



## wwPDB EM Validation Summary Report ⓘ

Apr 16, 2026 – 12:32 PM EDT

PDB ID : 9PE1 / pdb\_00009pe1  
EMDB ID : EMD-71550  
Title : Structure of beta-1,3-glucan synthase in complex with caspofungin, Rho1 and long glucan  
Authors : Ren, Z.; Lee, S.Y.  
Deposited on : 2025-07-01  
Resolution : 3.09 Å(reported)

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

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.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

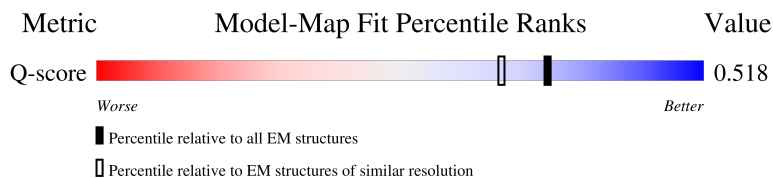
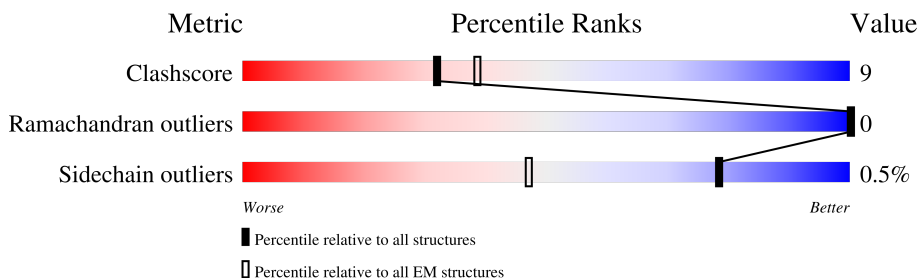
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.09 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14003 ( 2.59 - 3.59 )

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	1931	
2	E	235	
3	G	197	
4	H	6	

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Mol	Chain	Length	Quality of chain
5	D	17	 76%24%
6	K	5	 60%40%

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 32127 atoms, of which 15381 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 1,3-beta-glucan synthase component FKS1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1675	Total	C	H	N	O	S	0	0
			26592	8720	13201	2266	2330	75		

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1877	LEU	-	expression tag	UNP P38631
A	1878	GLU	-	expression tag	UNP P38631
A	1879	VAL	-	expression tag	UNP P38631
A	1880	LEU	-	expression tag	UNP P38631
A	1881	PHE	-	expression tag	UNP P38631
A	1882	GLN	-	expression tag	UNP P38631
A	1883	GLY	-	expression tag	UNP P38631
A	1884	PRO	-	expression tag	UNP P38631
A	1885	ALA	-	expression tag	UNP P38631
A	1886	ALA	-	expression tag	UNP P38631
A	1887	ALA	-	expression tag	UNP P38631
A	1888	GLY	-	expression tag	UNP P38631
A	1889	SER	-	expression tag	UNP P38631
A	1890	ALA	-	expression tag	UNP P38631
A	1891	GLY	-	expression tag	UNP P38631
A	1892	SER	-	expression tag	UNP P38631
A	1893	ALA	-	expression tag	UNP P38631
A	1894	ALA	-	expression tag	UNP P38631
A	1895	GLY	-	expression tag	UNP P38631
A	1896	SER	-	expression tag	UNP P38631
A	1897	GLY	-	expression tag	UNP P38631
A	1898	GLU	-	expression tag	UNP P38631
A	1899	PHE	-	expression tag	UNP P38631
A	1900	ASP	-	expression tag	UNP P38631
A	1901	TYR	-	expression tag	UNP P38631
A	1902	LYS	-	expression tag	UNP P38631
A	1903	ASP	-	expression tag	UNP P38631
A	1904	HIS	-	expression tag	UNP P38631

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1905	ASP	-	expression tag	UNP P38631
A	1906	GLY	-	expression tag	UNP P38631
A	1907	ASP	-	expression tag	UNP P38631
A	1908	TYR	-	expression tag	UNP P38631
A	1909	LYS	-	expression tag	UNP P38631
A	1910	ASP	-	expression tag	UNP P38631
A	1911	HIS	-	expression tag	UNP P38631
A	1912	ASP	-	expression tag	UNP P38631
A	1913	ILE	-	expression tag	UNP P38631
A	1914	ASP	-	expression tag	UNP P38631
A	1915	TYR	-	expression tag	UNP P38631
A	1916	LYS	-	expression tag	UNP P38631
A	1917	ASP	-	expression tag	UNP P38631
A	1918	ASP	-	expression tag	UNP P38631
A	1919	ASP	-	expression tag	UNP P38631
A	1920	ASP	-	expression tag	UNP P38631
A	1921	LYS	-	expression tag	UNP P38631
A	1922	HIS	-	expression tag	UNP P38631
A	1923	HIS	-	expression tag	UNP P38631
A	1924	HIS	-	expression tag	UNP P38631
A	1925	HIS	-	expression tag	UNP P38631
A	1926	HIS	-	expression tag	UNP P38631
A	1927	HIS	-	expression tag	UNP P38631
A	1928	HIS	-	expression tag	UNP P38631
A	1929	HIS	-	expression tag	UNP P38631
A	1930	HIS	-	expression tag	UNP P38631
A	1931	HIS	-	expression tag	UNP P38631

- Molecule 2 is a protein called GTP-binding protein RHO1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	E	179	Total	C	H	N	O	S	0	0
			2570	840	1250	227	249	4		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-25	MET	-	initiating methionine	UNP P06780
E	-24	GLY	-	expression tag	UNP P06780
E	-23	SER	-	expression tag	UNP P06780
E	-22	SER	-	expression tag	UNP P06780
E	-21	HIS	-	expression tag	UNP P06780

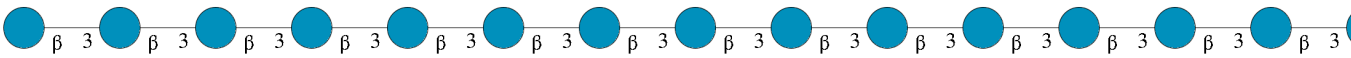
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-20	HIS	-	expression tag	UNP P06780
E	-19	HIS	-	expression tag	UNP P06780
E	-18	HIS	-	expression tag	UNP P06780
E	-17	HIS	-	expression tag	UNP P06780
E	-16	HIS	-	expression tag	UNP P06780
E	-15	SER	-	expression tag	UNP P06780
E	-14	SER	-	expression tag	UNP P06780
E	-13	GLY	-	expression tag	UNP P06780
E	-12	LEU	-	expression tag	UNP P06780
E	-11	VAL	-	expression tag	UNP P06780
E	-10	PRO	-	expression tag	UNP P06780
E	-9	ARG	-	expression tag	UNP P06780
E	-8	GLY	-	expression tag	UNP P06780
E	-7	SER	-	expression tag	UNP P06780
E	-6	HIS	-	expression tag	UNP P06780
E	-5	MET	-	expression tag	UNP P06780
E	-4	GLU	-	expression tag	UNP P06780
E	-3	ASN	-	expression tag	UNP P06780
E	-2	LEU	-	expression tag	UNP P06780
E	-1	TYR	-	expression tag	UNP P06780
E	0	PHE	-	expression tag	UNP P06780
E	1	GLN	-	expression tag	UNP P06780

- | Mol | Chain | Residues | Atoms |     |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|---|---------|-------|
| 3   | G     | 72       | Total | C   | H   | N  | O   | S | 0       | 0     |
|     |       |          | 1086  | 358 | 521 | 97 | 109 | 1 |         |       |

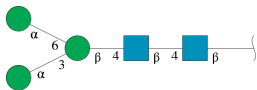
- | Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |   |
|-----|-------|----------|-------|----|----|----|---------|-------|---|
| 4   | H     | 6        | Total | C  | H  | N  | O       | 0     | 0 |
|     |       |          | 120   | 36 | 60 | 10 | 14      |       |   |

- 
- WORLD WIDE  
PDB  
PROTEIN DATA BANK



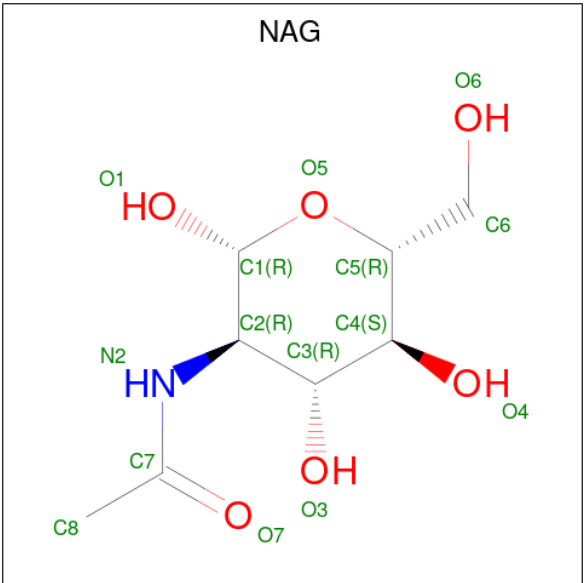
Mol	Chain	Residues	Atoms				AltConf	Trace
5	D	17	Total	C	H	O	0	0
			344	102	156	86		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	5	Total	C	H	N	O	0	0
			113	34	52	2	25		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	H	N	O	0
			27	8	13	1	5	

- # Y01

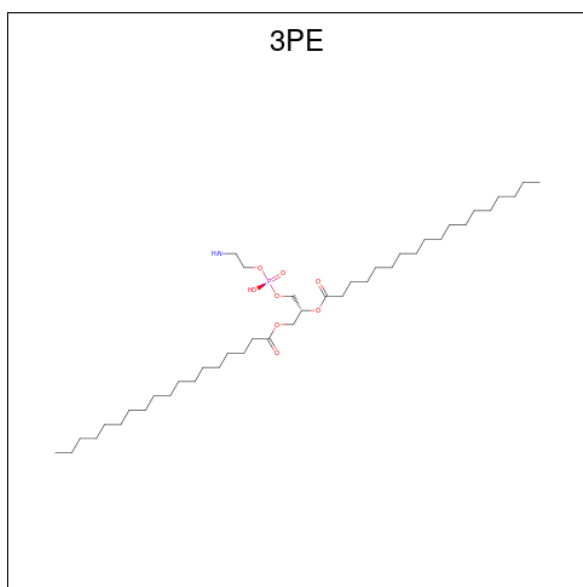
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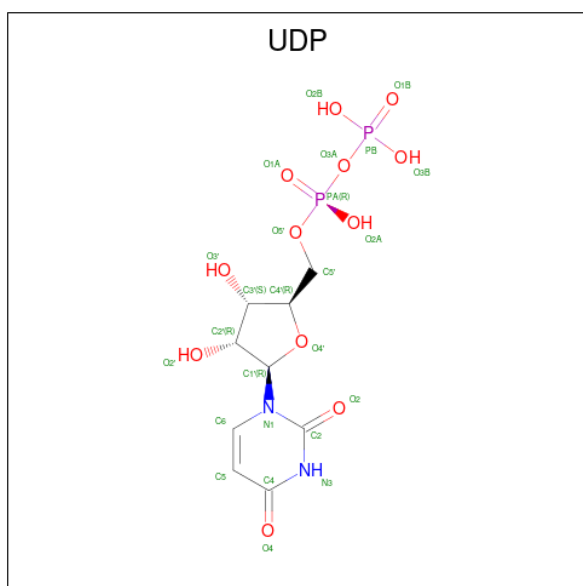
Mol	Chain	Residues	Atoms			AltConf
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31	4	
8	A	1	Total	C	O	0
			35	31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

- Molecule 9 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



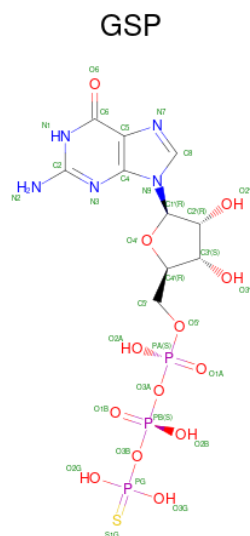
Mol	Chain	Residues	Atoms					AltConf	
9	A	1	Total	C	H	N	O	P	0
			123	39	74	1	8	1	

- Molecule 10 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula:  $C_9H_{14}N_2O_{12}P_2$ ) (labeled as "Ligand of Interest" by depositor).



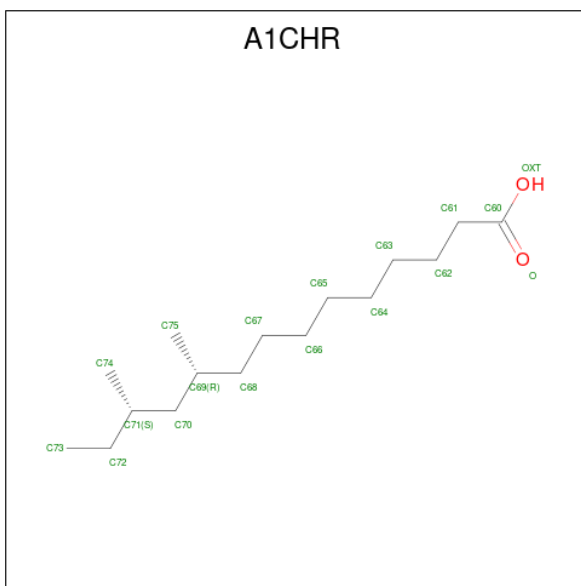
Mol	Chain	Residues	Atoms						AltConf
10	A	1	Total	C	H	N	O	P	0
			36	9	11	2	12	2	

- Molecule 11 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula:  $C_{10}H_{16}N_5O_{13}P_3S$ ).



Mol	Chain	Residues	Atoms								AltConf
11	E	1	Total	C	H	N	O	P	S	0	
			44	10	12	5	13	3	1		

- Molecule 12 is (10R,12S)-10,12-dimethyltetradecanoic acid (CCD ID: A1CHR) (formula:  $C_{16}H_{32}O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
12	H	1	Total	C	H	O	0
			48	16	31	1	

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
13	A	9	Total	O	0
			9	9	





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48860	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.867	Depositor
Minimum map value	-0.425	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.0792	Depositor
Map size (Å)	268.8, 268.8, 268.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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: 3PE, HYP, A1CHT, MAN, GSP, Y01, BMA, A1CHU, NAG, A1CHS, HY3, BGC, UDP, A1CHR

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	0.15	0/13750	0.30	0/18670
2	E	0.17	0/1345	0.32	0/1834
3	G	0.10	0/581	0.27	0/794
4	H	0.41	0/6	1.54	0/7
All	All	0.15	0/15682	0.30	0/21305

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
4	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	2	A1CHS	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	13391	13201	13201	112	0
2	E	1320	1250	1250	6	0
3	G	565	521	521	5	0
4	H	60	60	16	2	0
5	D	188	156	155	3	0
6	K	61	52	52	0	0
7	A	14	13	13	0	0
8	A	980	0	1372	198	0
8	H	35	0	49	7	0
9	A	49	74	75	2	0
10	A	25	11	10	0	0
11	E	32	12	12	0	0
12	H	17	31	0	0	0
13	A	9	0	0	0	0
All	All	16746	15381	16726	286	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 9.

The worst 5 of 286 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)
8:A:2002:Y01:HAD3	8:A:2013:Y01:HAI	1.43	0.96
8:A:2022:Y01:HAS1	8:H:102:Y01:HAK1	1.48	0.95
8:A:2014:Y01:HAL2	8:A:2016:Y01:HAL1	1.46	0.95
8:A:2010:Y01:HAB3	8:A:2015:Y01:HAA3	1.47	0.95
8:A:2002:Y01:HAU1	8:A:2004:Y01:HAB3	1.48	0.93

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1663/1931 (86%)	1636 (98%)	27 (2%)	0	100	100
2	E	177/235 (75%)	174 (98%)	3 (2%)	0	100	100
3	G	70/197 (36%)	65 (93%)	5 (7%)	0	100	100
4	H	1/6 (17%)	1 (100%)	0	0	100	100
All	All	1911/2369 (81%)	1876 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1400/1663 (84%)	1393 (100%)	7 (0%)	81	85
2	E	130/203 (64%)	130 (100%)	0	100	100
3	G	60/167 (36%)	60 (100%)	0	100	100
4	H	1/1 (100%)	0	1 (100%)	0	0
All	All	1591/2034 (78%)	1583 (100%)	8 (0%)	78	85

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	3	THR
1	A	1658	PHE
1	A	1133	TYR
1	A	1088	HIS
1	A	1195	HIS

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

Mol	Chain	Res	Type
1	A	1243	GLN
1	A	1779	GLN
1	A	1469	GLN

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Mol	Chain	Res	Type
2	E	155	GLN
1	A	1688	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
4	A1CHS	H	2	12,4	8,12,13	0.74	0	8,14,16	0.73	0
4	HYP	H	4	4	7,8,9	0.49	0	5,10,12	0.97	1 (20%)
4	A1CHU	H	6	4	6,8,9	0.43	0	4,9,11	1.06	1 (25%)
4	A1CHT	H	5	4	14,15,16	0.32	0	16,20,22	0.54	0
4	HY3	H	7	4	7,8,9	0.70	0	7,10,12	0.78	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
4	A1CHS	H	2	12,4	-	7/11/14/16	-
4	HYP	H	4	4	-	0/0/11/13	0/1/1/1
4	A1CHU	H	6	4	-	5/8/9/11	-
4	A1CHT	H	5	4	-	2/13/14/16	0/1/1/1
4	HY3	H	7	4	-	0/1/12/14	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	6	A1CHU	O-C-CA	-2.09	119.40	124.77
4	H	4	HYP	O-C-CA	-2.08	119.41	124.77

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	2	A1CHS	O-C-CA-CB
4	H	2	A1CHS	N-CA-CB-CG
4	H	2	A1CHS	N19-CD-CG-CB
4	H	2	A1CHS	N19-CD-CG-O58
4	H	2	A1CHS	NE-CD-CG-O58

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

22 monosaccharides 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	$\# Z  > 2$
5	BGC	D	1	5	12,12,12	1.25	1 (8%)	17,17,17	0.64	0
5	BGC	D	10	5	11,11,12	1.67	2 (18%)	15,15,17	0.85	1 (6%)
5	BGC	D	11	5	11,11,12	1.68	3 (27%)	15,15,17	0.85	0
5	BGC	D	12	5	11,11,12	1.62	2 (18%)	15,15,17	1.17	1 (6%)
5	BGC	D	13	5	11,11,12	1.69	2 (18%)	15,15,17	0.82	0
5	BGC	D	14	5	11,11,12	1.64	2 (18%)	15,15,17	0.86	0
5	BGC	D	15	5	11,11,12	1.51	2 (18%)	15,15,17	1.69	4 (26%)
5	BGC	D	16	5	11,11,12	1.61	2 (18%)	15,15,17	1.03	1 (6%)
5	BGC	D	17	5	11,11,12	1.65	2 (18%)	15,15,17	1.41	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BGC	D	2	5	11,11,12	1.58	2 (18%)	15,15,17	0.95	1 (6%)
5	BGC	D	3	5	11,11,12	1.60	2 (18%)	15,15,17	1.21	1 (6%)
5	BGC	D	4	5	11,11,12	1.63	2 (18%)	15,15,17	0.99	1 (6%)
5	BGC	D	5	5	11,11,12	1.60	2 (18%)	15,15,17	1.13	1 (6%)
5	BGC	D	6	5	11,11,12	1.62	2 (18%)	15,15,17	1.28	1 (6%)
5	BGC	D	7	5	11,11,12	1.57	2 (18%)	15,15,17	1.14	1 (6%)
5	BGC	D	8	5	11,11,12	1.56	2 (18%)	15,15,17	1.05	0
5	BGC	D	9	5	11,11,12	1.61	3 (27%)	15,15,17	0.74	0
6	NAG	K	1	1,6	14,14,15	0.42	0	17,19,21	0.71	0
6	NAG	K	2	6	14,14,15	0.39	0	17,19,21	0.91	1 (5%)
6	BMA	K	3	6	11,11,12	0.25	0	15,15,17	0.69	0
6	MAN	K	4	6	11,11,12	0.24	0	15,15,17	0.84	1 (6%)
6	MAN	K	5	6	11,11,12	0.28	0	15,15,17	0.56	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
5	BGC	D	1	5	-	0/2/22/22	0/1/1/1
5	BGC	D	10	5	-	0/2/19/22	0/1/1/1
5	BGC	D	11	5	-	0/2/19/22	0/1/1/1
5	BGC	D	12	5	-	0/2/19/22	0/1/1/1
5	BGC	D	13	5	-	0/2/19/22	0/1/1/1
5	BGC	D	14	5	-	1/2/19/22	0/1/1/1
5	BGC	D	15	5	-	0/2/19/22	0/1/1/1
5	BGC	D	16	5	-	0/2/19/22	0/1/1/1
5	BGC	D	17	5	-	1/2/19/22	0/1/1/1
5	BGC	D	2	5	-	0/2/19/22	0/1/1/1
5	BGC	D	3	5	-	0/2/19/22	0/1/1/1
5	BGC	D	4	5	-	1/2/19/22	0/1/1/1
5	BGC	D	5	5	-	1/2/19/22	0/1/1/1
5	BGC	D	6	5	-	0/2/19/22	0/1/1/1
5	BGC	D	7	5	-	1/2/19/22	0/1/1/1
5	BGC	D	8	5	-	0/2/19/22	0/1/1/1
5	BGC	D	9	5	-	0/2/19/22	0/1/1/1
6	NAG	K	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1
6	BMA	K	3	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	K	4	6	-	0/2/19/22	0/1/1/1
6	MAN	K	5	6	-	0/2/19/22	0/1/1/1

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	10	BGC	O5-C1	4.24	1.50	1.43
5	D	17	BGC	O5-C1	4.24	1.50	1.43
5	D	11	BGC	O5-C1	4.13	1.50	1.43
5	D	13	BGC	O5-C1	4.13	1.50	1.43
5	D	14	BGC	O5-C1	4.12	1.50	1.43

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	17	BGC	C1-C2-C3	4.27	115.86	109.64
5	D	15	BGC	C1-C2-C3	4.07	115.57	109.64
5	D	3	BGC	C1-C2-C3	3.27	114.41	109.64
5	D	7	BGC	C1-C2-C3	3.26	114.38	109.64
5	D	12	BGC	C1-C2-C3	3.03	114.06	109.64

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
5	D	4	BGC	O5-C5-C6-O6
5	D	7	BGC	O5-C5-C6-O6
5	D	5	BGC	O5-C5-C6-O6

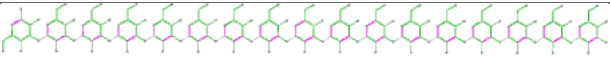
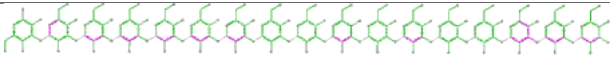
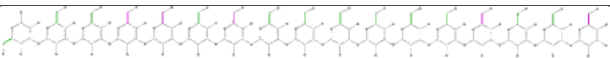
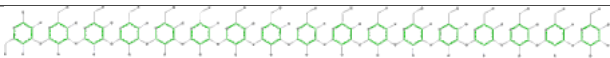
There are no ring outliers.

4 monomers are involved in 3 short contacts:

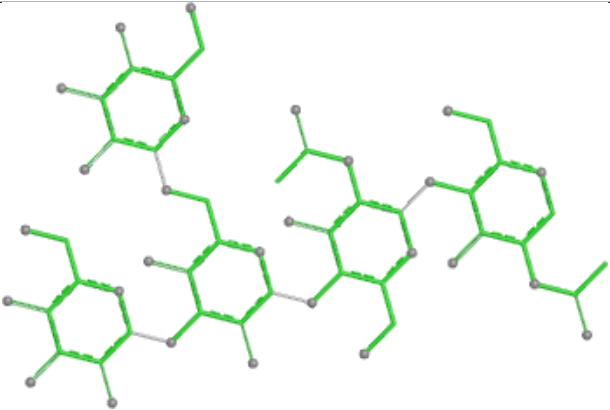
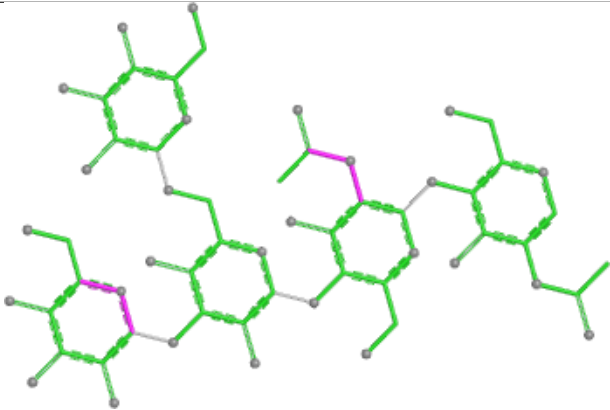
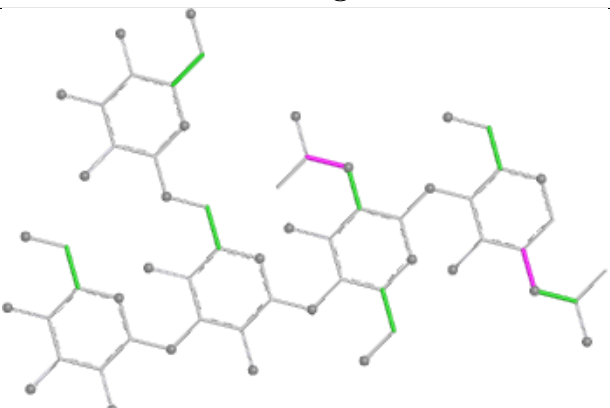
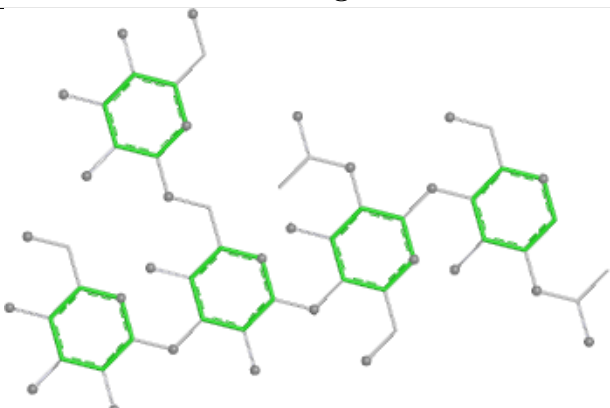
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	16	BGC	1	0
5	D	9	BGC	2	0
5	D	15	BGC	1	0
5	D	10	BGC	1	0

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

bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain D			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

Oligosaccharide Chain K			
			
Bond lengths		Bond angles	
			
Torsions		Rings	

## 5.6 Ligand geometry [i](#)

34 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
8	Y01	A	2010	-	38,38,38	1.08	3 (7%)	57,57,57	3.20	18 (31%)
8	Y01	A	2003	-	38,38,38	1.07	3 (7%)	57,57,57	3.15	21 (36%)
8	Y01	A	2002	-	38,38,38	1.06	3 (7%)	57,57,57	3.14	19 (33%)
8	Y01	A	2018	-	38,38,38	1.07	3 (7%)	57,57,57	3.19	19 (33%)
8	Y01	A	2004	-	38,38,38	1.10	3 (7%)	57,57,57	3.34	18 (31%)
8	Y01	A	2016	-	38,38,38	1.08	3 (7%)	57,57,57	3.22	19 (33%)
8	Y01	A	2009	-	38,38,38	1.09	3 (7%)	57,57,57	3.34	19 (33%)
8	Y01	A	2027	-	38,38,38	1.07	3 (7%)	57,57,57	3.13	18 (31%)
8	Y01	A	2007	-	38,38,38	1.10	3 (7%)	57,57,57	3.23	20 (35%)
8	Y01	A	2008	-	38,38,38	1.08	3 (7%)	57,57,57	3.41	23 (40%)
8	Y01	A	2026	-	38,38,38	1.09	3 (7%)	57,57,57	3.25	18 (31%)
8	Y01	A	2020	-	38,38,38	1.08	3 (7%)	57,57,57	3.26	17 (29%)
8	Y01	A	2019	-	38,38,38	1.08	3 (7%)	57,57,57	3.21	19 (33%)
9	3PE	A	2006	-	48,48,50	0.48	0	51,53,55	0.45	0
8	Y01	A	2012	-	38,38,38	1.08	3 (7%)	57,57,57	3.28	20 (35%)
8	Y01	A	2025	-	38,38,38	1.07	3 (7%)	57,57,57	3.19	18 (31%)
8	Y01	A	2022	-	38,38,38	1.07	3 (7%)	57,57,57	3.20	18 (31%)
8	Y01	A	2030	-	38,38,38	1.08	3 (7%)	57,57,57	3.25	20 (35%)
8	Y01	A	2011	-	38,38,38	1.09	3 (7%)	57,57,57	3.13	17 (29%)
8	Y01	A	2024	-	38,38,38	1.08	3 (7%)	57,57,57	3.17	20 (35%)
8	Y01	A	2023	-	38,38,38	1.06	3 (7%)	57,57,57	3.10	16 (28%)
8	Y01	H	102	-	38,38,38	1.07	3 (7%)	57,57,57	3.20	17 (29%)
8	Y01	A	2014	-	38,38,38	1.08	3 (7%)	57,57,57	3.28	22 (38%)
11	GSP	E	301	-	33,34,34	3.29	18 (54%)	47,54,54	2.16	11 (23%)
8	Y01	A	2005	-	38,38,38	1.10	3 (7%)	57,57,57	3.37	19 (33%)
7	NAG	A	2001	1	14,14,15	0.21	0	17,19,21	0.42	0
8	Y01	A	2017	-	38,38,38	1.09	3 (7%)	57,57,57	3.26	18 (31%)
8	Y01	A	2021	-	38,38,38	1.09	3 (7%)	57,57,57	3.31	20 (35%)
10	UDP	A	2031	-	25,26,26	3.80	14 (56%)	38,40,40	1.57	5 (13%)
8	Y01	A	2013	-	38,38,38	1.07	3 (7%)	57,57,57	3.32	20 (35%)
8	Y01	A	2015	-	38,38,38	1.09	3 (7%)	57,57,57	3.30	19 (33%)
8	Y01	A	2028	-	38,38,38	1.08	3 (7%)	57,57,57	3.12	15 (26%)
12	A1CHR	H	101	4	15,16,17	0.15	0	16,17,19	0.37	0
8	Y01	A	2029	-	38,38,38	1.10	3 (7%)	57,57,57	3.35	19 (33%)

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
8	Y01	A	2010	-	-	8/19/77/77	0/4/4/4
8	Y01	A	2003	-	-	13/19/77/77	0/4/4/4
8	Y01	A	2002	-	-	16/19/77/77	0/4/4/4
8	Y01	A	2018	-	-	16/19/77/77	0/4/4/4
8	Y01	A	2004	-	-	6/19/77/77	0/4/4/4
8	Y01	A	2016	-	-	9/19/77/77	0/4/4/4
8	Y01	A	2009	-	-	10/19/77/77	0/4/4/4
8	Y01	A	2027	-	-	16/19/77/77	0/4/4/4
8	Y01	A	2007	-	-	8/19/77/77	0/4/4/4
8	Y01	A	2008	-	-	10/19/77/77	0/4/4/4
8	Y01	A	2026	-	-	15/19/77/77	0/4/4/4
8	Y01	A	2020	-	-	10/19/77/77	0/4/4/4
8	Y01	A	2019	-	-	16/19/77/77	0/4/4/4
9	3PE	A	2006	-	-	21/52/52/54	-
8	Y01	A	2012	-	-	9/19/77/77	0/4/4/4
8	Y01	A	2025	-	-	12/19/77/77	0/4/4/4
8	Y01	A	2022	-	-	12/19/77/77	0/4/4/4
8	Y01	A	2030	-	-	9/19/77/77	0/4/4/4
8	Y01	A	2011	-	-	10/19/77/77	0/4/4/4
8	Y01	A	2024	-	-	12/19/77/77	0/4/4/4
8	Y01	A	2023	-	-	14/19/77/77	0/4/4/4
8	Y01	H	102	-	-	10/19/77/77	0/4/4/4
8	Y01	A	2014	-	-	12/19/77/77	0/4/4/4
11	GSP	E	301	-	-	6/21/38/38	0/3/3/3
8	Y01	A	2005	-	-	7/19/77/77	0/4/4/4
7	NAG	A	2001	1	-	0/6/23/26	0/1/1/1
8	Y01	A	2017	-	-	9/19/77/77	0/4/4/4
8	Y01	A	2021	-	-	12/19/77/77	0/4/4/4
10	UDP	A	2031	-	-	3/16/32/32	0/2/2/2
8	Y01	A	2013	-	-	12/19/77/77	0/4/4/4
8	Y01	A	2015	-	-	15/19/77/77	0/4/4/4
8	Y01	A	2028	-	-	7/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	A1CHR	H	101	4	-	6/16/16/17	-
8	Y01	A	2029	-	-	9/19/77/77	0/4/4/4

The worst 5 of 119 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	2031	UDP	O4'-C4'	7.41	1.61	1.45
10	A	2031	UDP	C3'-C4'	-7.25	1.34	1.53
10	A	2031	UDP	C2-N1	6.86	1.49	1.38
11	E	301	GSP	C4-N3	6.61	1.49	1.34
10	A	2031	UDP	C2-N3	6.60	1.49	1.38

The worst 5 of 562 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2027	Y01	CAT-CBH-CBF	-14.52	89.52	108.74
8	A	2020	Y01	CAT-CBH-CBF	-14.51	89.54	108.74
8	A	2023	Y01	CAT-CBH-CBF	-14.44	89.64	108.74
8	A	2002	Y01	CAT-CBH-CBF	-14.35	89.74	108.74
8	A	2016	Y01	CAT-CBH-CBF	-14.24	89.89	108.74

There are no chirality outliers.

5 of 360 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	2002	Y01	CAC-CBB-CBE-CBI
8	A	2003	Y01	CAM-CAY-OAW-CBC
8	A	2007	Y01	OAG-CAY-OAW-CBC
8	A	2007	Y01	CAM-CAY-OAW-CBC
8	A	2008	Y01	OAG-CAY-OAW-CBC

There are no ring outliers.

30 monomers are involved in 203 short contacts:

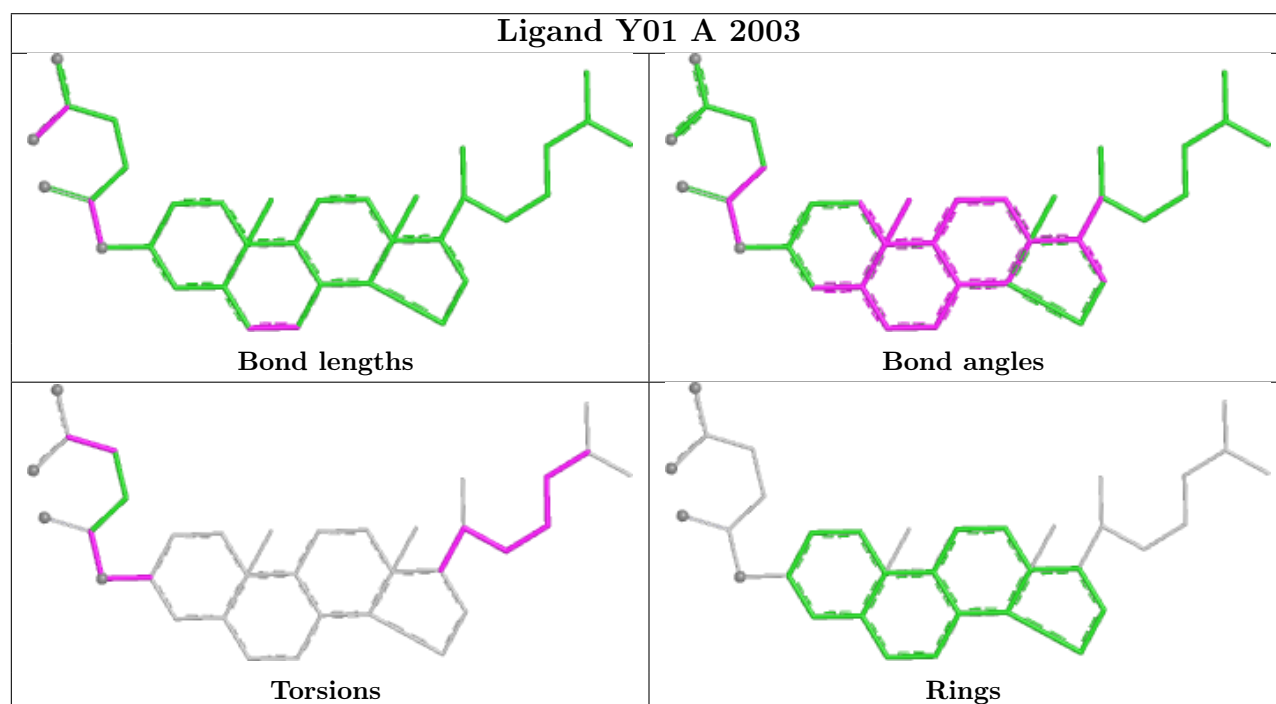
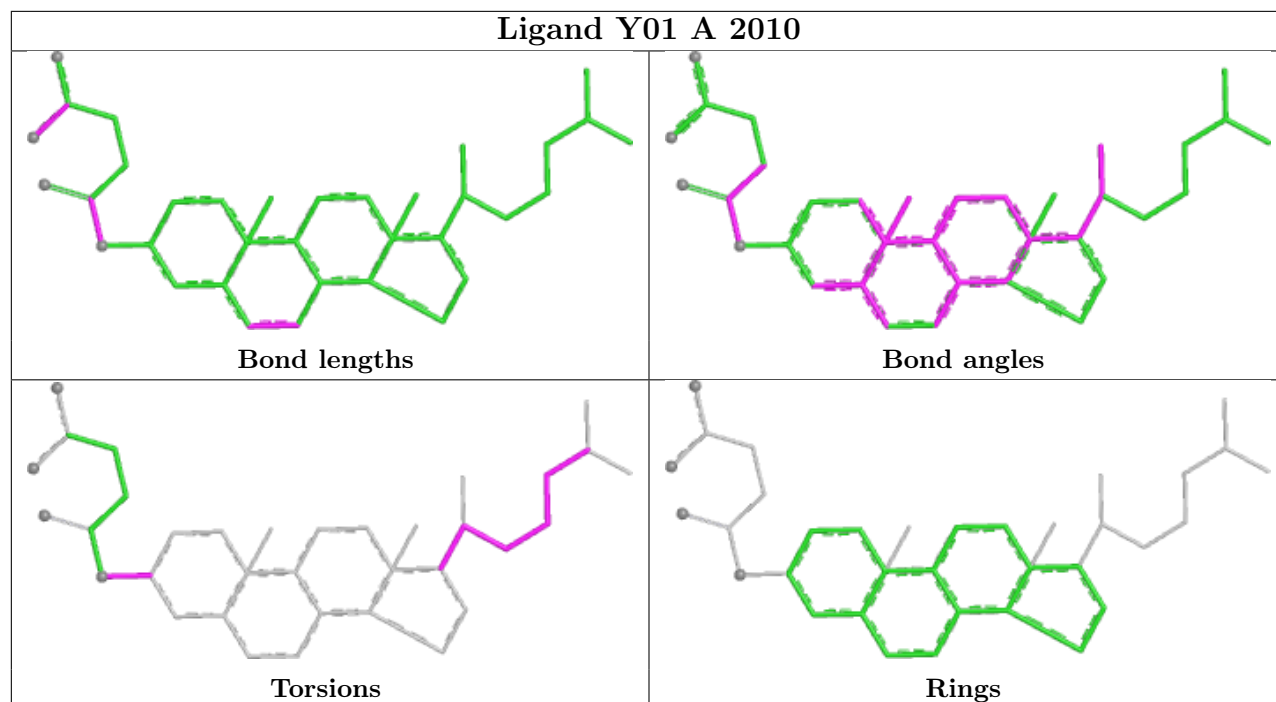
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2010	Y01	12	0
8	A	2003	Y01	13	0
8	A	2002	Y01	9	0
8	A	2018	Y01	13	0
8	A	2004	Y01	2	0

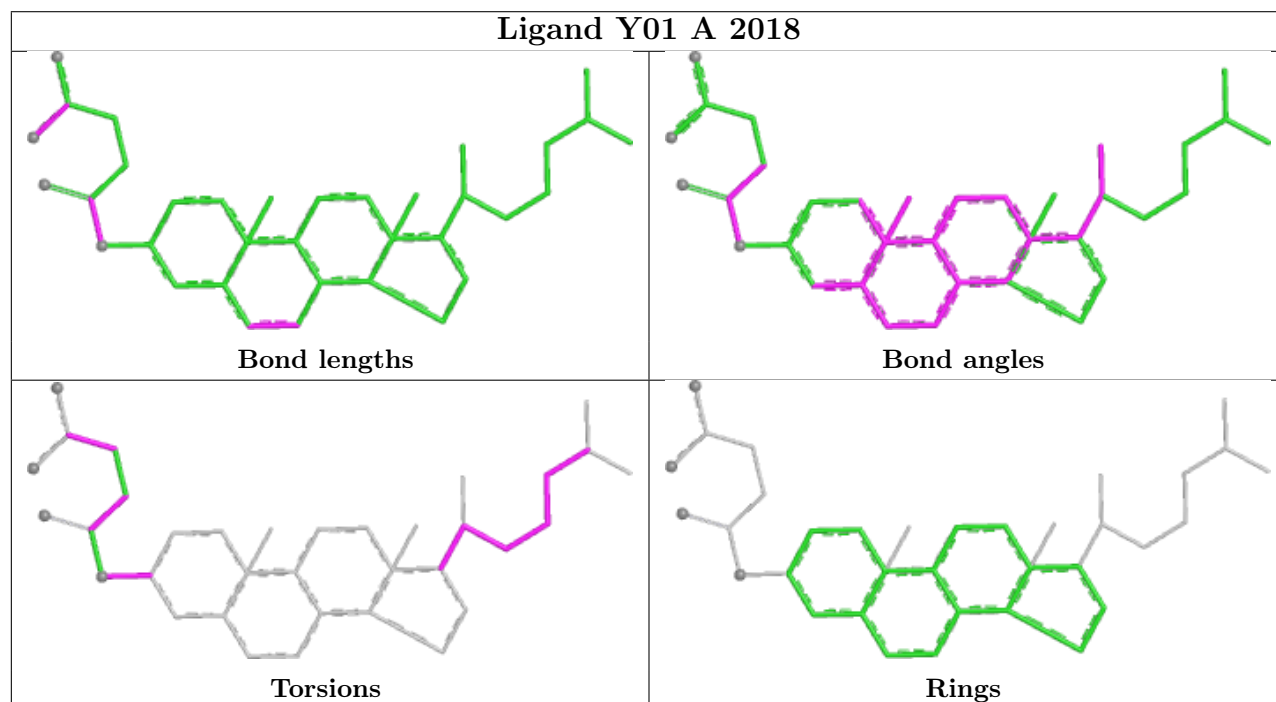
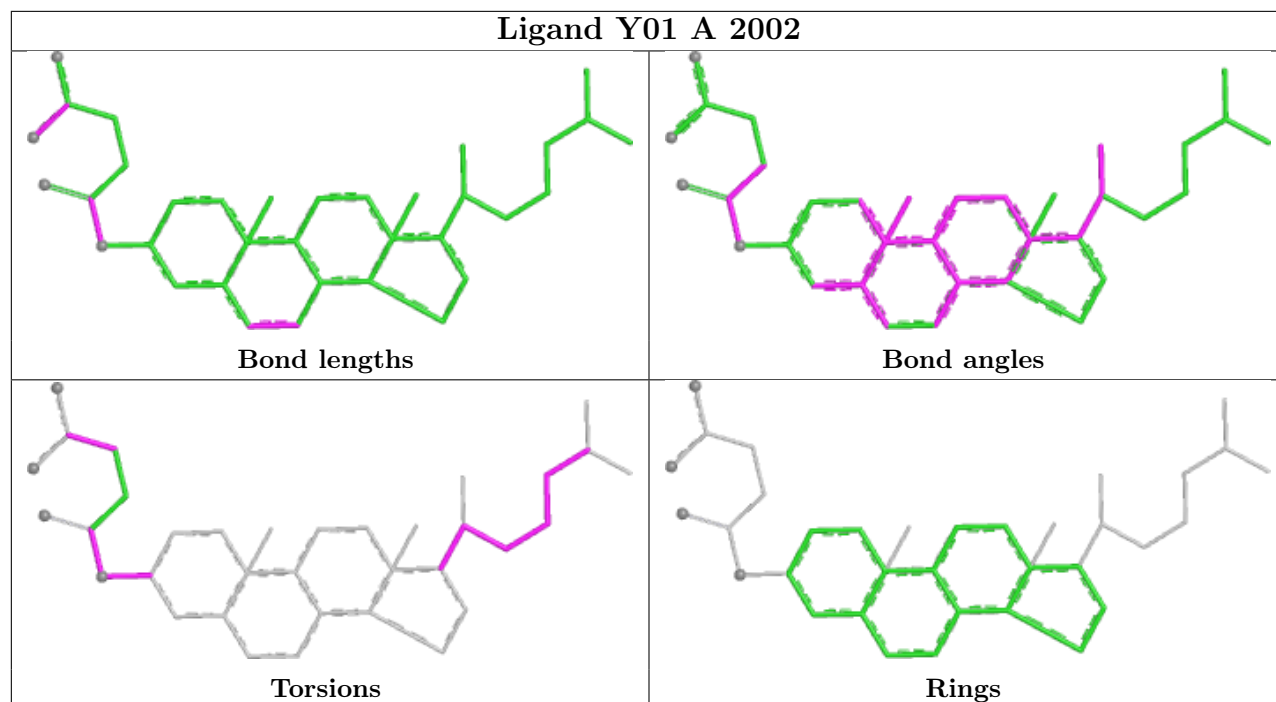
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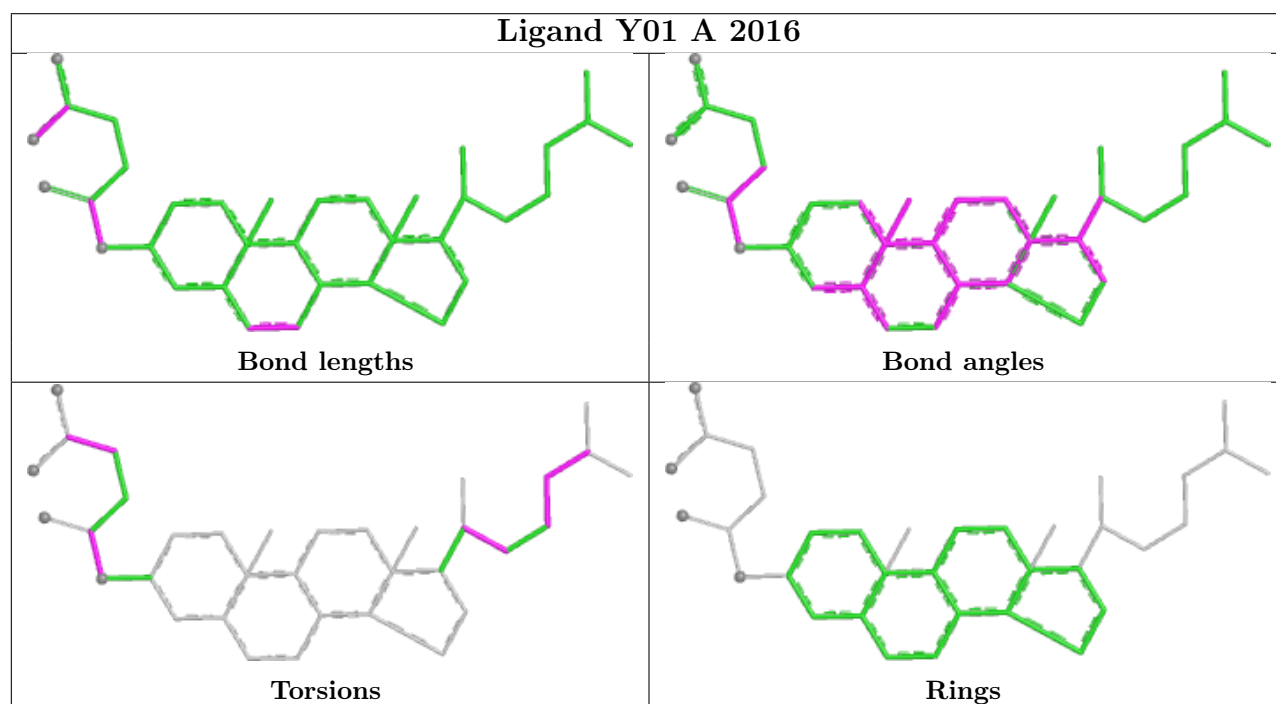
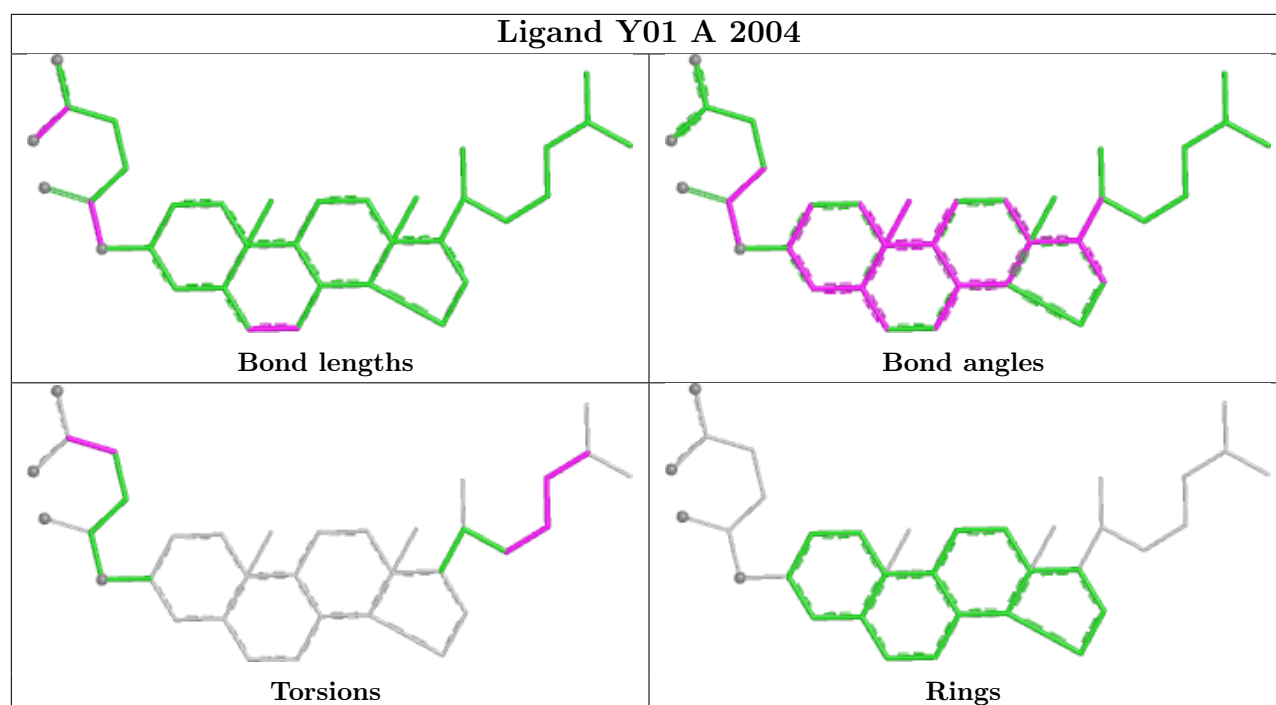
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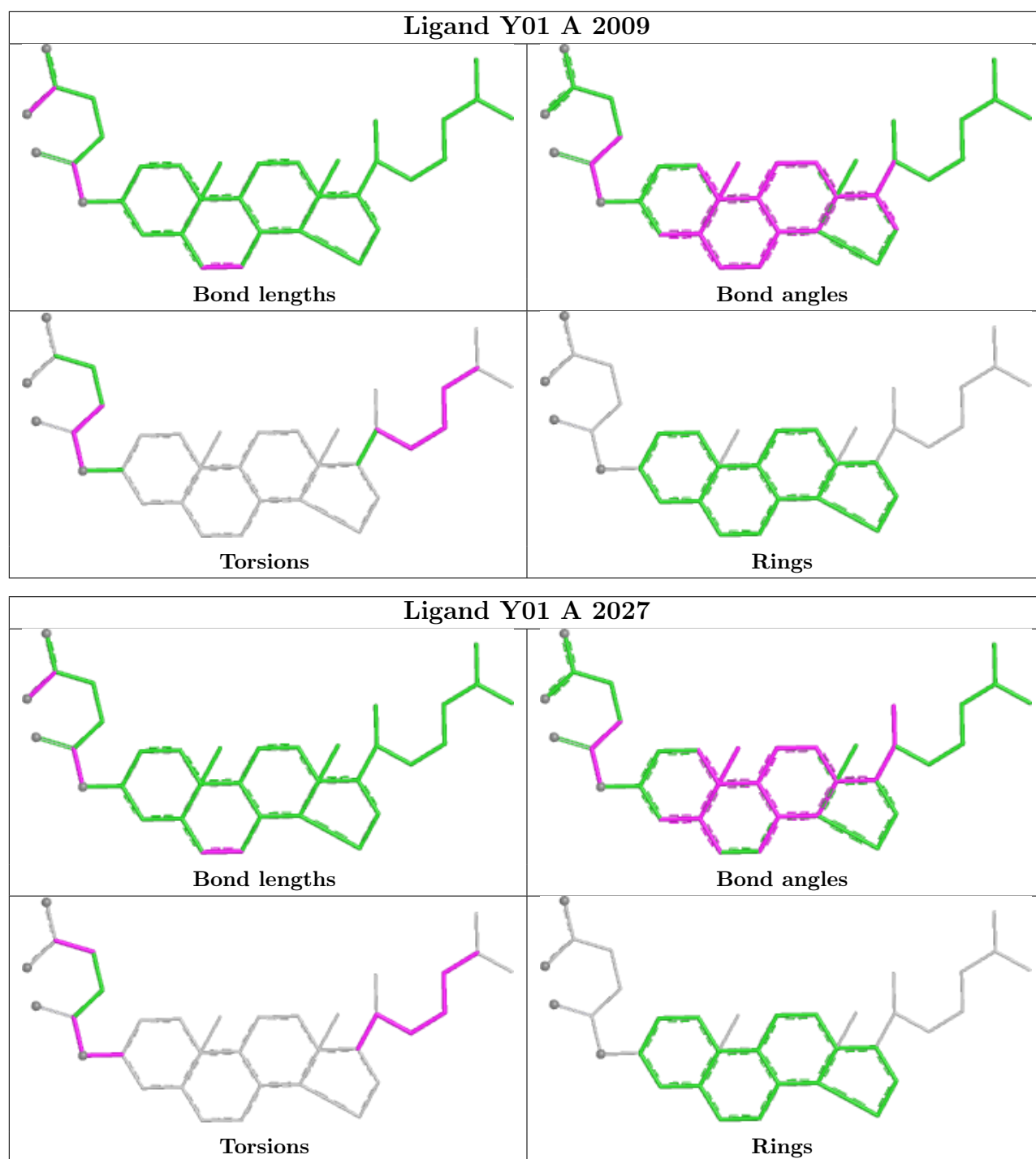
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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8	A	2009	Y01	9	0
8	A	2027	Y01	6	0
8	A	2007	Y01	8	0
8	A	2008	Y01	10	0
8	A	2026	Y01	5	0
8	A	2020	Y01	13	0
8	A	2019	Y01	7	0
9	A	2006	3PE	2	0
8	A	2012	Y01	12	0
8	A	2025	Y01	6	0
8	A	2022	Y01	10	0
8	A	2030	Y01	5	0
8	A	2011	Y01	6	0
8	A	2024	Y01	7	0
8	A	2023	Y01	9	0
8	H	102	Y01	7	0
8	A	2014	Y01	12	0
8	A	2005	Y01	11	0
8	A	2017	Y01	7	0
8	A	2021	Y01	5	0
8	A	2013	Y01	9	0
8	A	2015	Y01	9	0
8	A	2028	Y01	5	0
8	A	2029	Y01	7	0

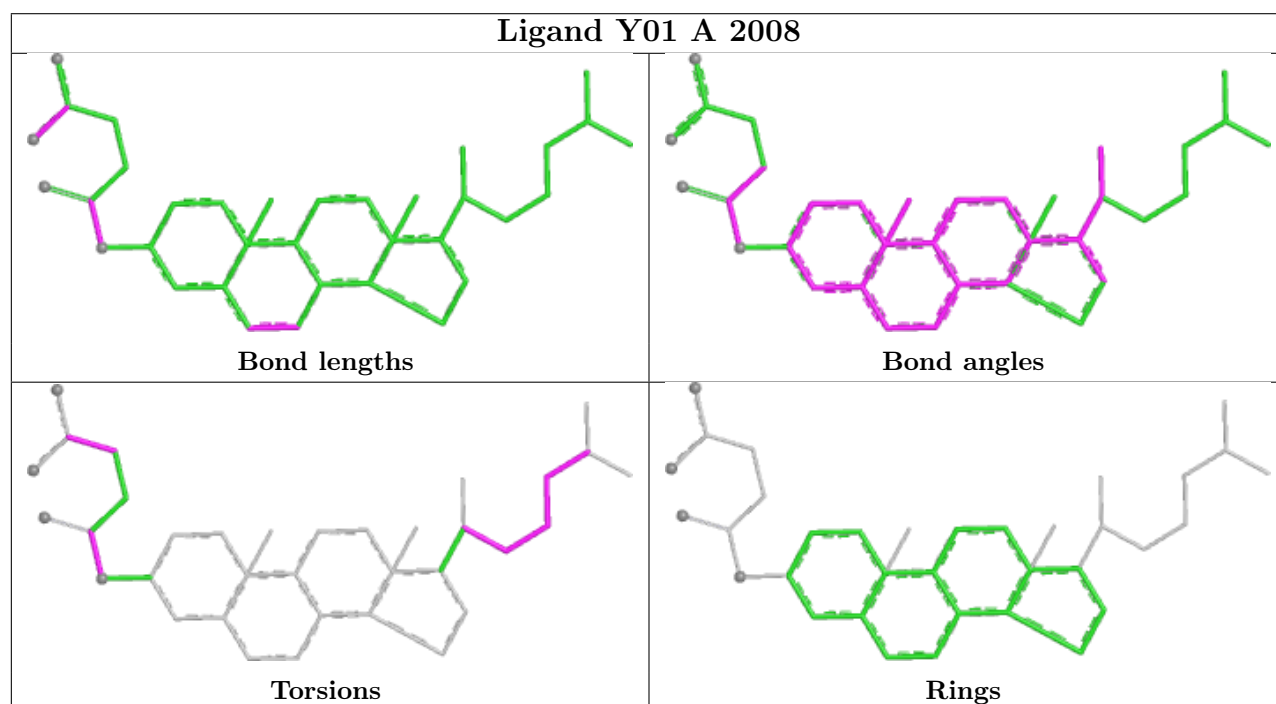
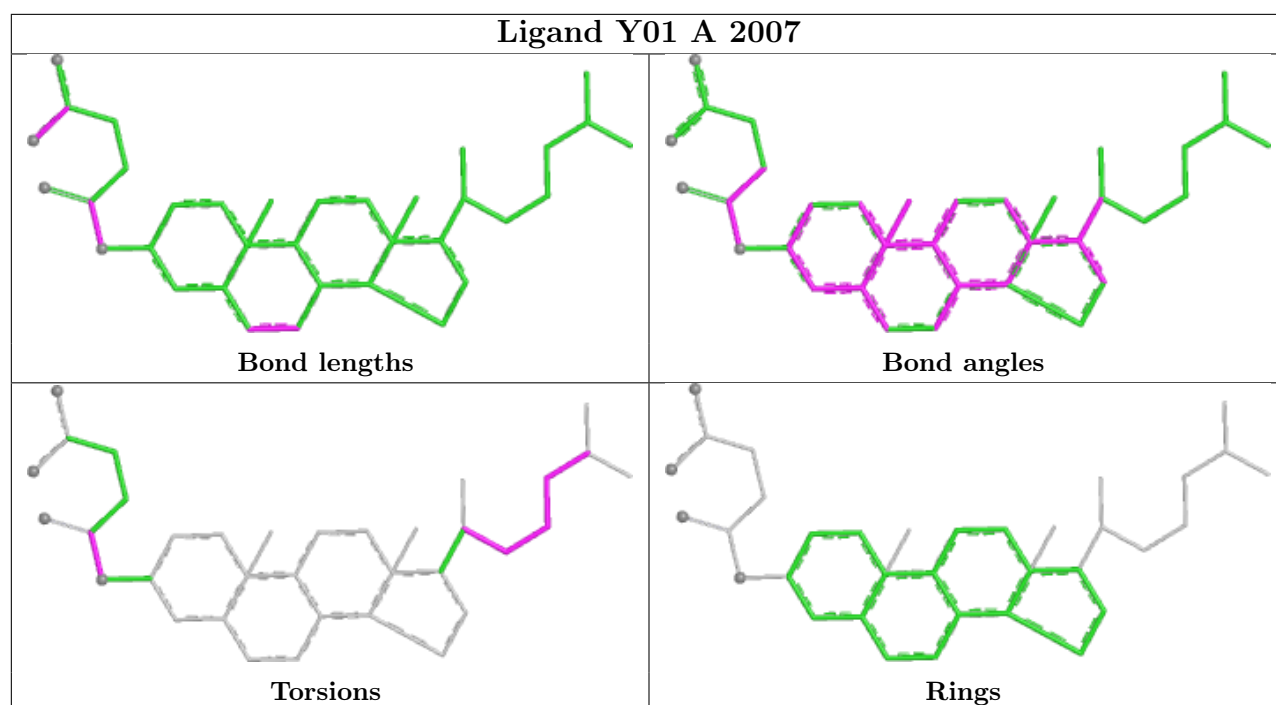
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



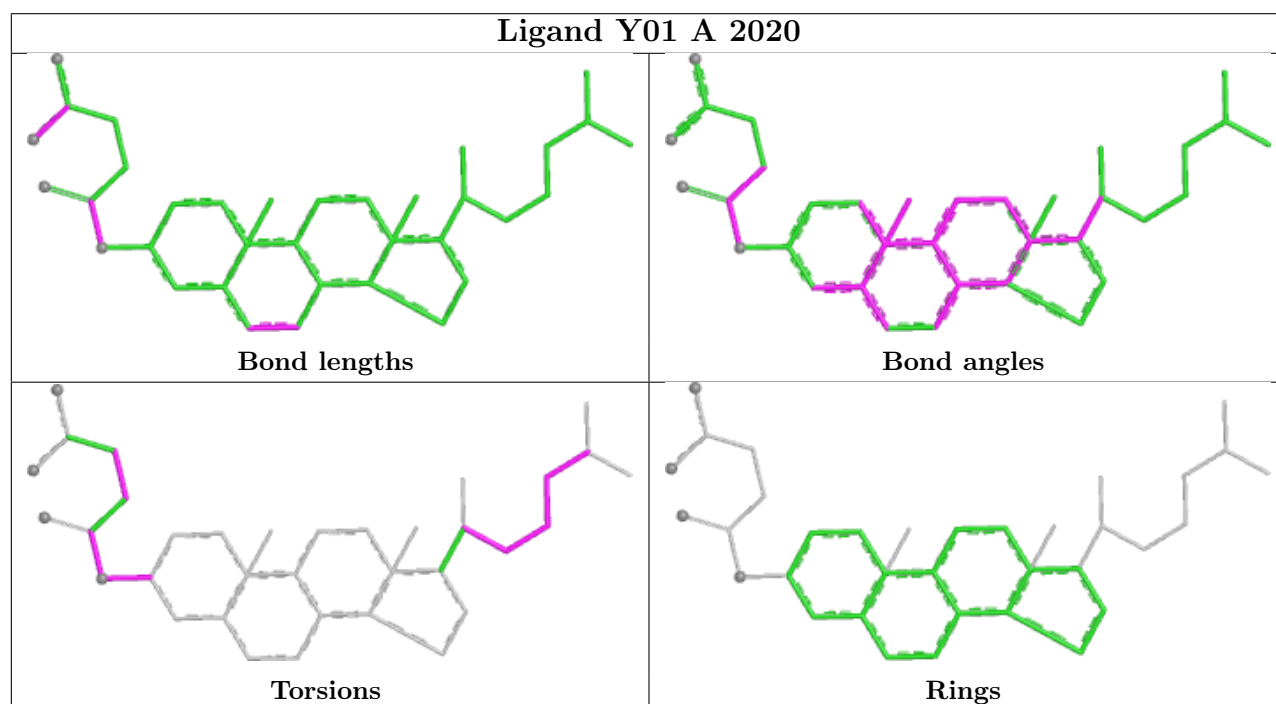
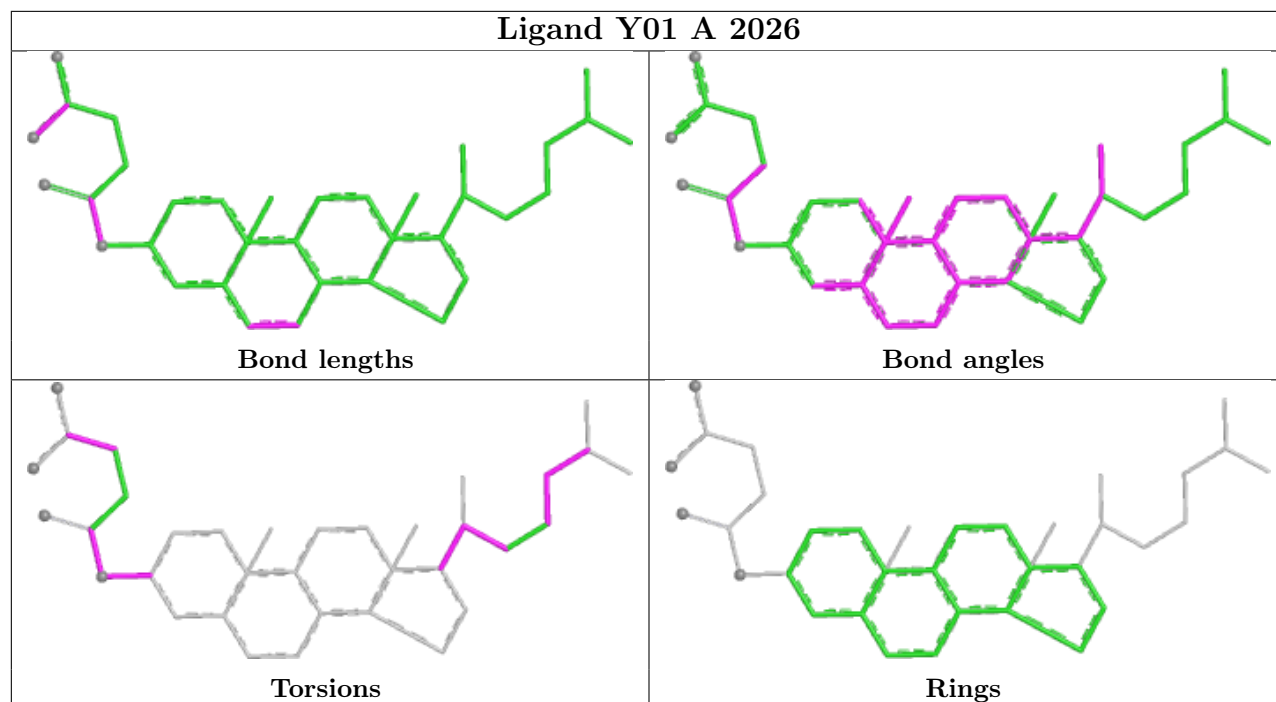


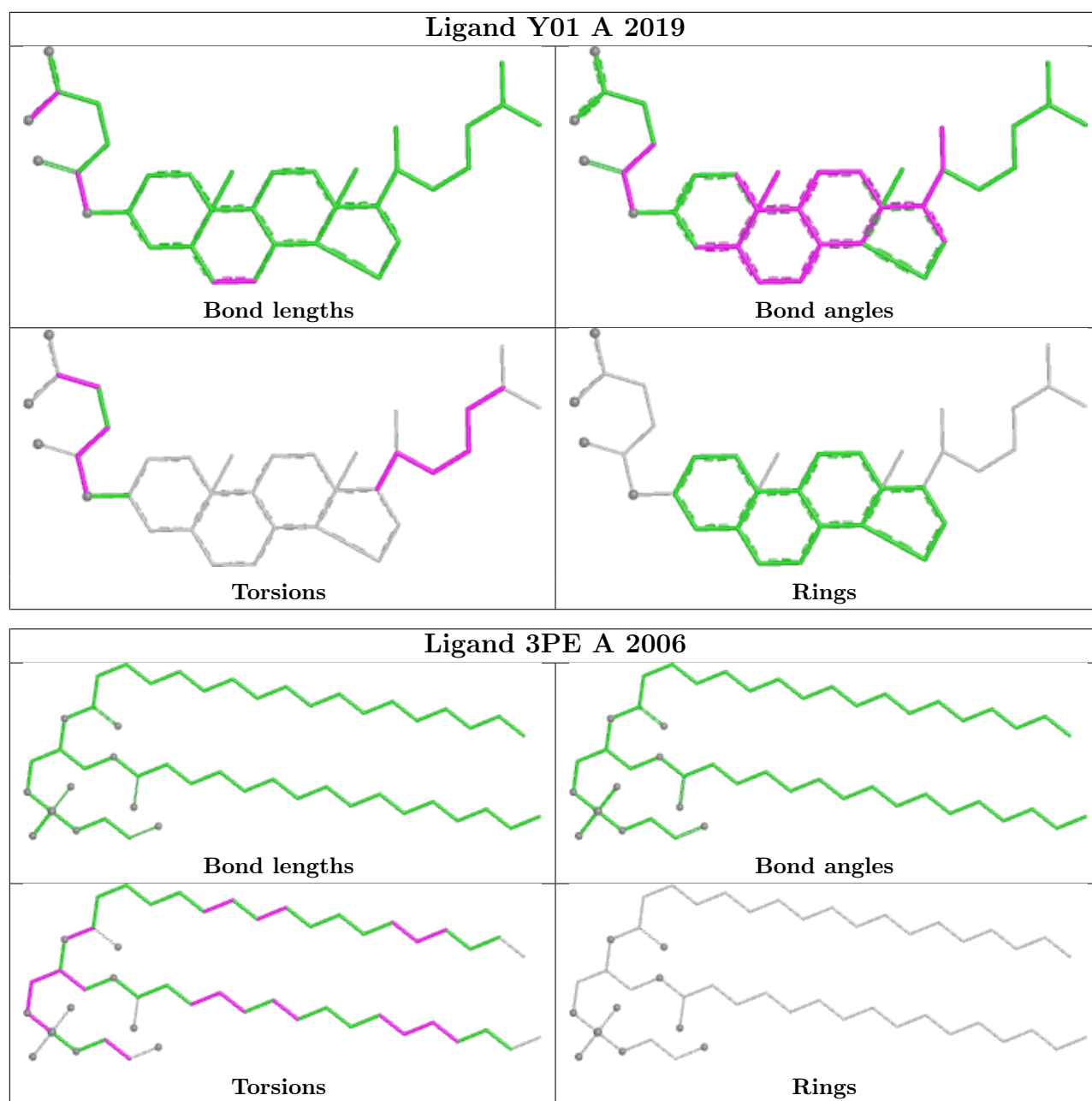


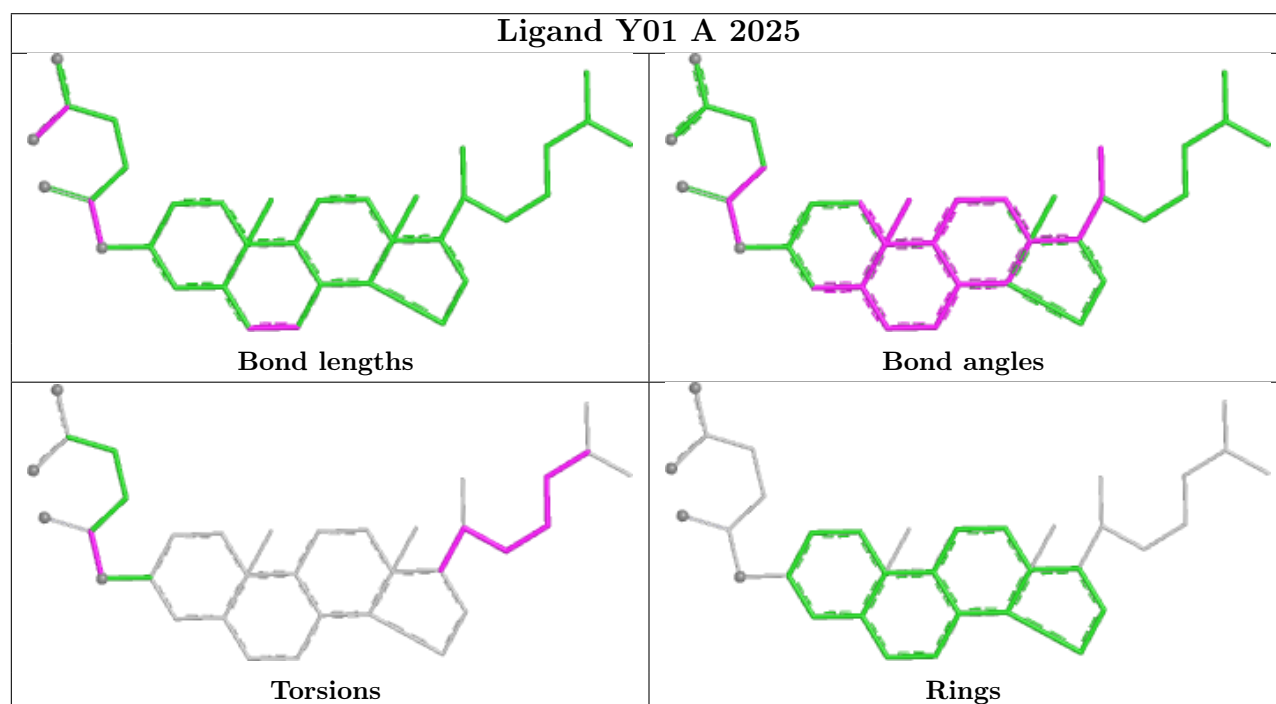
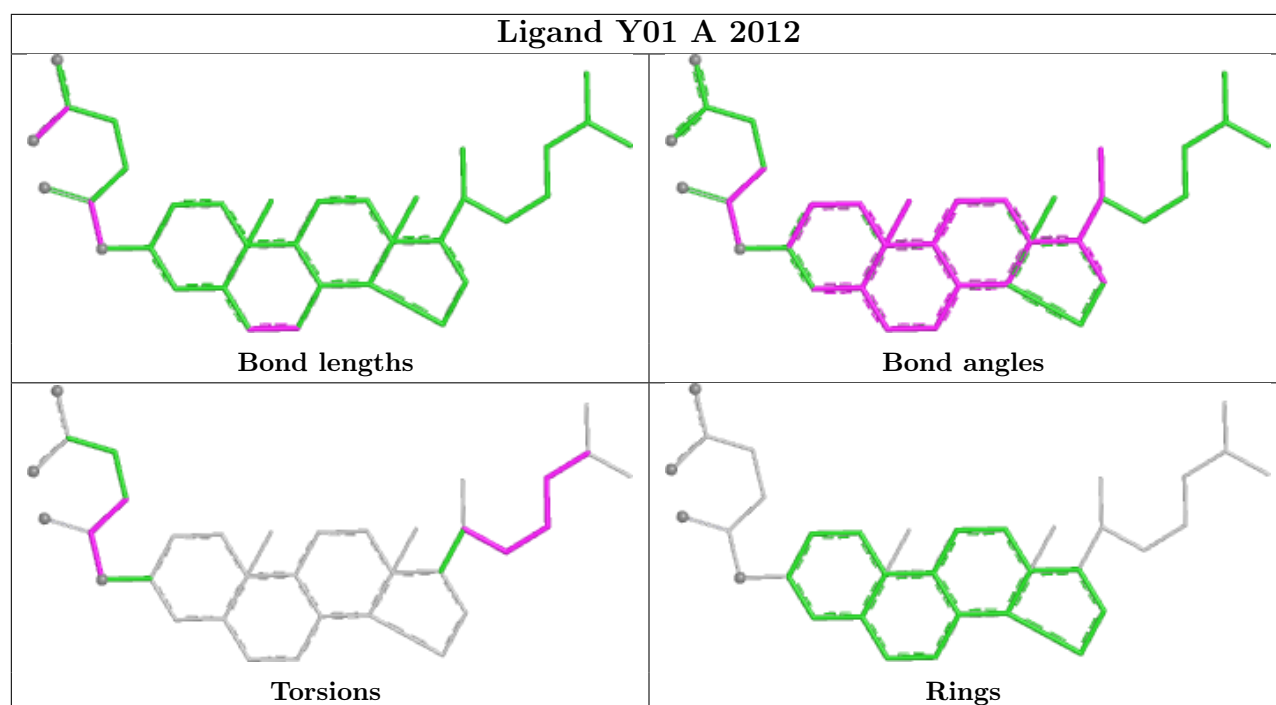


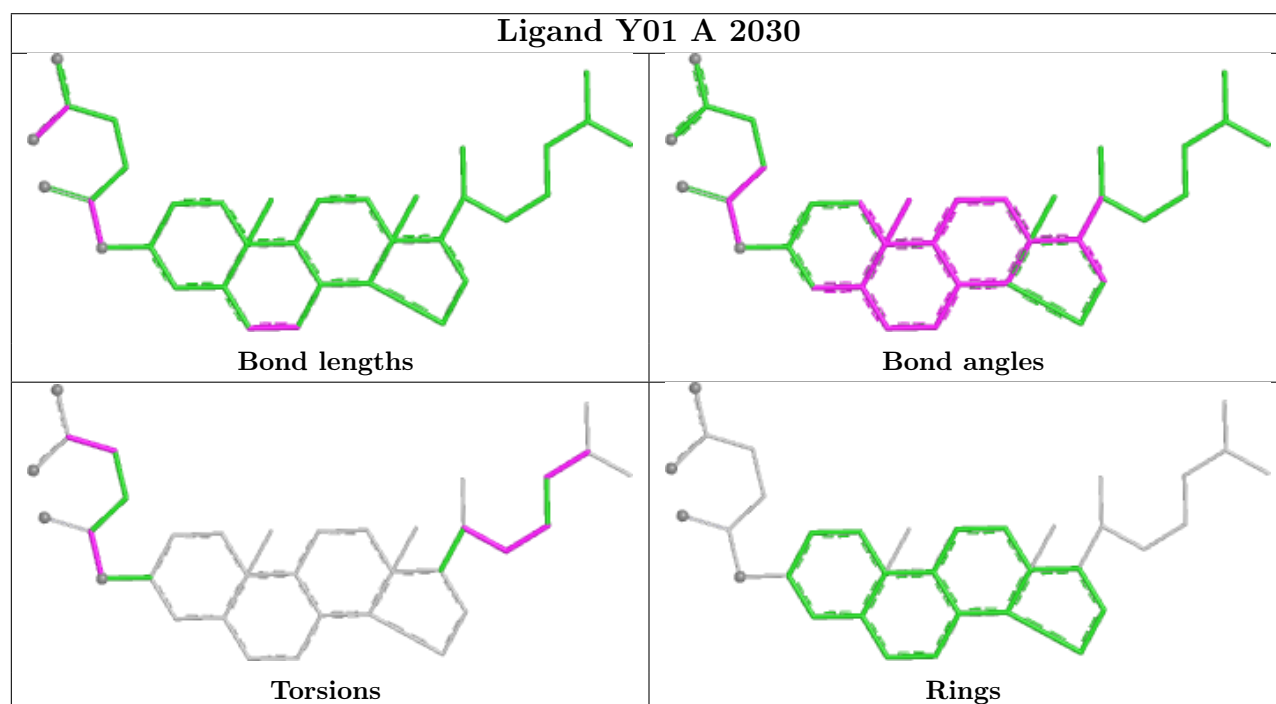
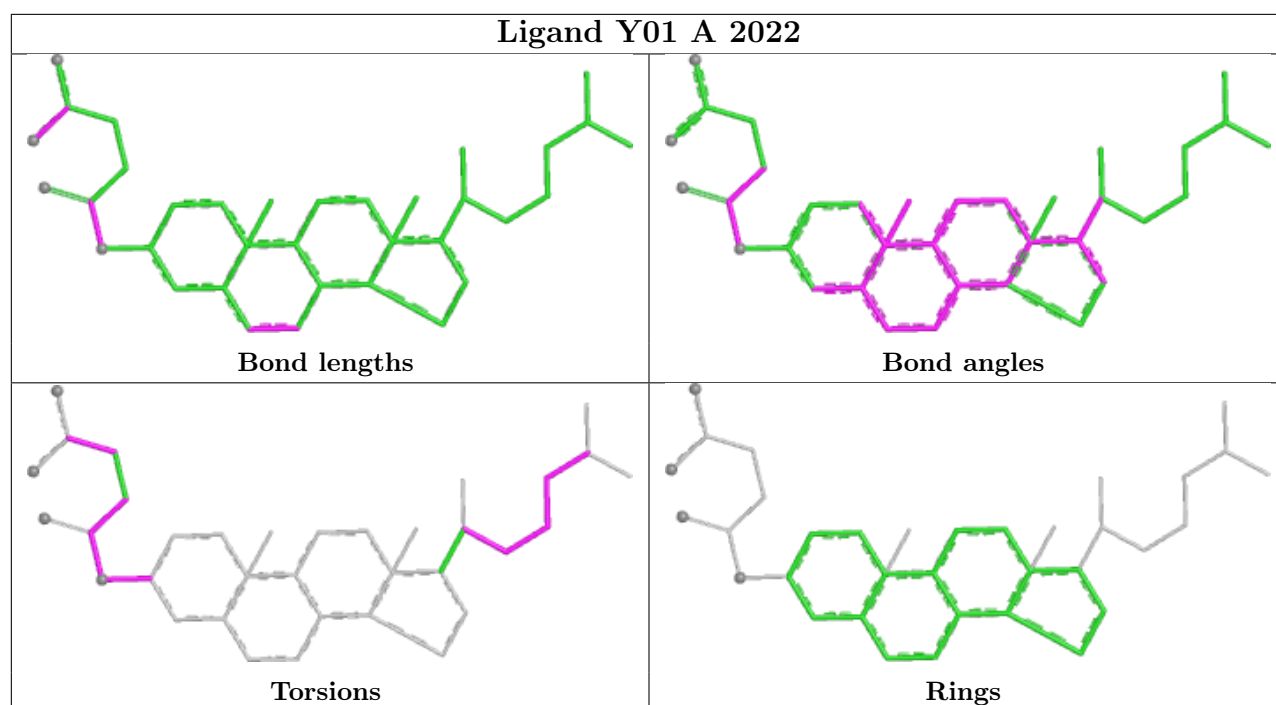


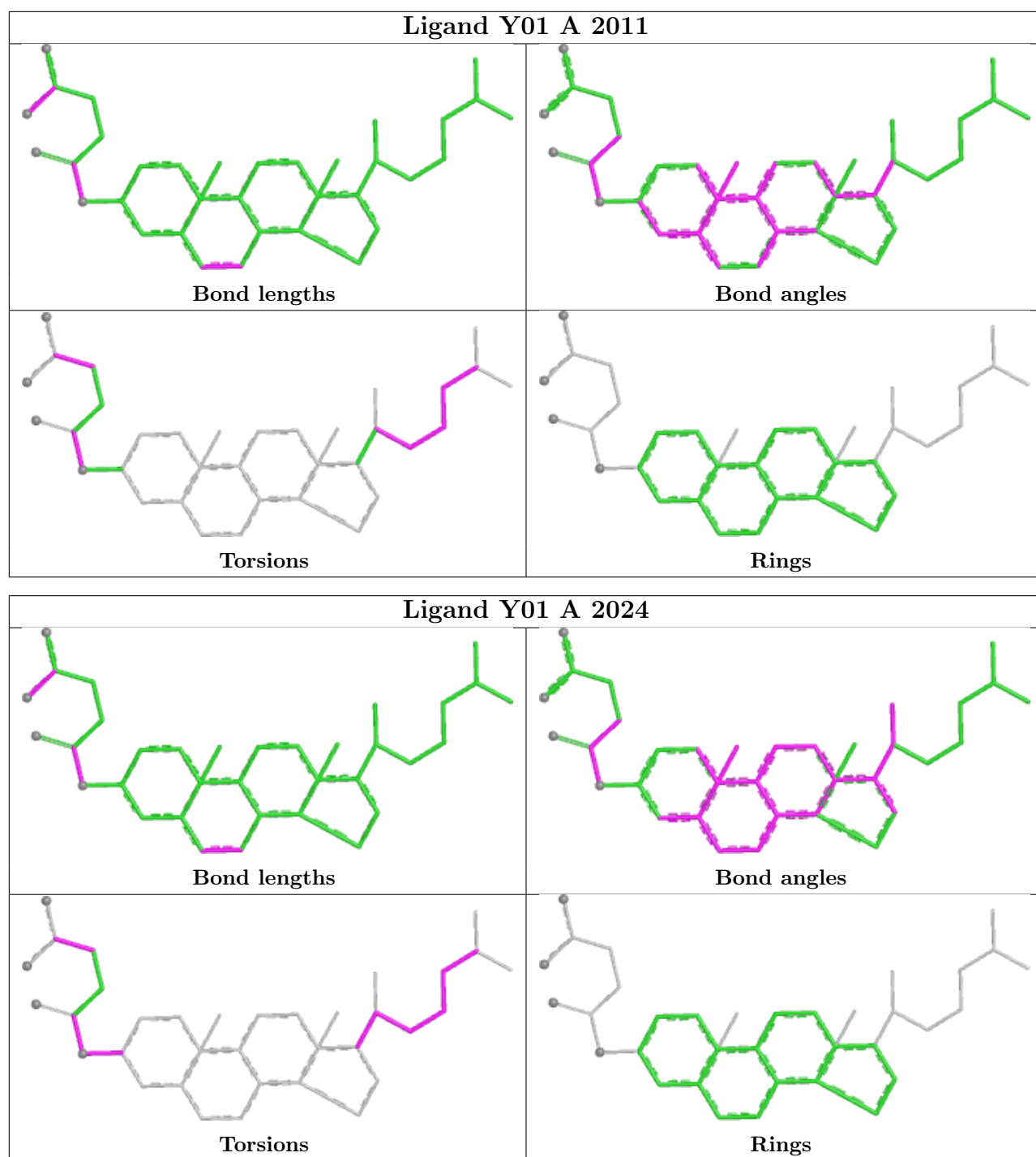


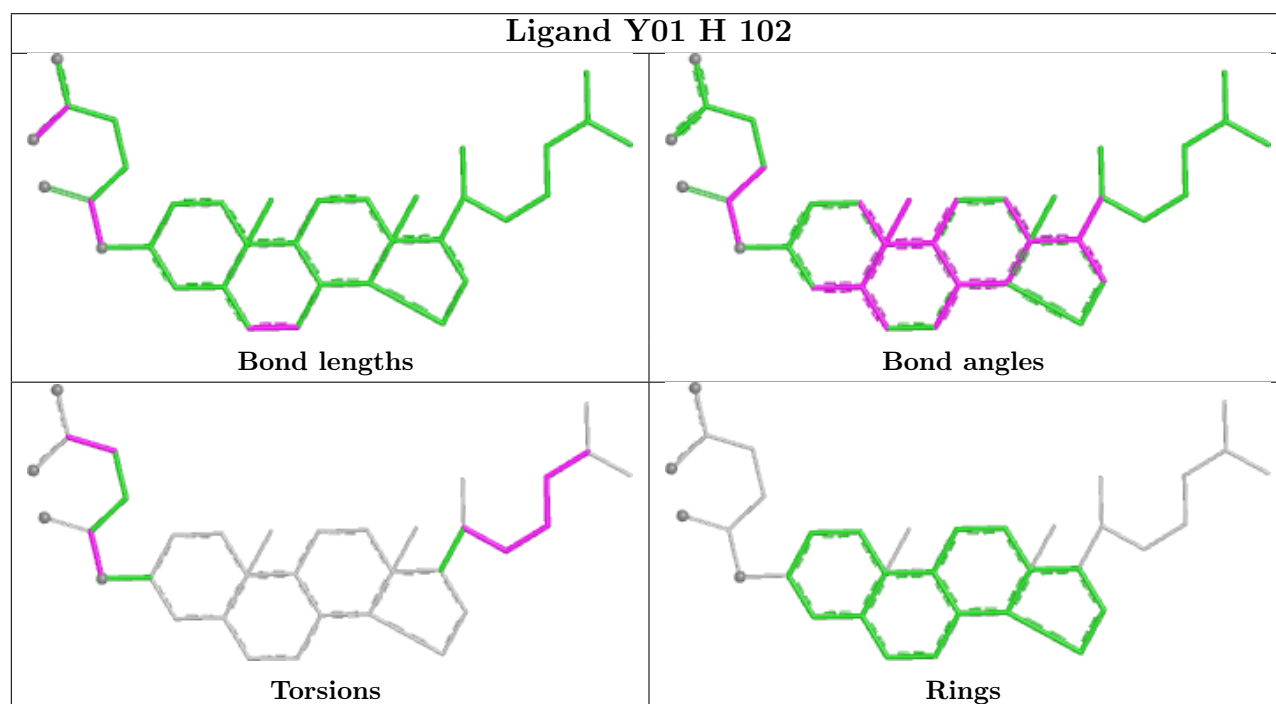
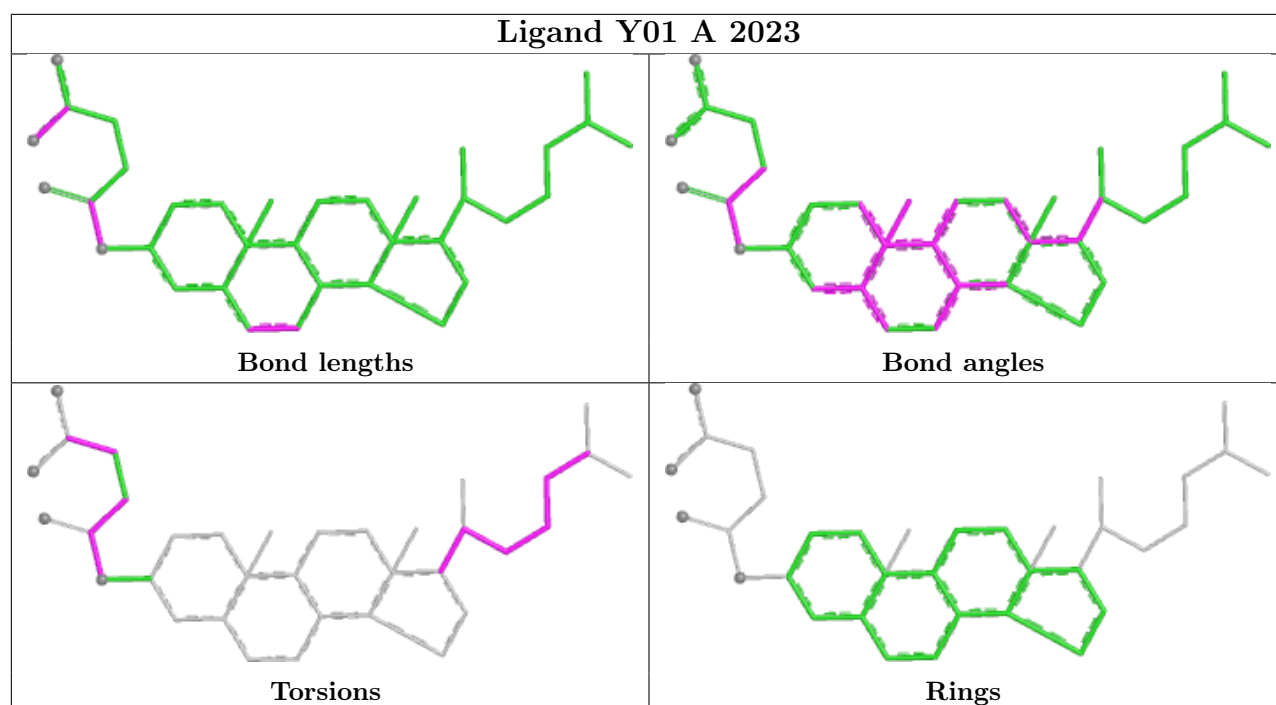


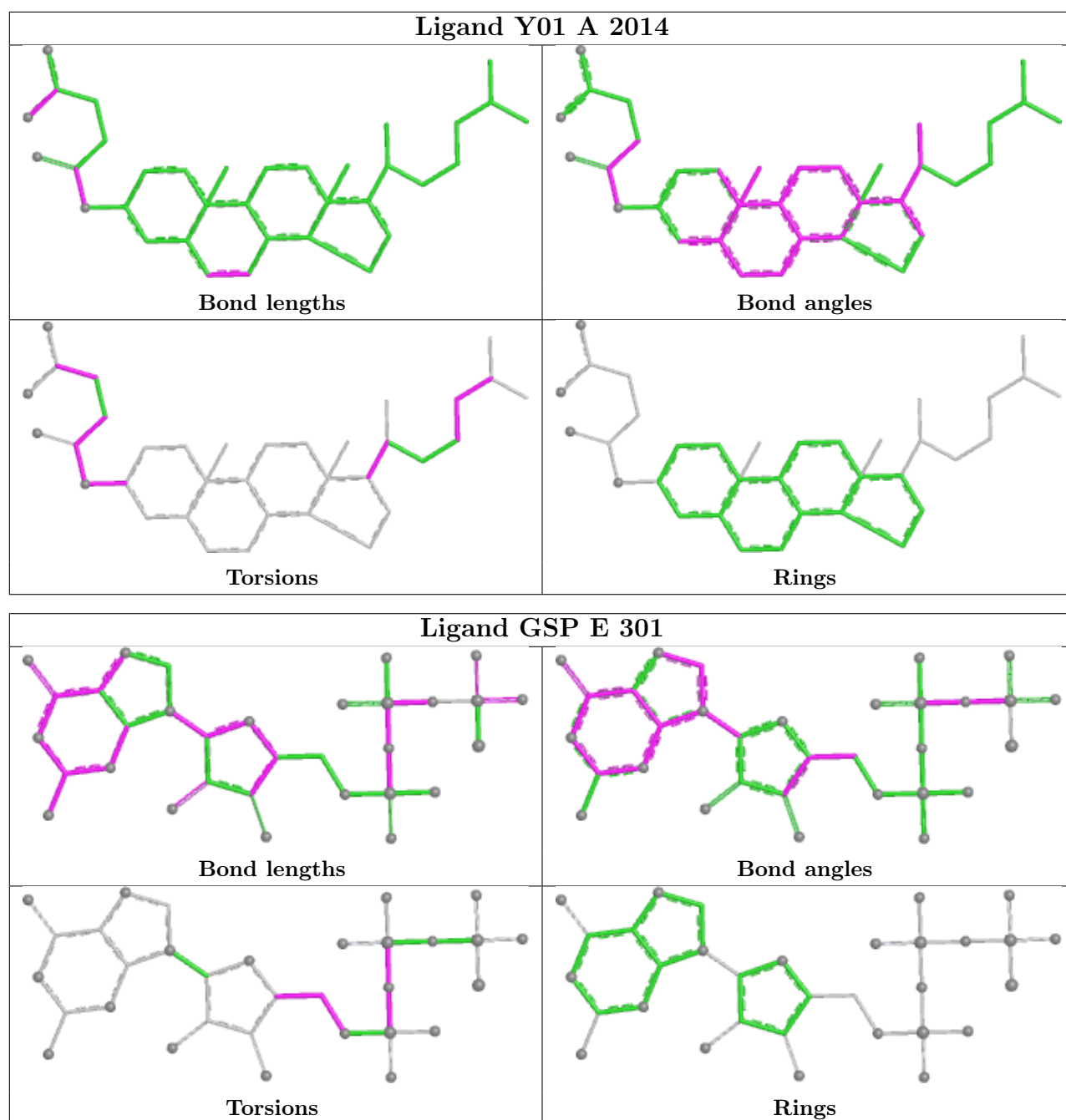


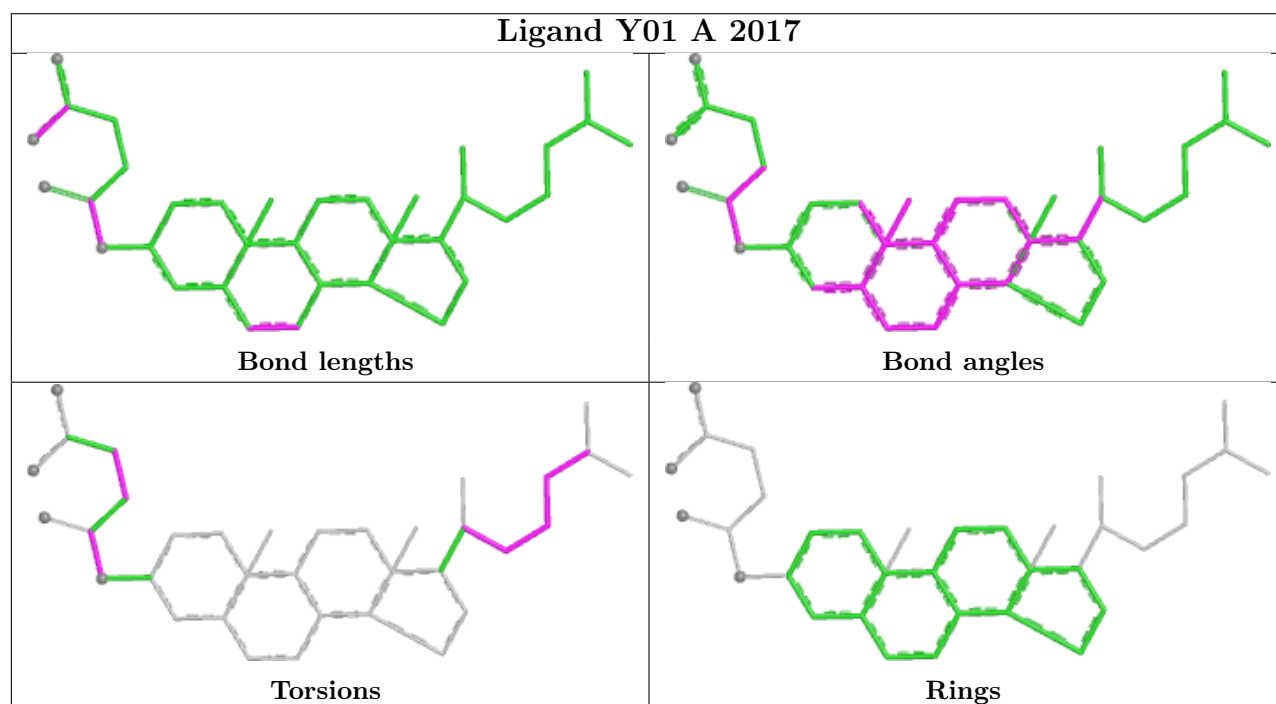
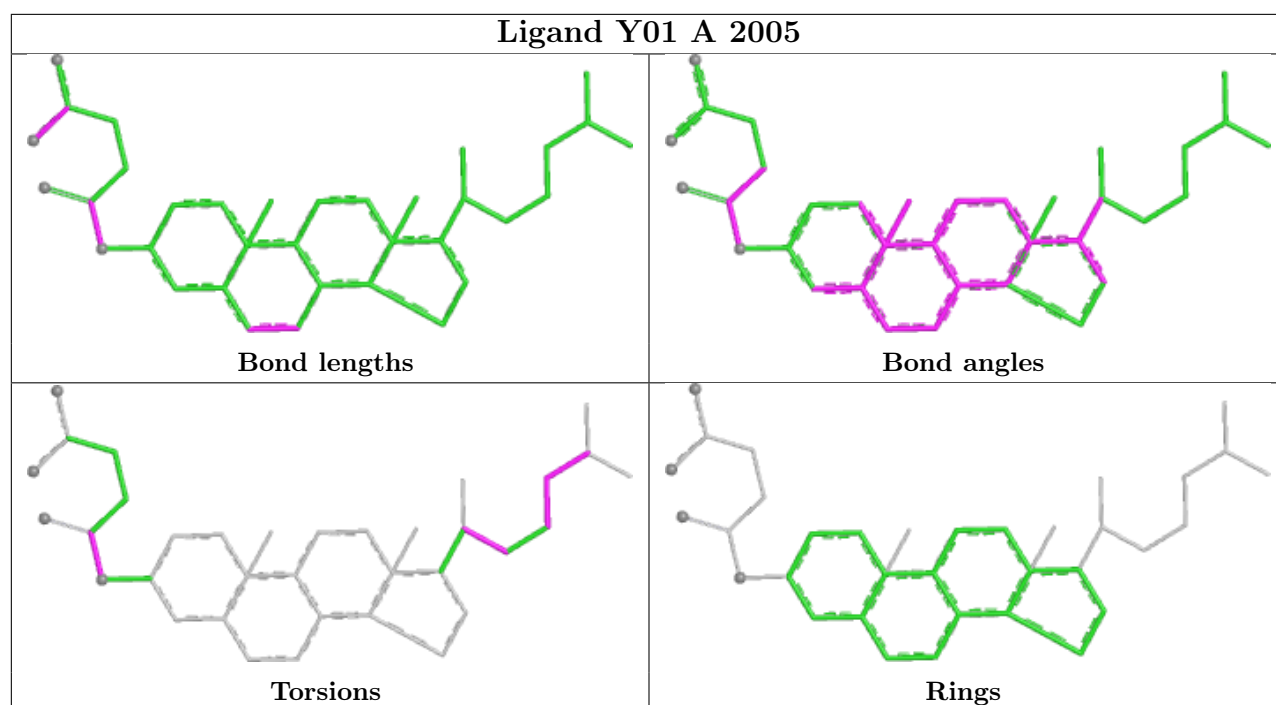




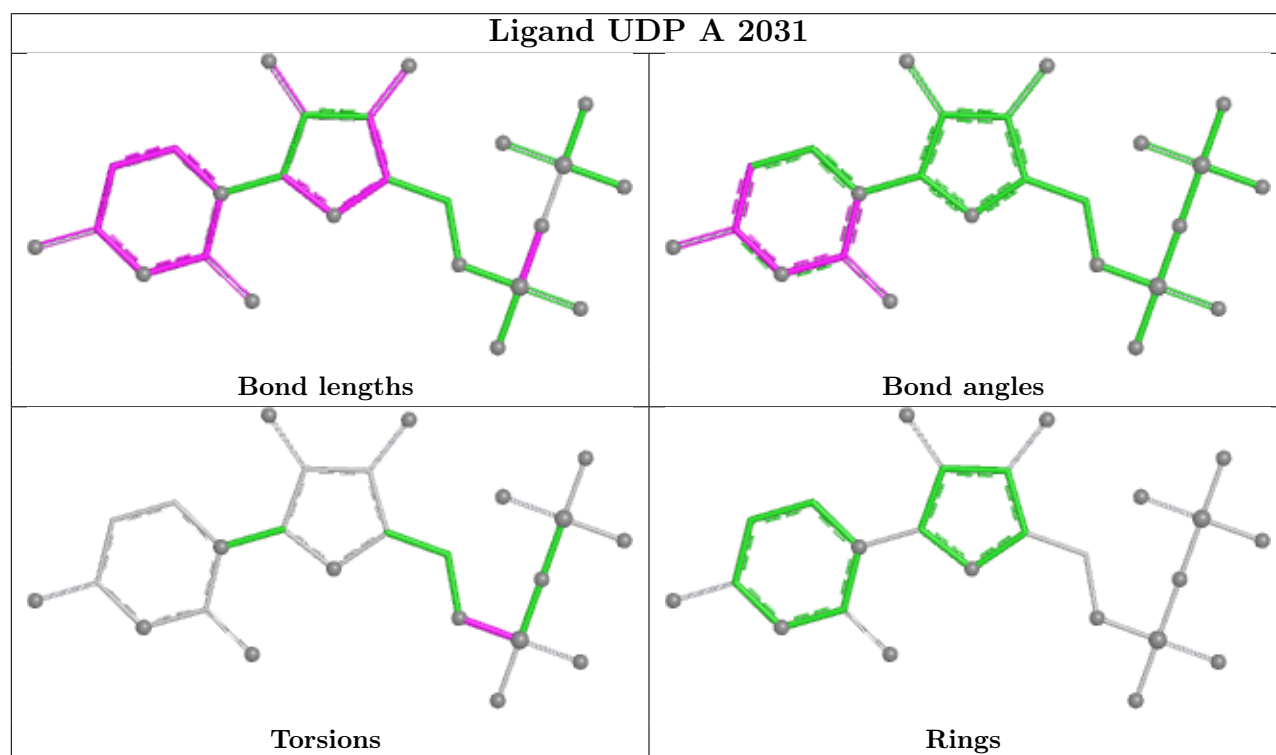
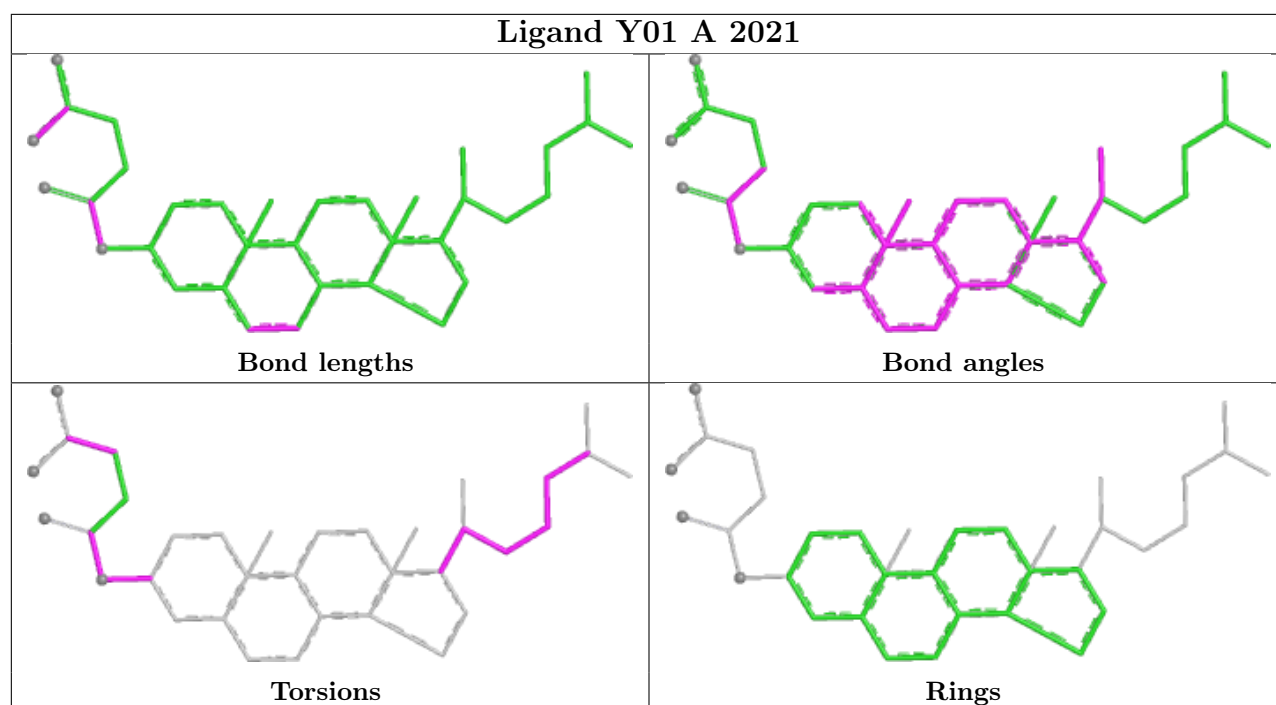


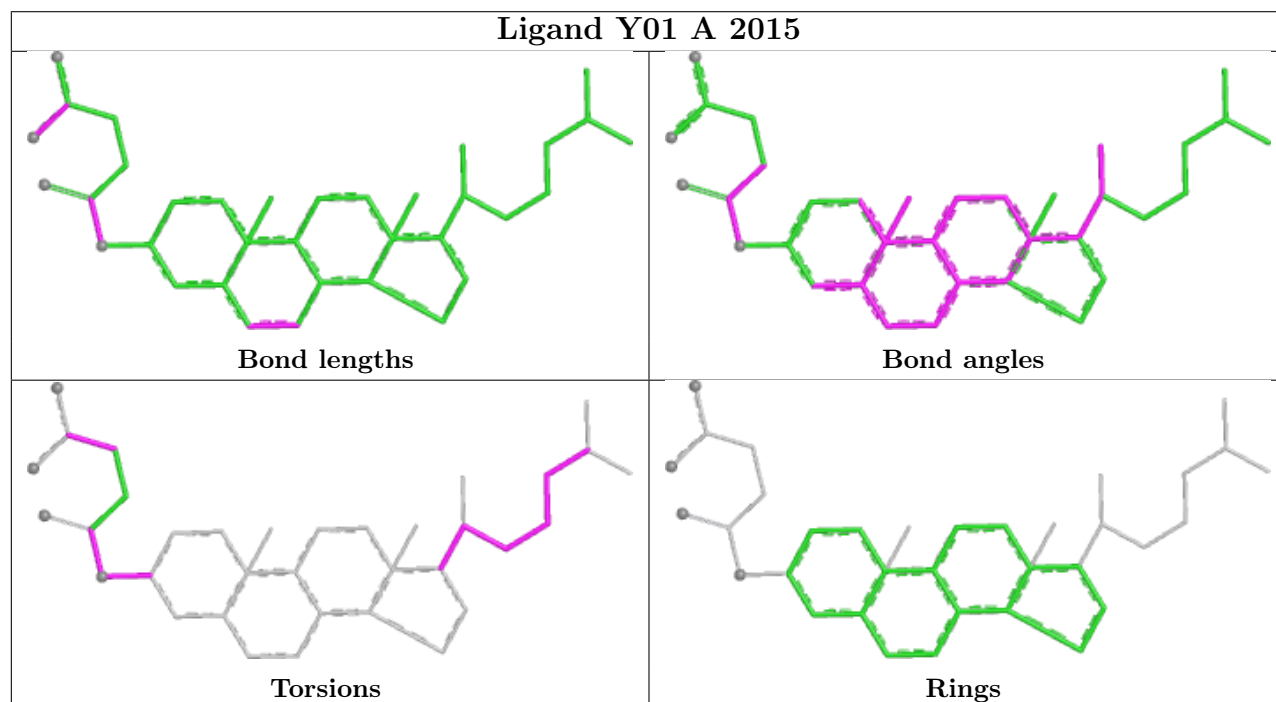
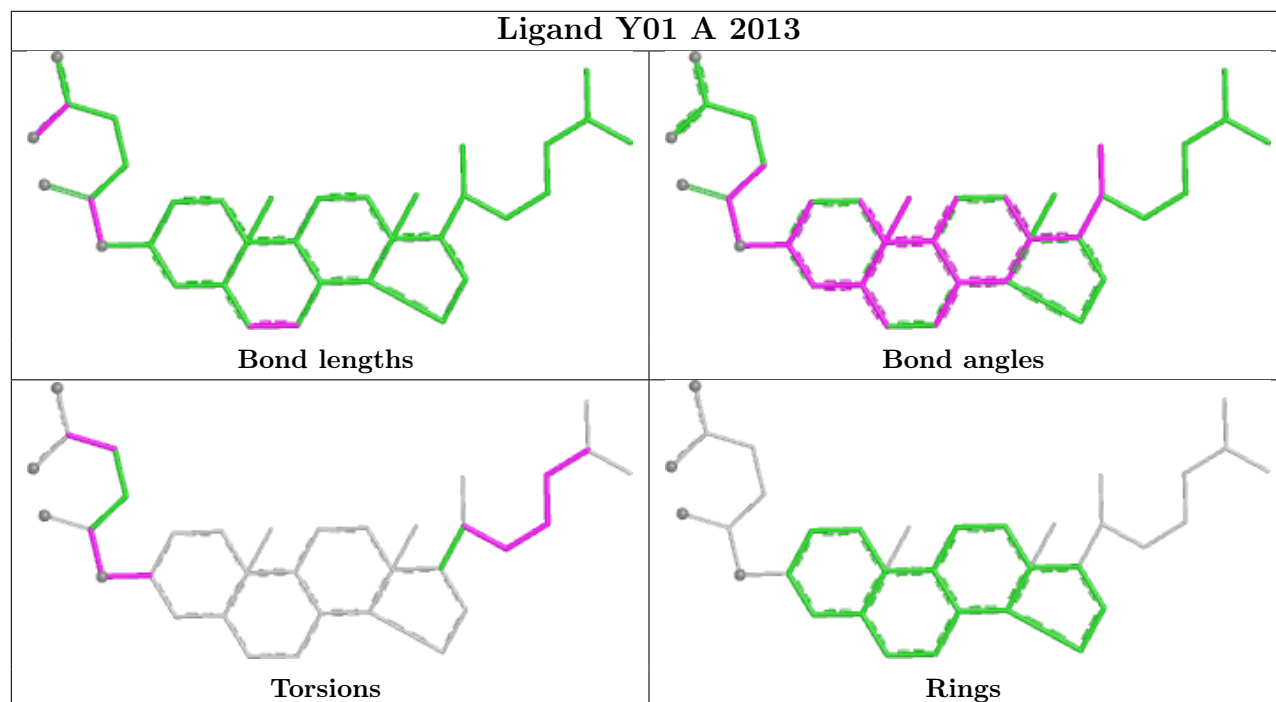


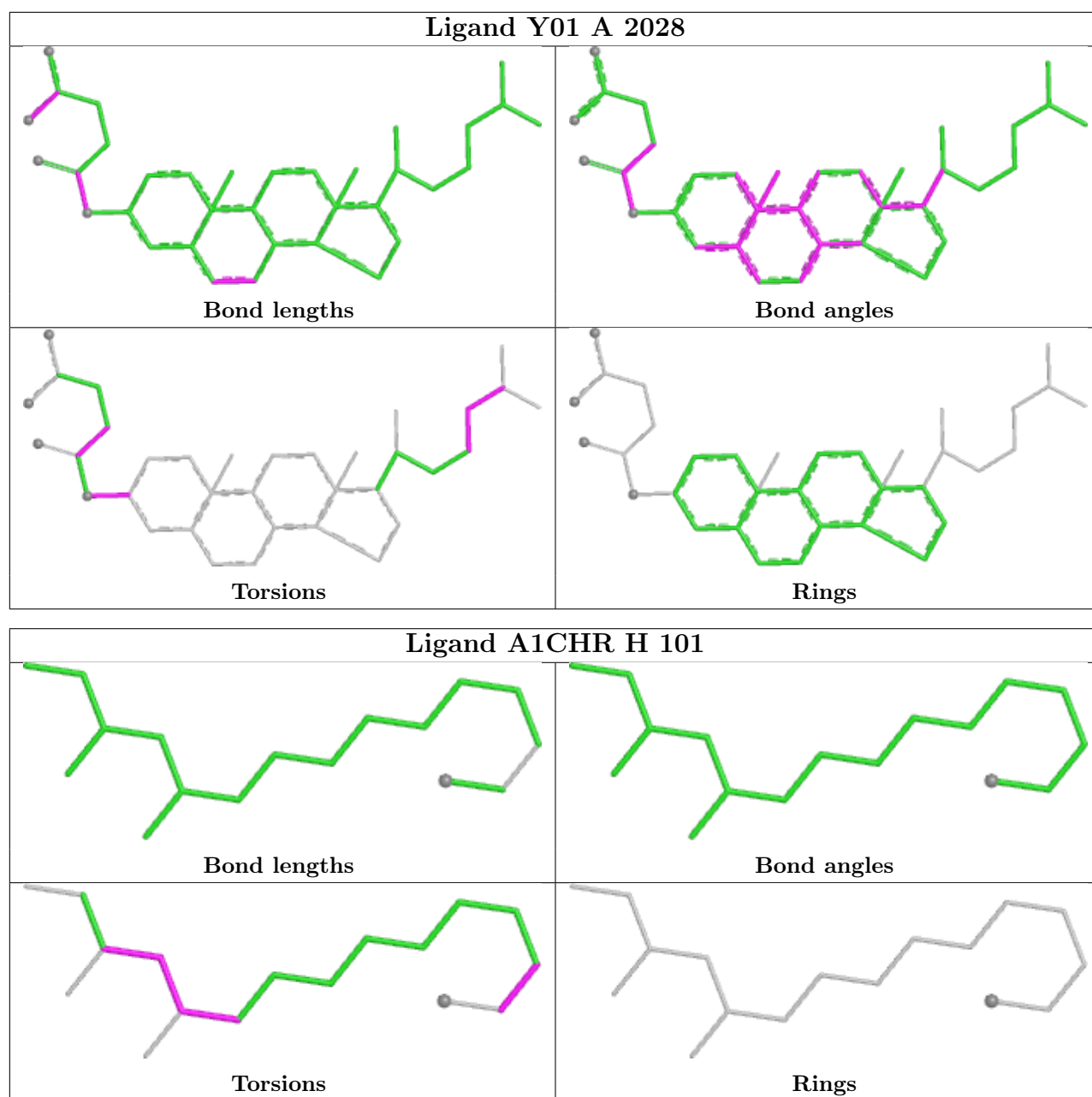


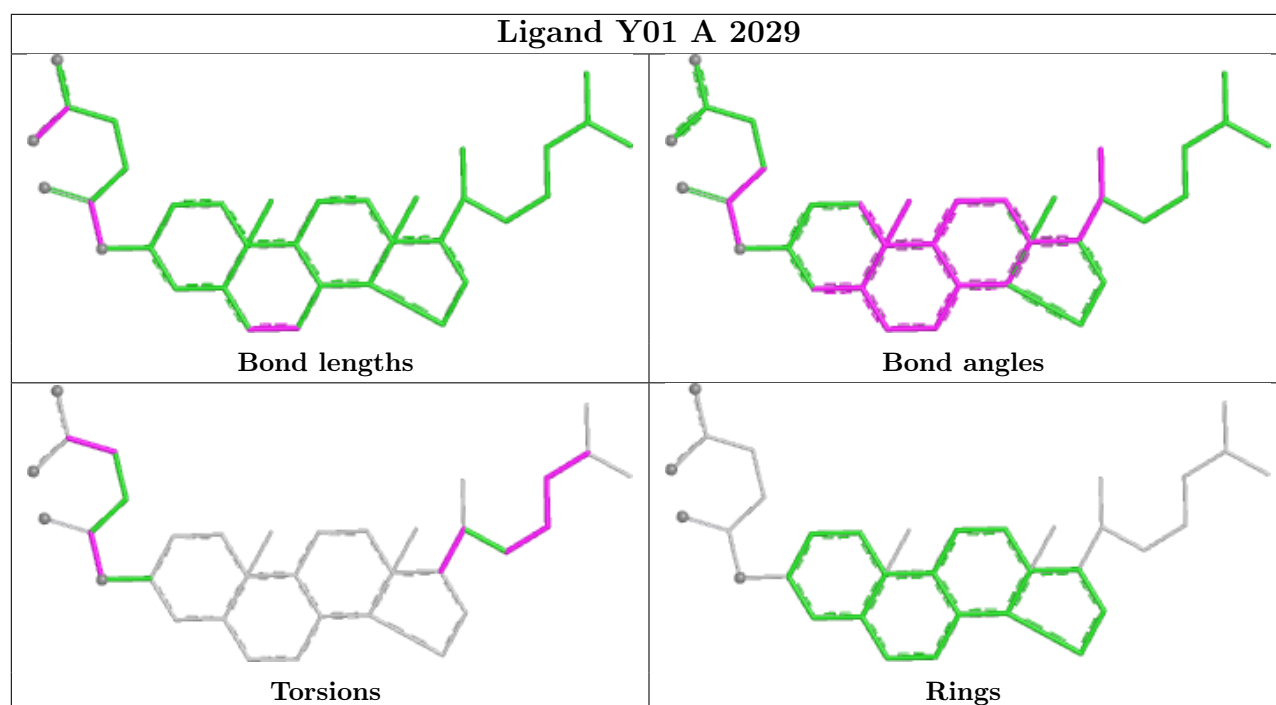












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

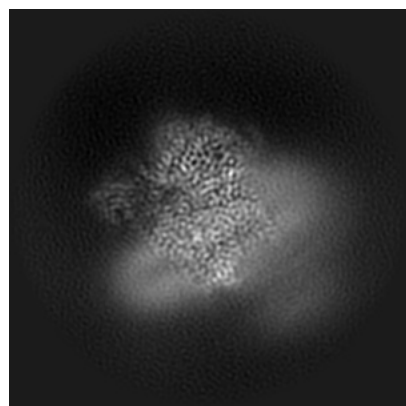
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71550. These allow visual inspection of the internal detail of the map and identification of artifacts.

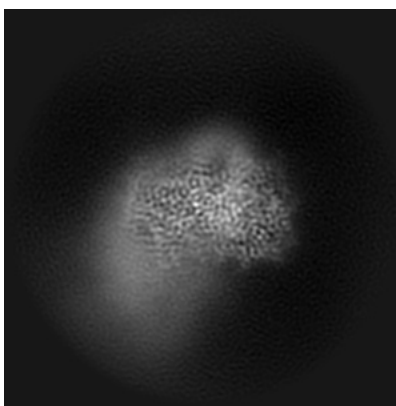
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

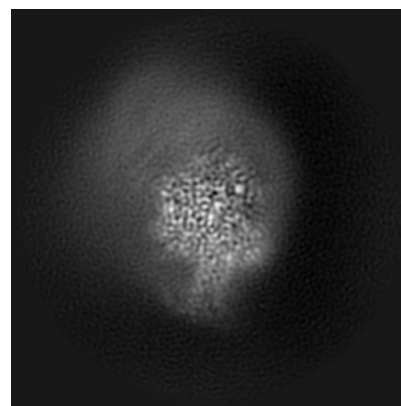
#### 6.1.1 Primary map



X

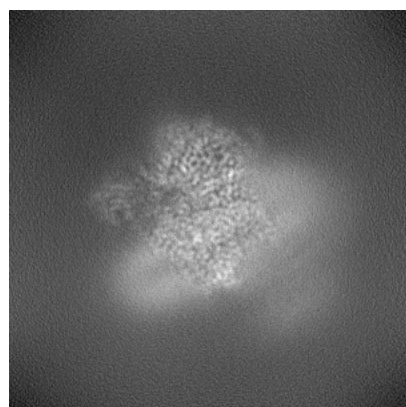


Y

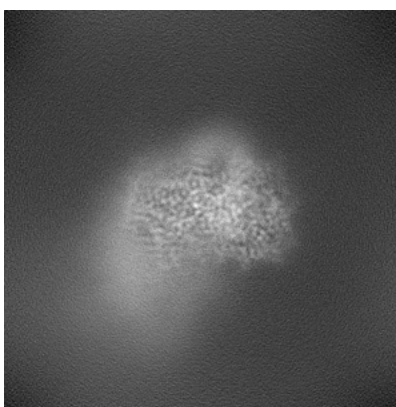


Z

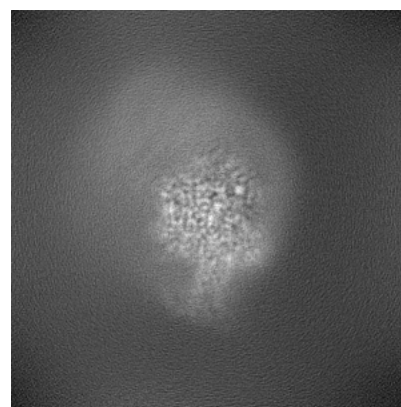
#### 6.1.2 Raw map



X



Y

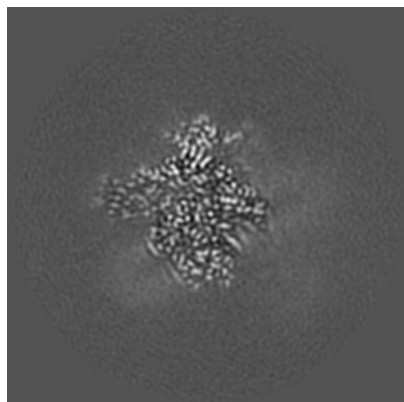


Z

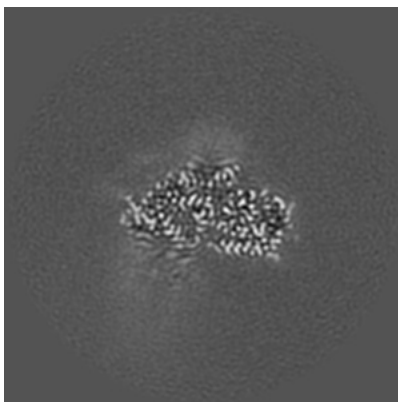
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

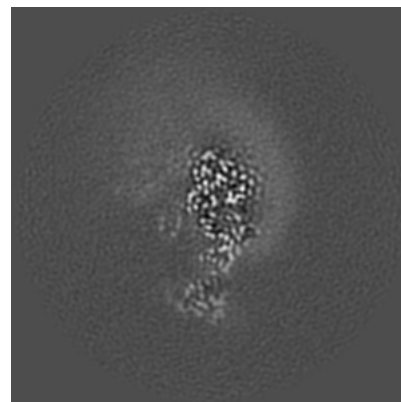
### 6.2.1 Primary map



X Index: 160

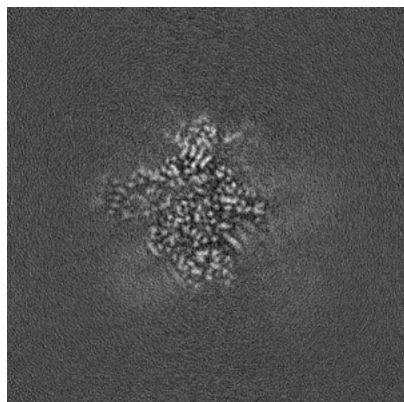


Y Index: 160

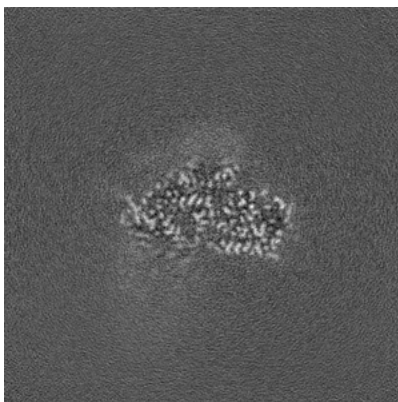


Z Index: 160

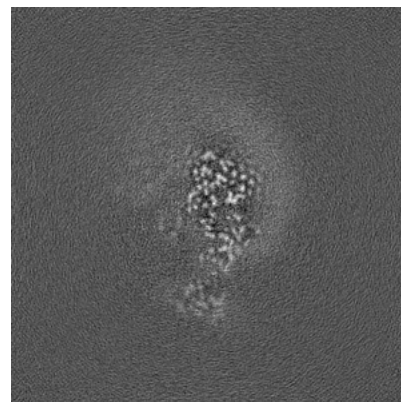
### 6.2.2 Raw map



X Index: 160



Y Index: 160



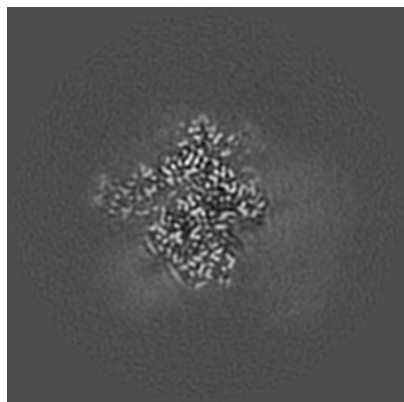
Z Index: 160

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

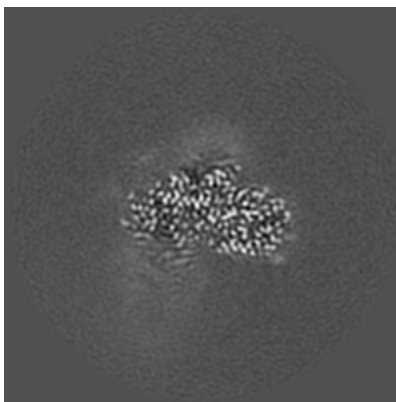


## 6.3 Largest variance slices [i](#)

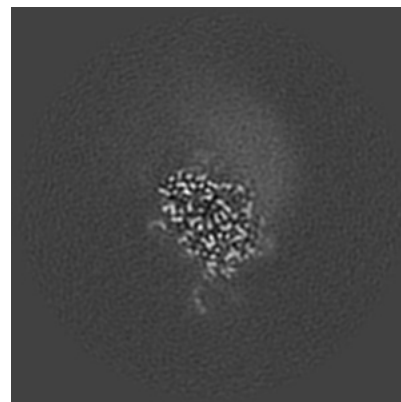
### 6.3.1 Primary map



X Index: 158

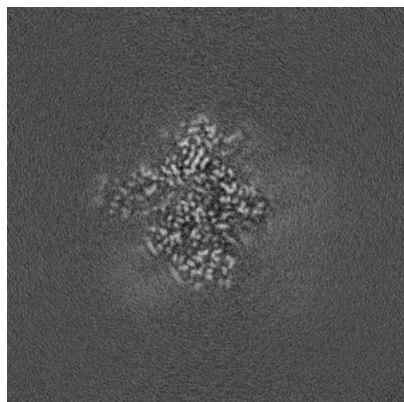


Y Index: 162

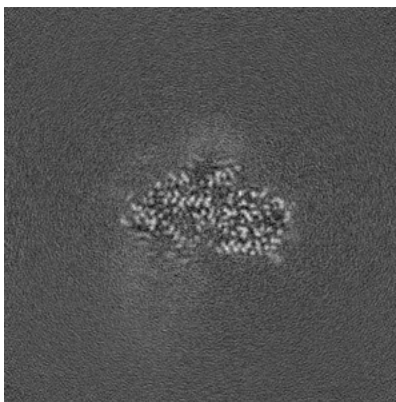


Z Index: 187

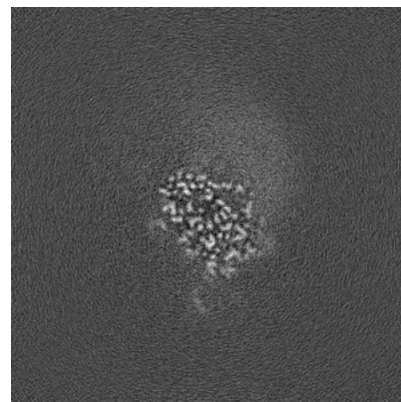
### 6.3.2 Raw map



X Index: 159



Y Index: 161

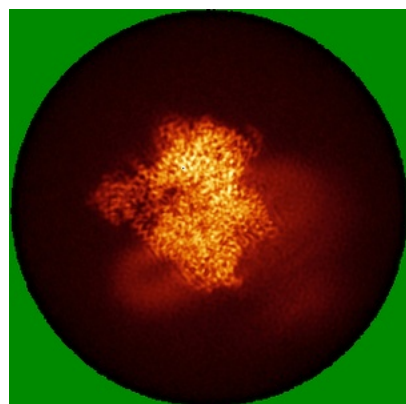


Z Index: 187

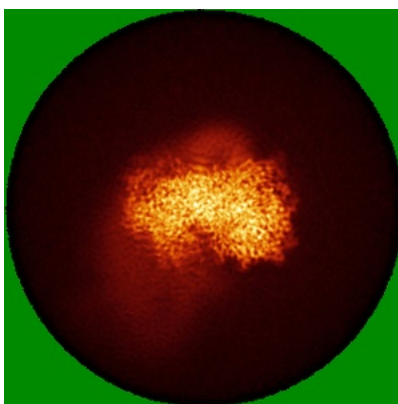
The images above show the largest variance slices of the map in three orthogonal directions.

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

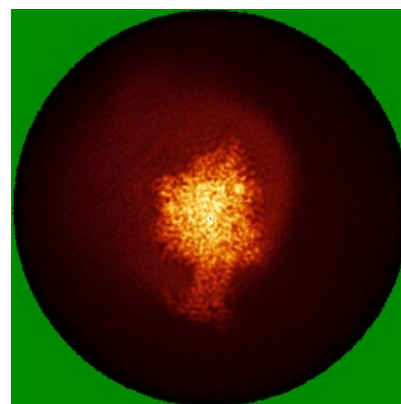
### 6.4.1 Primary map



X

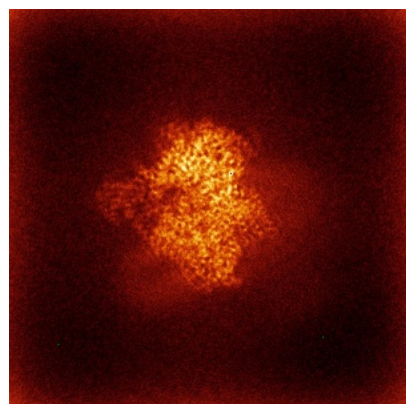


Y

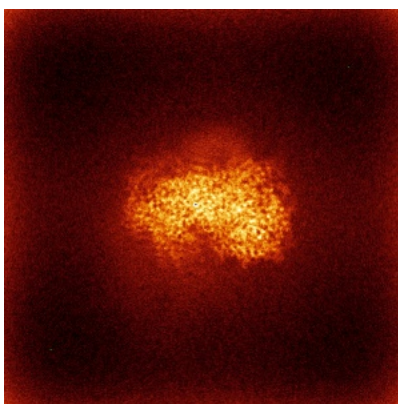


Z

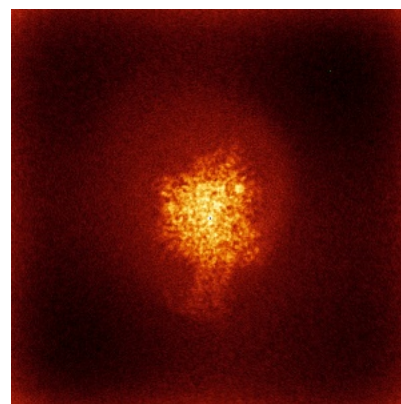
### 6.4.2 Raw map



X



Y



Z

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.



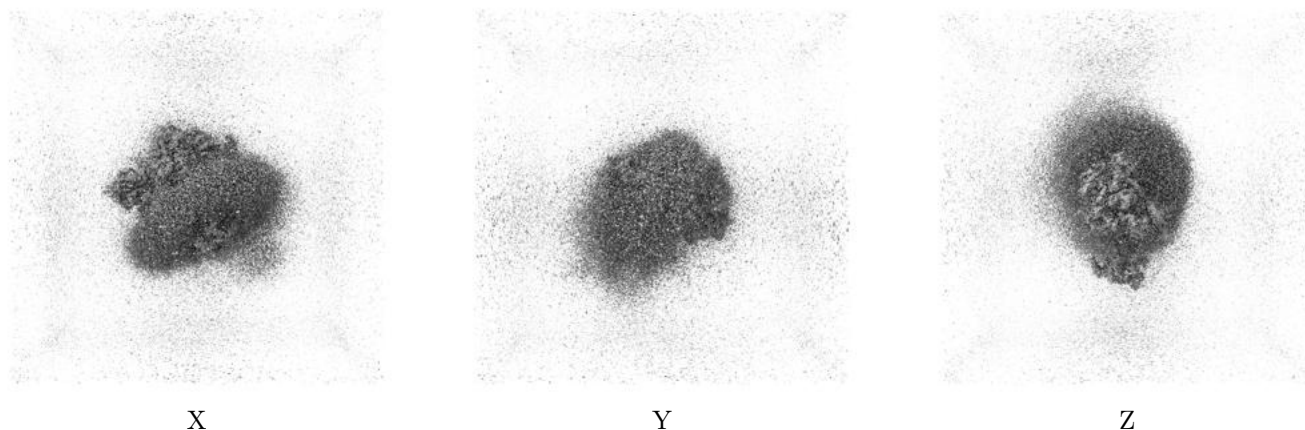
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0792. 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.

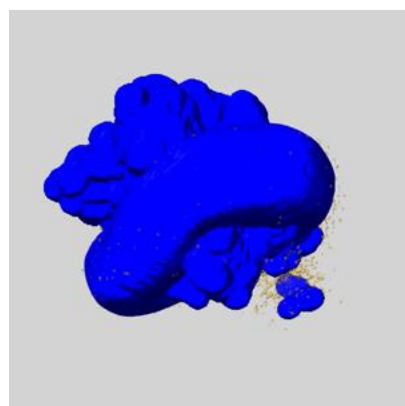
## 6.6 Mask visualisation [i](#)

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

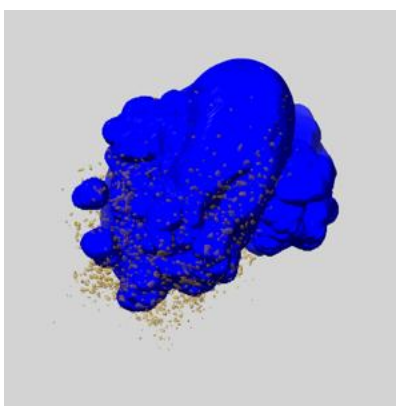
A mask typically either:

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

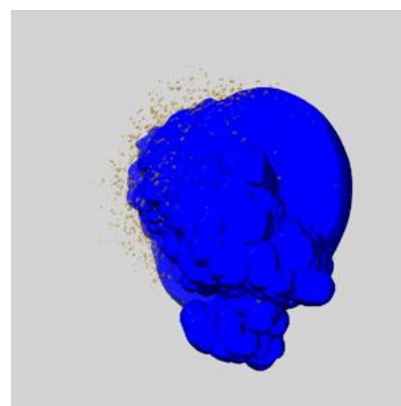
### 6.6.1 emd\_71550\_msk\_1.map [i](#)



X



Y

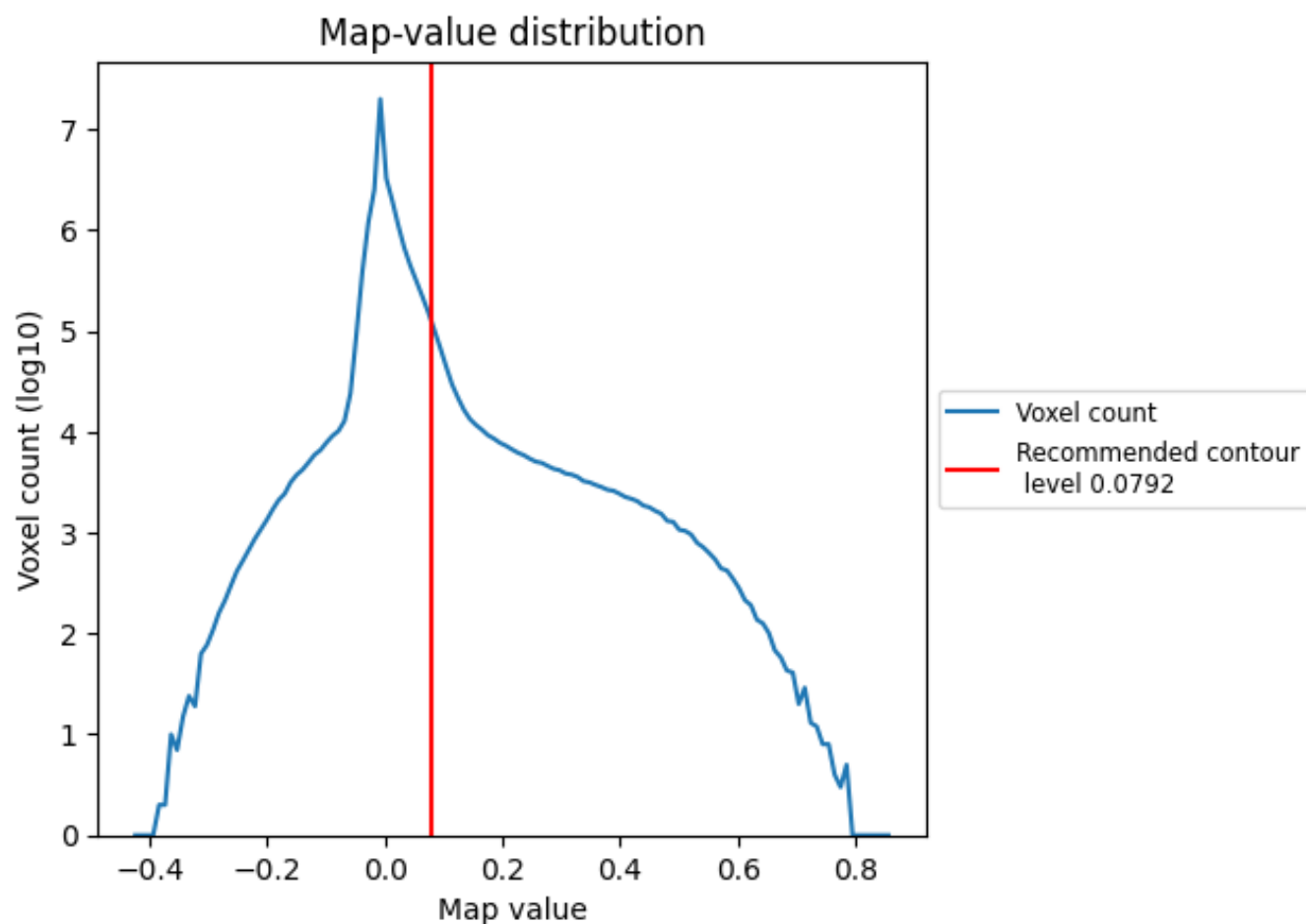


Z

## 7 Map analysis [i](#)

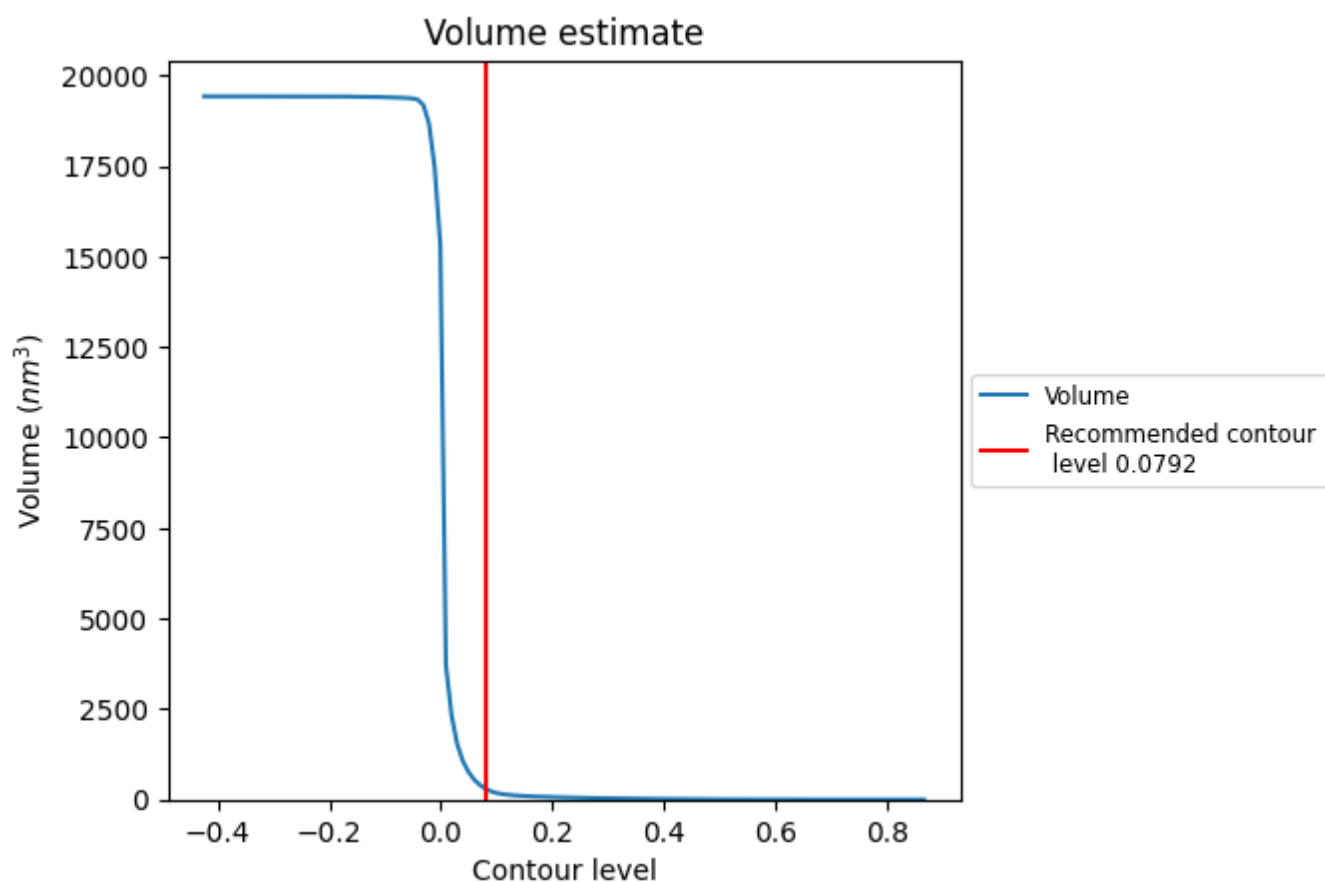
This section contains the results of statistical analysis of the map.

### 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.

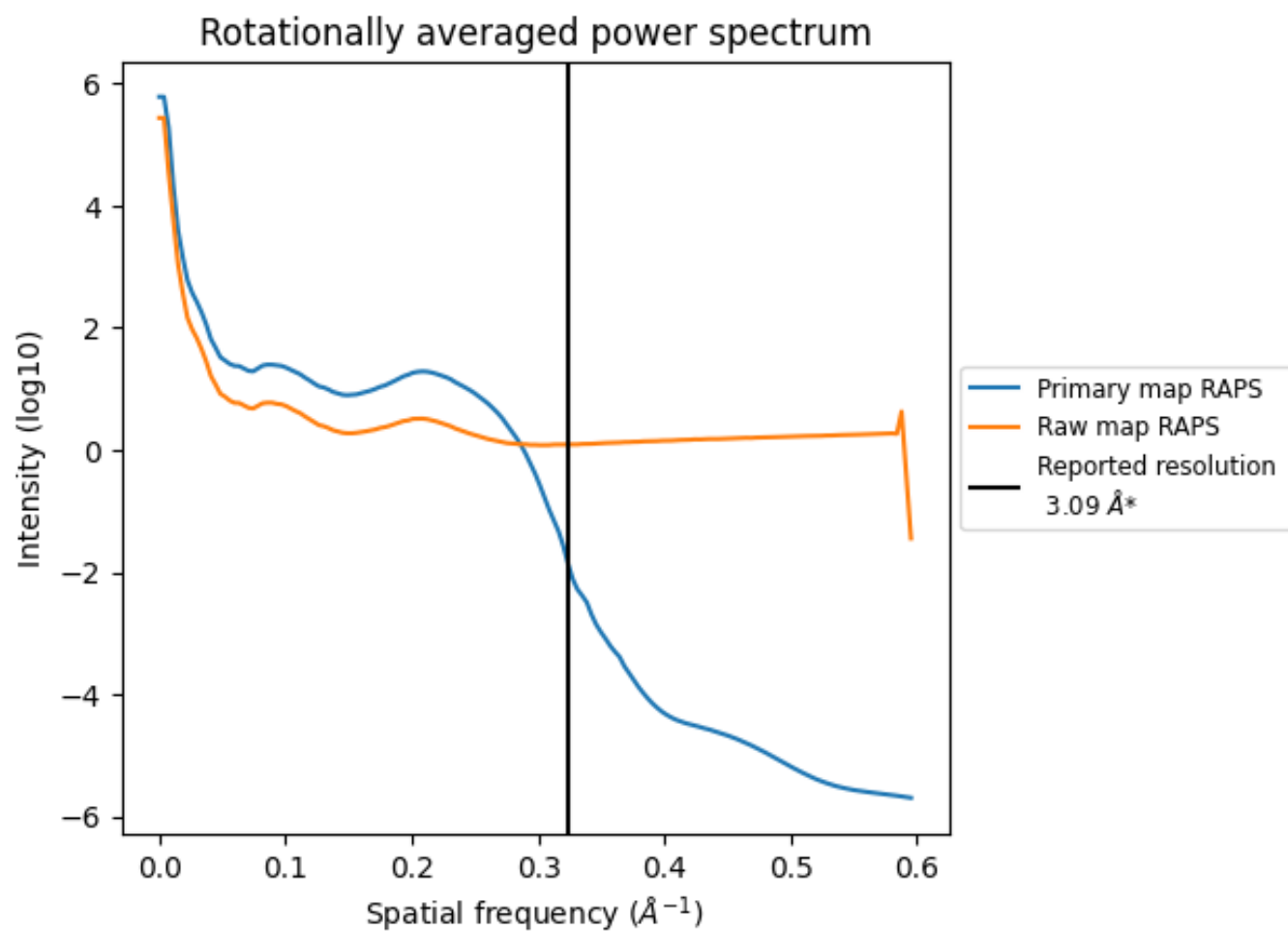
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 308 nm<sup>3</sup>; this corresponds to an approximate mass of 278 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 ⓘ

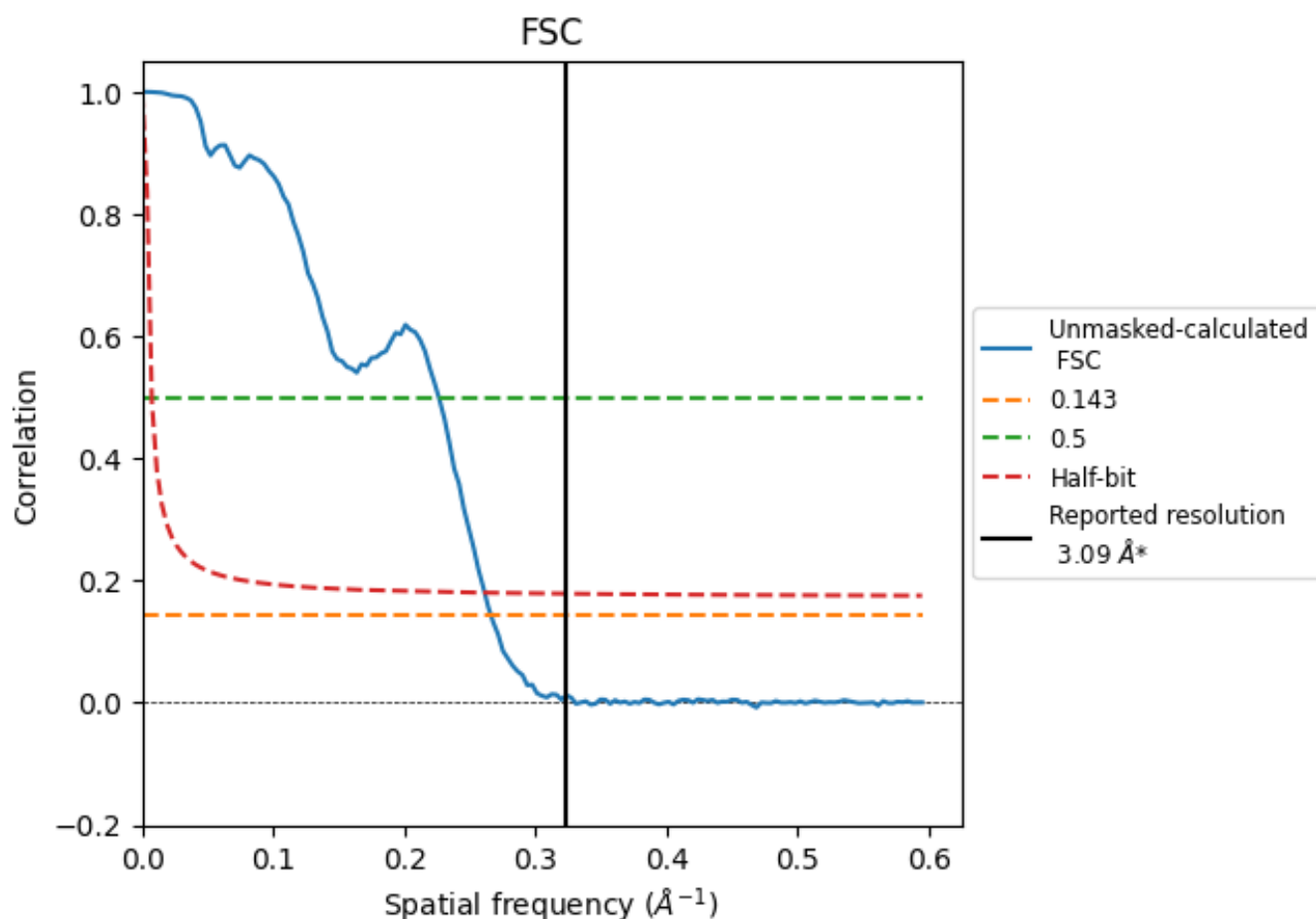


\*Reported resolution corresponds to spatial frequency of 0.324  $\text{\AA}^{-1}$

## 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 0.324  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

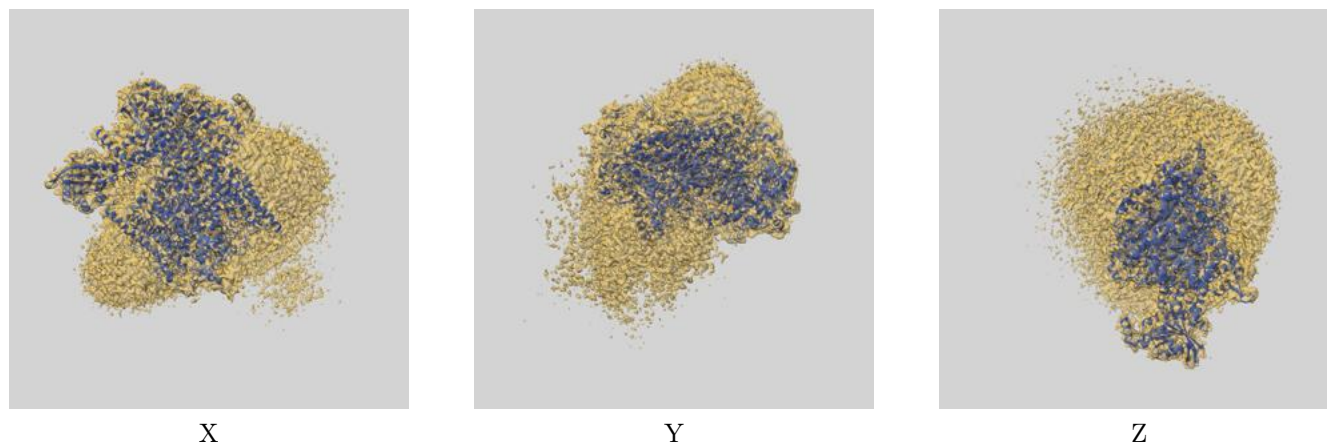
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.76	4.42	3.83

\*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 3.76 differs from the reported value 3.09 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-71550 and PDB model 9PE1. Per-residue inclusion information can be found in section [3](#) on page [13](#).

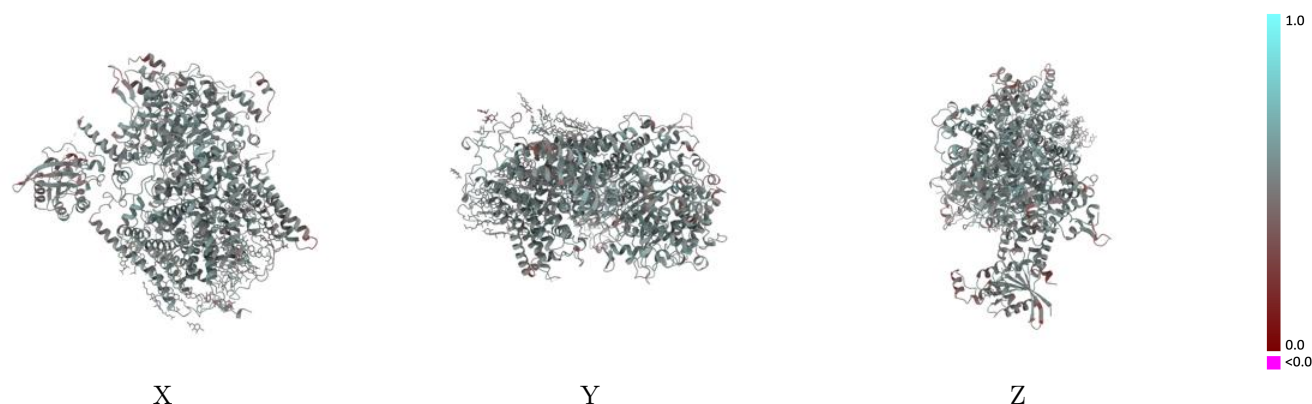
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0792 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.

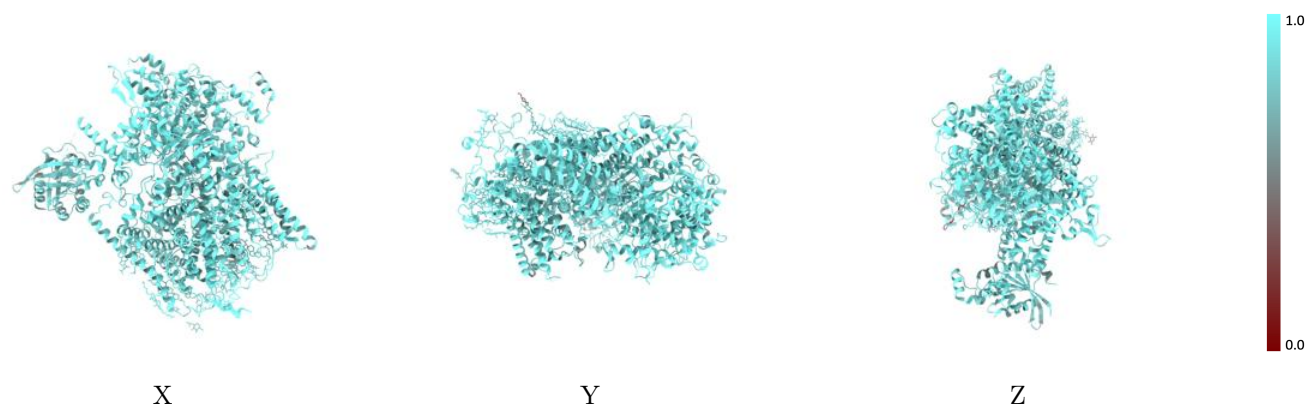


## 9.2 Q-score mapped to coordinate model [i](#)



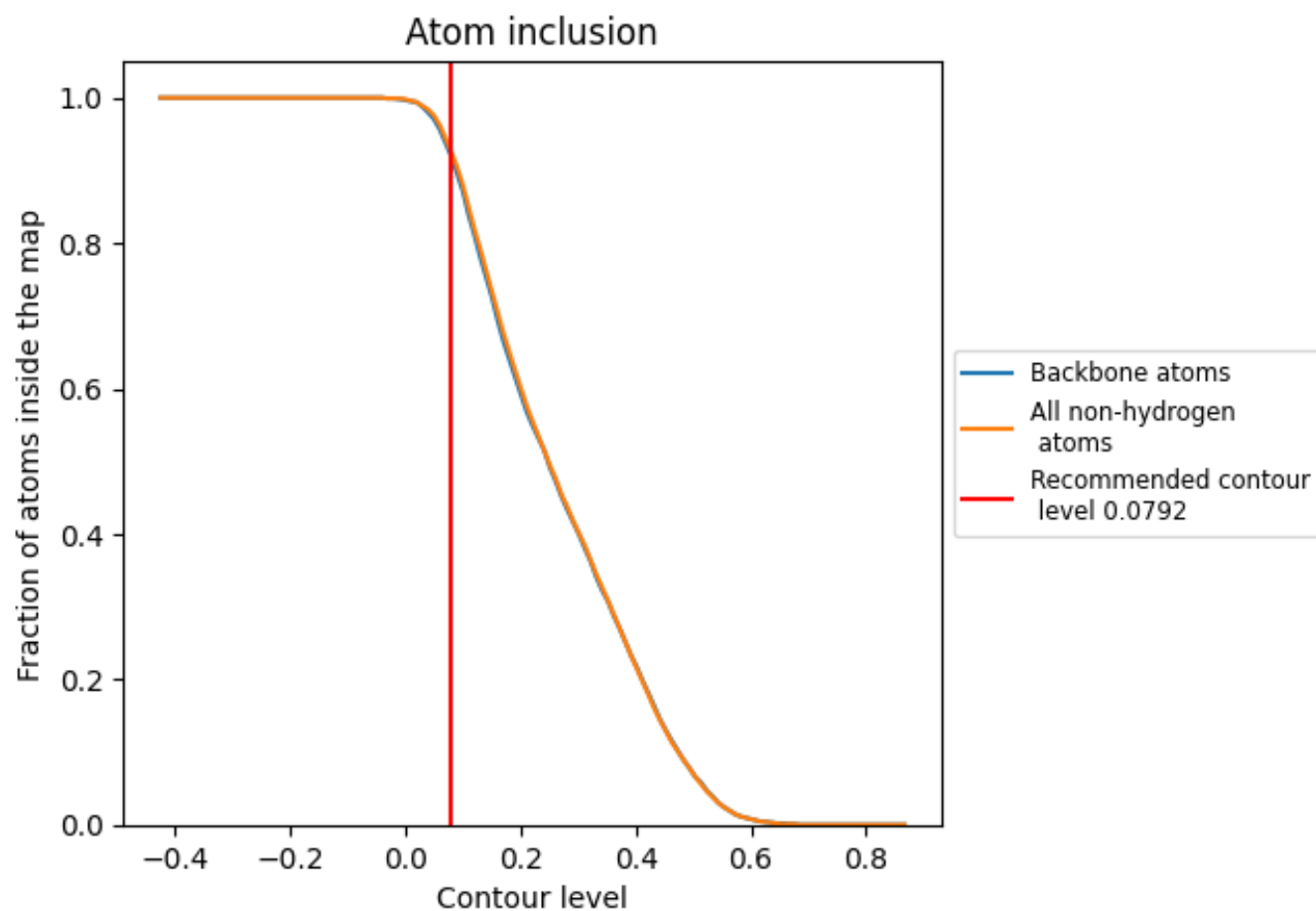
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0792).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0792) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9270	<div><div></div></div> 0.5180
A	<div><div></div></div> 0.9450	<div><div></div></div> 0.5230
D	<div><div></div></div> 0.9150	<div><div></div></div> 0.5280
E	<div><div></div></div> 0.8450	<div><div></div></div> 0.4790
G	<div><div></div></div> 0.8510	<div><div></div></div> 0.4880
H	<div><div></div></div> 0.9550	<div><div></div></div> 0.5060
K	<div><div></div></div> 0.9670	<div><div></div></div> 0.4310

1.0

0.0

<0.0