAE-CBI-CBE	2.42	116.23	111.71
2	A	1504	Y01	CAS-CBF-CBD	-2.41	108.28	111.75
2	A	1504	Y01	CAE-CBI-CAU	-2.41	106.79	110.59
2	A	1509	Y01	CAU-CAS-CBF	2.40	117.28	113.11
2	A	1507	Y01	CBI-CBE-CBB	-2.35	115.80	119.49
2	A	1506	Y01	CAU-CAS-CBF	2.31	117.11	113.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1501	Y01	CAQ-CAP-CBE	2.30	109.69	105.13
2	A	1505	Y01	CBH-CBF-CBD	-2.30	109.28	112.73
2	A	1508	Y01	CBH-CAZ-CAI	-2.29	119.39	122.90
2	A	1504	Y01	CAQ-CAP-CBE	2.29	109.68	105.13
2	A	1507	Y01	CAE-CBI-CBE	2.25	115.92	111.71
2	A	1502	Y01	CAD-CBH-CAT	2.24	112.97	109.43
2	A	1507	Y01	CAD-CBH-CAT	2.23	112.95	109.43
2	A	1506	Y01	CAK-CBD-CBF	2.23	112.41	109.71
2	A	1503	Y01	CAE-CBI-CBE	2.22	115.85	111.71
2	A	1509	Y01	CAQ-CBG-CBI	2.21	106.51	103.84
2	A	1502	Y01	CAU-CBI-CBG	2.21	110.70	107.27
2	A	1505	Y01	CAE-CBI-CBE	2.21	115.83	111.71
2	A	1509	Y01	CAK-CBD-CBF	2.20	112.37	109.71
2	A	1503	Y01	CAP-CBE-CBI	-2.20	101.20	103.84
2	A	1501	Y01	CAE-CBI-CBE	2.19	115.80	111.71
2	A	1503	Y01	CAD-CBH-CAT	2.17	112.85	109.43
2	A	1501	Y01	CBC-OAW-CAY	2.17	123.12	117.79
2	A	1505	Y01	CAQ-CBG-CBI	2.15	106.43	103.84
2	A	1504	Y01	CBH-CBF-CBD	-2.14	109.53	112.73
2	A	1509	Y01	CAT-CBH-CBF	2.11	111.68	108.73
2	A	1505	Y01	CAQ-CAP-CBE	2.11	109.31	105.13
2	A	1504	Y01	CBF-CBH-CAZ	-2.10	106.36	109.65
2	A	1504	Y01	CAT-CBH-CBF	2.10	111.66	108.73
3	A	1512	NAG	C2-N2-C7	2.09	125.88	122.90
2	A	1507	Y01	CBC-OAW-CAY	2.08	122.92	117.79
2	A	1509	Y01	CBC-OAW-CAY	2.06	122.86	117.79
2	A	1507	Y01	CAS-CBF-CBD	-2.06	108.79	111.75
2	A	1503	Y01	CBH-CAZ-CAI	-2.06	119.76	122.90
2	A	1509	Y01	CBH-CAZ-CAI	-2.05	119.77	122.90
2	A	1509	Y01	CAE-CBI-CBE	2.04	115.52	111.71
2	A	1506	Y01	CAE-CBI-CBE	2.04	115.52	111.71
2	A	1504	Y01	CAR-CAT-CBH	2.03	117.14	112.74

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1512	NAG	C1

All (70) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
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
2	A	1502	Y01	CAM-CAY-OAW-CBC
2	A	1507	Y01	OAG-CAY-OAW-CBC
2	A	1507	Y01	CAM-CAY-OAW-CBC
2	A	1509	Y01	OAG-CAY-OAW-CBC
2	A	1509	Y01	CAM-CAY-OAW-CBC
2	A	1503	Y01	OAG-CAY-OAW-CBC
2	A	1504	Y01	OAG-CAY-OAW-CBC
2	A	1504	Y01	CAM-CAY-OAW-CBC
2	A	1508	Y01	OAG-CAY-OAW-CBC
2	A	1508	Y01	CAM-CAY-OAW-CBC
2	A	1505	Y01	CAV-CBC-OAW-CAY
2	A	1505	Y01	OAG-CAY-OAW-CBC
2	A	1503	Y01	CAM-CAY-OAW-CBC
2	A	1505	Y01	CAM-CAY-OAW-CBC
3	A	1511	NAG	O5-C5-C6-O6
2	A	1503	Y01	CAJ-CAO-CBB-CBE
2	A	1504	Y01	CAJ-CAO-CBB-CBE
2	A	1507	Y01	CAJ-CAO-CBB-CBE
2	A	1505	Y01	CAJ-CAO-CBB-CBE
3	A	1511	NAG	C4-C5-C6-O6
3	A	1512	NAG	C8-C7-N2-C2
3	A	1512	NAG	O7-C7-N2-C2
2	A	1503	Y01	CAJ-CAO-CBB-CAC
2	A	1504	Y01	CAJ-CAO-CBB-CAC
2	A	1502	Y01	CAJ-CAO-CBB-CBE
2	A	1506	Y01	CAX-CAL-CAM-CAY
2	A	1504	Y01	CAX-CAL-CAM-CAY
2	A	1508	Y01	CAX-CAL-CAM-CAY
2	A	1509	Y01	CAJ-CAO-CBB-CBE
2	A	1502	Y01	CAJ-CAO-CBB-CAC
2	A	1507	Y01	CAJ-CAO-CBB-CAC
2	A	1509	Y01	CAJ-CAO-CBB-CAC
2	A	1505	Y01	CAJ-CAO-CBB-CAC
2	A	1504	Y01	CAN-CAJ-CAO-CBB
2	A	1505	Y01	CAO-CAJ-CAN-CBA
2	A	1501	Y01	CAN-CAJ-CAO-CBB
2	A	1506	Y01	CAJ-CAN-CBA-CAB
2	A	1506	Y01	CAJ-CAO-CBB-CBE

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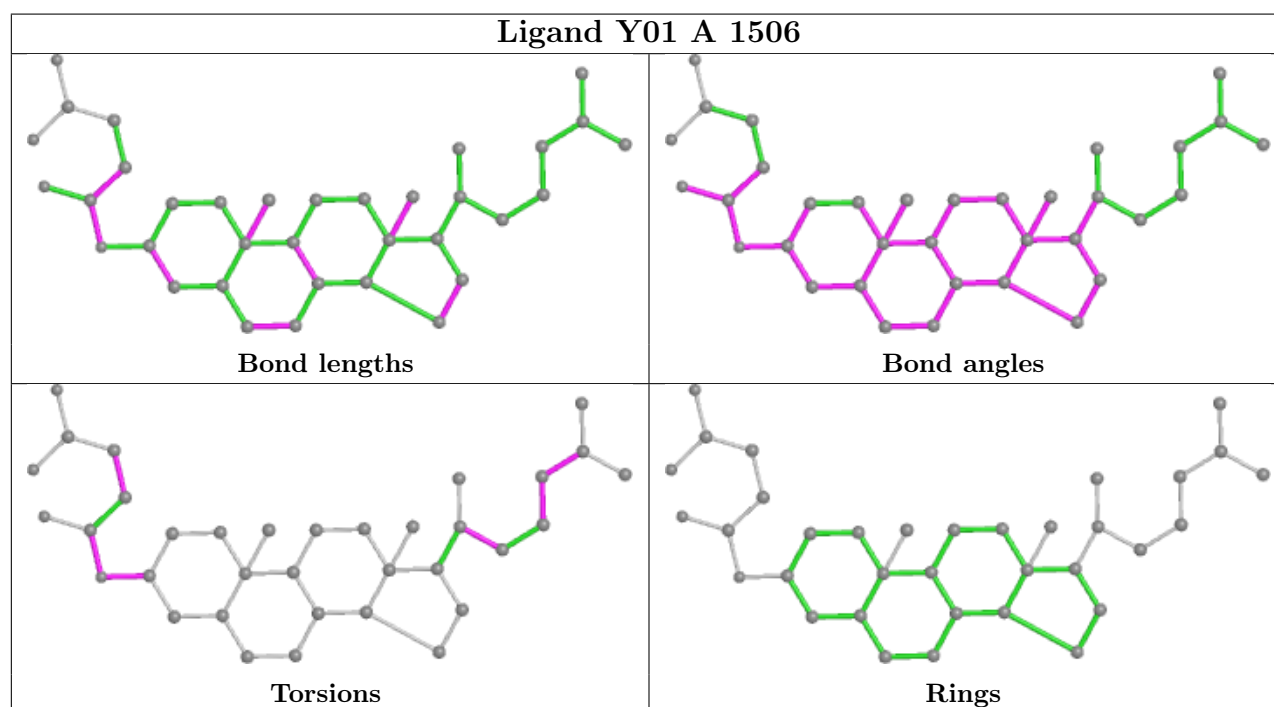
Mol	Chain	Res	Type	Atoms
2	A	1503	Y01	CAO-CAJ-CAN-CBA
2	A	1504	Y01	CAJ-CAN-CBA-CAA
2	A	1503	Y01	CAN-CAJ-CAO-CBB
2	A	1507	Y01	CAN-CAJ-CAO-CBB
2	A	1507	Y01	CAX-CAL-CAM-CAY
3	A	1512	NAG	O5-C5-C6-O6
2	A	1506	Y01	CAJ-CAN-CBA-CAA
2	A	1507	Y01	CAJ-CAN-CBA-CAB
2	A	1501	Y01	CAX-CAL-CAM-CAY
2	A	1507	Y01	CAJ-CAN-CBA-CAA
2	A	1506	Y01	CAR-CBC-OAW-CAY
2	A	1504	Y01	CAJ-CAN-CBA-CAB
2	A	1502	Y01	CAO-CAJ-CAN-CBA
2	A	1506	Y01	CAJ-CAO-CBB-CAC
2	A	1506	Y01	CAV-CBC-OAW-CAY
2	A	1501	Y01	CAJ-CAN-CBA-CAA
2	A	1504	Y01	CAO-CBB-CBE-CBI
2	A	1502	Y01	CAJ-CAN-CBA-CAA
2	A	1509	Y01	CAO-CAJ-CAN-CBA
2	A	1501	Y01	CAJ-CAN-CBA-CAB
2	A	1506	Y01	CAO-CAJ-CAN-CBA
2	A	1504	Y01	CAC-CBB-CBE-CBI
2	A	1504	Y01	CAL-CAM-CAY-OAW
2	A	1502	Y01	CAJ-CAN-CBA-CAB
2	A	1501	Y01	CAL-CAM-CAY-OAW
2	A	1507	Y01	CAL-CAM-CAY-OAW
2	A	1501	Y01	CAL-CAM-CAY-OAG

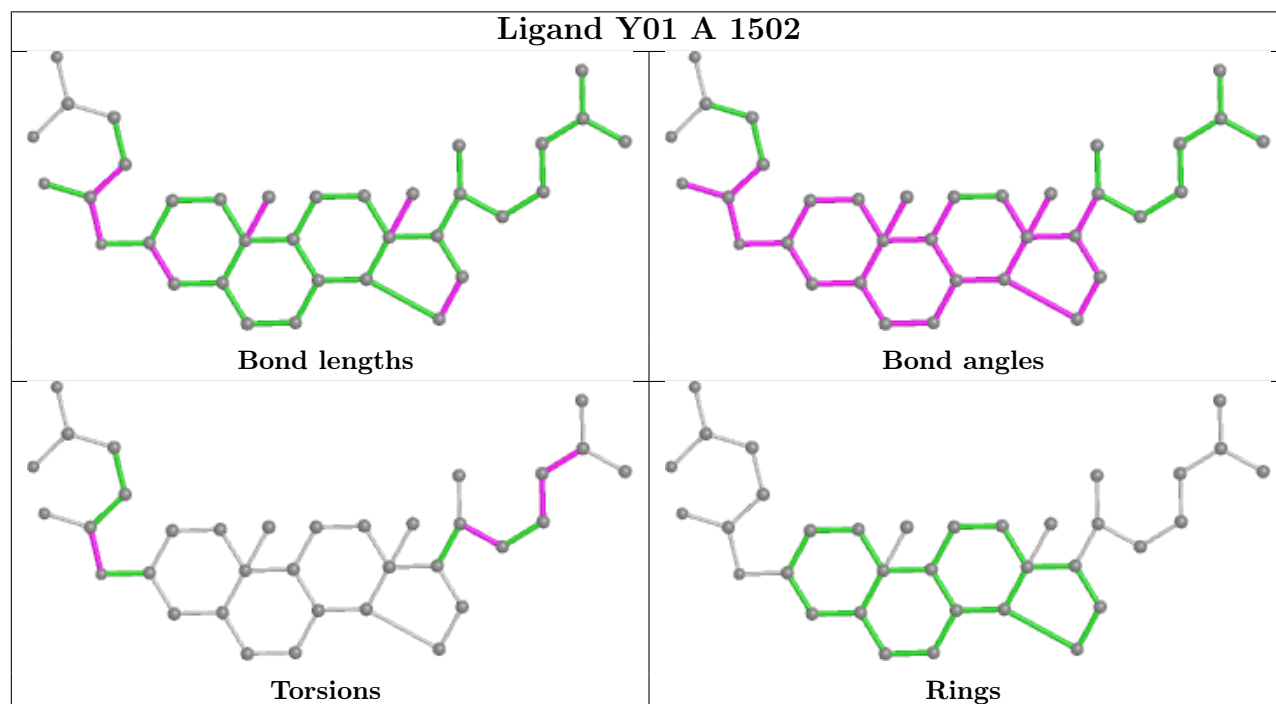
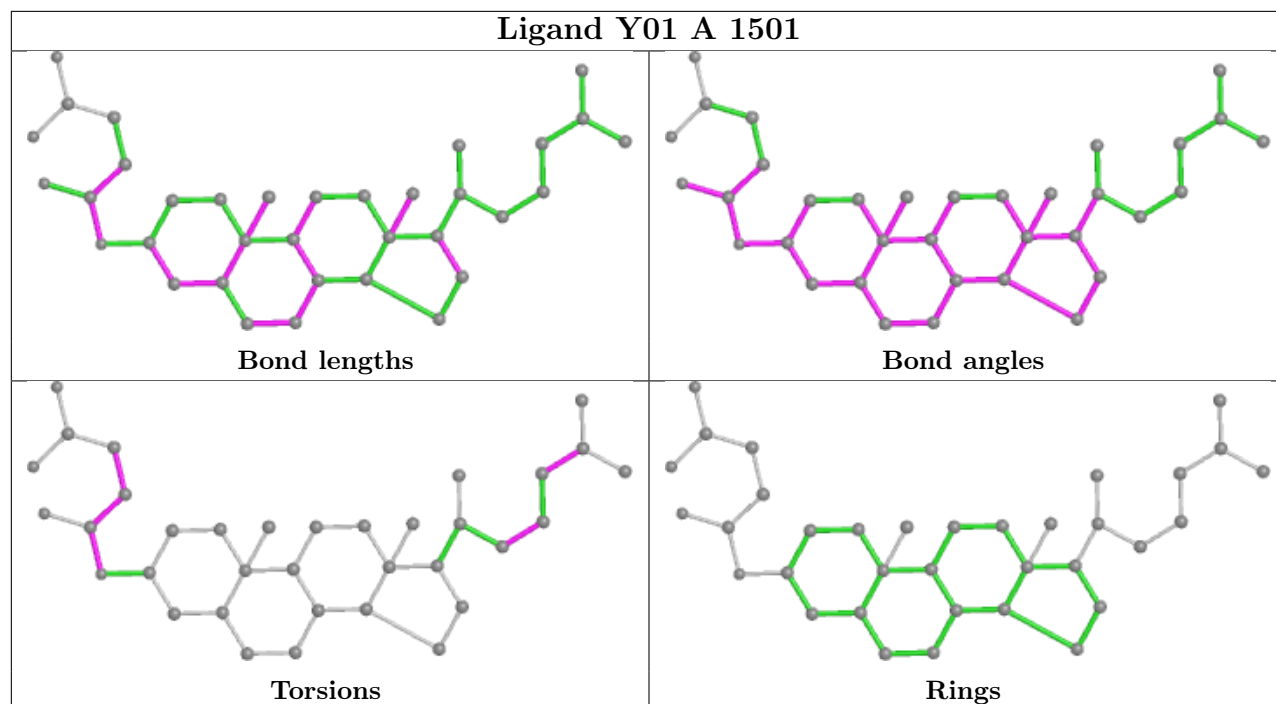
There are no ring outliers.

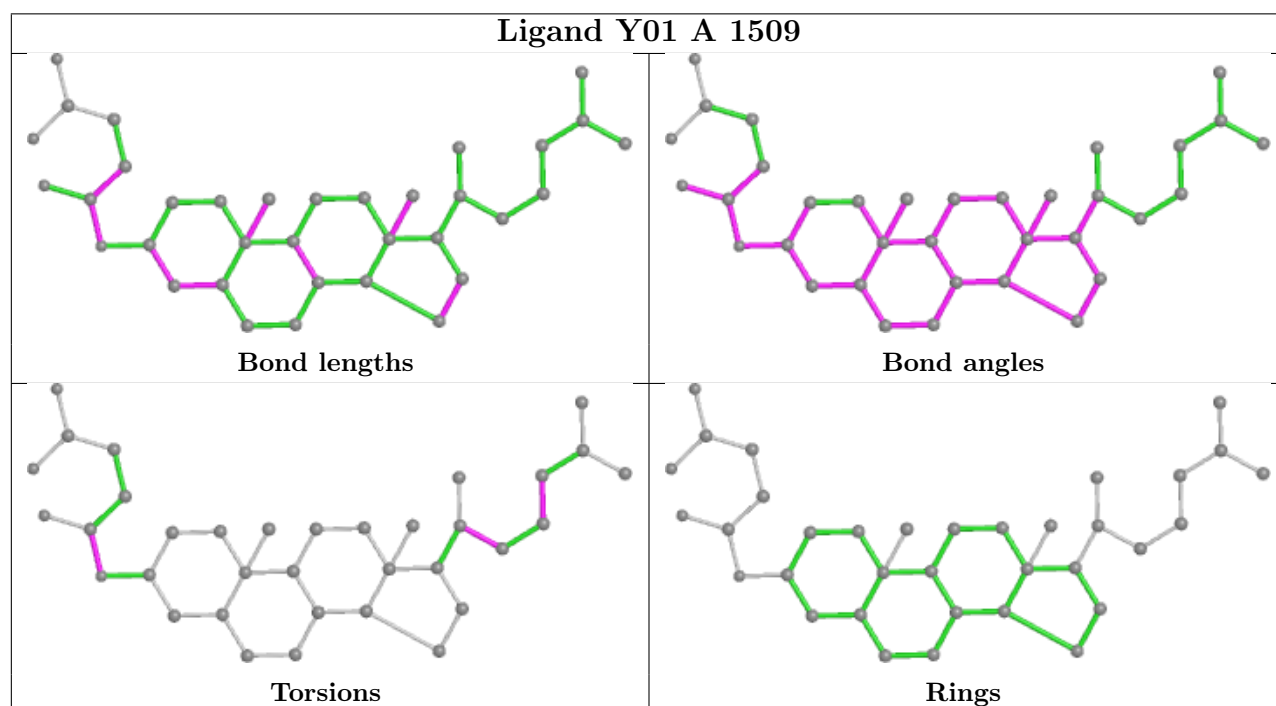
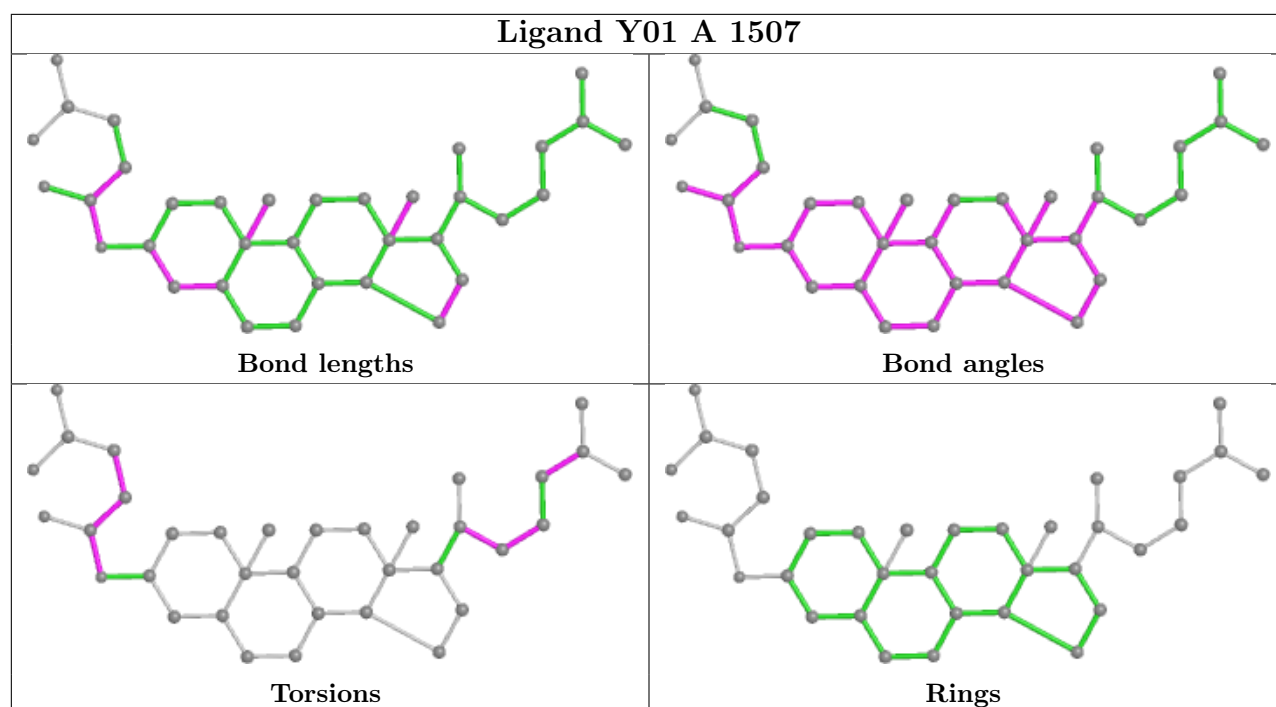
9 monomers are involved in 18 short contacts:

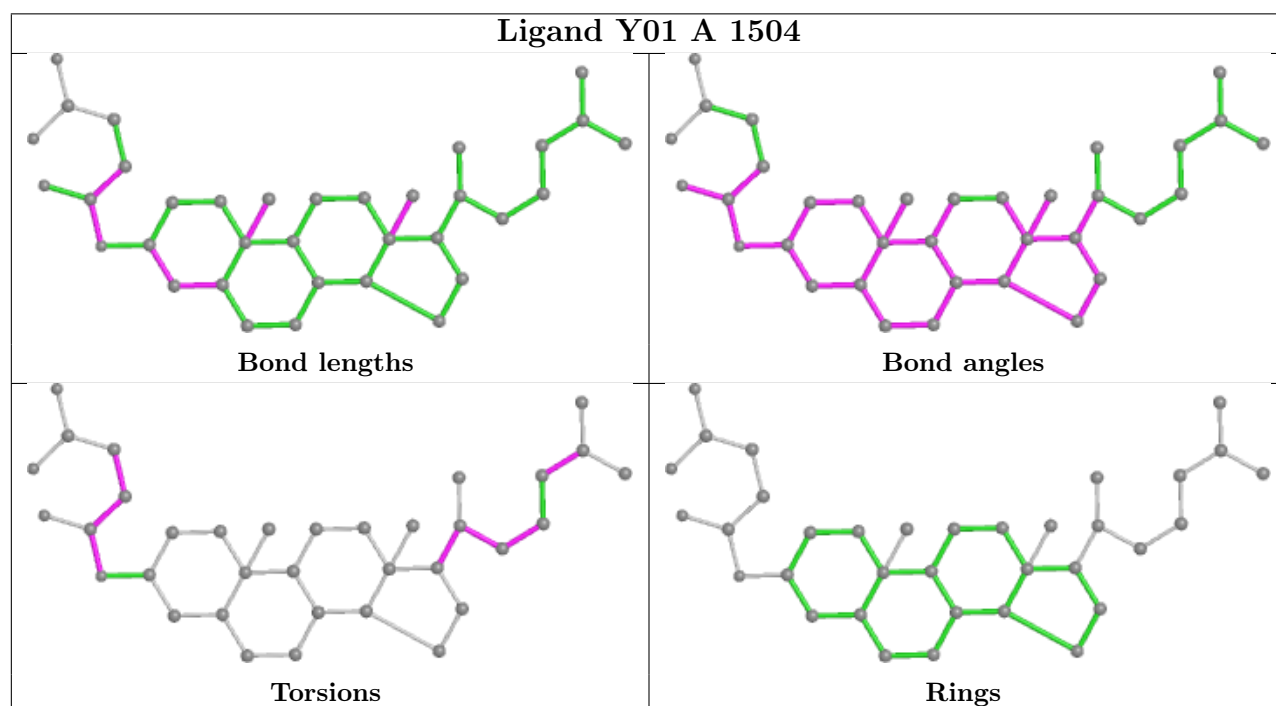
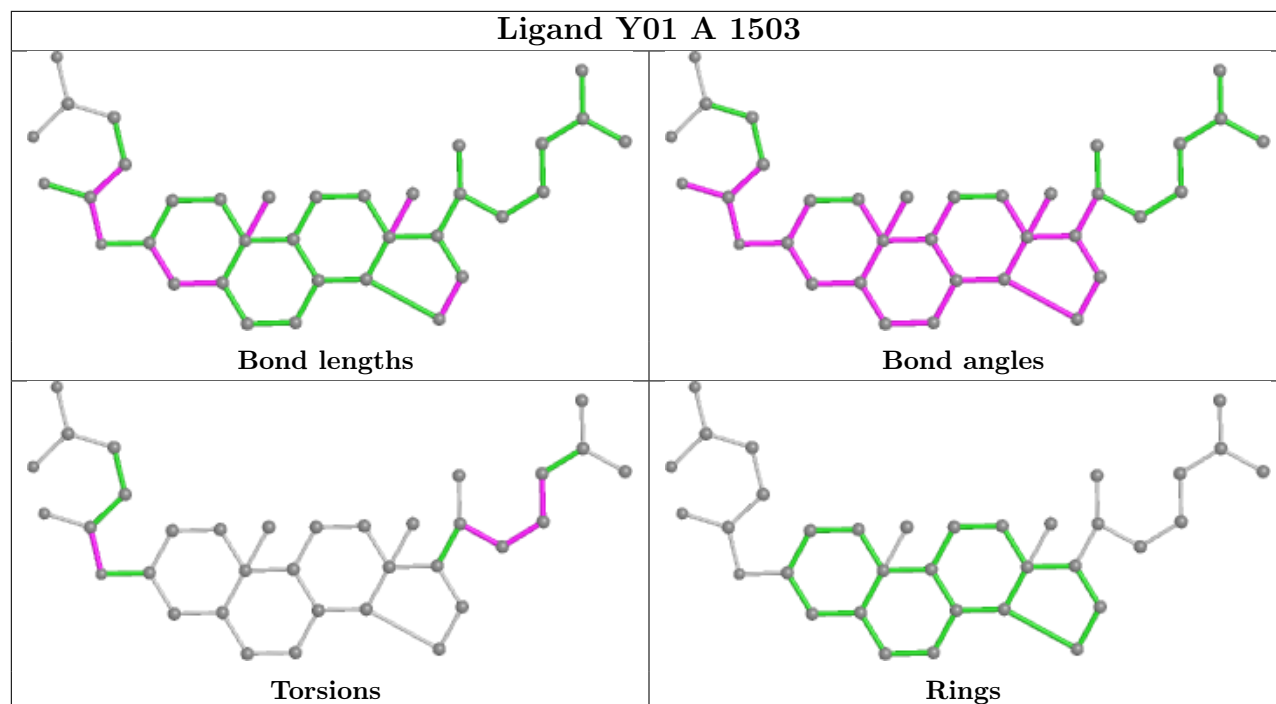
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1506	Y01	5	0
2	A	1501	Y01	2	0
2	A	1502	Y01	2	0
2	A	1507	Y01	2	0
2	A	1509	Y01	1	0
2	A	1503	Y01	1	0
2	A	1504	Y01	1	0
2	A	1508	Y01	1	0
2	A	1505	Y01	3	0

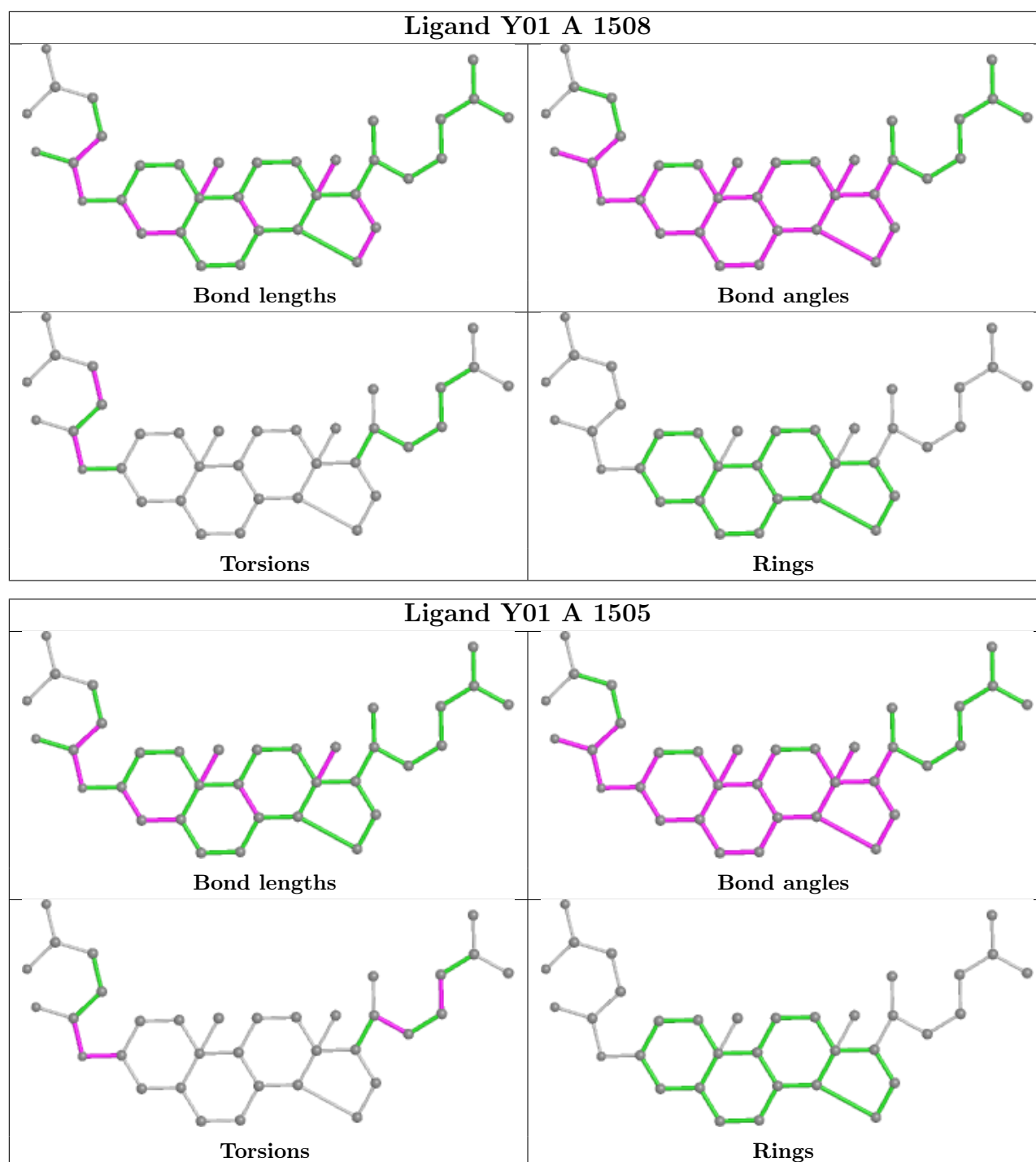
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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