



## Full wwPDB EM Validation Report ⓘ

Dec 5, 2023 – 02:35 PM EST

PDB ID : 7RPH  
EMDB ID : EMD-24614  
Title : Cryo-EM structure of murine Dispatched 'R' conformation  
Authors : Asarnow, D.; Wang, Q.; Ding, K.; Cheng, Y.; Beachy, P.A.  
Deposited on : 2021-08-03  
Resolution : 2.50 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

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

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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

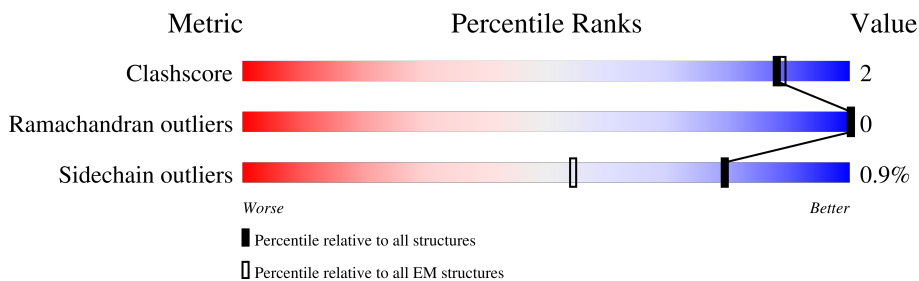
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.50 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 of 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1352	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8573 atoms, of which 0 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 homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	926	7366	4802	1180	1319	65	1	0

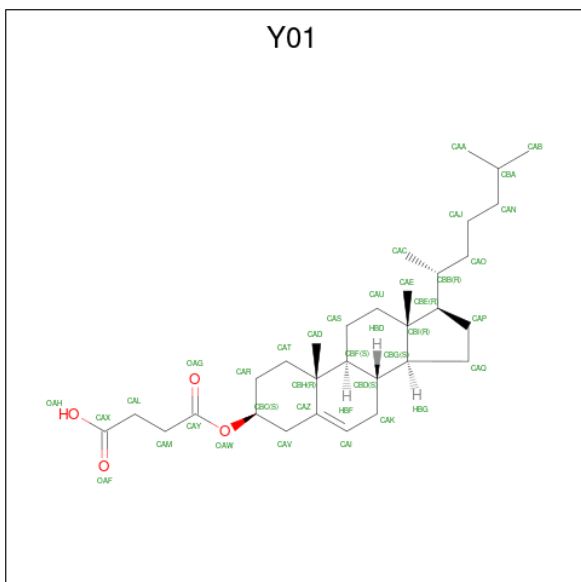
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	MET	-	expression tag	UNP Q3TDN0
A	171	ALA	-	expression tag	UNP Q3TDN0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	3	Total	Na	0
			3	3	

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C<sub>31</sub>H<sub>50</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



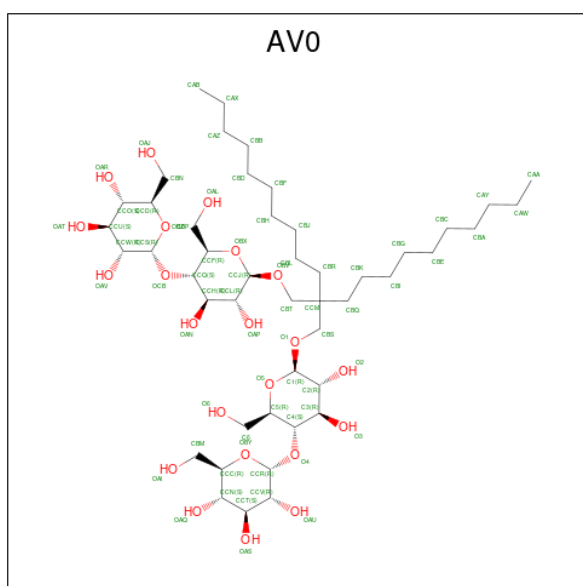
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	

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Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	

- Molecule 4 is Lauryl Maltose Neopentyl Glycol (three-letter code: AV0) (formula: C<sub>47</sub>H<sub>88</sub>O<sub>22</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			69	47	22	
4	A	1	Total	C	O	0
			69	47	22	

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	14	8	1	5	0
5	A	1	14	8	1	5	0
5	A	1	14	8	1	5	0
5	A	1	14	8	1	5	0
5	A	1	14	8	1	5	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
6	A	86	86	86	0



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	166203	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 ( $e^-/\text{\AA}^2$ )	66.7	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	59880	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	27.963	Depositor
Minimum map value	-17.711	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.579	Depositor
Recommended contour level	3.0	Depositor
Map size (Å)	267.19998, 267.19998, 267.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8349999, 0.8349999, 0.8349999	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, NA, AV0, Y01

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	0.70	0/7564	1.00	0/10290

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 [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	7366	0	7274	12	0
2	A	3	0	0	0	0
3	A	910	0	1274	26	0
4	A	138	0	0	0	0
5	A	70	0	65	0	0
6	A	86	0	0	0	0
All	All	8573	0	8613	33	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 2.

All (33) 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)
3:A:1605:Y01:HAE2	3:A:1605:Y01:CAC	2.13	0.79
1:A:557[B]:MET:HG2	1:A:1035:LEU:HD13	1.69	0.75
3:A:1605:Y01:HAE2	3:A:1605:Y01:HAC2	1.70	0.74
3:A:1609:Y01:HAC1	3:A:1609:Y01:HAU2	1.79	0.64
3:A:1624:Y01:HAC3	3:A:1624:Y01:CAN	2.34	0.57
3:A:1624:Y01:CAO	3:A:1624:Y01:CAE	2.85	0.54
3:A:1624:Y01:CAO	3:A:1624:Y01:HAE2	2.39	0.53
1:A:1097:PRO:O	3:A:1619:Y01:CAL	2.57	0.52
3:A:1605:Y01:CAC	3:A:1605:Y01:CAE	2.85	0.52
3:A:1608:Y01:HAC2	3:A:1608:Y01:HAE2	1.92	0.51
1:A:1097:PRO:O	3:A:1619:Y01:HAL1	2.12	0.50
3:A:1605:Y01:HAE2	3:A:1605:Y01:HAC1	1.92	0.50
1:A:613:THR:HG21	1:A:996:VAL:HG21	1.94	0.49
3:A:1606:Y01:HAC1	3:A:1606:Y01:HAU2	1.95	0.49
1:A:520:TYR:CE1	1:A:1083:MET:HG3	2.49	0.48
3:A:1618:Y01:HAC2	3:A:1618:Y01:HAE2	1.97	0.47
3:A:1624:Y01:CAE	3:A:1624:Y01:HAO2	2.46	0.46
3:A:1622:Y01:HAC1	3:A:1622:Y01:HAU2	1.98	0.45
3:A:1624:Y01:HAC3	3:A:1624:Y01:HAN1	1.97	0.45
1:A:560:THR:HG23	1:A:1106:LEU:HD22	1.99	0.44
1:A:520:TYR:CD1	1:A:1083:MET:HG3	2.53	0.44
1:A:1096:MET:HG3	3:A:1608:Y01:CAI	2.49	0.43
3:A:1617:Y01:HAC1	3:A:1617:Y01:HAU2	1.99	0.43
3:A:1615:Y01:HAU2	3:A:1615:Y01:HAC1	1.99	0.43
1:A:557[B]:MET:O	1:A:560:THR:HB	2.18	0.43
3:A:1620:Y01:HAU2	3:A:1620:Y01:HAC1	2.01	0.43
3:A:1629:Y01:HAC1	3:A:1629:Y01:HAU2	2.00	0.42
1:A:1097:PRO:O	3:A:1619:Y01:HAL2	2.20	0.42
3:A:1612:Y01:HAC1	3:A:1612:Y01:HAU2	2.01	0.42
1:A:613:THR:CG2	1:A:996:VAL:HG21	2.49	0.42
1:A:1097:PRO:HD3	3:A:1619:Y01:HBM	2.01	0.42
3:A:1624:Y01:CAN	3:A:1624:Y01:CAC	2.96	0.42
3:A:1624:Y01:HAO2	3:A:1624:Y01:HAE3	2.01	0.41

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	919/1352 (68%)	900 (98%)	19 (2%)	0	100 100

There are no Ramachandran outliers to report.

### 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	814/1190 (68%)	807 (99%)	7 (1%)	78 92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	289	SER
1	A	415	ARG
1	A	432	ASP
1	A	745	LEU
1	A	754	ARG
1	A	765	GLU
1	A	897	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 36 ligands modelled in this entry, 3 are monoatomic - leaving 33 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	Y01	A	1608	-	38,38,38	1.25	4 (10%)	57,57,57	0.89	1 (1%)
3	Y01	A	1615	-	38,38,38	1.18	3 (7%)	57,57,57	0.85	2 (3%)
3	Y01	A	1604	-	38,38,38	1.15	3 (7%)	57,57,57	0.98	4 (7%)
3	Y01	A	1614	-	38,38,38	1.28	5 (13%)	57,57,57	0.91	3 (5%)
3	Y01	A	1625	-	38,38,38	1.22	4 (10%)	57,57,57	0.78	0
3	Y01	A	1618	-	38,38,38	1.19	2 (5%)	57,57,57	0.91	4 (7%)
3	Y01	A	1616	-	38,38,38	1.19	4 (10%)	57,57,57	0.83	2 (3%)
5	NAG	A	1635	1	14,14,15	1.20	1 (7%)	17,19,21	0.77	0
3	Y01	A	1605	-	38,38,38	2.22	13 (34%)	57,57,57	1.33	5 (8%)
3	Y01	A	1613	-	38,38,38	1.27	5 (13%)	57,57,57	1.09	3 (5%)
3	Y01	A	1629	-	38,38,38	1.25	4 (10%)	57,57,57	0.79	1 (1%)
3	Y01	A	1609	-	38,38,38	1.09	2 (5%)	57,57,57	0.87	1 (1%)
3	Y01	A	1624	-	38,38,38	2.23	14 (36%)	57,57,57	1.64	8 (14%)
4	AV0	A	1630	-	72,72,72	1.02	3 (4%)	96,98,98	0.60	0
3	Y01	A	1606	-	38,38,38	1.21	2 (5%)	57,57,57	1.08	4 (7%)
3	Y01	A	1623	-	38,38,38	1.27	5 (13%)	57,57,57	1.05	3 (5%)
5	NAG	A	1632	1	14,14,15	1.27	2 (14%)	17,19,21	0.89	1 (5%)
3	Y01	A	1620	-	38,38,38	1.25	4 (10%)	57,57,57	0.99	3 (5%)
3	Y01	A	1619	-	38,38,38	1.25	3 (7%)	57,57,57	0.96	2 (3%)
3	Y01	A	1612	-	38,38,38	1.25	3 (7%)	57,57,57	1.14	5 (8%)
3	Y01	A	1611	-	38,38,38	1.17	3 (7%)	57,57,57	0.78	1 (1%)
3	Y01	A	1621	-	38,38,38	1.19	3 (7%)	57,57,57	0.81	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	Y01	A	1628	-	38,38,38	1.21	3 (7%)	57,57,57	0.90	2 (3%)
5	NAG	A	1636	1	14,14,15	1.26	1 (7%)	17,19,21	0.75	0
3	Y01	A	1622	-	38,38,38	1.22	4 (10%)	57,57,57	0.90	2 (3%)
3	Y01	A	1617	-	38,38,38	1.32	4 (10%)	57,57,57	1.10	4 (7%)
3	Y01	A	1626	-	38,38,38	1.27	3 (7%)	57,57,57	0.63	0
3	Y01	A	1610	-	38,38,38	1.29	4 (10%)	57,57,57	1.05	2 (3%)
3	Y01	A	1607	-	38,38,38	1.19	4 (10%)	57,57,57	1.21	3 (5%)
5	NAG	A	1633	1	14,14,15	1.24	2 (14%)	17,19,21	0.92	0
4	AV0	A	1631	-	72,72,72	1.07	5 (6%)	96,98,98	0.79	4 (4%)
5	NAG	A	1634	1	14,14,15	1.26	2 (14%)	17,19,21	0.85	1 (5%)
3	Y01	A	1627	-	38,38,38	1.26	3 (7%)	57,57,57	0.73	1 (1%)

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	Y01	A	1608	-	-	7/19/77/77	0/4/4/4
3	Y01	A	1615	-	-	6/19/77/77	0/4/4/4
3	Y01	A	1604	-	-	9/19/77/77	0/4/4/4
3	Y01	A	1614	-	-	12/19/77/77	0/4/4/4
3	Y01	A	1625	-	-	2/19/77/77	0/4/4/4
3	Y01	A	1618	-	-	8/19/77/77	0/4/4/4
3	Y01	A	1616	-	-	6/19/77/77	0/4/4/4
5	NAG	A	1635	1	-	1/6/23/26	0/1/1/1
3	Y01	A	1605	-	-	7/19/77/77	0/4/4/4
3	Y01	A	1613	-	-	5/19/77/77	0/4/4/4
3	Y01	A	1629	-	-	5/19/77/77	0/4/4/4
3	Y01	A	1609	-	-	0/19/77/77	0/4/4/4
3	Y01	A	1624	-	-	14/19/77/77	0/4/4/4
4	AV0	A	1630	-	-	8/50/130/130	0/4/4/4
3	Y01	A	1606	-	-	5/19/77/77	0/4/4/4
3	Y01	A	1623	-	-	9/19/77/77	0/4/4/4
5	NAG	A	1632	1	-	0/6/23/26	0/1/1/1
3	Y01	A	1620	-	-	4/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	Y01	A	1619	-	-	4/19/77/77	0/4/4/4
3	Y01	A	1612	-	-	7/19/77/77	0/4/4/4
3	Y01	A	1611	-	-	3/19/77/77	0/4/4/4
3	Y01	A	1621	-	-	11/19/77/77	0/4/4/4
3	Y01	A	1628	-	-	5/19/77/77	0/4/4/4
5	NAG	A	1636	1	-	0/6/23/26	0/1/1/1
3	Y01	A	1622	-	-	6/19/77/77	0/4/4/4
3	Y01	A	1617	-	-	8/19/77/77	0/4/4/4
3	Y01	A	1626	-	-	2/19/77/77	0/4/4/4
3	Y01	A	1610	-	-	3/19/77/77	0/4/4/4
3	Y01	A	1607	-	-	10/19/77/77	0/4/4/4
5	NAG	A	1633	1	-	2/6/23/26	0/1/1/1
4	AV0	A	1631	-	-	18/50/130/130	0/4/4/4
5	NAG	A	1634	1	-	0/6/23/26	0/1/1/1
3	Y01	A	1627	-	-	5/19/77/77	0/4/4/4

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1605	Y01	CAS-CBF	-6.50	1.42	1.53
3	A	1624	Y01	CAS-CBF	-6.10	1.43	1.53
3	A	1624	Y01	CAQ-CAP	4.86	1.67	1.54
3	A	1605	Y01	CAQ-CAP	4.33	1.65	1.54
3	A	1605	Y01	CAI-CAZ	-3.92	1.24	1.33
3	A	1624	Y01	CAI-CAZ	-3.88	1.24	1.33
3	A	1624	Y01	CBH-CAZ	-3.78	1.45	1.52
3	A	1624	Y01	CBD-CBF	3.56	1.60	1.53
3	A	1605	Y01	CBH-CAZ	-3.49	1.45	1.52
3	A	1605	Y01	CBD-CBF	3.48	1.60	1.53
3	A	1605	Y01	CAK-CBD	-3.47	1.47	1.53
3	A	1624	Y01	OAW-CAY	3.27	1.43	1.34
3	A	1605	Y01	OAW-CAY	3.26	1.43	1.34
3	A	1605	Y01	CAU-CAS	-3.23	1.46	1.53
3	A	1624	Y01	CAV-CAZ	3.22	1.58	1.51
3	A	1624	Y01	CAK-CBD	-3.08	1.47	1.53
3	A	1605	Y01	CAV-CAZ	2.92	1.58	1.51
3	A	1614	Y01	CAS-CBF	2.91	1.58	1.53
3	A	1624	Y01	CBI-CBE	-2.87	1.49	1.55
3	A	1627	Y01	CBB-CBE	2.84	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1624	Y01	CAU-CAS	-2.84	1.47	1.53
5	A	1632	NAG	O5-C5	2.74	1.49	1.43
3	A	1617	Y01	CBB-CBE	2.74	1.59	1.54
3	A	1610	Y01	CAS-CBF	2.74	1.58	1.53
3	A	1628	Y01	CAS-CBF	2.73	1.58	1.53
3	A	1605	Y01	CBI-CBE	-2.72	1.49	1.55
5	A	1634	NAG	O5-C5	2.70	1.48	1.43
3	A	1618	Y01	CBB-CBE	2.69	1.59	1.54
3	A	1614	Y01	CBB-CBE	2.68	1.59	1.54
3	A	1604	Y01	CAS-CBF	2.66	1.58	1.53
3	A	1606	Y01	CAS-CBF	2.66	1.58	1.53
3	A	1620	Y01	CAS-CBF	2.66	1.58	1.53
3	A	1627	Y01	OAH-CAX	-2.66	1.21	1.30
3	A	1629	Y01	CAS-CBF	2.65	1.58	1.53
3	A	1607	Y01	OAH-CAX	-2.61	1.22	1.30
3	A	1618	Y01	OAH-CAX	-2.60	1.22	1.30
5	A	1636	NAG	O5-C5	2.60	1.48	1.43
3	A	1621	Y01	OAH-CAX	-2.59	1.22	1.30
3	A	1625	Y01	CAS-CBF	2.57	1.58	1.53
5	A	1633	NAG	O5-C5	2.57	1.48	1.43
3	A	1623	Y01	CBB-CBE	2.57	1.58	1.54
3	A	1612	Y01	OAH-CAX	-2.56	1.22	1.30
3	A	1611	Y01	CBB-CBE	2.55	1.58	1.54
3	A	1619	Y01	OAH-CAX	-2.55	1.22	1.30
3	A	1604	Y01	OAH-CAX	-2.54	1.22	1.30
3	A	1628	Y01	OAH-CAX	-2.53	1.22	1.30
3	A	1617	Y01	OAH-CAX	-2.53	1.22	1.30
3	A	1626	Y01	OAH-CAX	-2.52	1.22	1.30
3	A	1625	Y01	OAH-CAX	-2.52	1.22	1.30
3	A	1611	Y01	OAH-CAX	-2.52	1.22	1.30
3	A	1622	Y01	OAH-CAX	-2.52	1.22	1.30
3	A	1615	Y01	OAH-CAX	-2.52	1.22	1.30
3	A	1610	Y01	OAH-CAX	-2.52	1.22	1.30
3	A	1613	Y01	CAS-CBF	2.51	1.58	1.53
3	A	1614	Y01	OAH-CAX	-2.51	1.22	1.30
3	A	1609	Y01	OAH-CAX	-2.51	1.22	1.30
3	A	1623	Y01	CAS-CBF	2.51	1.58	1.53
3	A	1613	Y01	OAH-CAX	-2.51	1.22	1.30
3	A	1608	Y01	OAH-CAX	-2.50	1.22	1.30
3	A	1610	Y01	CBB-CBE	2.50	1.58	1.54
3	A	1620	Y01	OAH-CAX	-2.49	1.22	1.30
3	A	1616	Y01	OAH-CAX	-2.49	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1606	Y01	OAH-CAX	-2.47	1.22	1.30
3	A	1623	Y01	OAH-CAX	-2.46	1.22	1.30
3	A	1629	Y01	OAH-CAX	-2.46	1.22	1.30
3	A	1622	Y01	CAS-CBF	2.45	1.57	1.53
3	A	1612	Y01	CBB-CBE	2.45	1.58	1.54
3	A	1617	Y01	CAS-CBF	2.42	1.57	1.53
3	A	1608	Y01	CBB-CBE	2.42	1.58	1.54
3	A	1620	Y01	CBB-CBE	2.40	1.58	1.54
3	A	1626	Y01	CBB-CBE	2.38	1.58	1.54
3	A	1613	Y01	CBB-CBE	2.37	1.58	1.54
3	A	1611	Y01	CAS-CBF	2.37	1.57	1.53
5	A	1635	NAG	O5-C5	2.37	1.48	1.43
3	A	1626	Y01	CAS-CBF	2.37	1.57	1.53
4	A	1631	AV0	OBV-CCJ	2.36	1.44	1.40
3	A	1607	Y01	CBB-CBE	2.36	1.58	1.54
3	A	1625	Y01	CBB-CBE	2.36	1.58	1.54
3	A	1608	Y01	CAS-CBF	2.36	1.57	1.53
3	A	1616	Y01	CBB-CBE	2.31	1.58	1.54
4	A	1631	AV0	O1-C1	2.31	1.44	1.40
4	A	1630	AV0	OBV-CCJ	2.31	1.44	1.40
3	A	1621	Y01	CBB-CBE	2.30	1.58	1.54
3	A	1624	Y01	CBD-CBG	2.27	1.57	1.53
3	A	1614	Y01	CAE-CBI	2.27	1.58	1.54
3	A	1629	Y01	CBB-CBE	2.26	1.58	1.54
3	A	1615	Y01	CBB-CBE	2.26	1.58	1.54
3	A	1623	Y01	CAE-CBI	2.23	1.58	1.54
3	A	1627	Y01	CAS-CBF	2.22	1.57	1.53
3	A	1622	Y01	CBB-CBE	2.22	1.58	1.54
3	A	1625	Y01	CBH-CBF	2.21	1.59	1.56
3	A	1605	Y01	CBD-CBG	2.21	1.57	1.53
3	A	1620	Y01	CBD-CBF	2.21	1.57	1.53
3	A	1624	Y01	CAM-CAY	2.21	1.57	1.50
3	A	1628	Y01	CBB-CBE	2.20	1.58	1.54
3	A	1607	Y01	CAS-CBF	2.18	1.57	1.53
3	A	1621	Y01	CAS-CBF	2.18	1.57	1.53
3	A	1619	Y01	CAS-CBF	2.17	1.57	1.53
3	A	1605	Y01	OAW-CBC	-2.16	1.41	1.46
3	A	1615	Y01	CAS-CBF	2.16	1.57	1.53
4	A	1631	AV0	CBR-CCM	2.15	1.58	1.54
3	A	1616	Y01	CAS-CBF	2.15	1.57	1.53
4	A	1630	AV0	CCN-CCC	2.14	1.57	1.53
3	A	1623	Y01	CBD-CBF	2.12	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1633	NAG	C1-C2	2.11	1.55	1.52
3	A	1607	Y01	CAE-CBI	2.11	1.58	1.54
3	A	1612	Y01	CAS-CBF	2.10	1.57	1.53
3	A	1619	Y01	CAT-CBH	2.10	1.58	1.54
4	A	1631	AV0	CBS-CCM	2.10	1.58	1.53
3	A	1629	Y01	CAE-CBI	2.10	1.58	1.54
5	A	1634	NAG	O5-C1	2.09	1.47	1.43
3	A	1617	Y01	CAE-CBI	2.08	1.58	1.54
5	A	1632	NAG	O5-C1	2.08	1.47	1.43
3	A	1613	Y01	CBD-CBF	2.07	1.57	1.53
3	A	1605	Y01	CAM-CAY	2.06	1.56	1.50
3	A	1616	Y01	CAT-CBH	2.06	1.58	1.54
3	A	1604	Y01	CBB-CBE	2.04	1.58	1.54
3	A	1614	Y01	CBH-CBF	2.04	1.59	1.56
3	A	1610	Y01	CBH-CBF	2.04	1.59	1.56
3	A	1622	Y01	CAE-CBI	2.02	1.57	1.54
3	A	1624	Y01	CBI-CBG	-2.01	1.51	1.55
3	A	1608	Y01	CBH-CBF	2.01	1.59	1.56
3	A	1609	Y01	CAE-CBI	2.01	1.57	1.54
3	A	1624	Y01	OAW-CBC	-2.01	1.41	1.46
4	A	1631	AV0	CBQ-CCM	2.00	1.58	1.54
4	A	1630	AV0	O1-C1	2.00	1.43	1.40
3	A	1613	Y01	CAE-CBI	2.00	1.57	1.54

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1607	Y01	CAP-CBE-CBB	5.73	121.02	112.15
3	A	1624	Y01	CBI-CBE-CBB	-4.88	111.85	119.49
3	A	1623	Y01	CAP-CBE-CBB	4.52	119.14	112.15
3	A	1624	Y01	CBI-CBG-CBD	-4.49	107.73	114.38
3	A	1617	Y01	CBC-OAW-CAY	3.94	127.50	117.79
3	A	1605	Y01	OAW-CAY-CAM	3.89	119.89	111.50
3	A	1628	Y01	CAP-CBE-CBB	3.86	118.12	112.15
3	A	1607	Y01	CAO-CBB-CBE	3.81	118.16	110.28
3	A	1624	Y01	OAW-CAY-CAM	3.73	119.54	111.50
3	A	1619	Y01	CBC-OAW-CAY	3.67	126.83	117.79
3	A	1605	Y01	CBH-CBF-CBD	-3.52	107.46	112.73
3	A	1622	Y01	CBC-OAW-CAY	3.29	125.88	117.79
3	A	1612	Y01	CBC-OAW-CAY	3.28	125.87	117.79
3	A	1624	Y01	CAC-CBB-CBE	-3.26	107.94	112.92
3	A	1606	Y01	CBC-OAW-CAY	3.18	125.61	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1617	Y01	CBC-CAV-CAZ	3.16	116.43	111.52
3	A	1605	Y01	CBI-CBG-CBD	-3.16	109.70	114.38
3	A	1604	Y01	CAP-CBE-CBB	3.13	116.99	112.15
3	A	1614	Y01	CAP-CBE-CBB	3.13	116.99	112.15
3	A	1607	Y01	CBI-CBE-CBB	-3.08	114.66	119.49
3	A	1624	Y01	CBH-CBF-CBD	-3.04	108.18	112.73
3	A	1611	Y01	CBC-OAW-CAY	2.91	124.96	117.79
3	A	1610	Y01	CBC-OAW-CAY	2.90	124.93	117.79
3	A	1616	Y01	CBC-OAW-CAY	2.89	124.91	117.79
3	A	1613	Y01	CBC-OAW-CAY	2.78	124.64	117.79
3	A	1606	Y01	CBC-CAV-CAZ	2.78	115.84	111.52
3	A	1624	Y01	CAP-CAQ-CBG	-2.78	99.62	105.13
3	A	1612	Y01	OAW-CAY-CAM	2.73	117.38	111.50
3	A	1606	Y01	CAR-CBC-CAV	2.72	115.04	110.99
3	A	1622	Y01	OAW-CAY-CAM	2.67	117.25	111.50
3	A	1612	Y01	CBC-CAV-CAZ	2.65	115.64	111.52
3	A	1624	Y01	CBG-CBI-CBE	2.64	103.20	100.07
3	A	1618	Y01	CAP-CBE-CBB	2.63	116.22	112.15
3	A	1615	Y01	CBC-OAW-CAY	2.61	124.22	117.79
3	A	1615	Y01	OAW-CBC-CAV	2.61	113.45	108.12
3	A	1613	Y01	CAS-CBF-CBD	2.61	115.51	111.75
3	A	1612	Y01	CAT-CAR-CBC	2.57	114.72	110.33
3	A	1604	Y01	CBC-OAW-CAY	2.57	124.12	117.79
5	A	1634	NAG	C1-O5-C5	2.56	115.66	112.19
3	A	1604	Y01	CAC-CBB-CBE	-2.54	109.03	112.92
3	A	1619	Y01	OAW-CAY-CAM	2.50	116.89	111.50
3	A	1608	Y01	CAC-CBB-CBE	2.50	116.75	112.92
3	A	1606	Y01	CAT-CAR-CBC	2.49	114.57	110.33
3	A	1618	Y01	CAC-CBB-CBE	2.46	116.69	112.92
3	A	1623	Y01	CBI-CBE-CBB	-2.44	115.66	119.49
3	A	1620	Y01	CBC-OAW-CAY	2.41	123.72	117.79
3	A	1623	Y01	CAC-CBB-CBE	-2.39	109.26	112.92
3	A	1620	Y01	CAO-CBB-CBE	2.39	115.22	110.28
3	A	1627	Y01	CAP-CBE-CBB	2.39	115.84	112.15
3	A	1617	Y01	CAO-CBB-CBE	2.35	115.15	110.28
3	A	1614	Y01	CBC-OAW-CAY	2.34	123.56	117.79
3	A	1628	Y01	CAO-CBB-CBE	2.34	115.12	110.28
3	A	1618	Y01	CAS-CBF-CBD	2.34	115.12	111.75
3	A	1612	Y01	CAS-CBF-CBD	2.32	115.10	111.75
3	A	1620	Y01	CAS-CBF-CBD	2.30	115.07	111.75
3	A	1617	Y01	OAW-CAY-CAM	2.28	116.42	111.50
3	A	1621	Y01	CAC-CBB-CBE	2.24	116.35	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1616	Y01	OAW-CBC-CAV	2.21	112.64	108.12
3	A	1605	Y01	CAP-CAQ-CBG	-2.21	100.76	105.13
3	A	1614	Y01	CAO-CBB-CBE	2.19	114.82	110.28
3	A	1624	Y01	CBF-CBD-CBG	-2.19	106.16	109.09
5	A	1632	NAG	C1-O5-C5	2.16	115.12	112.19
4	A	1631	AV0	C1-O5-C5	2.16	117.93	113.69
3	A	1618	Y01	CBC-OAW-CAY	2.13	123.05	117.79
3	A	1604	Y01	CAO-CBB-CBE	2.12	114.67	110.28
3	A	1621	Y01	CAP-CBE-CBB	2.10	115.39	112.15
3	A	1605	Y01	CAV-CAZ-CBH	2.08	119.18	116.42
3	A	1629	Y01	CBC-OAW-CAY	2.07	122.90	117.79
3	A	1609	Y01	CAO-CBB-CBE	2.05	114.53	110.28
4	A	1631	AV0	O4-C4-C3	2.04	112.70	107.28
4	A	1631	AV0	O5-C5-C6	2.03	111.48	106.44
4	A	1631	AV0	O1-C1-C2	2.03	111.47	108.30
3	A	1610	Y01	OAW-CAY-CAM	2.01	115.83	111.50
3	A	1613	Y01	CBG-CBI-CBE	2.01	102.45	100.07

There are no chirality outliers.

All (192) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1605	Y01	CAO-CBB-CBE-CAP
3	A	1606	Y01	OAG-CAY-OAW-CBC
3	A	1606	Y01	CAM-CAY-OAW-CBC
3	A	1607	Y01	CAO-CBB-CBE-CBI
3	A	1607	Y01	CAC-CBB-CBE-CBI
3	A	1607	Y01	OAG-CAY-OAW-CBC
3	A	1607	Y01	CAM-CAY-OAW-CBC
3	A	1610	Y01	OAG-CAY-OAW-CBC
3	A	1610	Y01	CAM-CAY-OAW-CBC
3	A	1612	Y01	OAG-CAY-OAW-CBC
3	A	1612	Y01	CAM-CAY-OAW-CBC
3	A	1613	Y01	OAG-CAY-OAW-CBC
3	A	1613	Y01	CAM-CAY-OAW-CBC
3	A	1614	Y01	OAG-CAY-OAW-CBC
3	A	1614	Y01	CAM-CAY-OAW-CBC
3	A	1615	Y01	CAR-CBC-OAW-CAY
3	A	1616	Y01	CAV-CBC-OAW-CAY
3	A	1617	Y01	OAG-CAY-OAW-CBC
3	A	1617	Y01	CAM-CAY-OAW-CBC
3	A	1618	Y01	OAG-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
3	A	1618	Y01	CAM-CAY-OAW-CBC
3	A	1619	Y01	OAG-CAY-OAW-CBC
3	A	1619	Y01	CAM-CAY-OAW-CBC
3	A	1621	Y01	OAG-CAY-OAW-CBC
3	A	1621	Y01	CAM-CAY-OAW-CBC
3	A	1622	Y01	OAG-CAY-OAW-CBC
3	A	1622	Y01	CAM-CAY-OAW-CBC
3	A	1627	Y01	CAO-CBB-CBE-CBI
3	A	1629	Y01	OAG-CAY-OAW-CBC
3	A	1629	Y01	CAM-CAY-OAW-CBC
4	A	1630	AV0	C2-C1-O1-CBS
4	A	1630	AV0	O5-C1-O1-CBS
4	A	1631	AV0	C2-C1-O1-CBS
4	A	1631	AV0	O5-C1-O1-CBS
4	A	1631	AV0	O1-CBS-CCM-CBQ
3	A	1607	Y01	CAC-CBB-CBE-CAP
3	A	1623	Y01	CAC-CBB-CBE-CBI
3	A	1624	Y01	CAJ-CAO-CBB-CAC
3	A	1623	Y01	CAC-CBB-CBE-CAP
3	A	1607	Y01	CAO-CBB-CBE-CAP
3	A	1623	Y01	CAO-CBB-CBE-CAP
3	A	1614	Y01	CAO-CBB-CBE-CBI
3	A	1623	Y01	CAO-CBB-CBE-CBI
3	A	1614	Y01	CAC-CBB-CBE-CAP
3	A	1621	Y01	CAO-CBB-CBE-CBI
3	A	1614	Y01	CAO-CBB-CBE-CAP
4	A	1631	AV0	O5-C5-C6-O6
3	A	1614	Y01	CAJ-CAO-CBB-CBE
3	A	1615	Y01	CAJ-CAO-CBB-CBE
3	A	1624	Y01	CAJ-CAO-CBB-CBE
3	A	1614	Y01	CAC-CBB-CBE-CBI
3	A	1605	Y01	CAO-CBB-CBE-CBI
3	A	1628	Y01	CAO-CBB-CBE-CBI
3	A	1608	Y01	CAO-CBB-CBE-CAP
3	A	1604	Y01	CAO-CBB-CBE-CBI
3	A	1618	Y01	CAO-CBB-CBE-CBI
3	A	1624	Y01	CAO-CBB-CBE-CBI
3	A	1614	Y01	CAJ-CAO-CBB-CAC
3	A	1615	Y01	CAJ-CAO-CBB-CAC
3	A	1624	Y01	CAO-CAJ-CAN-CBA
3	A	1604	Y01	CAC-CBB-CBE-CAP
3	A	1628	Y01	CAC-CBB-CBE-CAP

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Mol	Chain	Res	Type	Atoms
3	A	1605	Y01	CAN-CAJ-CAO-CBB
3	A	1624	Y01	CAC-CBB-CBE-CAP
3	A	1627	Y01	CAC-CBB-CBE-CAP
3	A	1618	Y01	CAO-CBB-CBE-CAP
3	A	1621	Y01	CAO-CBB-CBE-CAP
3	A	1627	Y01	CAO-CBB-CBE-CAP
4	A	1631	AV0	OBX-CCJ-OBV-CBT
3	A	1605	Y01	CAC-CBB-CBE-CAP
3	A	1604	Y01	CAC-CBB-CBE-CBI
3	A	1624	Y01	CAC-CBB-CBE-CBI
3	A	1628	Y01	CAC-CBB-CBE-CBI
3	A	1608	Y01	CAO-CBB-CBE-CBI
3	A	1621	Y01	CAN-CAJ-CAO-CBB
3	A	1604	Y01	CAN-CAJ-CAO-CBB
4	A	1631	AV0	CBJ-CBL-CBR-CCM
3	A	1608	Y01	CAC-CBB-CBE-CAP
3	A	1621	Y01	CAC-CBB-CBE-CAP
3	A	1611	Y01	CAR-CBC-OAW-CAY
3	A	1608	Y01	CAM-CAY-OAW-CBC
4	A	1631	AV0	O1-CBS-CCM-CBT
3	A	1617	Y01	CAV-CBC-OAW-CAY
4	A	1631	AV0	CCL-CCJ-OBV-CBT
3	A	1607	Y01	CAO-CAJ-CAN-CBA
4	A	1630	AV0	CBH-CBJ-CBL-CBR
3	A	1618	Y01	CAC-CBB-CBE-CAP
3	A	1616	Y01	CAJ-CAO-CBB-CAC
3	A	1616	Y01	CAJ-CAO-CBB-CBE
4	A	1631	AV0	CAX-CAZ-CBB-CBD
3	A	1617	Y01	CAR-CBC-OAW-CAY
3	A	1605	Y01	CAC-CBB-CBE-CBI
3	A	1616	Y01	CAO-CAJ-CAN-CBA
3	A	1621	Y01	CAJ-CAN-CBA-CAA
3	A	1624	Y01	CAJ-CAN-CBA-CAA
3	A	1617	Y01	CAJ-CAN-CBA-CAA
3	A	1608	Y01	OAG-CAY-OAW-CBC
3	A	1624	Y01	CAM-CAY-OAW-CBC
3	A	1604	Y01	CAR-CBC-OAW-CAY
3	A	1624	Y01	CAJ-CAN-CBA-CAB
3	A	1620	Y01	CAV-CBC-OAW-CAY
5	A	1635	NAG	O5-C5-C6-O6
3	A	1624	Y01	CAL-CAM-CAY-OAW
4	A	1630	AV0	CCF-CCQ-OCB-CCS

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Mol	Chain	Res	Type	Atoms
3	A	1627	Y01	CAC-CBB-CBE-CBI
3	A	1604	Y01	CAO-CBB-CBE-CAP
3	A	1611	Y01	CAV-CBC-OAW-CAY
4	A	1630	AV0	CCH-CCQ-OCB-CCS
3	A	1628	Y01	CAO-CBB-CBE-CAP
3	A	1624	Y01	OAG-CAY-OAW-CBC
4	A	1631	AV0	C5-C4-O4-CCR
3	A	1613	Y01	CAJ-CAO-CBB-CAC
4	A	1631	AV0	CBA-CBC-CBE-CBG
3	A	1604	Y01	CAV-CBC-OAW-CAY
3	A	1620	Y01	CAR-CBC-OAW-CAY
3	A	1621	Y01	CAJ-CAN-CBA-CAB
3	A	1617	Y01	CAJ-CAN-CBA-CAB
3	A	1621	Y01	CAC-CBB-CBE-CBI
4	A	1631	AV0	C3-C4-O4-CCR
4	A	1631	AV0	O1-CBS-CCM-CBR
3	A	1629	Y01	CAJ-CAN-CBA-CAB
3	A	1606	Y01	CAJ-CAN-CBA-CAA
4	A	1630	AV0	CAA-CAW-CAY-CBA
4	A	1631	AV0	CCM-CBS-O1-C1
4	A	1631	AV0	C4-C5-C6-O6
3	A	1607	Y01	CAJ-CAO-CBB-CBE
3	A	1629	Y01	CAJ-CAN-CBA-CAA
5	A	1633	NAG	C1-C2-N2-C7
3	A	1614	Y01	CAM-CAL-CAX-OAF
3	A	1606	Y01	CAJ-CAN-CBA-CAB
3	A	1624	Y01	CAL-CAM-CAY-OAG
3	A	1604	Y01	CAM-CAL-CAX-OAF
3	A	1616	Y01	CAM-CAL-CAX-OAF
3	A	1624	Y01	CAM-CAL-CAX-OAF
3	A	1623	Y01	CAM-CAL-CAX-OAF
3	A	1612	Y01	CAN-CAJ-CAO-CBB
3	A	1625	Y01	CAM-CAL-CAX-OAF
3	A	1617	Y01	CAM-CAL-CAX-OAH
4	A	1630	AV0	CCW-CCS-OCB-CCQ
3	A	1607	Y01	CAM-CAL-CAX-OAH
3	A	1605	Y01	CAJ-CAN-CBA-CAB
3	A	1604	Y01	CAM-CAL-CAX-OAH
3	A	1607	Y01	CAM-CAL-CAX-OAF
3	A	1617	Y01	CAM-CAL-CAX-OAF
3	A	1622	Y01	CAM-CAL-CAX-OAF
3	A	1612	Y01	CAM-CAL-CAX-OAF

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Mol	Chain	Res	Type	Atoms
3	A	1616	Y01	CAM-CAL-CAX-OAH
3	A	1624	Y01	CAM-CAL-CAX-OAH
3	A	1605	Y01	CAJ-CAN-CBA-CAA
3	A	1614	Y01	CAO-CAJ-CAN-CBA
3	A	1615	Y01	CAM-CAL-CAX-OAF
3	A	1625	Y01	CAM-CAL-CAX-OAH
3	A	1615	Y01	CAM-CAL-CAX-OAH
3	A	1608	Y01	CAJ-CAO-CBB-CAC
3	A	1614	Y01	CAM-CAL-CAX-OAH
3	A	1622	Y01	CAM-CAL-CAX-OAH
3	A	1623	Y01	CAV-CBC-OAW-CAY
3	A	1618	Y01	CAV-CBC-OAW-CAY
3	A	1623	Y01	CAM-CAL-CAX-OAH
3	A	1612	Y01	CAX-CAL-CAM-CAY
3	A	1620	Y01	CAM-CAL-CAX-OAF
3	A	1621	Y01	CAM-CAL-CAX-OAH
3	A	1627	Y01	CAN-CAJ-CAO-CBB
4	A	1631	AV0	CCV-CCR-O4-C4
4	A	1630	AV0	OBZ-CCS-OCB-CCQ
3	A	1612	Y01	CAM-CAL-CAX-OAH
3	A	1626	Y01	CAM-CAL-CAX-OAF
3	A	1622	Y01	CAL-CAM-CAY-OAW
3	A	1618	Y01	CAM-CAL-CAX-OAH
3	A	1626	Y01	CAM-CAL-CAX-OAH
3	A	1620	Y01	CAM-CAL-CAX-OAH
3	A	1619	Y01	CAJ-CAO-CBB-CBE
3	A	1612	Y01	CAL-CAM-CAY-OAW
3	A	1618	Y01	CAM-CAL-CAX-OAF
4	A	1631	AV0	CCF-CCQ-OCB-CCS
3	A	1615	Y01	CAL-CAM-CAY-OAW
3	A	1621	Y01	CAM-CAL-CAX-OAF
5	A	1633	NAG	C3-C2-N2-C7
3	A	1622	Y01	CAL-CAM-CAY-OAG
3	A	1606	Y01	CAV-CBC-OAW-CAY
3	A	1611	Y01	CAM-CAL-CAX-OAH
3	A	1623	Y01	CAR-CBC-OAW-CAY
3	A	1628	Y01	CAM-CAL-CAX-OAF
3	A	1619	Y01	CAM-CAL-CAX-OAH
3	A	1608	Y01	CAL-CAM-CAY-OAW
3	A	1629	Y01	CAV-CBC-OAW-CAY
3	A	1613	Y01	CAM-CAL-CAX-OAH
3	A	1613	Y01	CAM-CAL-CAX-OAF

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Mol	Chain	Res	Type	Atoms
4	A	1631	AV0	CCH-CCQ-OCB-CCS
3	A	1623	Y01	CAJ-CAO-CBB-CAC
3	A	1614	Y01	CAN-CAJ-CAO-CBB
3	A	1610	Y01	CAL-CAM-CAY-OAG

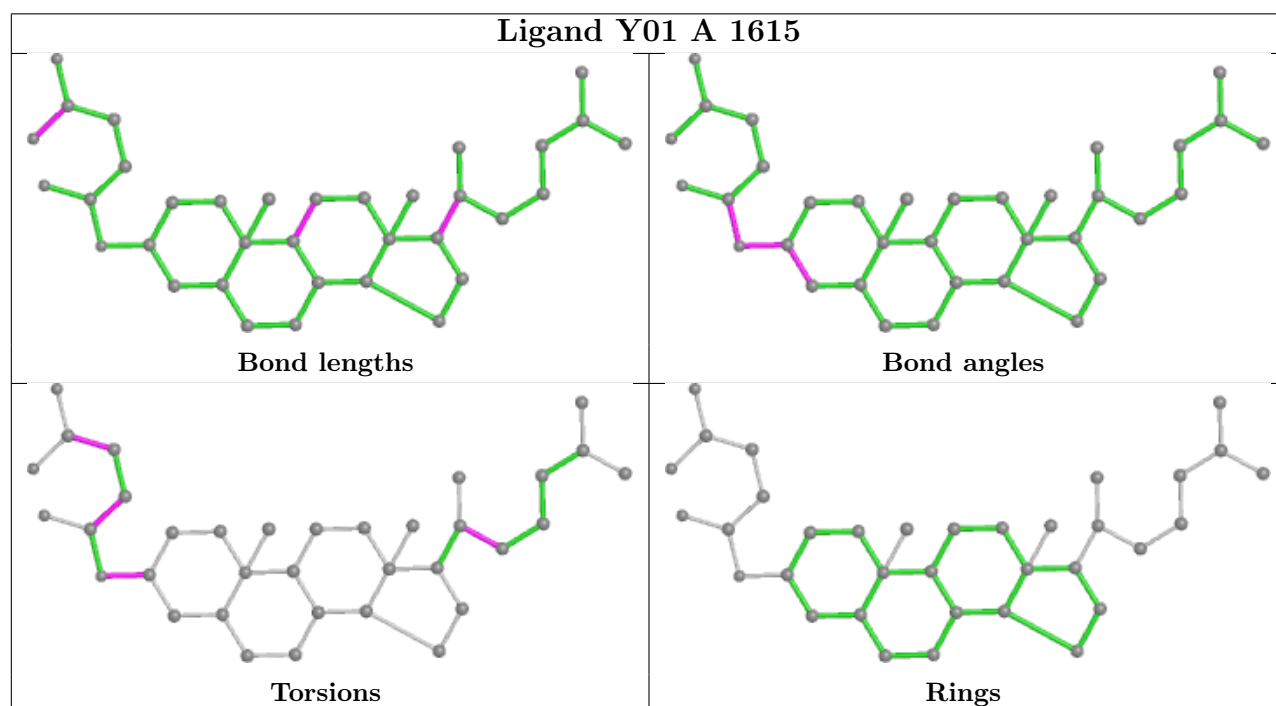
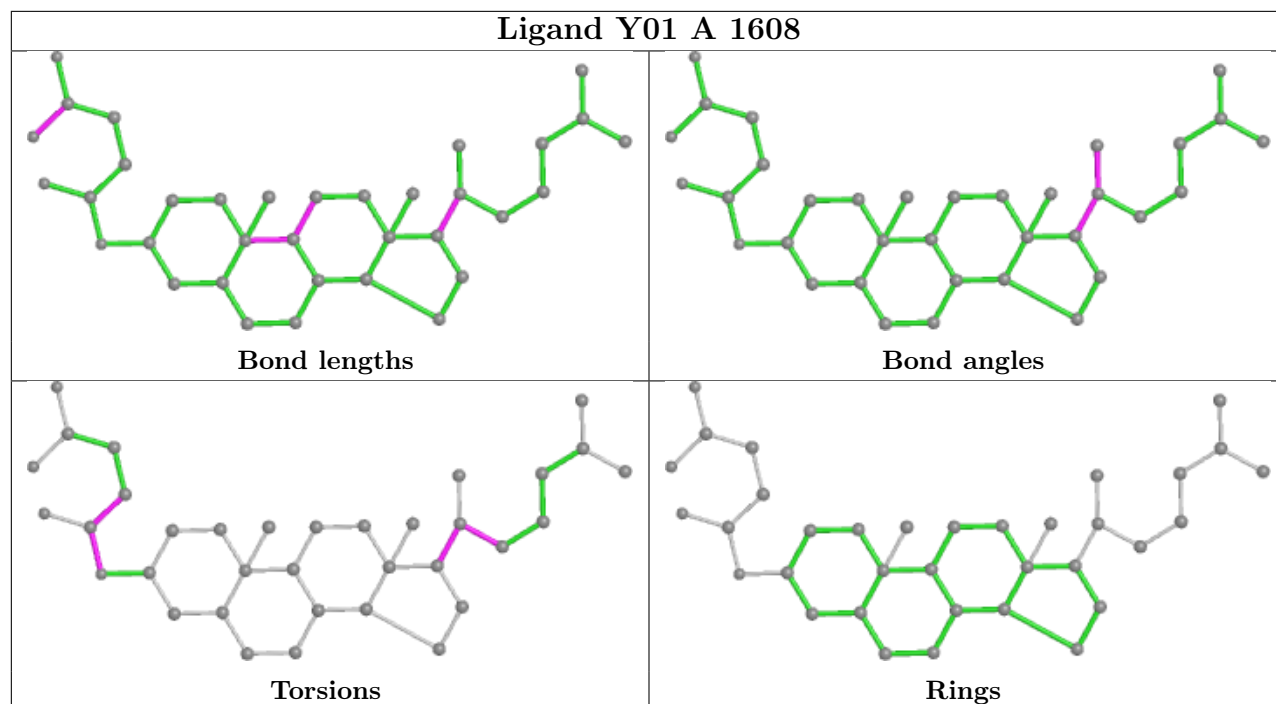
There are no ring outliers.

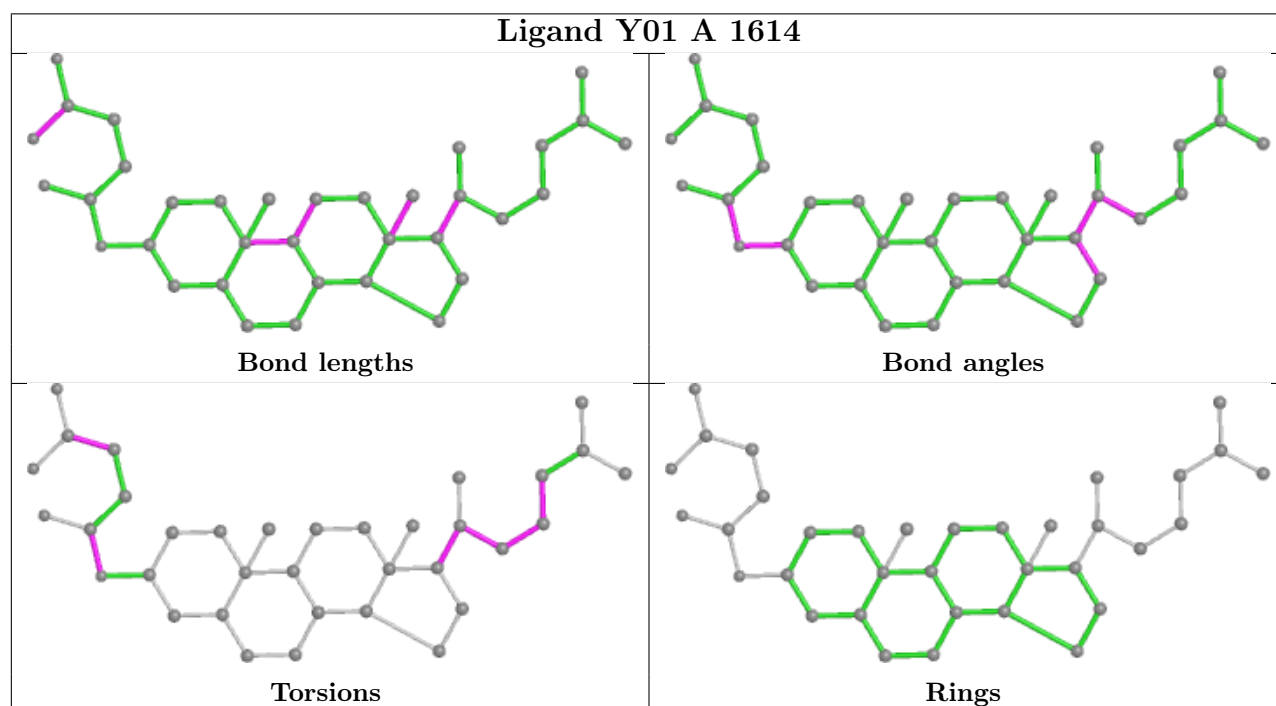
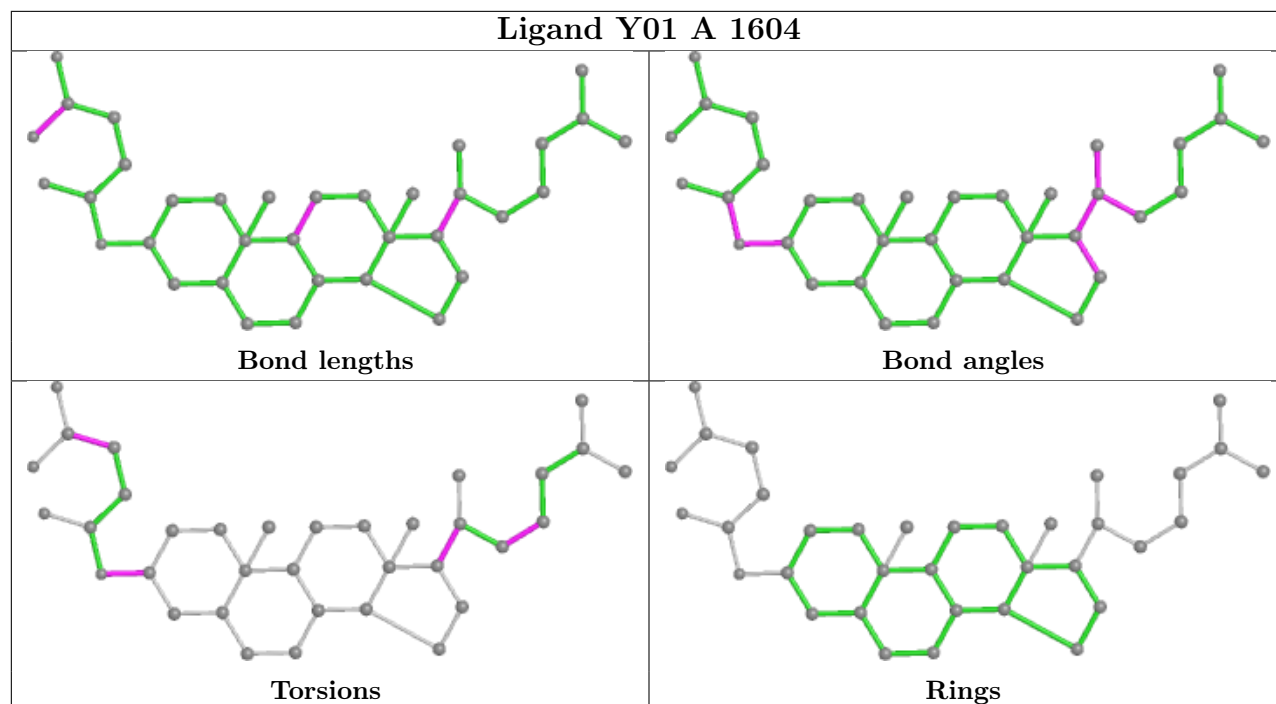
13 monomers are involved in 26 short contacts:

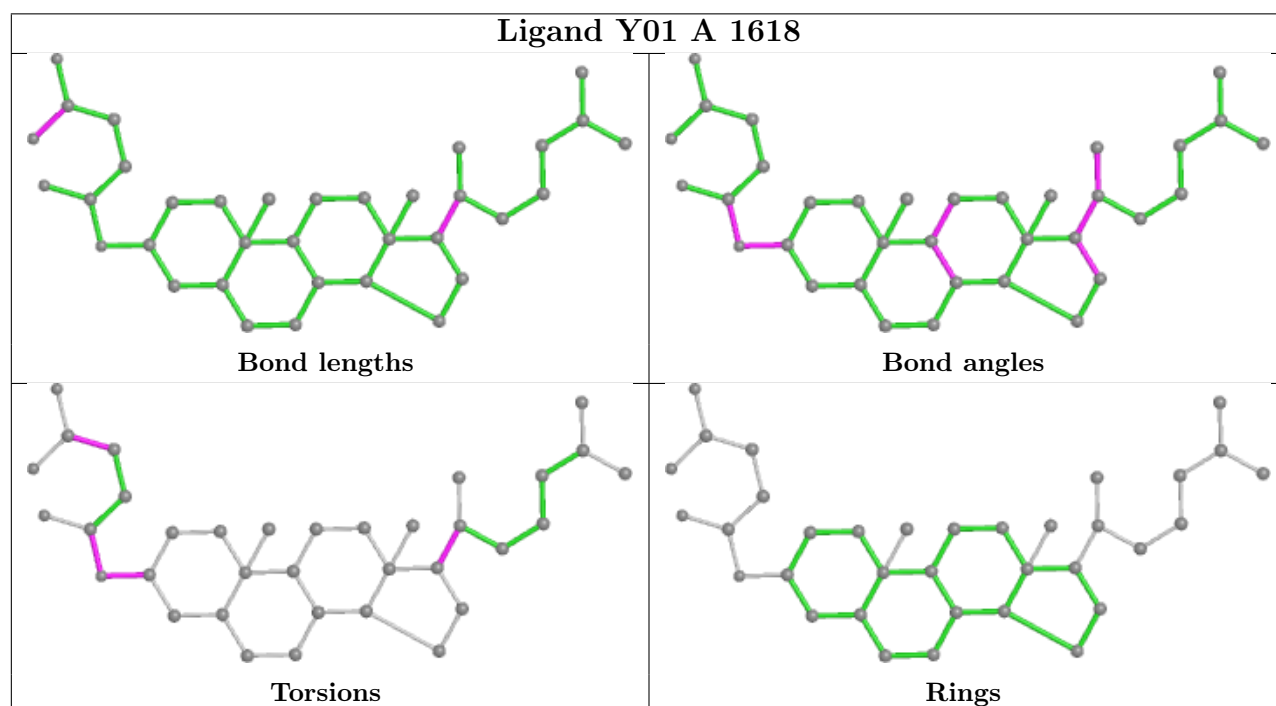
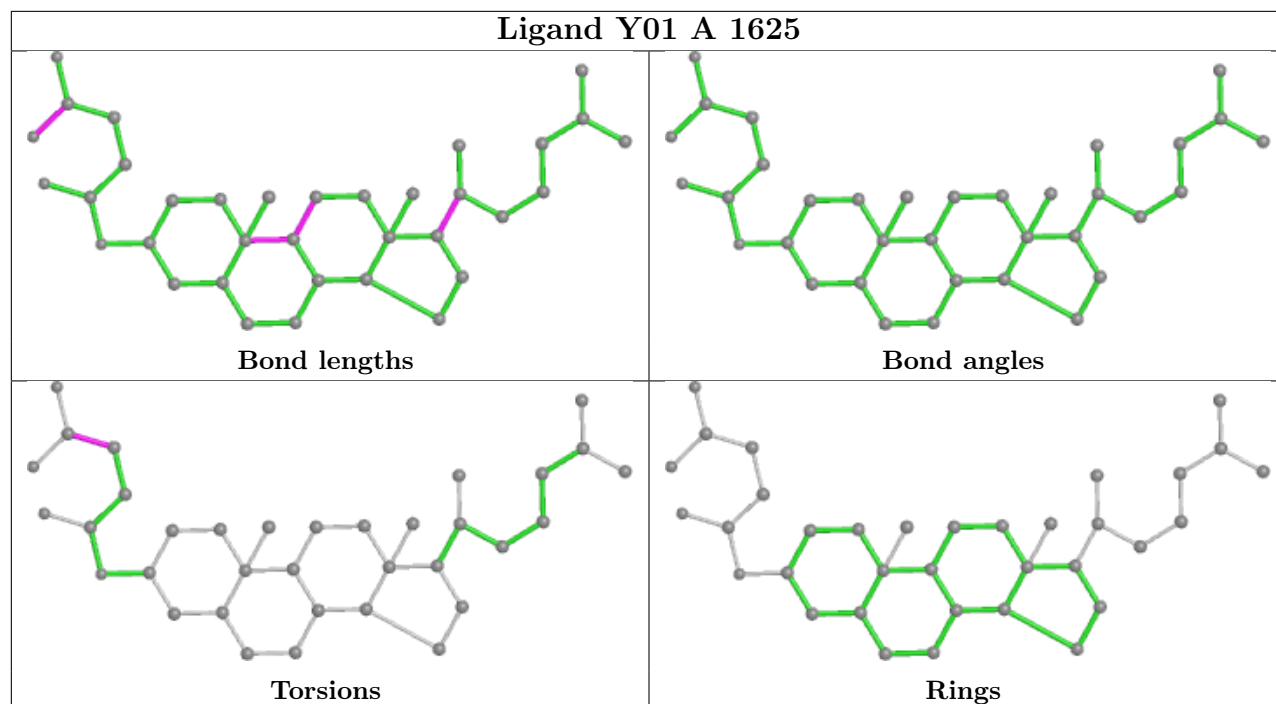
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1608	Y01	2	0
3	A	1615	Y01	1	0
3	A	1618	Y01	1	0
3	A	1605	Y01	4	0
3	A	1629	Y01	1	0
3	A	1609	Y01	1	0
3	A	1624	Y01	7	0
3	A	1606	Y01	1	0
3	A	1620	Y01	1	0
3	A	1619	Y01	4	0
3	A	1612	Y01	1	0
3	A	1622	Y01	1	0
3	A	1617	Y01	1	0

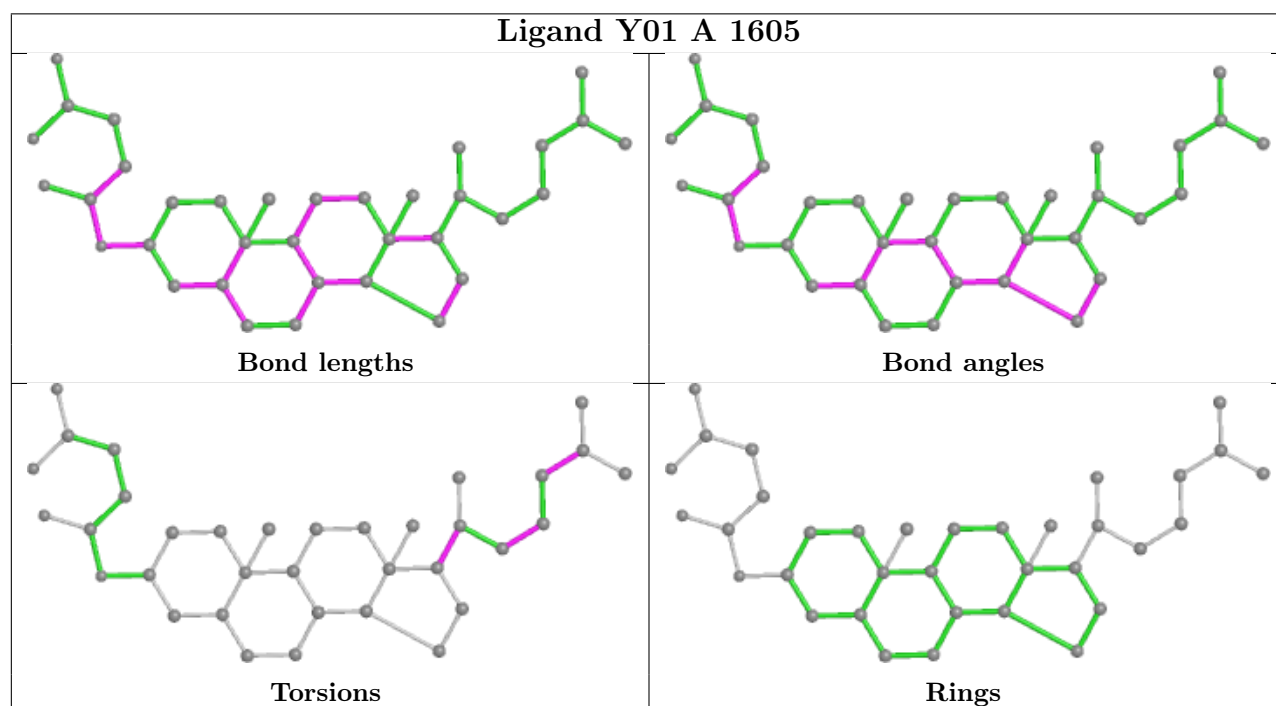
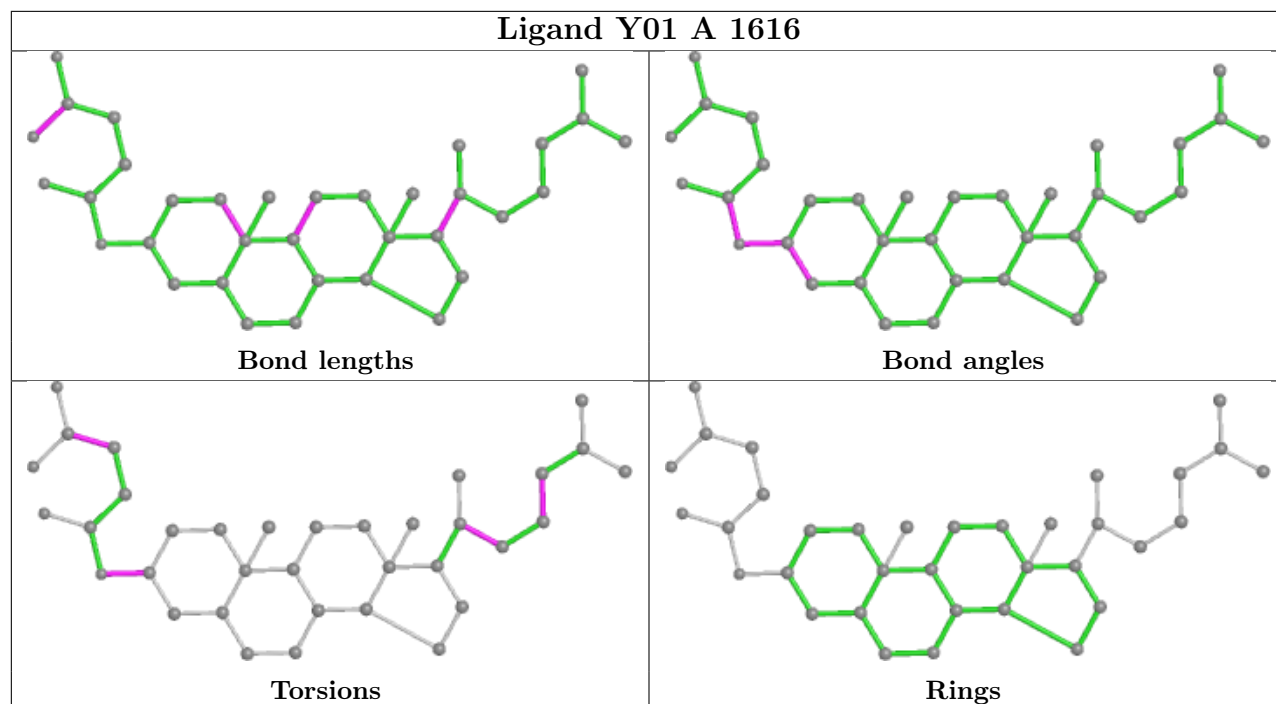
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

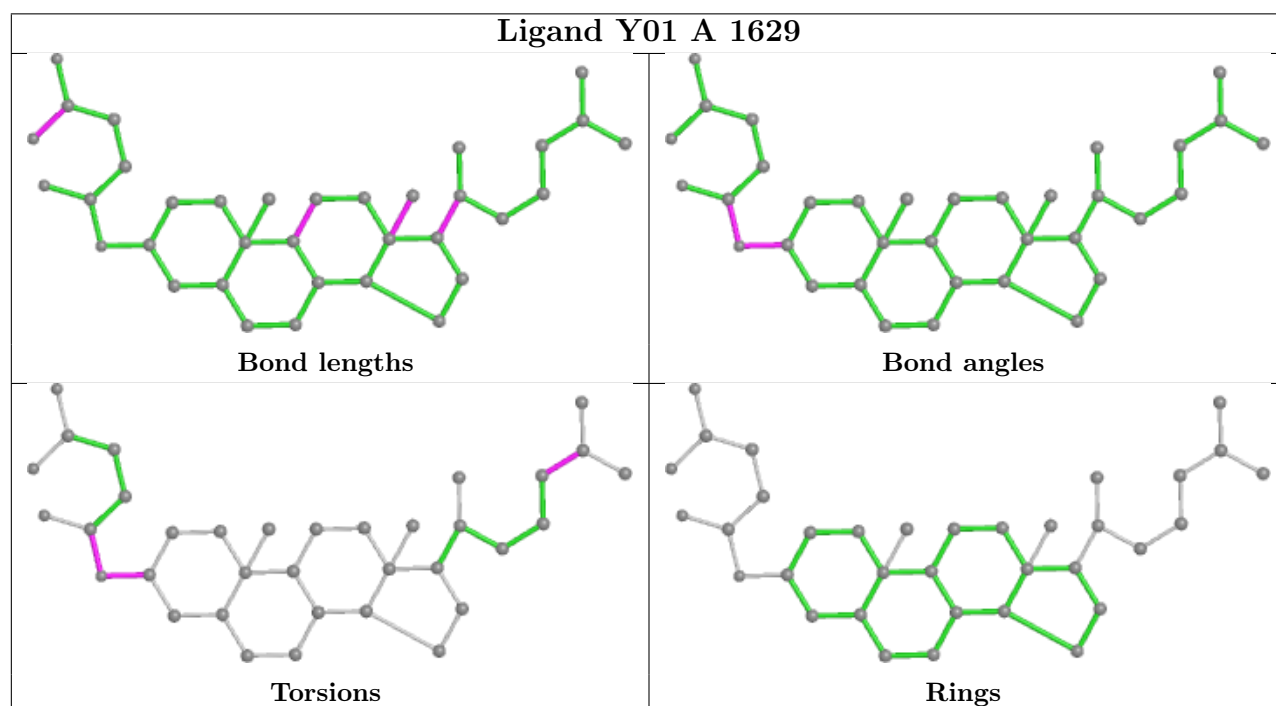
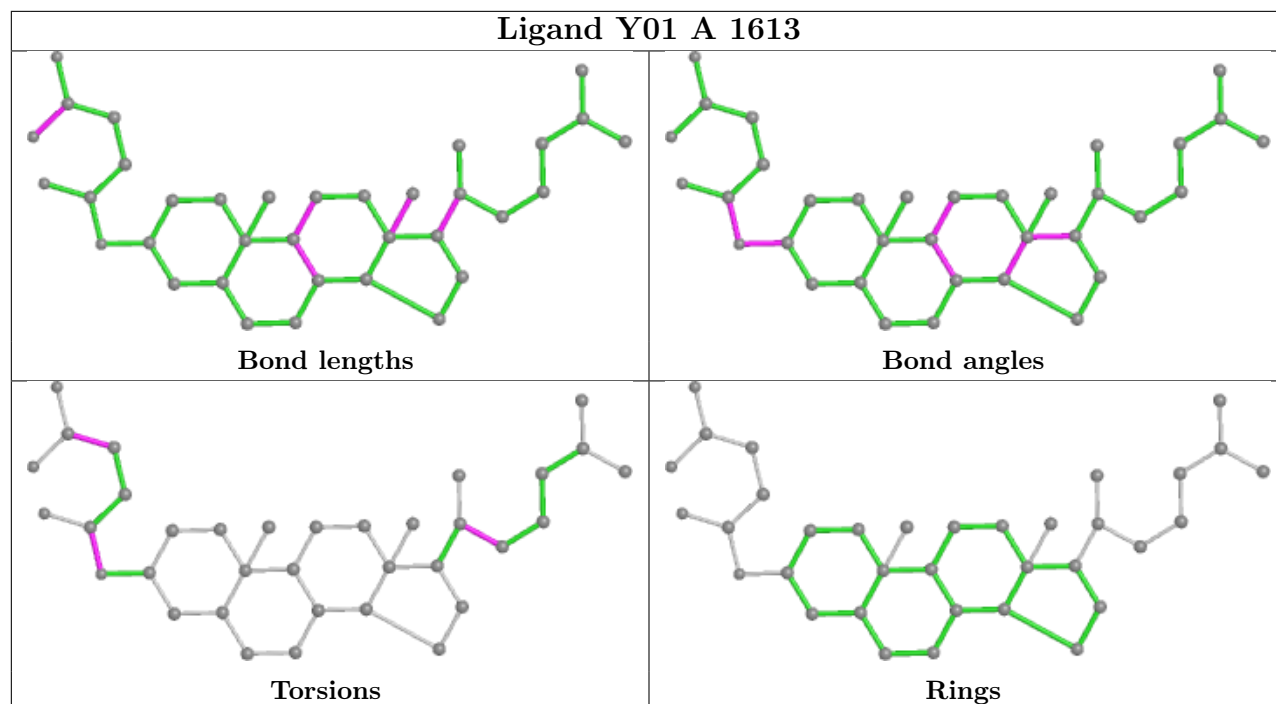


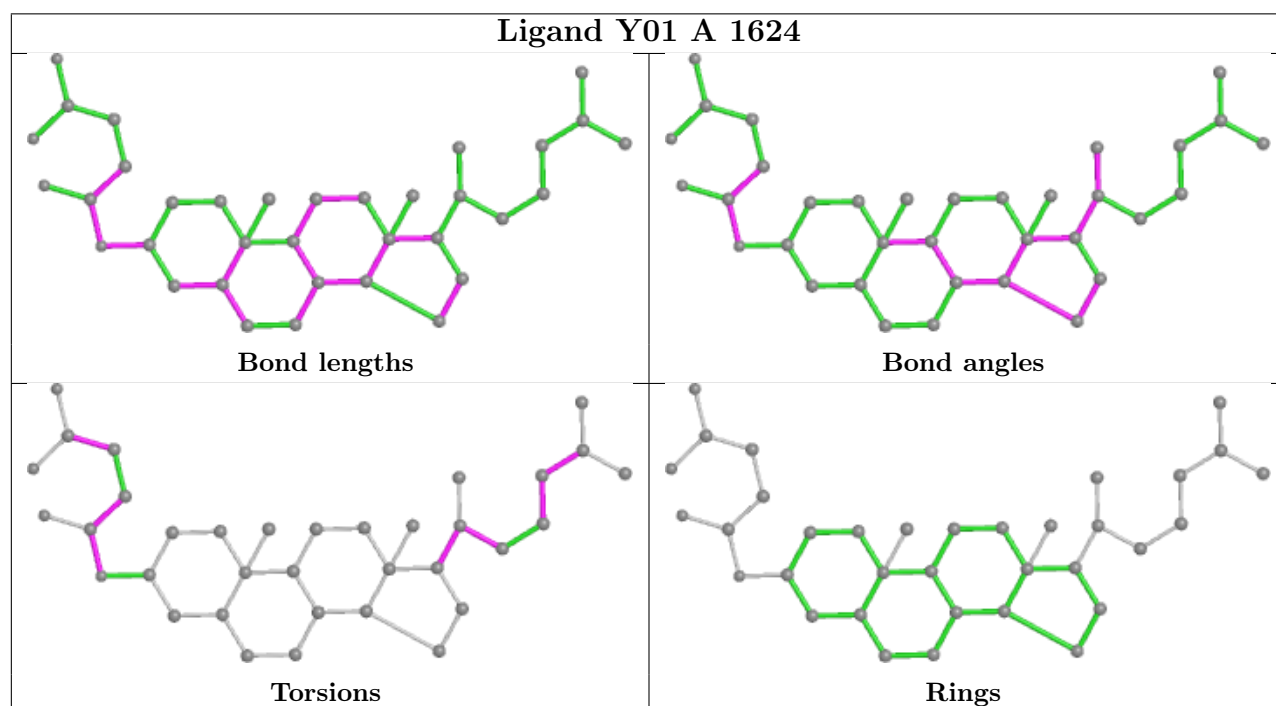
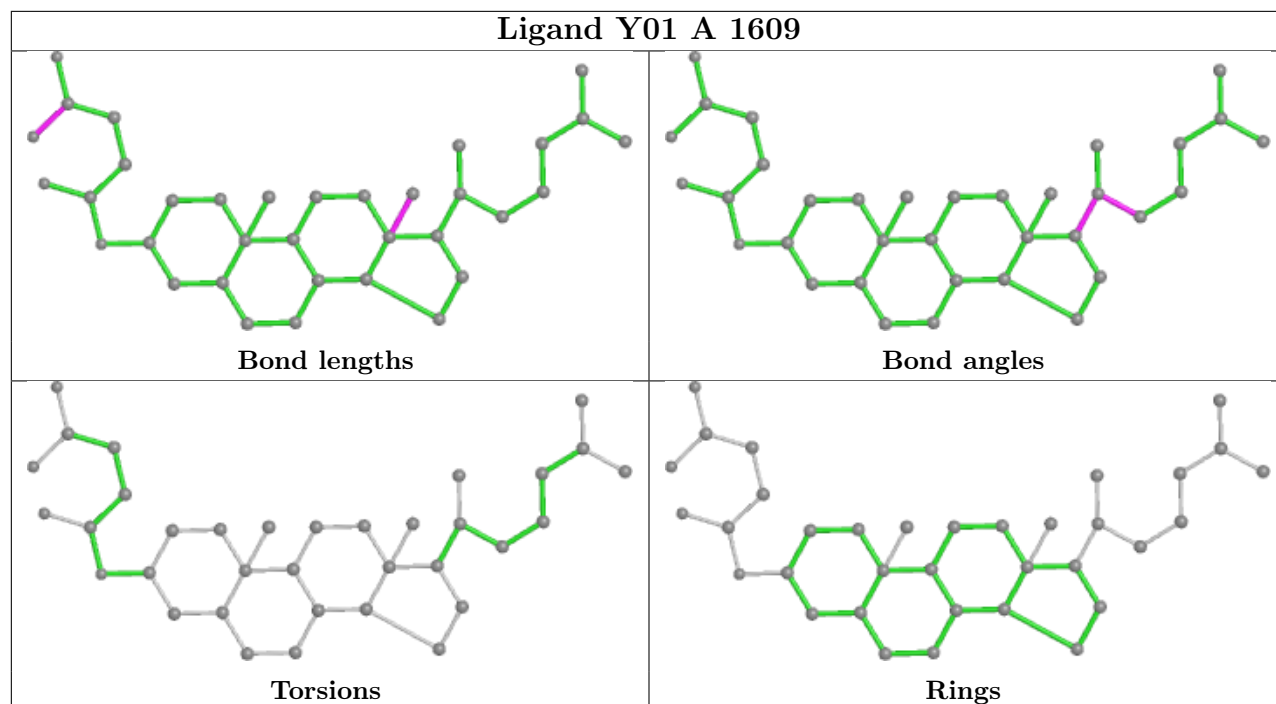


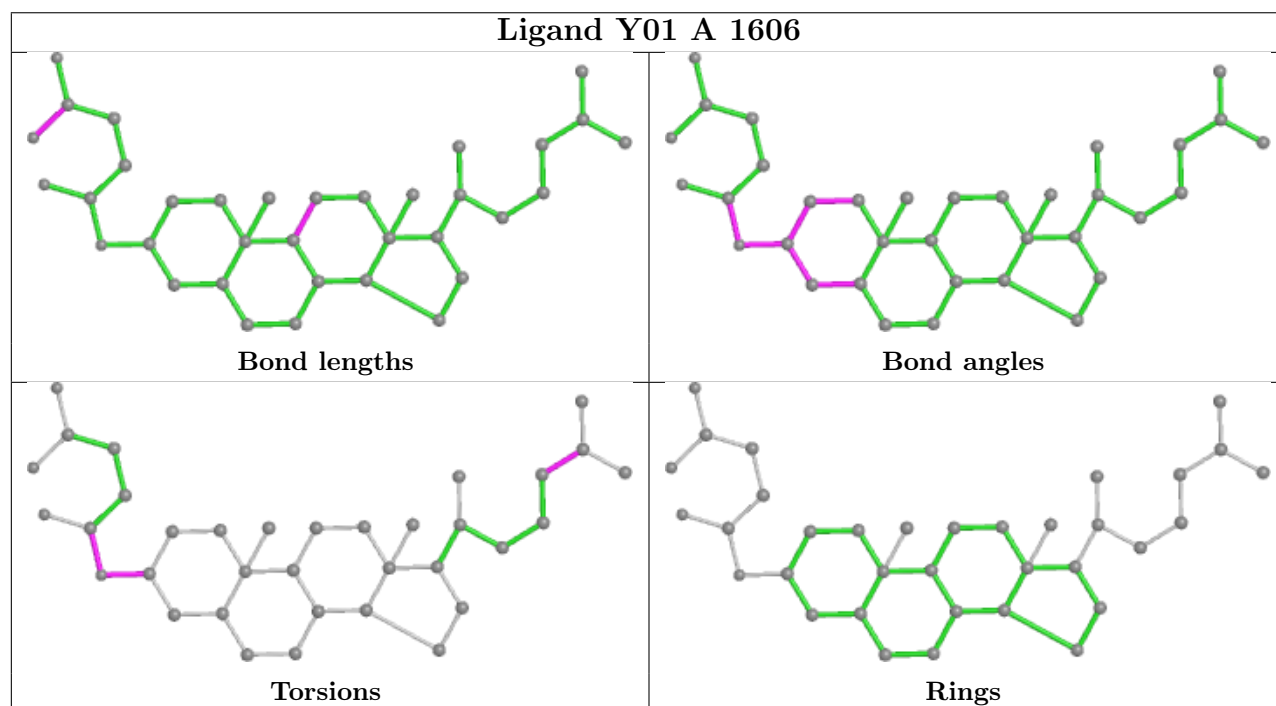
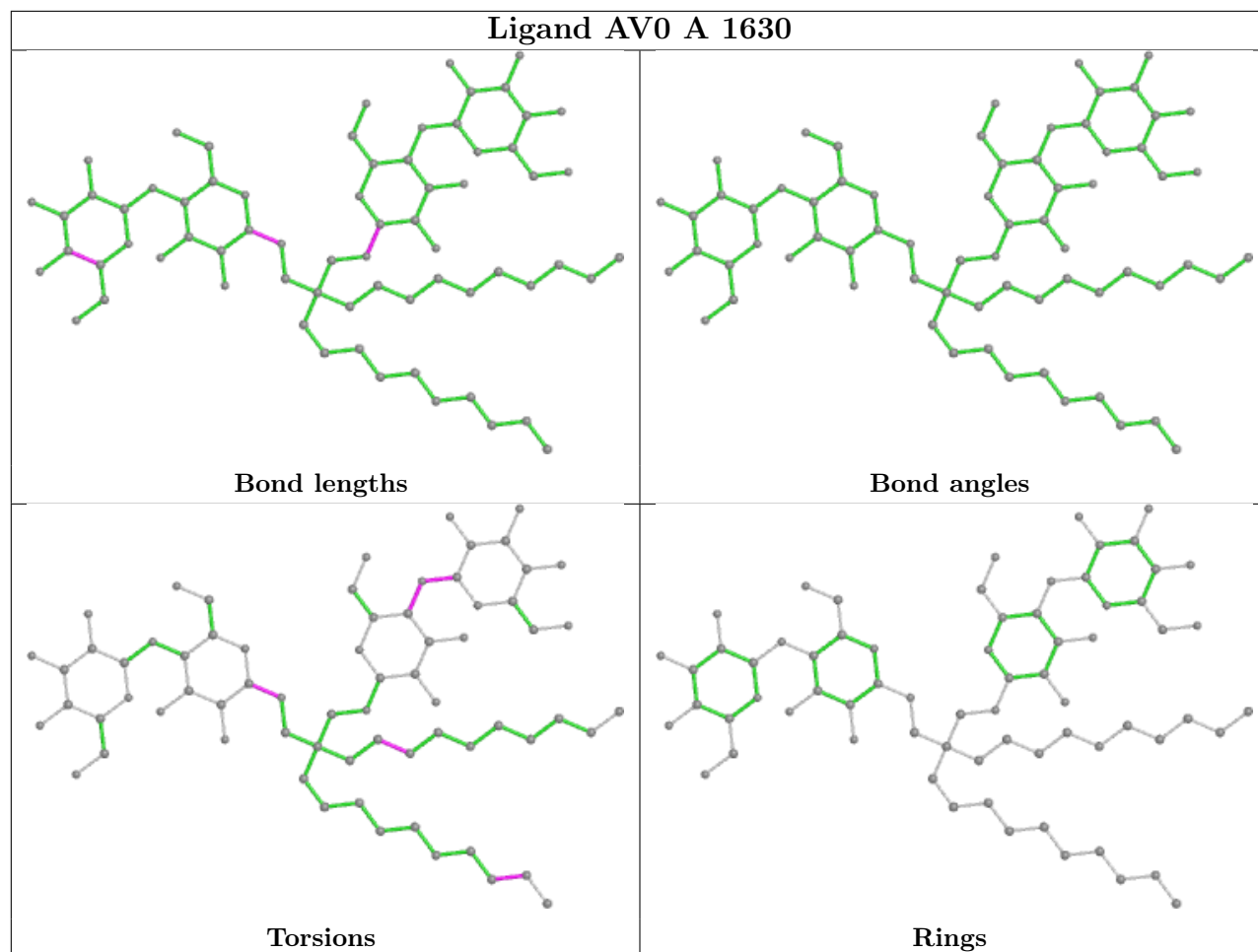


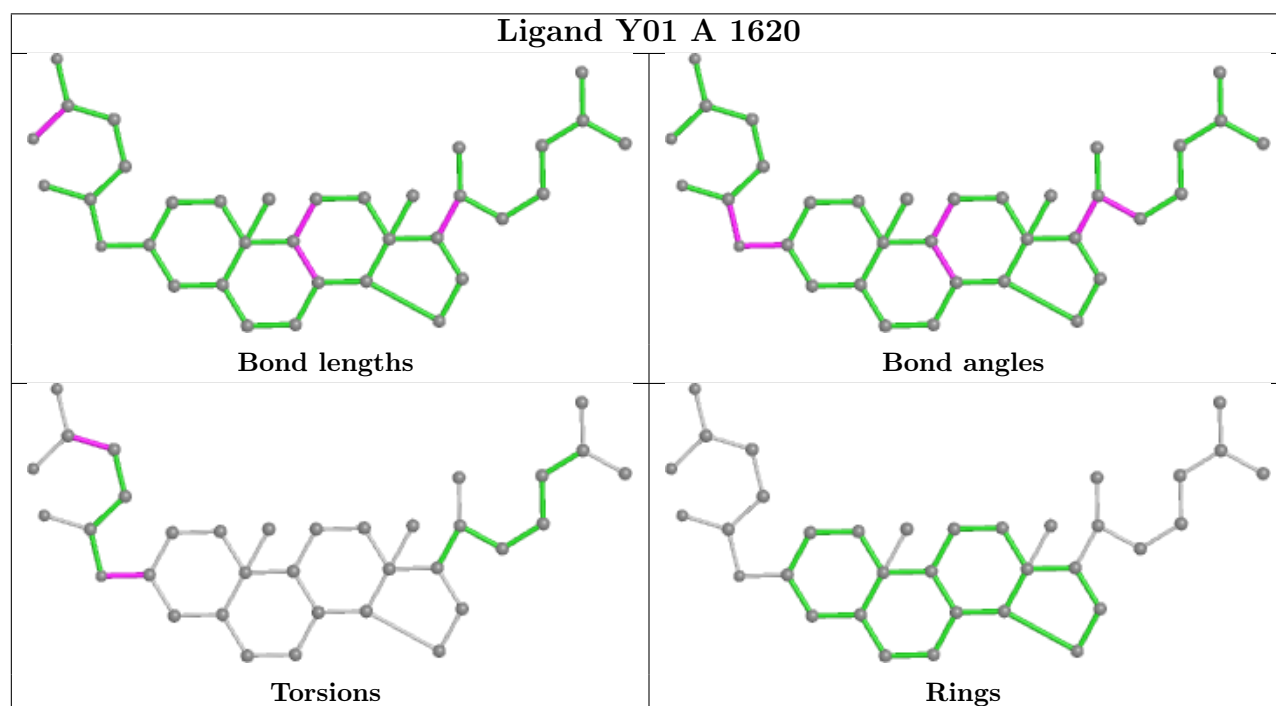
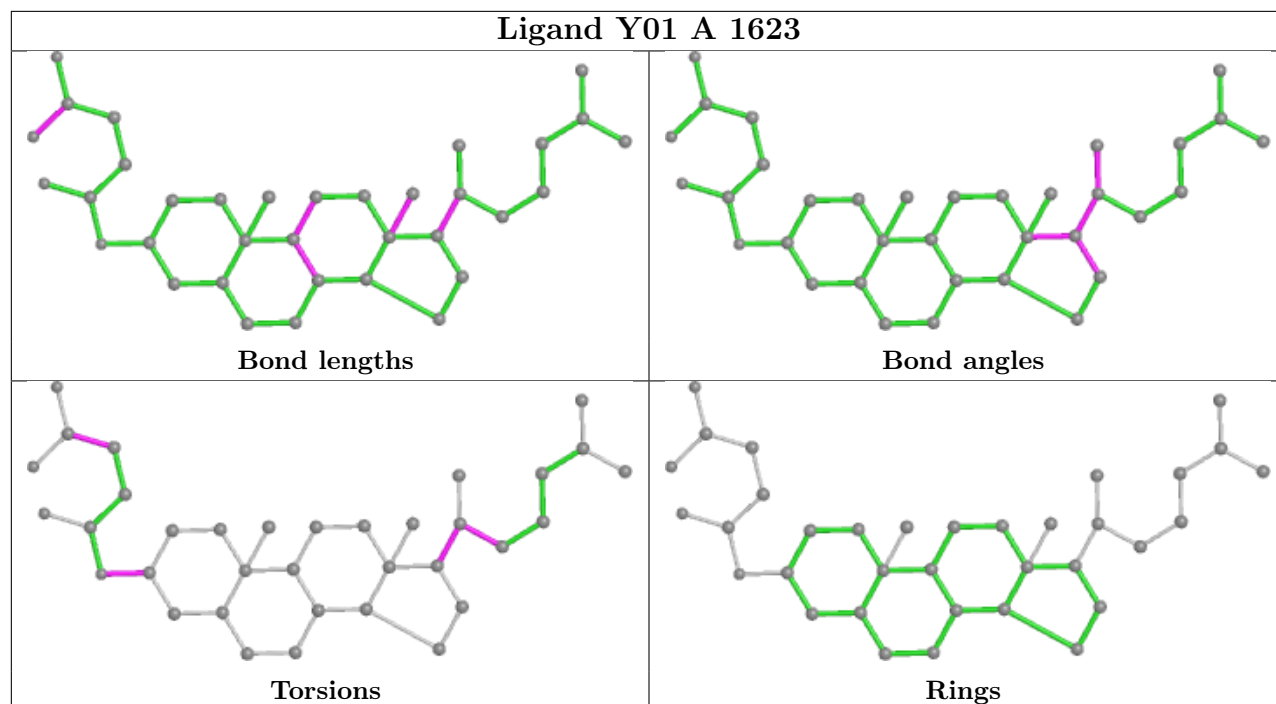




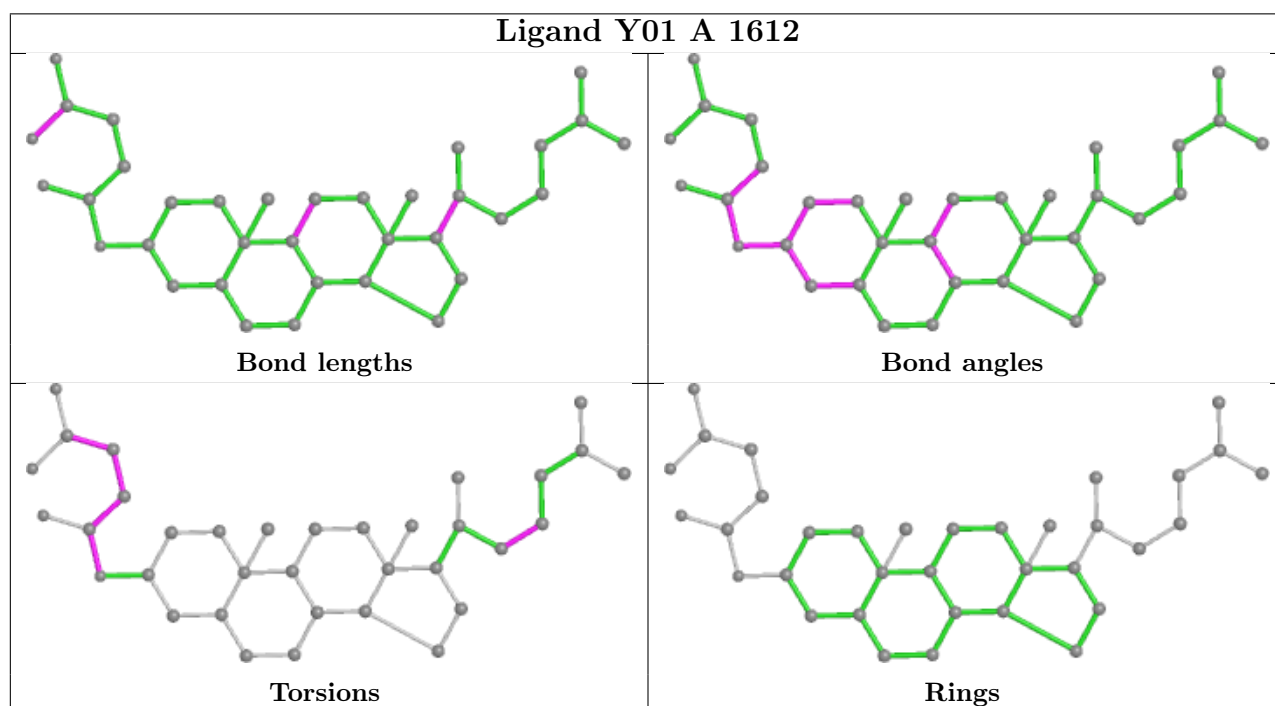
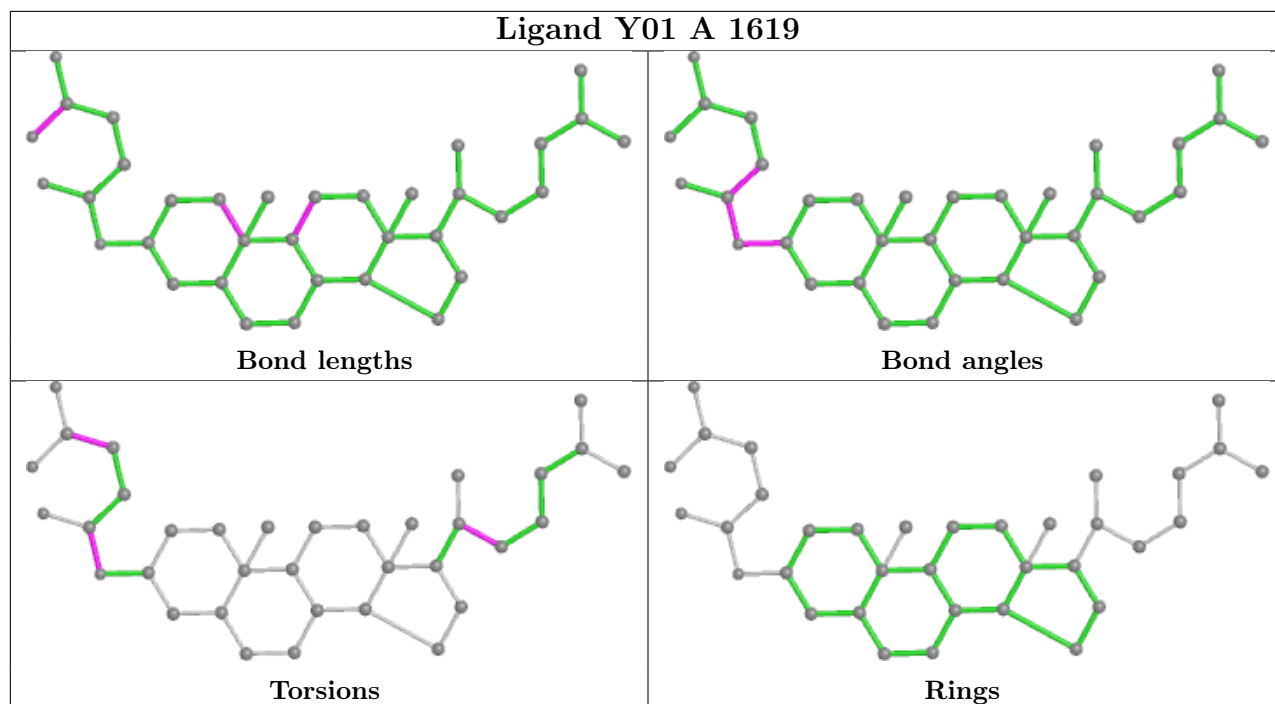


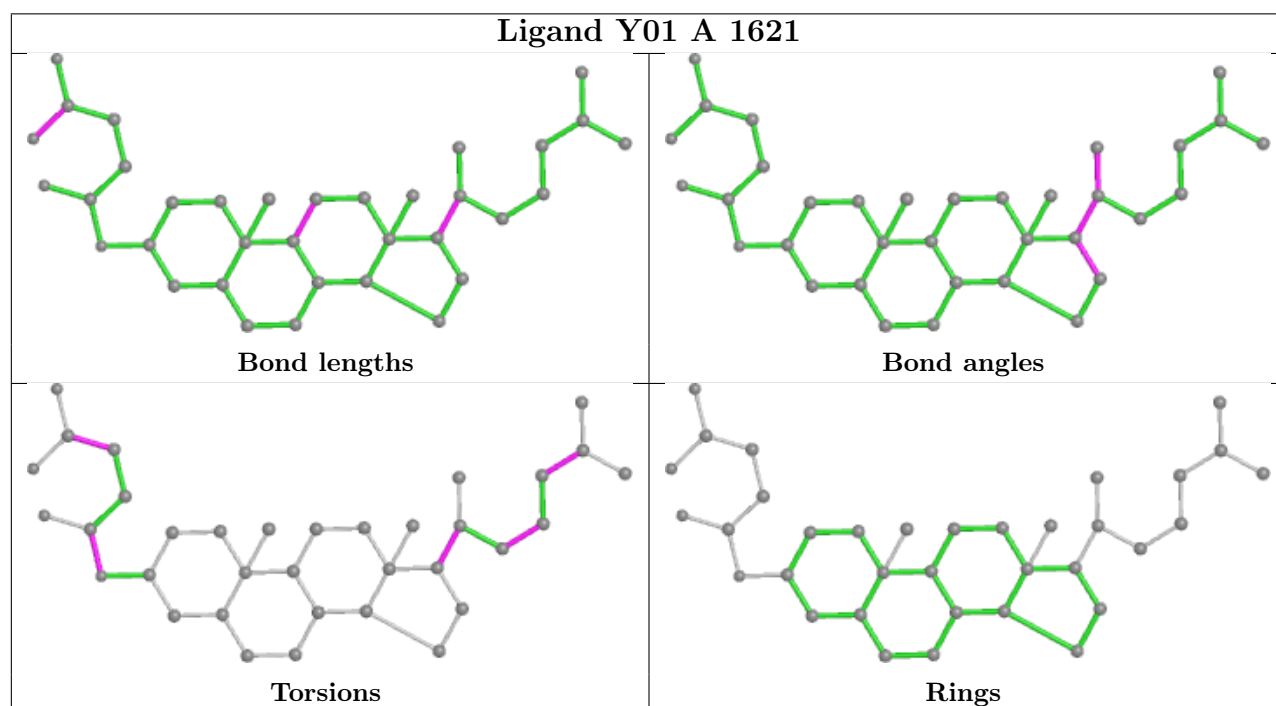
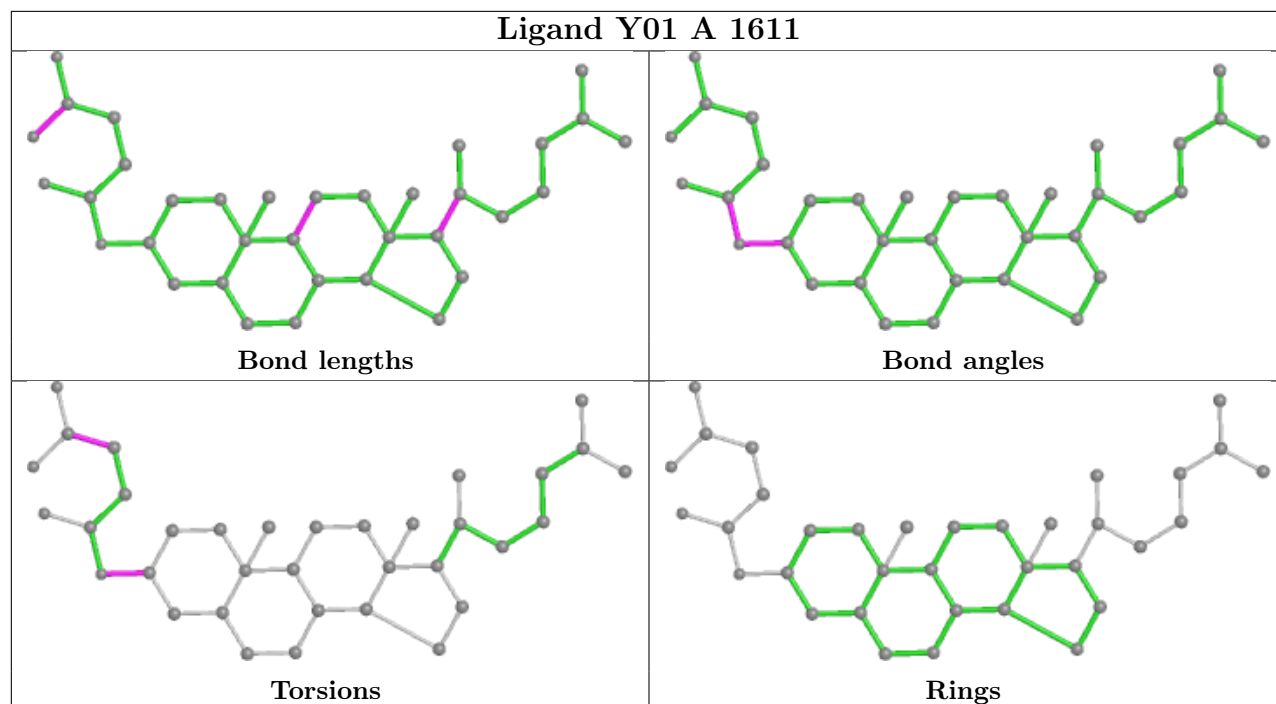


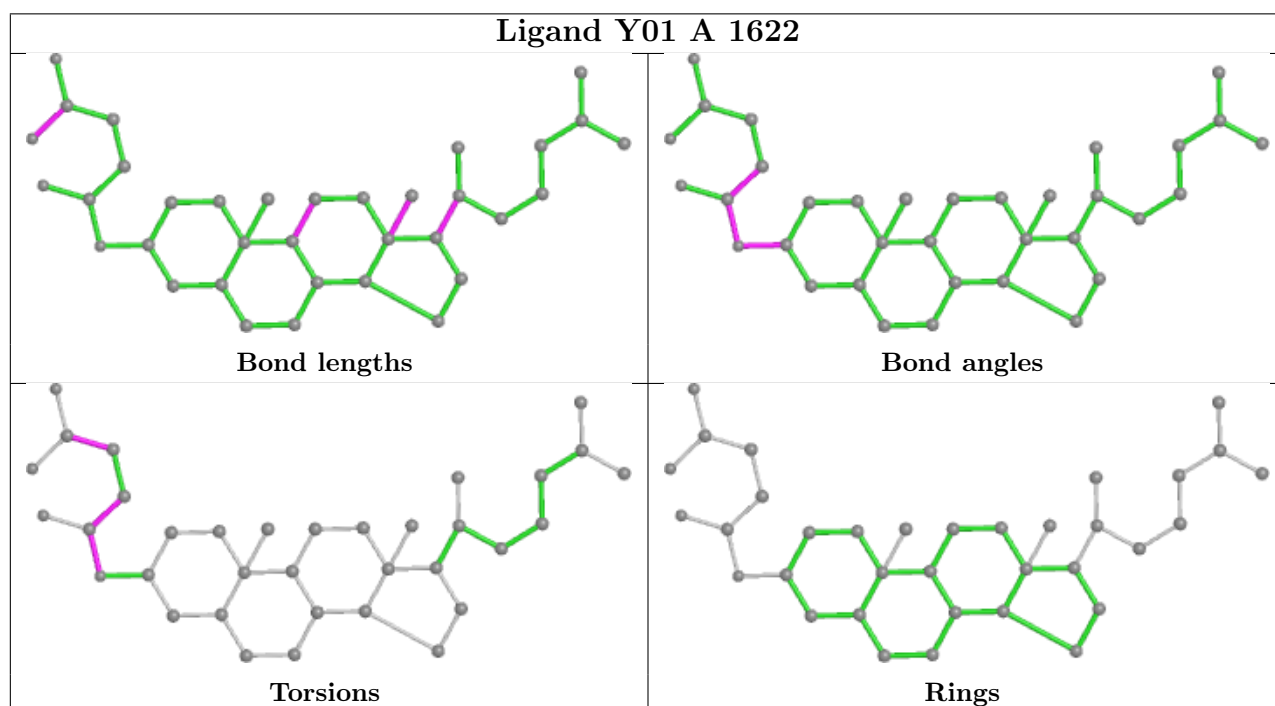
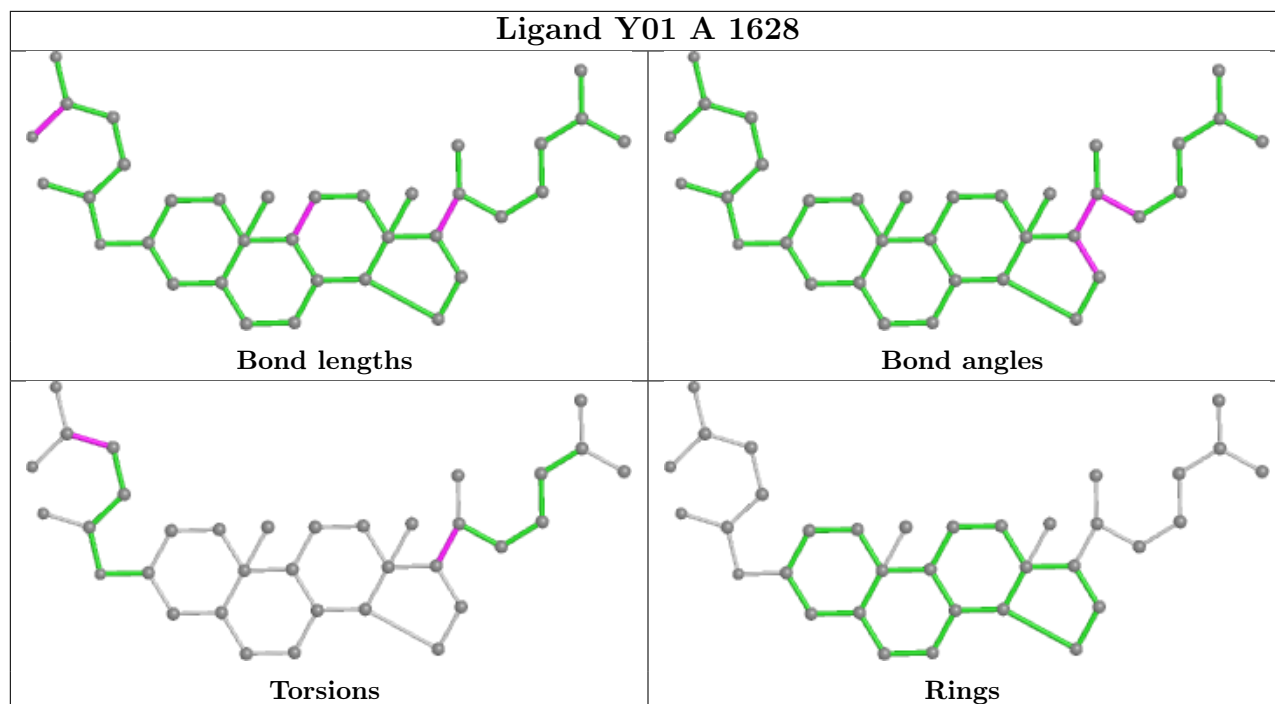


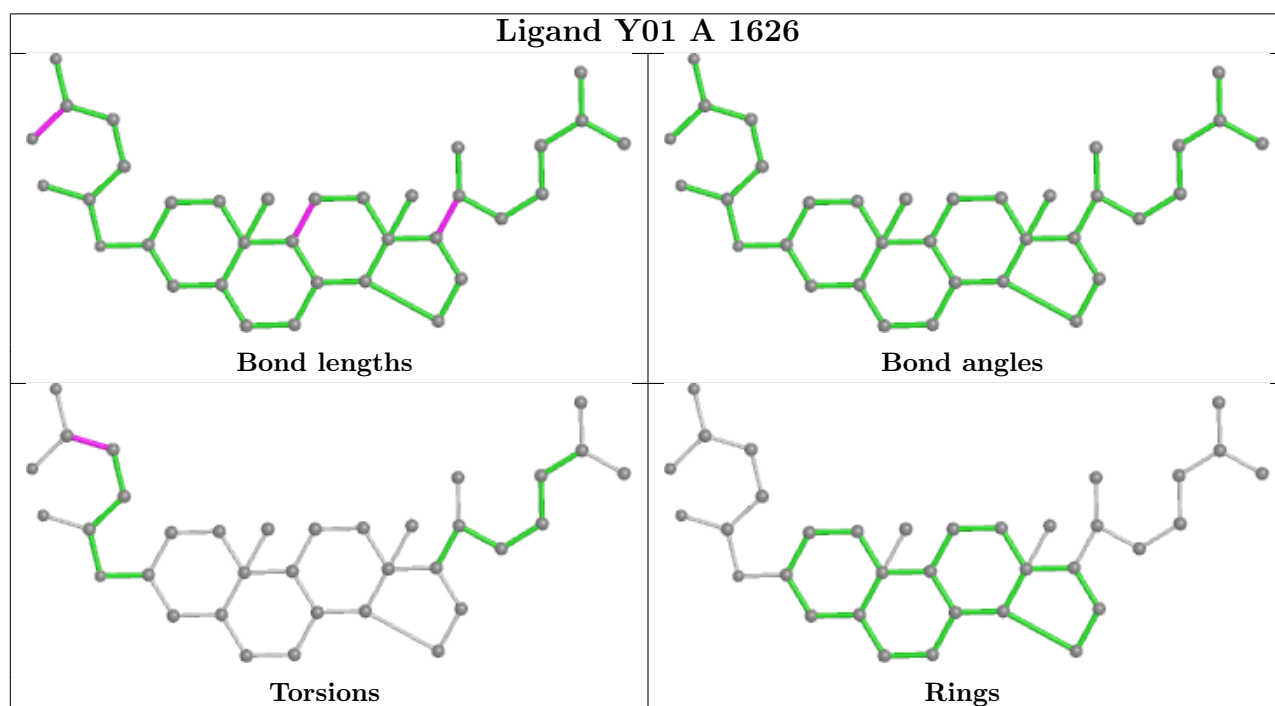
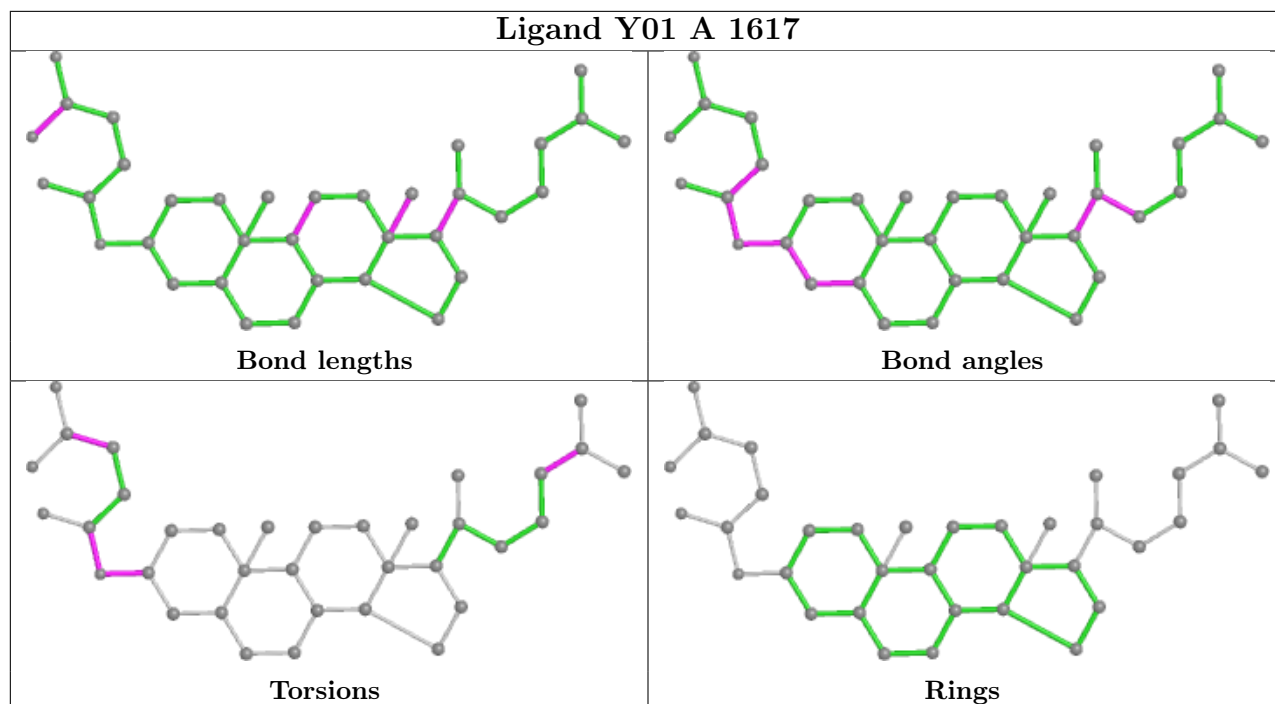


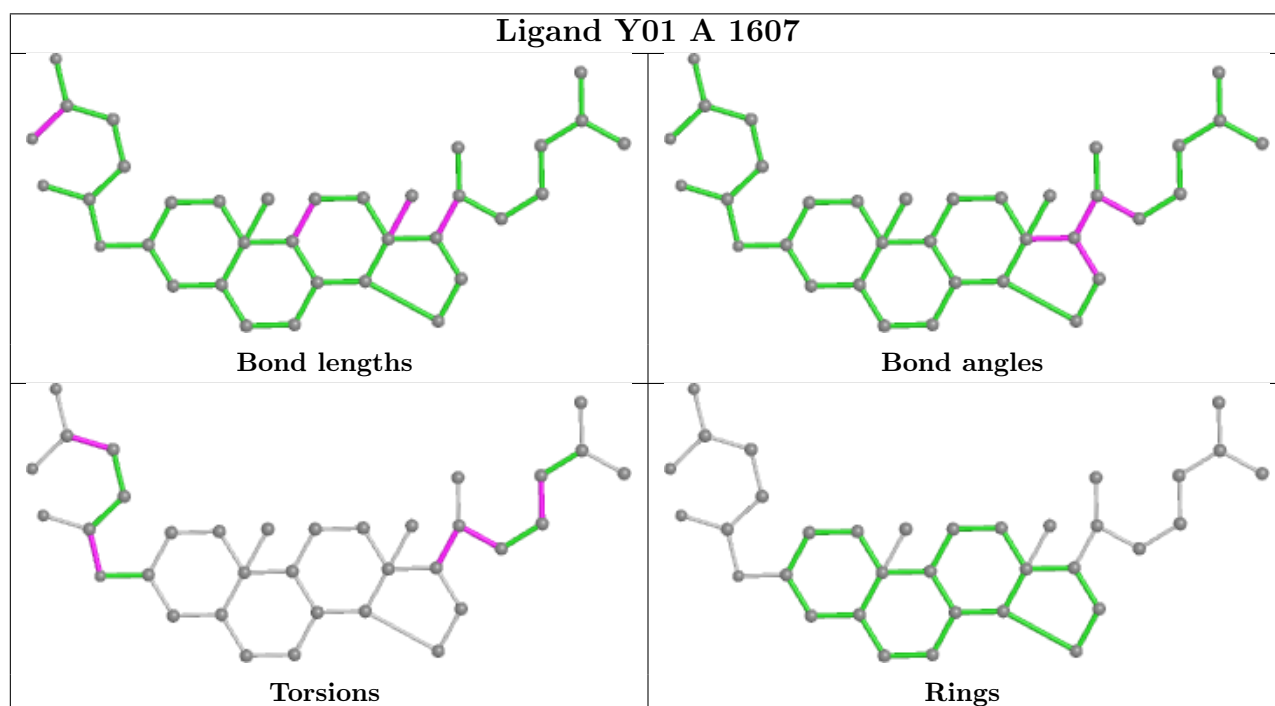
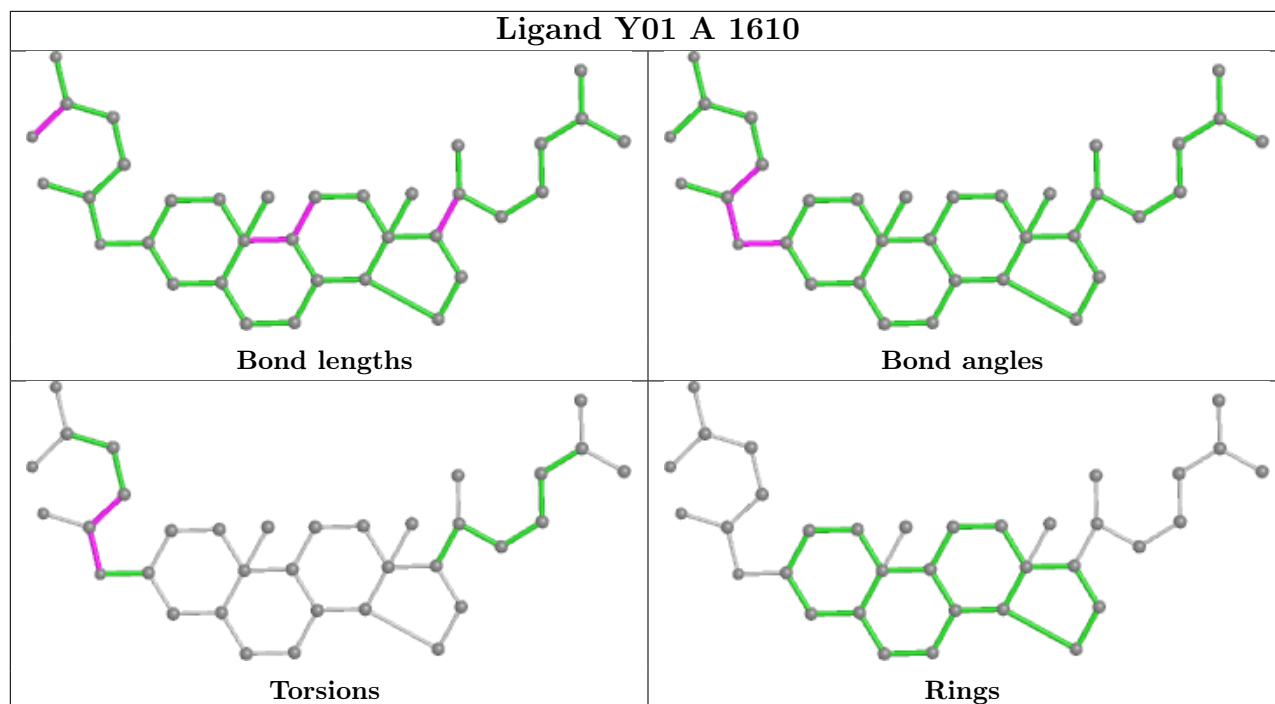


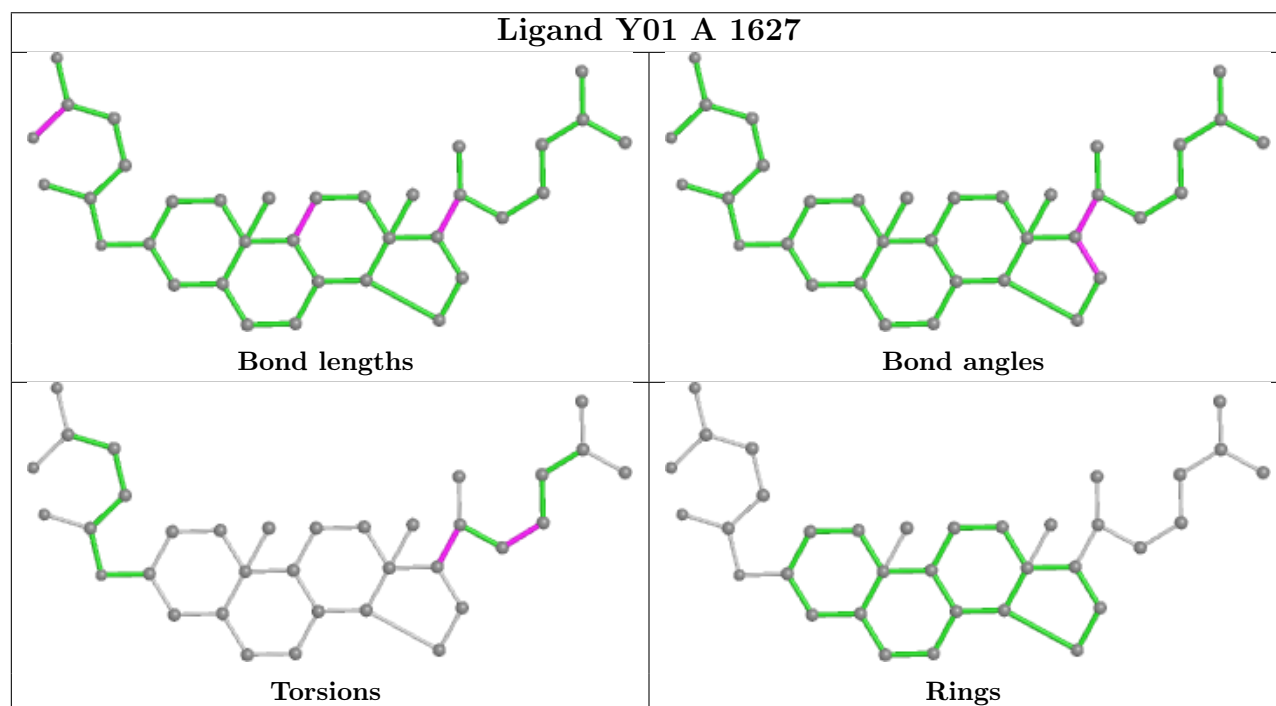
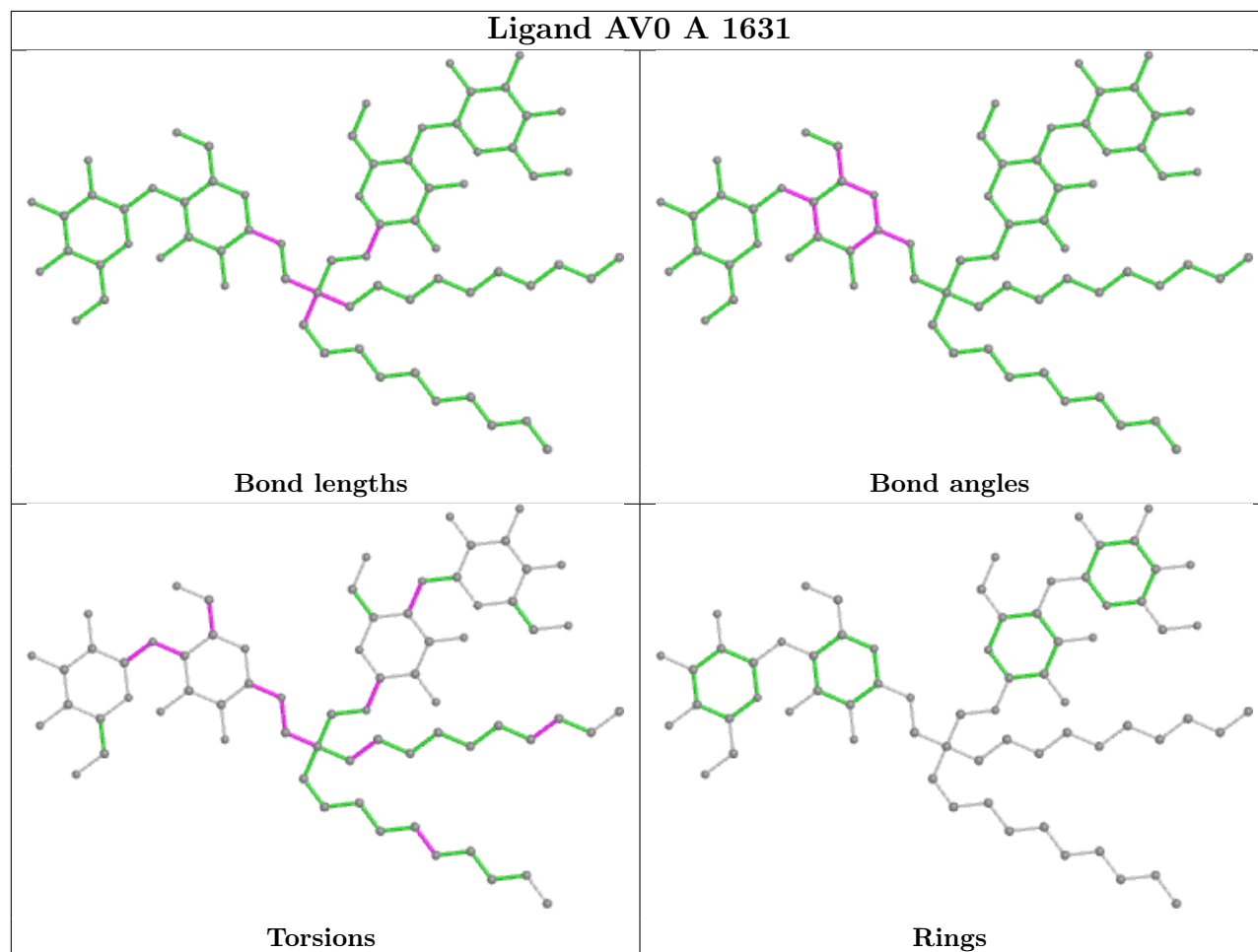












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

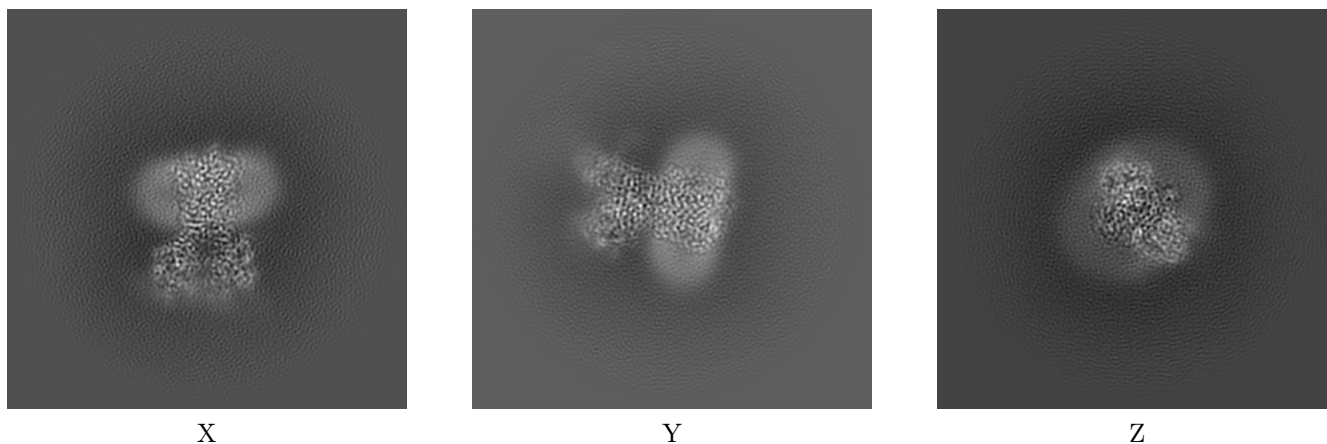
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24614. These allow visual inspection of the internal detail of the map and identification of artifacts.

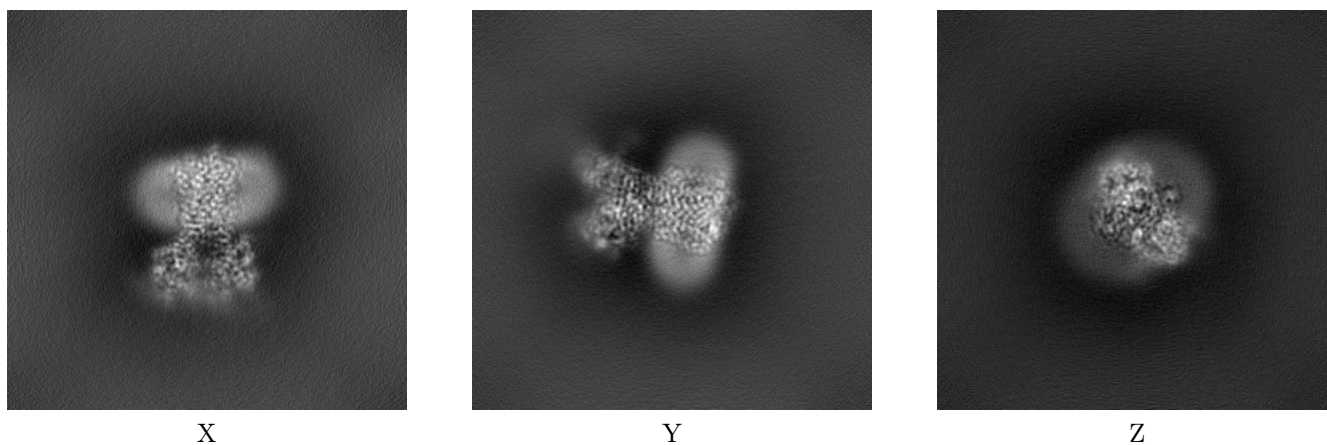
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



#### 6.1.2 Raw map

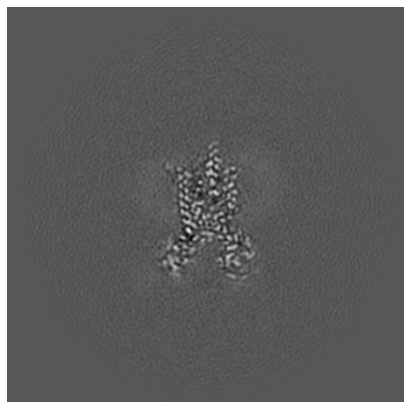


The images above show the map projected in three orthogonal directions.

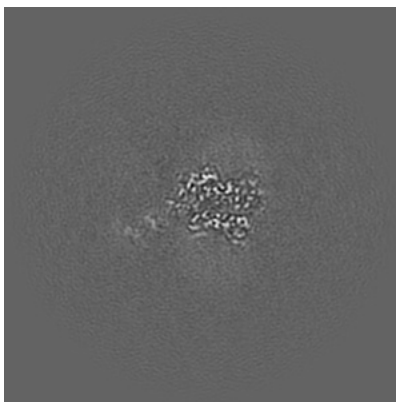


## 6.2 Central slices [i](#)

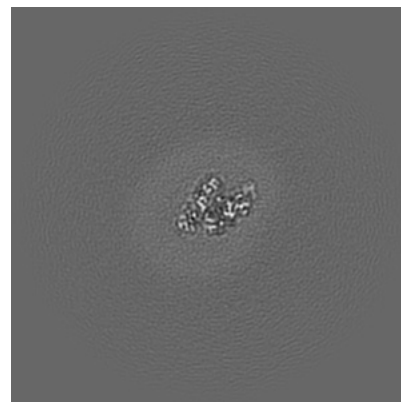
### 6.2.1 Primary map



X Index: 160

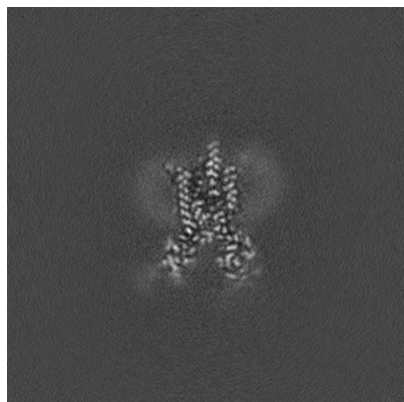


Y Index: 160

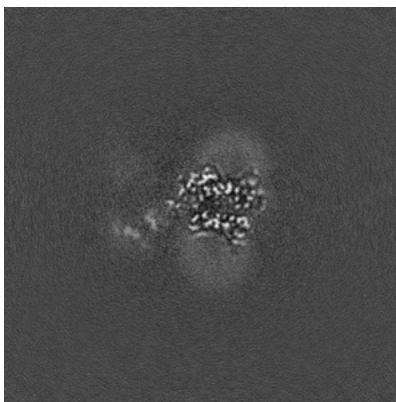


Z Index: 160

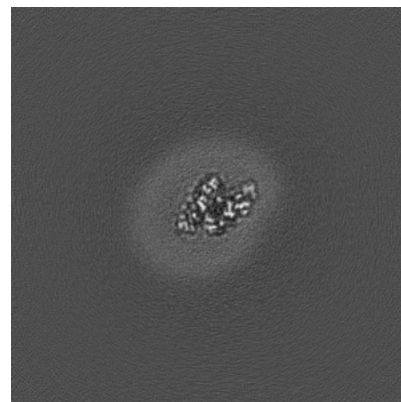
### 6.2.2 Raw map



X Index: 160



Y Index: 160

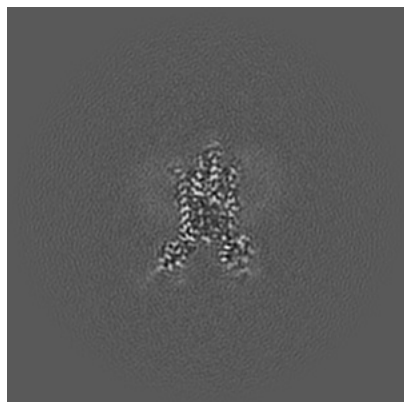


Z Index: 160

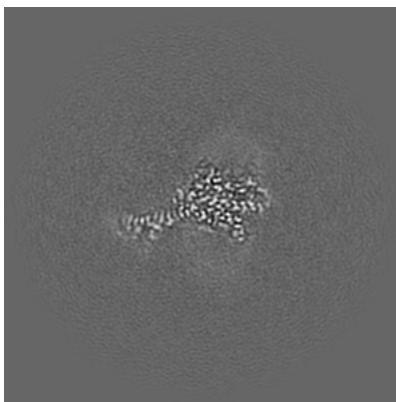
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

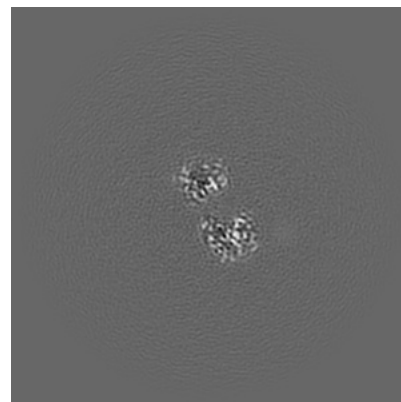
### 6.3.1 Primary map



X Index: 163

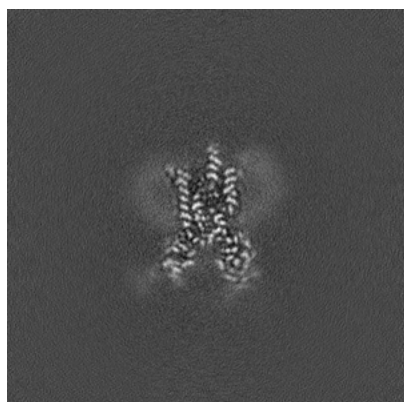


Y Index: 166

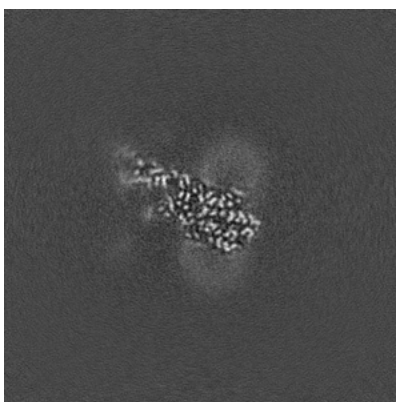


Z Index: 127

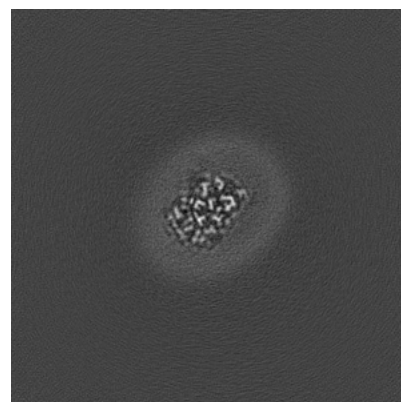
### 6.3.2 Raw map



X Index: 159



Y Index: 149

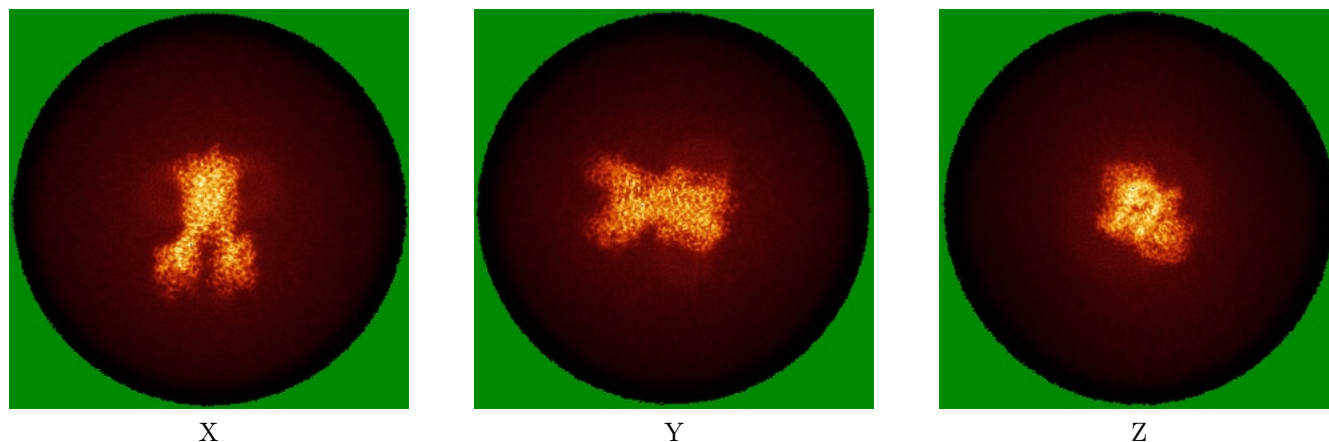


Z Index: 186

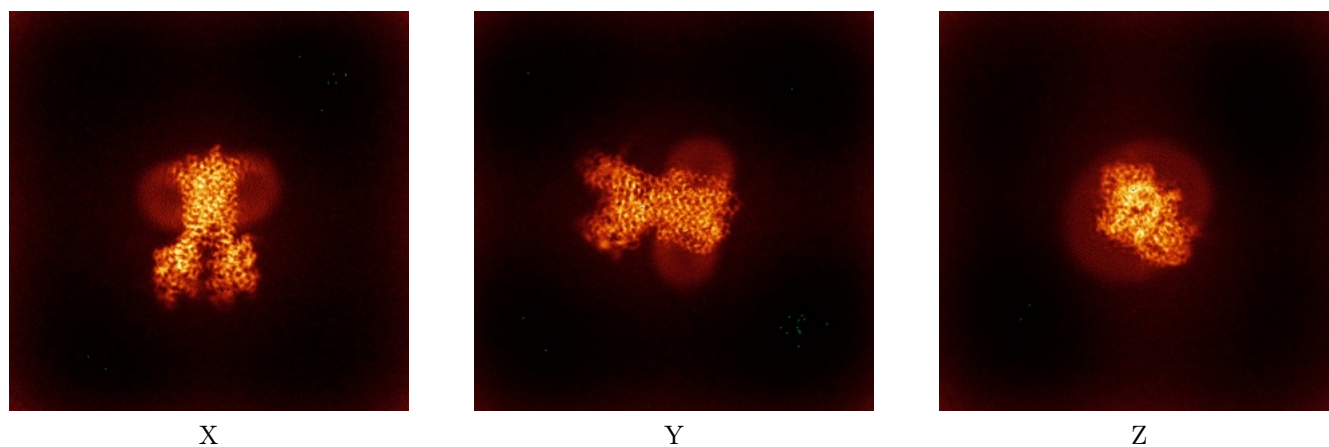
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



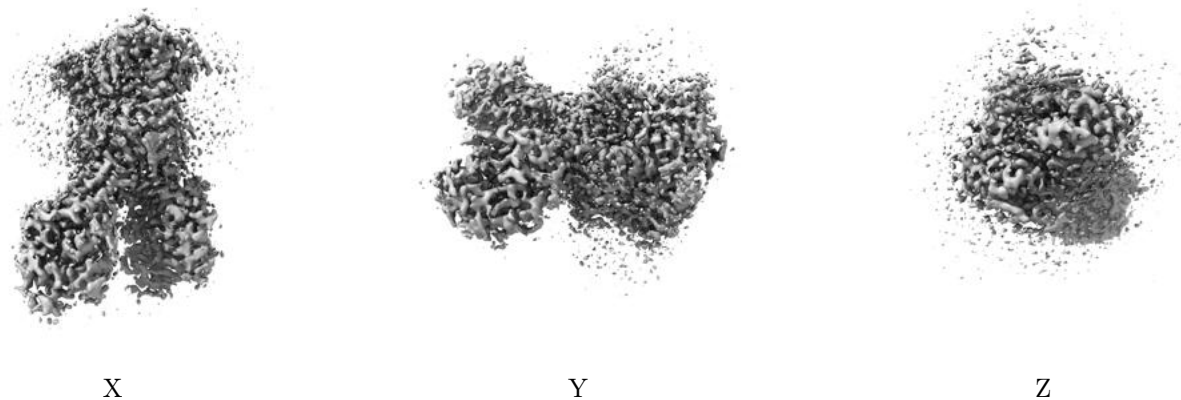
### 6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

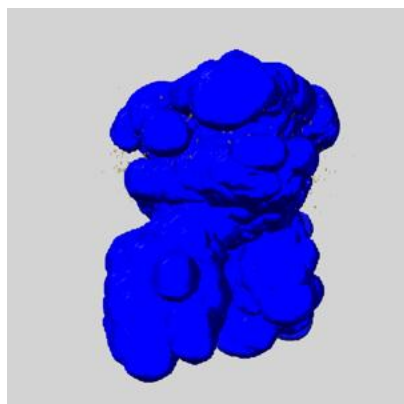
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

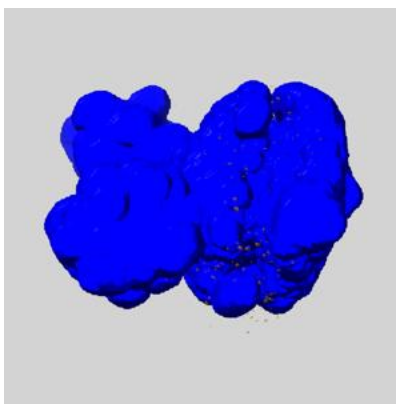
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

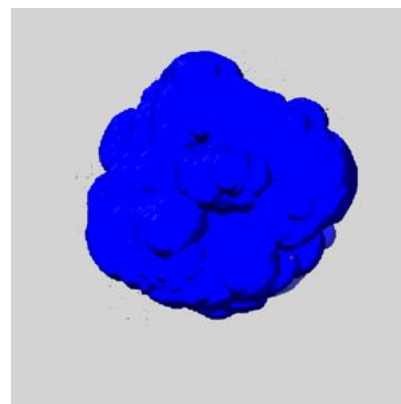
### 6.6.1 emd\_24614\_msk\_1.map [i](#)



X

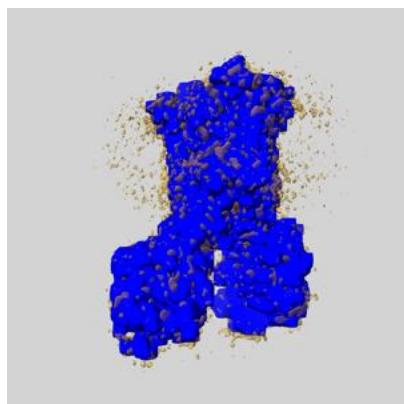


Y

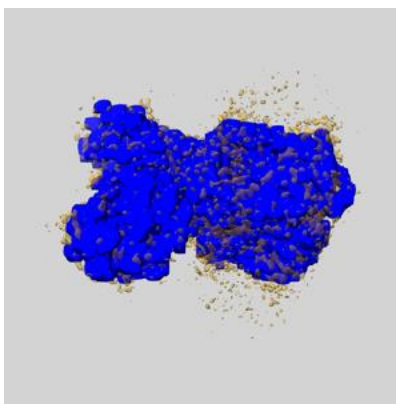


Z

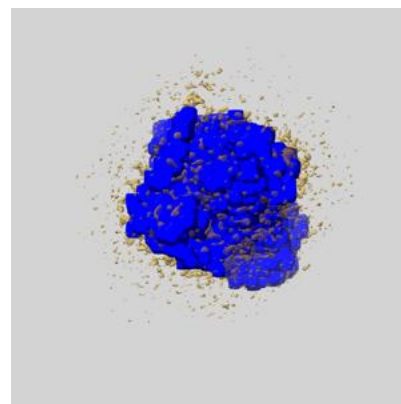
### 6.6.2 emd\_24614\_msk\_2.map [i](#)



X



Y

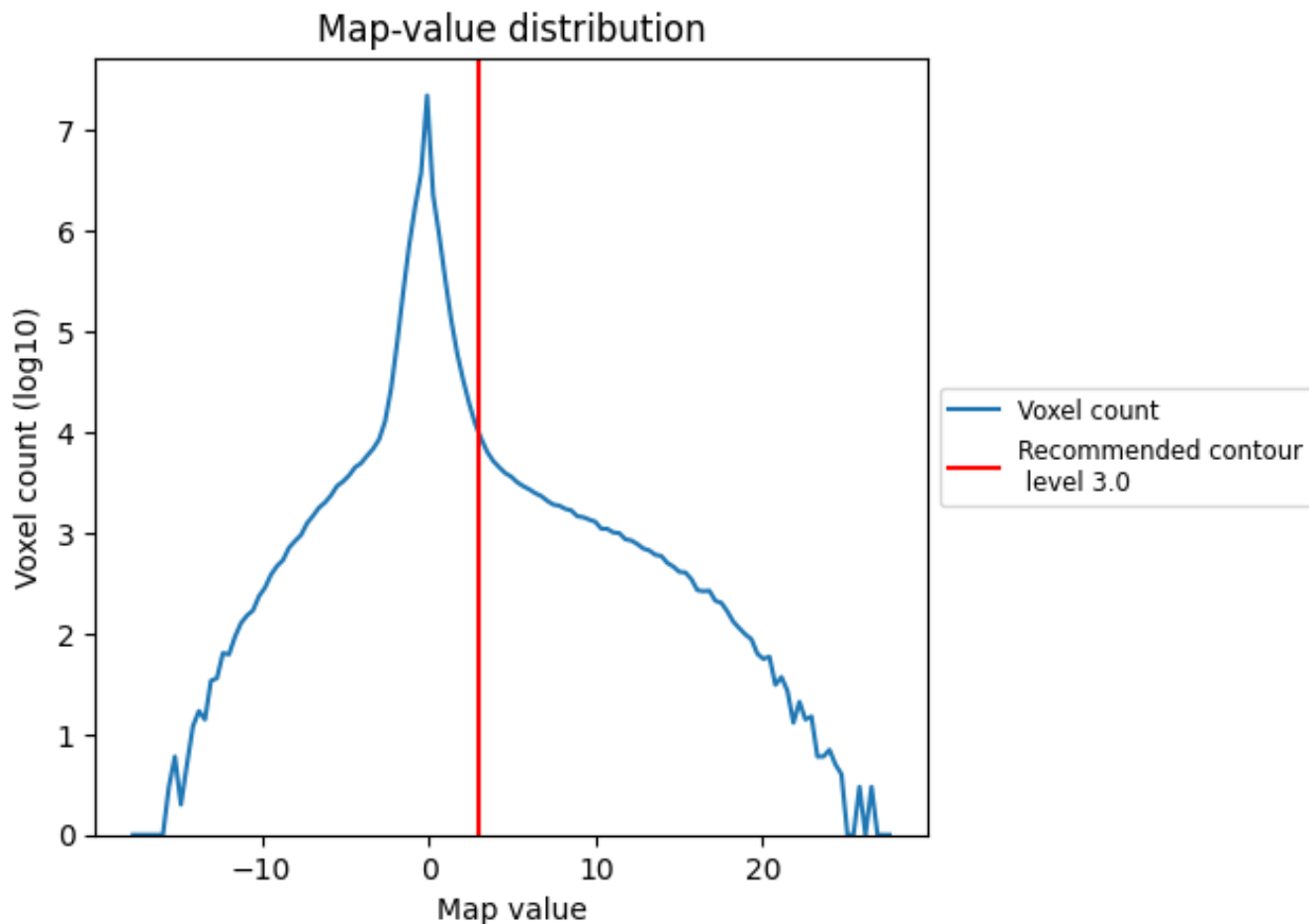


Z

## 7 Map analysis [i](#)

This section contains the results of statistical analysis of the map.

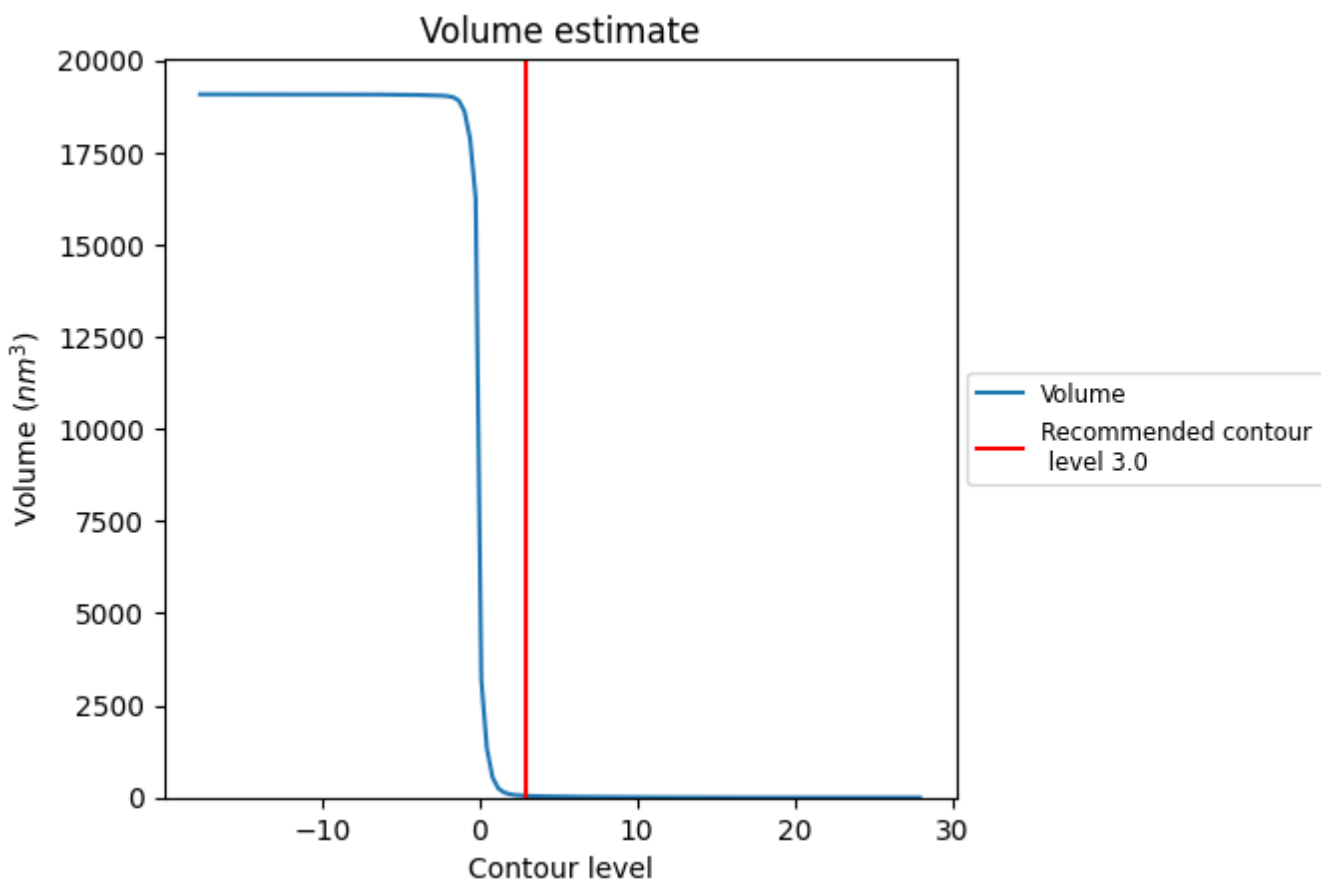
### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



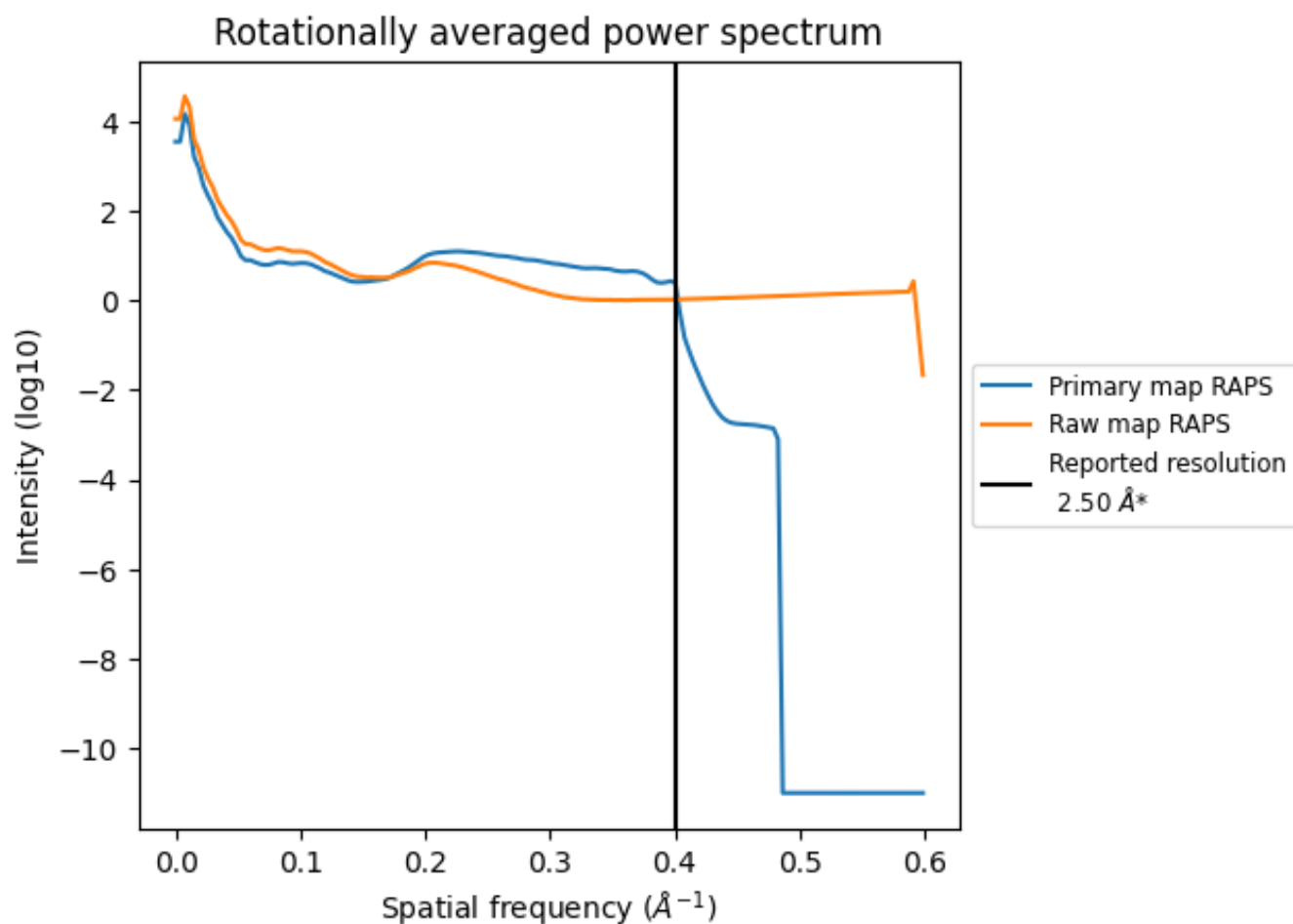
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46  $\text{nm}^3$ ; this corresponds to an approximate mass of 41 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)



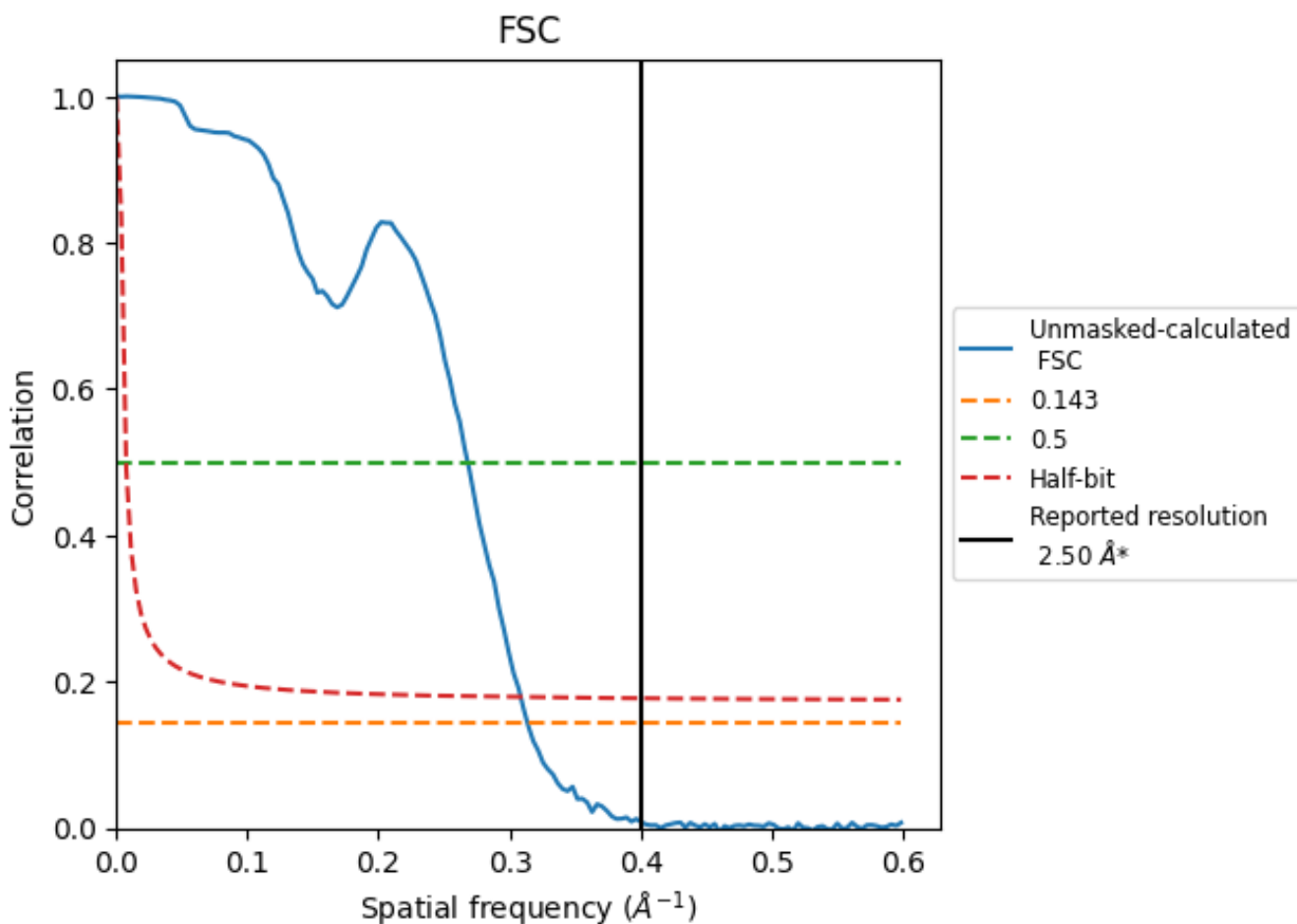
\*Reported resolution corresponds to spatial frequency of 0.400 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.400 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

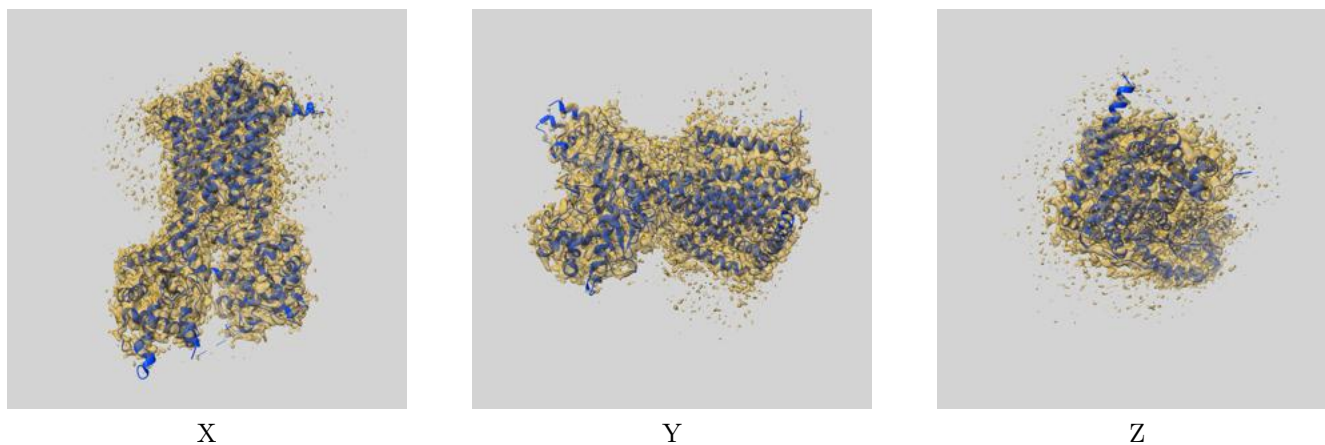
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.19	3.73	3.24

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.19 differs from the reported value 2.5 by more than 10 %

## 9 Map-model fit [i](#)

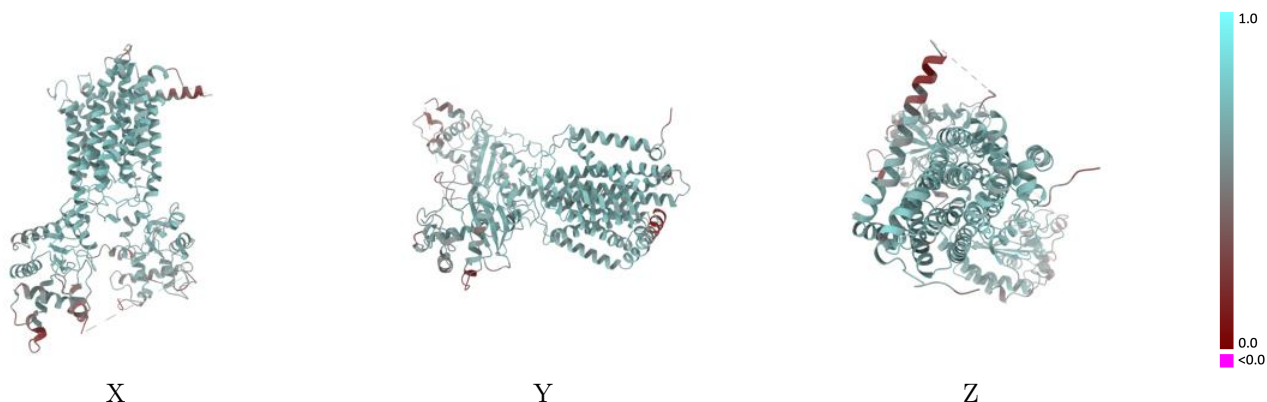
This section contains information regarding the fit between EMDB map EMD-24614 and PDB model 7RPH. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay [i](#)



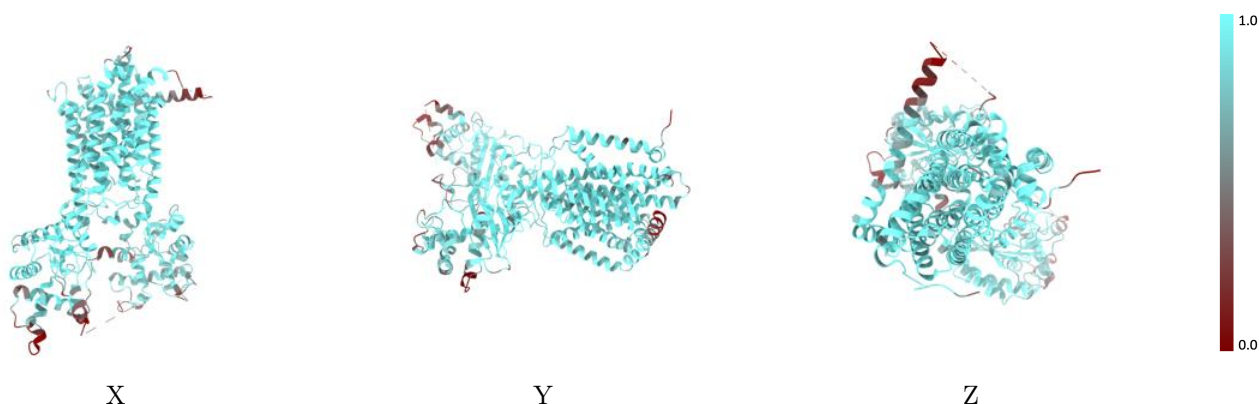
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [\(i\)](#)



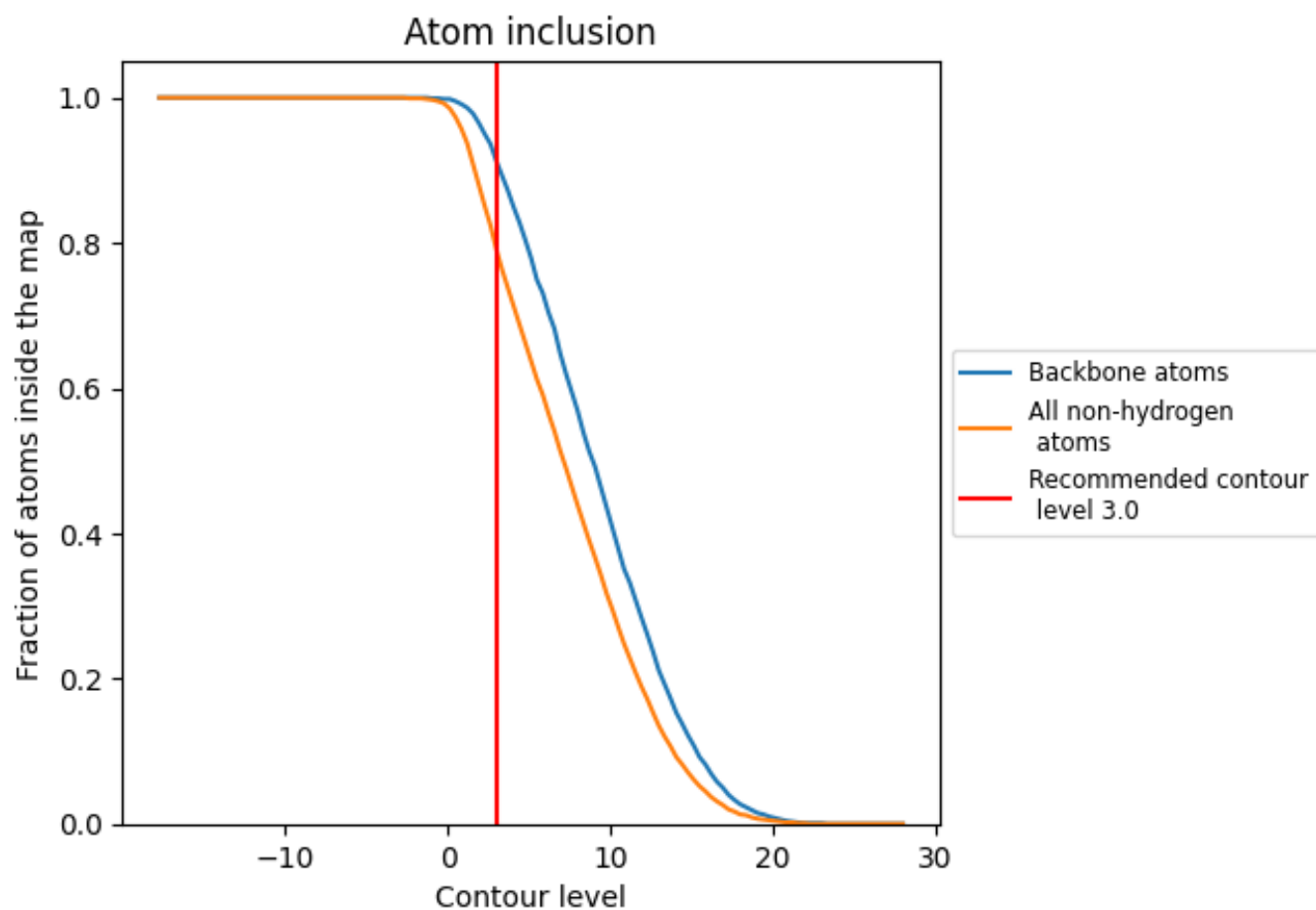
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.0).





## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7900	 0.5700
A	 0.7900	 0.5700

