



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 01:33 AM UTC

PDB ID : 7RPK / pdb_00007rpk
EMDB ID : EMD-24617
Title : Cryo-EM structure of murine Dispatched in complex with Sonic hedgehog
Authors : Asarnow, D.; Wang, Q.; Ding, K.; Cheng, Y.; Beachy, P.A.
Deposited on : 2021-08-03
Resolution : 2.70 Å(reported)

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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>.

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

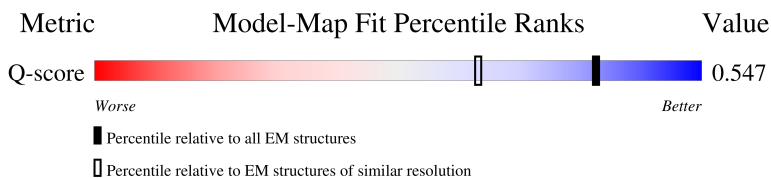
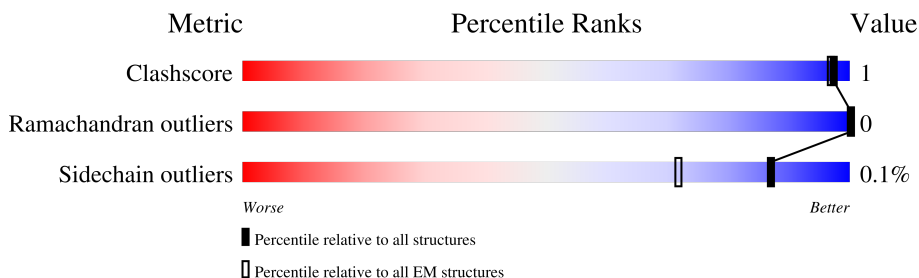
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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 ≥ 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	H	164	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 10018 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	953	7606	4942	1233	1366	65	1	0

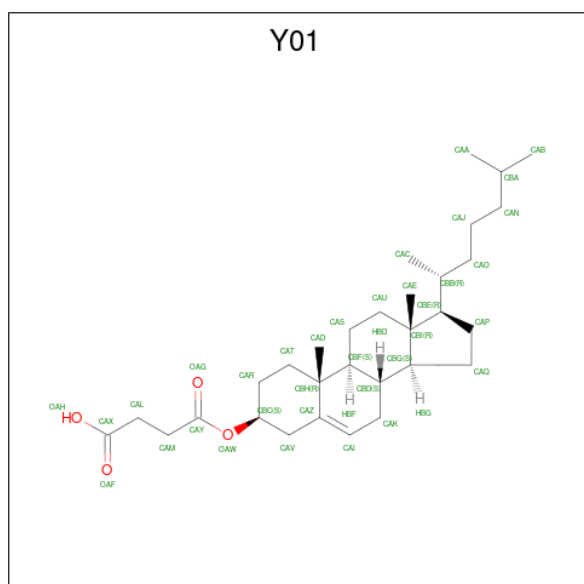
There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Sonic hedgehog protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	151	1215	760	216	234	5	0	0

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$) (labeled as "Ligand of Interest" by depositor).

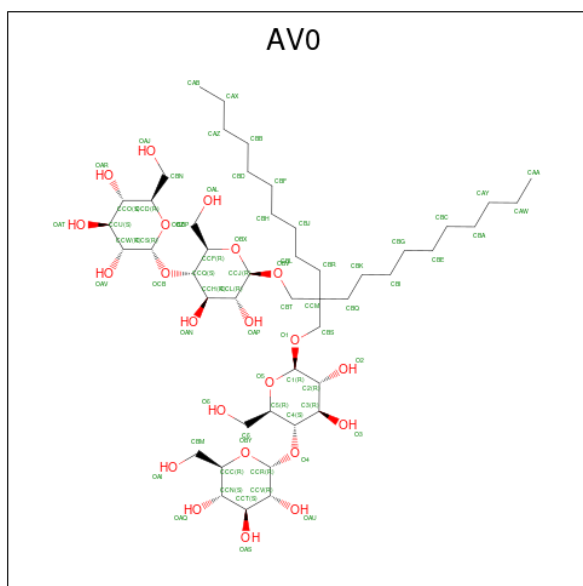


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Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	
3	A	1	Total	C	O	0
			35	31	4	

- Molecule 4 is Lauryl Maltose Neopentyl Glycol (CCD ID: AV0) (formula: C₄₇H₈₈O₂₂) (labeled as "Ligand of Interest" by depositor).

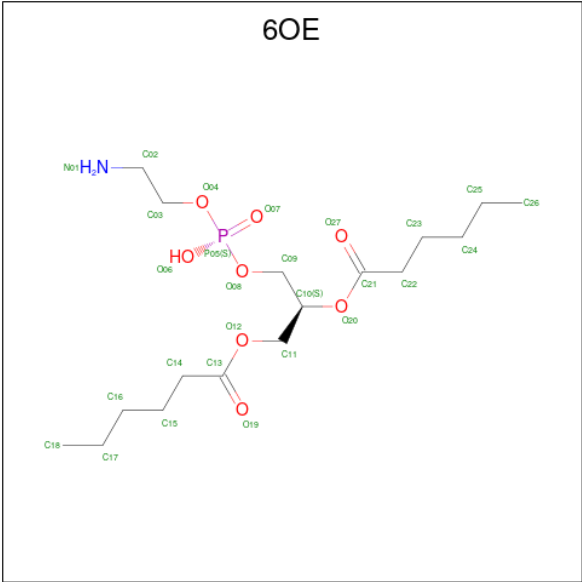


Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			69	47	22	
4	A	1	Total	C	O	0
			69	47	22	

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

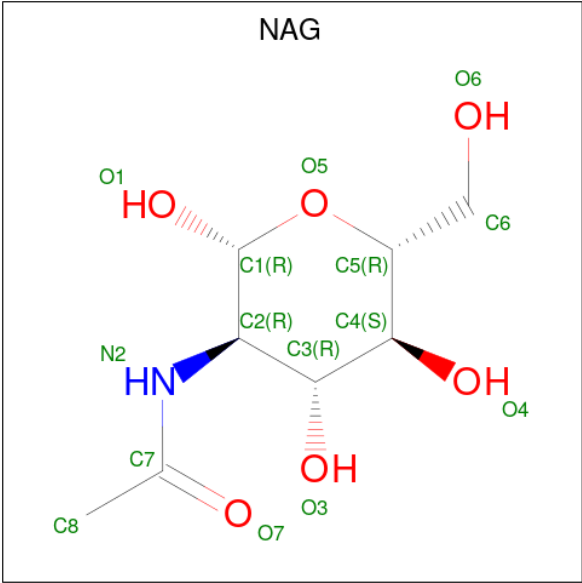
Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total	Na	0
			2	2	

- Molecule 6 is (2S)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(hexanoyloxy)propyl hexanoate (CCD ID: 6OE) (formula: C₁₇H₃₄NO₈P).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			27	17	1	8	1	

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

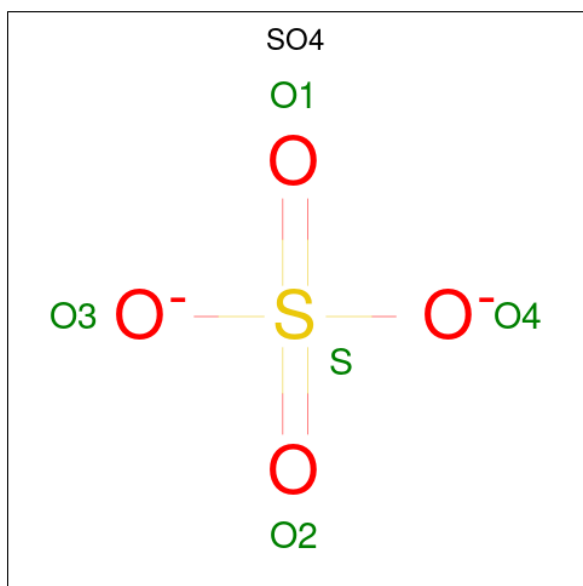
- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
8	H	2	Total	Ca	0
			2	2	

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	H	1	Total	Zn	0
			1	1	

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			AltConf
10	H	1	Total	O	S	0
			5	4	1	

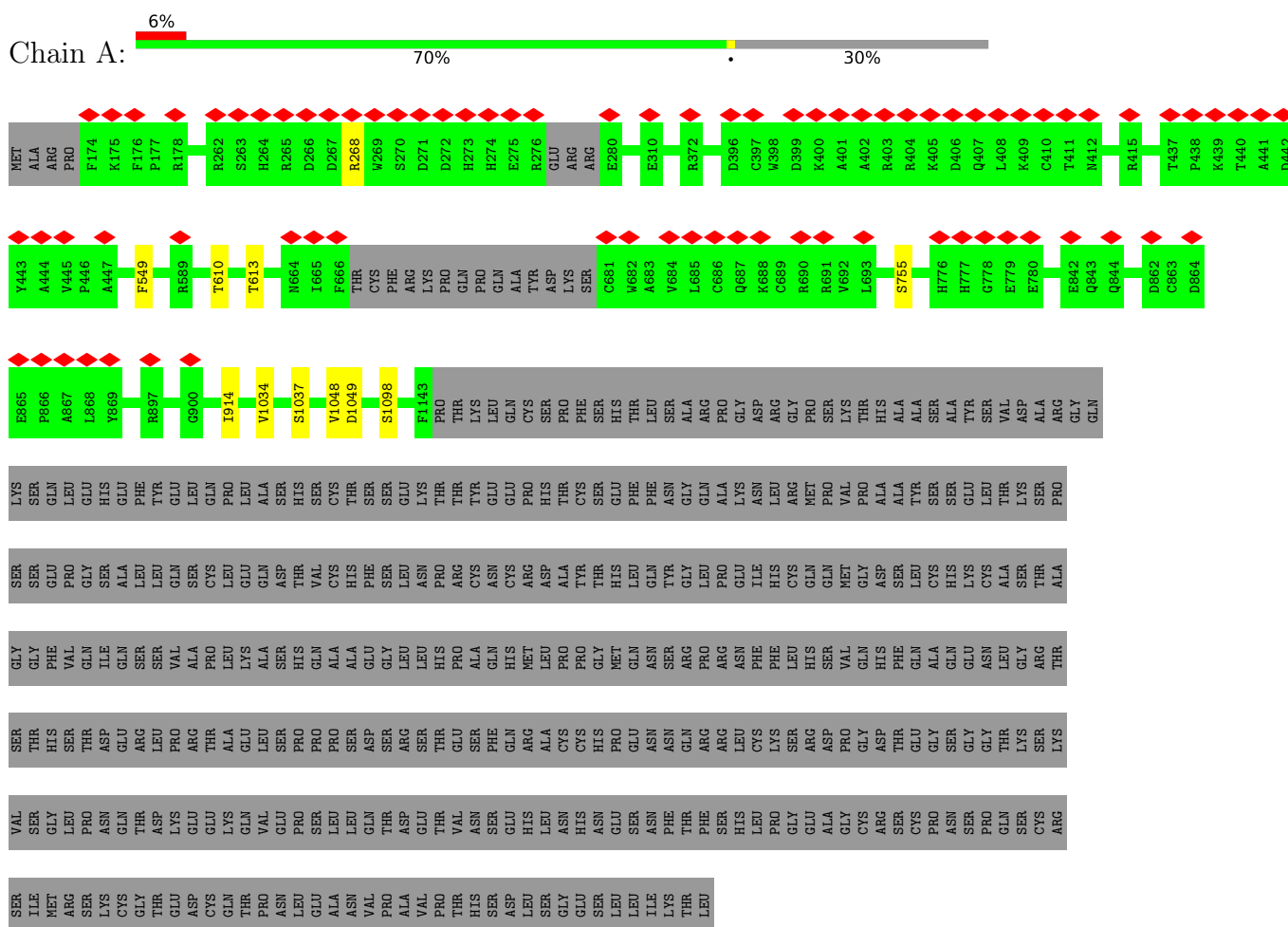
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		AltConf
11	A	42	Total 42	O 42	0

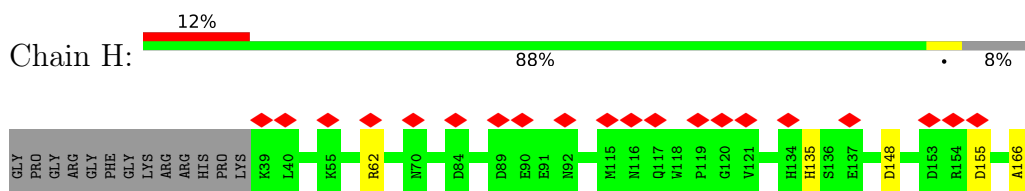
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Protein dispatched homolog 1



• Molecule 2: Sonic hedgehog protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	204786	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	22.779	Depositor
Minimum map value	-14.416	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.574	Depositor
Recommended contour level	3	Depositor
Map size (Å)	240.48, 240.48, 240.48	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6OE, SO4, AV0, Y01, CA, ZN, NA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.74	2/7810 (0.0%)	1.25	4/10620 (0.0%)
2	H	0.82	1/1241 (0.1%)	1.30	5/1674 (0.3%)
All	All	0.75	3/9051 (0.0%)	1.25	9/12294 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1037	SER	C-O	-6.52	1.16	1.24
2	H	166	ALA	CA-CB	-6.38	1.43	1.53
1	A	268	ARG	C-O	-5.25	1.17	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1034	VAL	N-CA-C	9.84	119.78	110.53
2	H	62	ARG	N-CA-C	6.57	119.89	110.10
2	H	155	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	1098	SER	CA-C-N	5.51	130.00	120.58
1	A	1098	SER	C-N-CA	5.51	130.00	120.58
2	H	183	HIS	CB-CG-CD2	-5.50	124.05	131.20
2	H	135	HIS	CB-CG-CD2	-5.42	124.15	131.20
2	H	148	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	549	PHE	CA-CB-CG	5.06	118.86	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7606	0	7492	3	0
2	H	1215	0	1179	0	0
3	A	910	0	1274	9	0
4	A	138	0	0	0	0
5	A	2	0	0	0	0
6	A	27	0	0	0	0
7	A	70	0	65	0	0
8	H	2	0	0	0	0
9	H	1	0	0	0	0
10	H	5	0	0	0	0
11	A	42	0	0	0	0
All	All	10018	0	10010	12	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 1.

All (12) 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:2124:Y01:HAC2	3:A:2124:Y01:HAE2	1.88	0.55
3:A:2102:Y01:HAC1	3:A:2102:Y01:HAU2	1.90	0.51
1:A:610:THR:HG22	1:A:1049:ASP:HA	1.92	0.51
1:A:613:THR:HG21	1:A:1048:VAL:HG11	1.94	0.50
3:A:2106:Y01:HAC1	3:A:2106:Y01:HAU2	1.95	0.47
3:A:2118:Y01:HAC1	3:A:2118:Y01:HAU2	1.96	0.47
1:A:914:ILE:HD12	1:A:914:ILE:H	1.82	0.44
3:A:2107:Y01:HAC1	3:A:2107:Y01:HAU2	2.00	0.43
3:A:2112:Y01:HAU2	3:A:2112:Y01:HAC1	2.02	0.41
3:A:2114:Y01:HAC1	3:A:2114:Y01:HAU2	2.02	0.41
3:A:2116:Y01:HAC1	3:A:2116:Y01:HAU2	2.03	0.41
3:A:2126:Y01:HAC1	3:A:2126:Y01:HAU2	2.01	0.41

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	948/1352 (70%)	920 (97%)	28 (3%)	0	100	100
2	H	149/164 (91%)	144 (97%)	5 (3%)	0	100	100
All	All	1097/1516 (72%)	1064 (97%)	33 (3%)	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	839/1190 (70%)	838 (100%)	1 (0%)	88	96
2	H	129/138 (94%)	129 (100%)	0	100	100
All	All	968/1328 (73%)	967 (100%)	1 (0%)	87	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	755	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	361	ASN
1	A	367	GLN

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Mol	Chain	Res	Type
1	A	621	ASN
1	A	751	GLN
1	A	827	HIS
1	A	839	HIS
1	A	968	ASN
1	A	1105	GLN
1	A	1135	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 5 are monoatomic - leaving 35 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	2120	-	38,38,38	1.23	5 (13%)	57,57,57	1.11	4 (7%)
3	Y01	A	2102	-	38,38,38	1.17	3 (7%)	57,57,57	0.95	1 (1%)
3	Y01	A	2115	-	38,38,38	1.36	4 (10%)	57,57,57	1.16	3 (5%)
3	Y01	A	2124	-	38,38,38	1.30	5 (13%)	57,57,57	0.78	2 (3%)
4	AV0	A	2127	-	72,72,72	1.06	2 (2%)	92,98,98	0.86	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	Y01	A	2126	-	38,38,38	1.30	5 (13%)	57,57,57	0.90	3 (5%)
3	Y01	A	2123	-	38,38,38	1.24	4 (10%)	57,57,57	0.78	0
3	Y01	A	2122	-	38,38,38	1.30	5 (13%)	57,57,57	0.97	2 (3%)
7	NAG	A	2135	1	14,14,15	1.30	2 (14%)	17,19,21	0.93	1 (5%)
10	SO4	H	204	-	4,4,4	0.26	0	6,6,6	0.26	0
3	Y01	A	2117	-	38,38,38	1.28	4 (10%)	57,57,57	0.96	2 (3%)
3	Y01	A	2121	-	38,38,38	1.25	4 (10%)	57,57,57	0.80	1 (1%)
4	AV0	A	2128	-	72,72,72	1.10	4 (5%)	92,98,98	0.74	3 (3%)
3	Y01	A	2103	-	38,38,38	1.23	4 (10%)	57,57,57	0.92	3 (5%)
3	Y01	A	2119	-	38,38,38	1.32	5 (13%)	57,57,57	1.01	2 (3%)
7	NAG	A	2132	1	14,14,15	1.31	2 (14%)	17,19,21	0.83	0
7	NAG	A	2136	1	14,14,15	1.30	1 (7%)	17,19,21	0.69	0
3	Y01	A	2107	-	38,38,38	1.29	4 (10%)	57,57,57	1.07	3 (5%)
3	Y01	A	2116	-	38,38,38	1.24	2 (5%)	57,57,57	0.74	1 (1%)
7	NAG	A	2133	1	14,14,15	1.29	2 (14%)	17,19,21	0.86	0
3	Y01	A	2111	-	38,38,38	1.25	3 (7%)	57,57,57	0.88	0
3	Y01	A	2118	-	38,38,38	1.23	3 (7%)	57,57,57	0.95	2 (3%)
3	Y01	A	2109	-	38,38,38	1.35	6 (15%)	57,57,57	1.20	6 (10%)
3	Y01	A	2110	-	38,38,38	1.29	4 (10%)	57,57,57	0.92	2 (3%)
3	Y01	A	2112	-	38,38,38	1.14	2 (5%)	57,57,57	0.83	2 (3%)
3	Y01	A	2108	-	38,38,38	1.20	4 (10%)	57,57,57	0.84	2 (3%)
3	Y01	A	2106	-	38,38,38	1.12	2 (5%)	57,57,57	0.75	0
7	NAG	A	2134	1	14,14,15	1.29	2 (14%)	17,19,21	0.84	1 (5%)
3	Y01	A	2125	-	38,38,38	1.26	4 (10%)	57,57,57	0.72	0
3	Y01	A	2104	-	38,38,38	1.19	4 (10%)	57,57,57	1.26	4 (7%)
3	Y01	A	2113	-	38,38,38	1.31	5 (13%)	57,57,57	0.94	3 (5%)
3	Y01	A	2105	-	38,38,38	1.23	3 (7%)	57,57,57	0.97	4 (7%)
3	Y01	A	2114	-	38,38,38	1.26	4 (10%)	57,57,57	0.93	2 (3%)
3	Y01	A	2101	-	38,38,38	1.20	3 (7%)	57,57,57	0.94	2 (3%)
6	6OE	A	2131	-	26,26,26	0.83	0	29,31,31	0.43	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
3	Y01	A	2120	-	-	9/19/77/77	0/4/4/4
3	Y01	A	2102	-	-	2/19/77/77	0/4/4/4
3	Y01	A	2115	-	-	12/19/77/77	0/4/4/4
3	Y01	A	2124	-	-	7/19/77/77	0/4/4/4
4	AV0	A	2127	-	-	6/50/130/130	0/4/4/4
3	Y01	A	2126	-	-	7/19/77/77	0/4/4/4
3	Y01	A	2123	-	-	4/19/77/77	0/4/4/4
3	Y01	A	2122	-	-	7/19/77/77	0/4/4/4
7	NAG	A	2135	1	-	0/6/23/26	0/1/1/1
3	Y01	A	2117	-	-	7/19/77/77	0/4/4/4
3	Y01	A	2121	-	-	7/19/77/77	0/4/4/4
4	AV0	A	2128	-	-	16/50/130/130	0/4/4/4
3	Y01	A	2103	-	-	5/19/77/77	0/4/4/4
3	Y01	A	2119	-	-	8/19/77/77	0/4/4/4
7	NAG	A	2132	1	-	0/6/23/26	0/1/1/1
7	NAG	A	2136	1	-	0/6/23/26	0/1/1/1
3	Y01	A	2107	-	-	4/19/77/77	0/4/4/4
3	Y01	A	2116	-	-	5/19/77/77	0/4/4/4
7	NAG	A	2133	1	-	0/6/23/26	0/1/1/1
3	Y01	A	2111	-	-	7/19/77/77	0/4/4/4
3	Y01	A	2118	-	-	11/19/77/77	0/4/4/4
3	Y01	A	2109	-	-	7/19/77/77	0/4/4/4
3	Y01	A	2110	-	-	4/19/77/77	0/4/4/4
3	Y01	A	2112	-	-	7/19/77/77	0/4/4/4
3	Y01	A	2108	-	-	5/19/77/77	0/4/4/4
3	Y01	A	2106	-	-	2/19/77/77	0/4/4/4
7	NAG	A	2134	1	-	0/6/23/26	0/1/1/1
3	Y01	A	2125	-	-	3/19/77/77	0/4/4/4
3	Y01	A	2104	-	-	10/19/77/77	0/4/4/4
3	Y01	A	2113	-	-	4/19/77/77	0/4/4/4
3	Y01	A	2105	-	-	7/19/77/77	0/4/4/4
3	Y01	A	2114	-	-	6/19/77/77	0/4/4/4
3	Y01	A	2101	-	-	6/19/77/77	0/4/4/4
6	6OE	A	2131	-	-	0/30/30/30	-

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2115	Y01	CBB-CBE	3.69	1.60	1.54
4	A	2128	AV0	O1-C1	3.15	1.45	1.40
3	A	2105	Y01	CAS-CBF	2.87	1.58	1.53
3	A	2126	Y01	CAS-CBF	2.86	1.58	1.53
7	A	2136	NAG	O5-C5	2.84	1.49	1.43
3	A	2107	Y01	CAS-CBF	2.82	1.58	1.53
3	A	2119	Y01	CAS-CBF	2.80	1.58	1.53
7	A	2133	NAG	O5-C5	2.80	1.48	1.43
4	A	2128	AV0	CBS-CCM	2.77	1.59	1.53
3	A	2110	Y01	CAS-CBF	2.76	1.58	1.53
4	A	2127	AV0	O1-C1	2.76	1.44	1.40
7	A	2132	NAG	O5-C5	2.75	1.48	1.43
3	A	2117	Y01	CBB-CBE	2.74	1.59	1.54
3	A	2124	Y01	OAH-CAX	-2.74	1.21	1.30
7	A	2134	NAG	O5-C5	2.70	1.48	1.43
3	A	2111	Y01	CAS-CBF	2.70	1.58	1.53
3	A	2115	Y01	OAH-CAX	-2.69	1.21	1.30
3	A	2102	Y01	OAH-CAX	-2.67	1.22	1.30
3	A	2117	Y01	CAS-CBF	2.66	1.58	1.53
3	A	2106	Y01	OAH-CAX	-2.64	1.22	1.30
3	A	2112	Y01	OAH-CAX	-2.64	1.22	1.30
3	A	2120	Y01	CBB-CBE	2.64	1.58	1.54
3	A	2119	Y01	OAH-CAX	-2.63	1.22	1.30
3	A	2118	Y01	OAH-CAX	-2.62	1.22	1.30
3	A	2111	Y01	OAH-CAX	-2.62	1.22	1.30
3	A	2107	Y01	OAH-CAX	-2.62	1.22	1.30
4	A	2128	AV0	CBQ-CCM	2.61	1.59	1.54
3	A	2121	Y01	CAS-CBF	2.61	1.58	1.53
3	A	2110	Y01	OAH-CAX	-2.61	1.22	1.30
3	A	2113	Y01	CAS-CBF	2.61	1.58	1.53
3	A	2109	Y01	OAH-CAX	-2.61	1.22	1.30
3	A	2108	Y01	OAH-CAX	-2.60	1.22	1.30
3	A	2122	Y01	OAH-CAX	-2.60	1.22	1.30
3	A	2125	Y01	OAH-CAX	-2.59	1.22	1.30
3	A	2117	Y01	OAH-CAX	-2.58	1.22	1.30
3	A	2124	Y01	CAS-CBF	2.57	1.58	1.53
3	A	2114	Y01	OAH-CAX	-2.57	1.22	1.30
3	A	2126	Y01	OAH-CAX	-2.56	1.22	1.30
3	A	2105	Y01	OAH-CAX	-2.56	1.22	1.30
4	A	2128	AV0	CBR-CCM	2.56	1.58	1.54
3	A	2121	Y01	OAH-CAX	-2.56	1.22	1.30
3	A	2122	Y01	CAS-CBF	2.56	1.58	1.53
3	A	2101	Y01	OAH-CAX	-2.55	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2120	Y01	OAH-CAX	-2.54	1.22	1.30
3	A	2104	Y01	OAH-CAX	-2.54	1.22	1.30
3	A	2113	Y01	CBB-CBE	2.53	1.58	1.54
3	A	2113	Y01	OAH-CAX	-2.53	1.22	1.30
3	A	2103	Y01	OAH-CAX	-2.53	1.22	1.30
3	A	2123	Y01	OAH-CAX	-2.52	1.22	1.30
3	A	2116	Y01	OAH-CAX	-2.51	1.22	1.30
7	A	2135	NAG	O5-C5	2.50	1.48	1.43
3	A	2101	Y01	CAS-CBF	2.48	1.57	1.53
7	A	2135	NAG	C1-C2	2.48	1.55	1.52
3	A	2104	Y01	CBB-CBE	2.47	1.58	1.54
3	A	2125	Y01	CBB-CBE	2.47	1.58	1.54
3	A	2124	Y01	CBB-CBE	2.46	1.58	1.54
3	A	2102	Y01	CBB-CBE	2.46	1.58	1.54
3	A	2114	Y01	CBB-CBE	2.45	1.58	1.54
3	A	2108	Y01	CBB-CBE	2.45	1.58	1.54
3	A	2125	Y01	CAS-CBF	2.44	1.57	1.53
3	A	2114	Y01	CAS-CBF	2.44	1.57	1.53
3	A	2112	Y01	CAS-CBF	2.43	1.57	1.53
3	A	2120	Y01	CAS-CBF	2.42	1.57	1.53
3	A	2109	Y01	CBB-CBE	2.41	1.58	1.54
3	A	2116	Y01	CAS-CBF	2.41	1.57	1.53
3	A	2126	Y01	CBB-CBE	2.40	1.58	1.54
3	A	2105	Y01	CBB-CBE	2.38	1.58	1.54
3	A	2106	Y01	CBB-CBE	2.38	1.58	1.54
3	A	2109	Y01	CAS-CBF	2.37	1.57	1.53
3	A	2110	Y01	CBB-CBE	2.37	1.58	1.54
3	A	2115	Y01	CAS-CBF	2.36	1.57	1.53
3	A	2111	Y01	CBB-CBE	2.35	1.58	1.54
3	A	2104	Y01	CAE-CBI	2.31	1.58	1.54
3	A	2113	Y01	CAE-CBI	2.30	1.58	1.54
3	A	2115	Y01	CAE-CBI	2.30	1.58	1.54
3	A	2119	Y01	CBB-CBE	2.30	1.58	1.54
3	A	2120	Y01	CAE-CBI	2.29	1.58	1.54
3	A	2103	Y01	CAS-CBF	2.28	1.57	1.53
3	A	2121	Y01	CBB-CBE	2.26	1.58	1.54
3	A	2123	Y01	CAS-CBF	2.25	1.57	1.53
7	A	2133	NAG	C1-C2	2.24	1.55	1.52
7	A	2132	NAG	C1-C2	2.22	1.55	1.52
3	A	2122	Y01	CBB-CBE	2.21	1.58	1.54
3	A	2125	Y01	CAE-CBI	2.19	1.57	1.54
4	A	2127	AV0	OBV-CCJ	2.18	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2119	Y01	CAE-CBI	2.18	1.57	1.54
3	A	2104	Y01	CAS-CBF	2.16	1.57	1.53
3	A	2108	Y01	CAE-CBI	2.16	1.57	1.54
3	A	2124	Y01	CBH-CBF	2.16	1.59	1.56
3	A	2118	Y01	CAE-CBI	2.16	1.57	1.54
3	A	2114	Y01	CAE-CBI	2.15	1.57	1.54
3	A	2110	Y01	CAE-CBI	2.14	1.57	1.54
3	A	2118	Y01	CBB-CBE	2.13	1.58	1.54
3	A	2109	Y01	CAR-CBC	2.13	1.56	1.51
3	A	2123	Y01	CBB-CBE	2.12	1.58	1.54
7	A	2134	NAG	C1-C2	2.12	1.55	1.52
3	A	2126	Y01	CBH-CBF	2.12	1.59	1.56
3	A	2103	Y01	CBB-CBE	2.11	1.58	1.54
3	A	2122	Y01	CAE-CBI	2.11	1.57	1.54
3	A	2108	Y01	CAS-CBF	2.11	1.57	1.53
3	A	2121	Y01	CBH-CBF	2.09	1.59	1.56
3	A	2109	Y01	CBD-CBF	2.09	1.57	1.53
3	A	2126	Y01	CAE-CBI	2.08	1.57	1.54
3	A	2107	Y01	CBB-CBE	2.08	1.57	1.54
3	A	2107	Y01	CBH-CBF	2.07	1.59	1.56
3	A	2109	Y01	CAE-CBI	2.07	1.57	1.54
3	A	2119	Y01	CBH-CBF	2.06	1.59	1.56
3	A	2120	Y01	CBD-CBF	2.06	1.57	1.53
3	A	2124	Y01	CBD-CBF	2.06	1.57	1.53
3	A	2122	Y01	CBH-CBF	2.03	1.59	1.56
3	A	2123	Y01	CAE-CBI	2.03	1.57	1.54
3	A	2113	Y01	CBH-CBF	2.03	1.59	1.56
3	A	2117	Y01	CBH-CBF	2.02	1.59	1.56
3	A	2101	Y01	CBB-CBE	2.01	1.57	1.54
3	A	2102	Y01	CAS-CBF	2.01	1.57	1.53
3	A	2103	Y01	CAT-CBH	2.00	1.57	1.54

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2104	Y01	CAP-CBE-CBB	6.07	121.36	112.18
3	A	2120	Y01	CAP-CBE-CBB	4.92	119.62	112.18
4	A	2127	AV0	CCR-OBY-CCC	3.79	121.11	113.72
3	A	2104	Y01	CAO-CBB-CBE	3.75	118.10	110.33
3	A	2122	Y01	CBC-OAW-CAY	3.66	126.57	117.80
3	A	2115	Y01	CAO-CBB-CBE	3.64	117.87	110.33
3	A	2119	Y01	CBC-OAW-CAY	3.57	126.34	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2113	Y01	CAC-CBB-CAO	-3.25	105.31	110.34
3	A	2109	Y01	CBC-OAW-CAY	3.16	125.36	117.80
3	A	2104	Y01	CBI-CBE-CBB	-3.16	114.62	119.50
3	A	2122	Y01	CBC-CAV-CAZ	3.00	115.88	111.45
3	A	2118	Y01	CBC-OAW-CAY	2.95	124.86	117.80
3	A	2108	Y01	CBC-OAW-CAY	2.91	124.77	117.80
3	A	2109	Y01	CBC-CAV-CAZ	2.91	115.75	111.45
3	A	2115	Y01	CAS-CBF-CBD	2.89	115.81	111.78
3	A	2113	Y01	CBC-OAW-CAY	2.88	124.69	117.80
3	A	2102	Y01	CAS-CBF-CBD	2.82	115.71	111.78
3	A	2110	Y01	CBC-OAW-CAY	2.78	124.46	117.80
3	A	2117	Y01	CBC-OAW-CAY	2.77	124.43	117.80
3	A	2103	Y01	CBC-OAW-CAY	2.74	124.35	117.80
3	A	2119	Y01	OAW-CAY-CAM	2.72	117.37	111.48
3	A	2103	Y01	CAK-CBD-CBF	2.71	112.86	109.72
4	A	2128	AV0	C1-O5-C5	2.70	119.00	113.72
3	A	2114	Y01	CBC-OAW-CAY	2.69	124.23	117.80
3	A	2112	Y01	CBC-OAW-CAY	2.67	124.20	117.80
3	A	2120	Y01	CAO-CBB-CBE	2.67	115.86	110.33
3	A	2101	Y01	CBC-OAW-CAY	2.66	124.17	117.80
3	A	2117	Y01	CAO-CBB-CBE	2.66	115.84	110.33
3	A	2105	Y01	CAC-CBB-CBE	-2.65	108.90	112.88
3	A	2107	Y01	CBC-OAW-CAY	2.64	124.12	117.80
3	A	2121	Y01	CBC-OAW-CAY	2.61	124.05	117.80
7	A	2135	NAG	C1-O5-C5	2.60	115.68	112.19
3	A	2120	Y01	CBI-CBE-CBB	-2.60	115.48	119.50
3	A	2126	Y01	CBC-OAW-CAY	2.58	123.97	117.80
3	A	2105	Y01	CAO-CBB-CBE	2.57	115.66	110.33
3	A	2108	Y01	OAW-CBC-CAV	2.57	113.33	108.04
3	A	2105	Y01	CAP-CBE-CBB	2.57	116.06	112.18
4	A	2127	AV0	O1-C1-C2	2.56	112.15	108.27
7	A	2134	NAG	C1-O5-C5	2.51	115.54	112.19
3	A	2109	Y01	CAT-CAR-CBC	2.48	114.38	110.33
3	A	2118	Y01	OAW-CAY-CAM	2.45	116.79	111.48
4	A	2127	AV0	O4-CCR-OB	-2.45	104.25	110.69
3	A	2109	Y01	CBF-CBH-CAZ	-2.42	106.11	109.65
3	A	2101	Y01	CAR-CBC-CAV	2.42	114.34	110.97
3	A	2116	Y01	CBC-OAW-CAY	2.42	123.58	117.80
3	A	2124	Y01	CAC-CBB-CBE	2.36	116.43	112.88
3	A	2112	Y01	OAW-CBC-CAV	2.35	112.87	108.04
3	A	2115	Y01	CBC-OAW-CAY	2.32	123.36	117.80
3	A	2120	Y01	CAS-CBF-CBD	2.31	115.00	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2103	Y01	CBF-CBD-CBG	-2.23	106.17	109.09
3	A	2114	Y01	CAS-CBF-CBD	2.20	114.84	111.78
3	A	2109	Y01	CBH-CBF-CBD	-2.17	109.54	112.71
3	A	2124	Y01	CBI-CBE-CBB	2.17	122.85	119.50
4	A	2128	AV0	CBS-O1-C1	2.16	118.79	113.31
3	A	2126	Y01	CAO-CBB-CBE	2.15	114.79	110.33
3	A	2105	Y01	CBC-CAV-CAZ	2.10	114.55	111.45
3	A	2107	Y01	CAO-CBB-CBE	2.06	114.60	110.33
3	A	2109	Y01	OAW-CAY-CAM	2.03	115.88	111.48
3	A	2126	Y01	OAW-CAY-CAM	2.03	115.88	111.48
4	A	2128	AV0	CCS-OCB-CCQ	-2.03	113.16	117.98
3	A	2113	Y01	CAO-CBB-CBE	2.02	114.52	110.33
3	A	2107	Y01	CAS-CBF-CBD	2.02	114.59	111.78
3	A	2104	Y01	CAU-CBI-CBE	-2.01	113.64	116.60
3	A	2110	Y01	CBG-CBI-CBE	2.00	102.40	100.10

There are no chirality outliers.

All (185) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2104	Y01	CAO-CBB-CBE-CAP
3	A	2104	Y01	OAG-CAY-OAW-CBC
3	A	2104	Y01	CAM-CAY-OAW-CBC
3	A	2107	Y01	OAG-CAY-OAW-CBC
3	A	2107	Y01	CAM-CAY-OAW-CBC
3	A	2109	Y01	OAG-CAY-OAW-CBC
3	A	2109	Y01	CAM-CAY-OAW-CBC
3	A	2110	Y01	OAG-CAY-OAW-CBC
3	A	2110	Y01	CAM-CAY-OAW-CBC
3	A	2111	Y01	OAG-CAY-OAW-CBC
3	A	2111	Y01	CAM-CAY-OAW-CBC
3	A	2114	Y01	OAG-CAY-OAW-CBC
3	A	2114	Y01	CAM-CAY-OAW-CBC
3	A	2115	Y01	CAO-CBB-CBE-CBI
3	A	2115	Y01	OAG-CAY-OAW-CBC
3	A	2115	Y01	CAM-CAY-OAW-CBC
3	A	2116	Y01	OAG-CAY-OAW-CBC
3	A	2116	Y01	CAM-CAY-OAW-CBC
3	A	2118	Y01	OAG-CAY-OAW-CBC
3	A	2118	Y01	CAM-CAY-OAW-CBC
3	A	2119	Y01	OAG-CAY-OAW-CBC
3	A	2119	Y01	CAM-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
3	A	2120	Y01	CAO-CBB-CBE-CAP
3	A	2120	Y01	CAC-CBB-CBE-CBI
3	A	2122	Y01	OAG-CAY-OAW-CBC
3	A	2122	Y01	CAM-CAY-OAW-CBC
3	A	2126	Y01	OAG-CAY-OAW-CBC
3	A	2126	Y01	CAM-CAY-OAW-CBC
4	A	2127	AV0	O5-C1-O1-CBS
4	A	2128	AV0	CBL-CBR-CCM-CBQ
4	A	2128	AV0	CBL-CBR-CCM-CBS
4	A	2128	AV0	CBL-CBR-CCM-CBT
4	A	2128	AV0	O1-CBS-CCM-CBQ
4	A	2128	AV0	O1-CBS-CCM-CBR
3	A	2104	Y01	CAC-CBB-CBE-CAP
3	A	2120	Y01	CAC-CBB-CBE-CAP
3	A	2104	Y01	CAC-CBB-CBE-CBI
3	A	2104	Y01	CAO-CBB-CBE-CBI
3	A	2120	Y01	CAO-CBB-CBE-CBI
3	A	2112	Y01	CAR-CBC-OAW-CAY
3	A	2113	Y01	CAV-CBC-OAW-CAY
3	A	2115	Y01	CAC-CBB-CBE-CAP
3	A	2115	Y01	CAC-CBB-CBE-CBI
3	A	2124	Y01	CAO-CBB-CBE-CAP
4	A	2128	AV0	O1-CBS-CCM-CBT
3	A	2115	Y01	CAJ-CAO-CBB-CAC
3	A	2115	Y01	CAO-CBB-CBE-CAP
3	A	2120	Y01	CAJ-CAO-CBB-CBE
3	A	2103	Y01	CAJ-CAO-CBB-CAC
4	A	2128	AV0	O5-C1-O1-CBS
3	A	2103	Y01	CAJ-CAO-CBB-CBE
3	A	2104	Y01	CAJ-CAO-CBB-CBE
3	A	2116	Y01	CAJ-CAO-CBB-CBE
3	A	2118	Y01	CAX-CAL-CAM-CAY
4	A	2128	AV0	C2-C1-O1-CBS
3	A	2122	Y01	CAV-CBC-OAW-CAY
3	A	2120	Y01	CAJ-CAO-CBB-CAC
3	A	2124	Y01	CAO-CBB-CBE-CBI
3	A	2112	Y01	CAJ-CAO-CBB-CBE
3	A	2119	Y01	CAN-CAJ-CAO-CBB
3	A	2116	Y01	CAJ-CAO-CBB-CAC
3	A	2103	Y01	CAR-CBC-OAW-CAY
3	A	2124	Y01	CAC-CBB-CBE-CAP
3	A	2103	Y01	CAO-CAJ-CAN-CBA

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Mol	Chain	Res	Type	Atoms
3	A	2113	Y01	CAO-CAJ-CAN-CBA
3	A	2112	Y01	CAJ-CAO-CBB-CAC
4	A	2127	AV0	CBI-CBK-CBQ-CCM
3	A	2105	Y01	CAC-CBB-CBE-CBI
3	A	2105	Y01	CAO-CBB-CBE-CBI
3	A	2108	Y01	CAR-CBC-OAW-CAY
3	A	2105	Y01	CAC-CBB-CBE-CAP
3	A	2101	Y01	CAR-CBC-OAW-CAY
3	A	2118	Y01	CAJ-CAN-CBA-CAB
3	A	2117	Y01	CAV-CBC-OAW-CAY
3	A	2121	Y01	CAR-CBC-OAW-CAY
3	A	2118	Y01	CAJ-CAN-CBA-CAA
3	A	2118	Y01	CAO-CAJ-CAN-CBA
3	A	2111	Y01	CAJ-CAO-CBB-CBE
3	A	2122	Y01	CAR-CBC-OAW-CAY
3	A	2119	Y01	CAJ-CAO-CBB-CBE
4	A	2128	AV0	C5-C4-O4-CCR
3	A	2124	Y01	CAJ-CAO-CBB-CAC
3	A	2115	Y01	CAJ-CAO-CBB-CBE
4	A	2128	AV0	C3-C4-O4-CCR
3	A	2118	Y01	CAV-CBC-OAW-CAY
3	A	2104	Y01	CAO-CAJ-CAN-CBA
4	A	2128	AV0	O5-C5-C6-O6
3	A	2105	Y01	CAJ-CAO-CBB-CAC
3	A	2126	Y01	CAJ-CAN-CBA-CAB
3	A	2112	Y01	CAM-CAY-OAW-CBC
4	A	2127	AV0	CBH-CBJ-CBL-CBR
4	A	2127	AV0	C2-C1-O1-CBS
3	A	2114	Y01	CAJ-CAN-CBA-CAB
3	A	2123	Y01	CAJ-CAN-CBA-CAB
3	A	2117	Y01	CAR-CBC-OAW-CAY
3	A	2111	Y01	CAJ-CAO-CBB-CAC
3	A	2117	Y01	CAO-CBB-CBE-CBI
3	A	2105	Y01	CAJ-CAO-CBB-CBE
4	A	2127	AV0	CCF-CCQ-OCB-CCS
3	A	2107	Y01	CAN-CAJ-CAO-CBB
4	A	2127	AV0	CCH-CCQ-OCB-CCS
3	A	2120	Y01	CAN-CAJ-CAO-CBB
3	A	2121	Y01	CAJ-CAO-CBB-CBE
3	A	2123	Y01	CAN-CAJ-CAO-CBB
3	A	2108	Y01	CAV-CBC-OAW-CAY
3	A	2126	Y01	CAJ-CAN-CBA-CAA

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Mol	Chain	Res	Type	Atoms
3	A	2108	Y01	CAJ-CAN-CBA-CAB
3	A	2117	Y01	CAO-CBB-CBE-CAP
3	A	2101	Y01	CAC-CBB-CBE-CBI
3	A	2114	Y01	CAJ-CAN-CBA-CAA
4	A	2128	AV0	CCM-CBS-O1-C1
3	A	2123	Y01	CAJ-CAN-CBA-CAA
3	A	2113	Y01	CAJ-CAO-CBB-CAC
3	A	2101	Y01	CAO-CBB-CBE-CAP
3	A	2101	Y01	CAO-CBB-CBE-CBI
3	A	2125	Y01	CAN-CAJ-CAO-CBB
3	A	2103	Y01	CAV-CBC-OAW-CAY
3	A	2101	Y01	CAC-CBB-CBE-CAP
3	A	2108	Y01	CAJ-CAN-CBA-CAA
3	A	2121	Y01	CAV-CBC-OAW-CAY
3	A	2117	Y01	CAM-CAL-CAX-OAF
3	A	2125	Y01	CAM-CAL-CAX-OAH
3	A	2115	Y01	CAV-CBC-OAW-CAY
3	A	2126	Y01	CAM-CAL-CAX-OAF
3	A	2106	Y01	CAM-CAL-CAX-OAH
3	A	2126	Y01	CAM-CAL-CAX-OAH
3	A	2102	Y01	CAM-CAL-CAX-OAH
3	A	2117	Y01	CAM-CAL-CAX-OAH
3	A	2118	Y01	CAM-CAL-CAX-OAF
3	A	2118	Y01	CAR-CBC-OAW-CAY
3	A	2102	Y01	CAM-CAL-CAX-OAF
3	A	2112	Y01	CAM-CAL-CAX-OAF
3	A	2120	Y01	CAM-CAL-CAX-OAH
3	A	2123	Y01	CAJ-CAO-CBB-CAC
3	A	2101	Y01	CAV-CBC-OAW-CAY
3	A	2105	Y01	CAM-CAL-CAX-OAF
3	A	2109	Y01	CAJ-CAN-CBA-CAB
3	A	2105	Y01	CAM-CAL-CAX-OAH
3	A	2117	Y01	CAC-CBB-CBE-CBI
3	A	2104	Y01	CAV-CBC-OAW-CAY
3	A	2122	Y01	CAM-CAL-CAX-OAF
4	A	2128	AV0	CBD-CBF-CBH-CBJ
3	A	2120	Y01	CAM-CAL-CAX-OAF
3	A	2115	Y01	CAM-CAL-CAX-OAH
3	A	2106	Y01	CAM-CAL-CAX-OAF
3	A	2121	Y01	CAM-CAL-CAX-OAF
3	A	2122	Y01	CAM-CAL-CAX-OAH
3	A	2125	Y01	CAM-CAL-CAX-OAF

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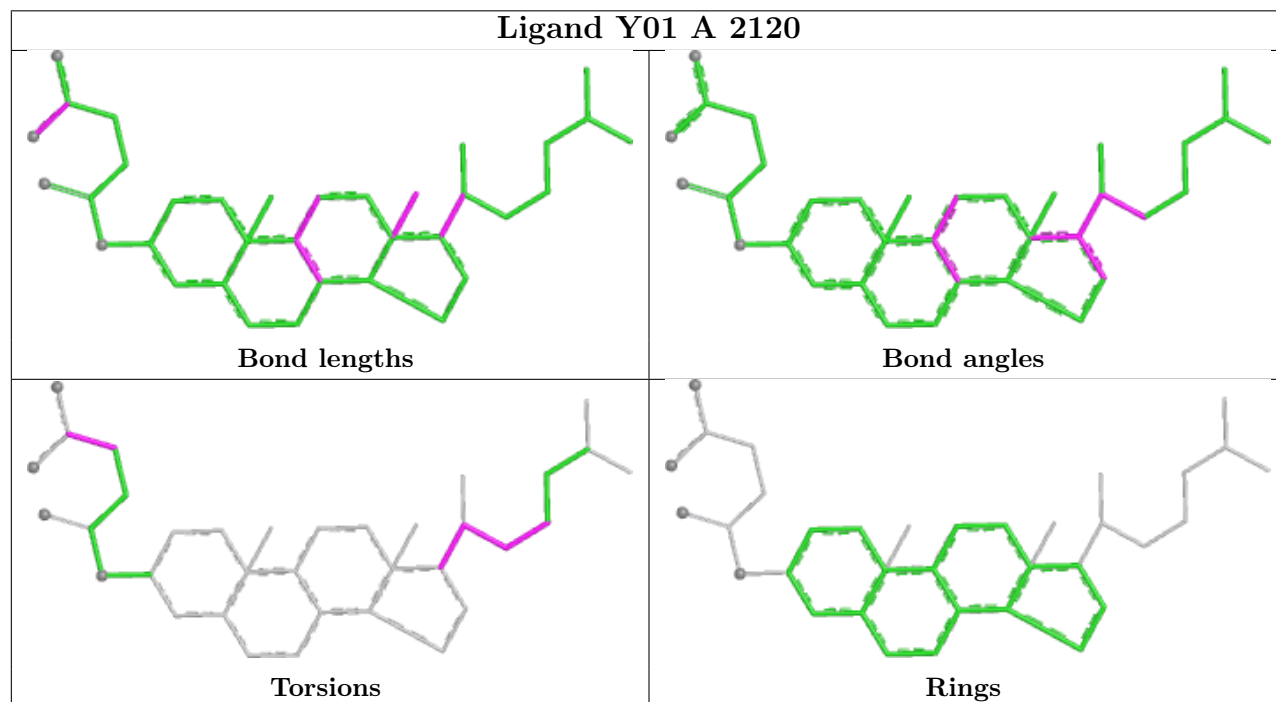
Mol	Chain	Res	Type	Atoms
4	A	2128	AV0	CBA-CBC-CBE-CBG
3	A	2119	Y01	CAM-CAL-CAX-OAF
3	A	2114	Y01	CAM-CAL-CAX-OAF
3	A	2111	Y01	CAM-CAL-CAX-OAH
3	A	2114	Y01	CAM-CAL-CAX-OAH
3	A	2121	Y01	CAM-CAL-CAX-OAH
3	A	2112	Y01	CAM-CAL-CAX-OAH
4	A	2128	AV0	OBX-CCJ-OBV-CBT
3	A	2108	Y01	CAO-CAJ-CAN-CBA
3	A	2122	Y01	CAO-CAJ-CAN-CBA
3	A	2119	Y01	CAM-CAL-CAX-OAH
3	A	2115	Y01	CAM-CAL-CAX-OAF
3	A	2115	Y01	CAR-CBC-OAW-CAY
3	A	2111	Y01	CAM-CAL-CAX-OAF
3	A	2124	Y01	CAL-CAM-CAY-OAW
3	A	2109	Y01	CAJ-CAN-CBA-CAA
3	A	2119	Y01	CAL-CAM-CAY-OAW
3	A	2111	Y01	CAL-CAM-CAY-OAW
3	A	2121	Y01	CAL-CAM-CAY-OAW
4	A	2128	AV0	CBF-CBH-CBJ-CBL
3	A	2124	Y01	CAM-CAL-CAX-OAF
3	A	2110	Y01	CAM-CAL-CAX-OAF
3	A	2118	Y01	CAM-CAL-CAX-OAH
3	A	2109	Y01	CAM-CAL-CAX-OAH
3	A	2110	Y01	CAM-CAL-CAX-OAH
3	A	2112	Y01	CAV-CBC-OAW-CAY
3	A	2124	Y01	CAM-CAL-CAX-OAH
3	A	2119	Y01	CAL-CAM-CAY-OAG
3	A	2109	Y01	CAO-CAJ-CAN-CBA
3	A	2118	Y01	CAN-CAJ-CAO-CBB
3	A	2121	Y01	CAL-CAM-CAY-OAG
3	A	2126	Y01	CAL-CAM-CAY-OAG
3	A	2104	Y01	CAM-CAL-CAX-OAH
3	A	2107	Y01	CAM-CAL-CAX-OAH
3	A	2109	Y01	CAN-CAJ-CAO-CBB
3	A	2113	Y01	CAN-CAJ-CAO-CBB
3	A	2116	Y01	CAV-CBC-OAW-CAY

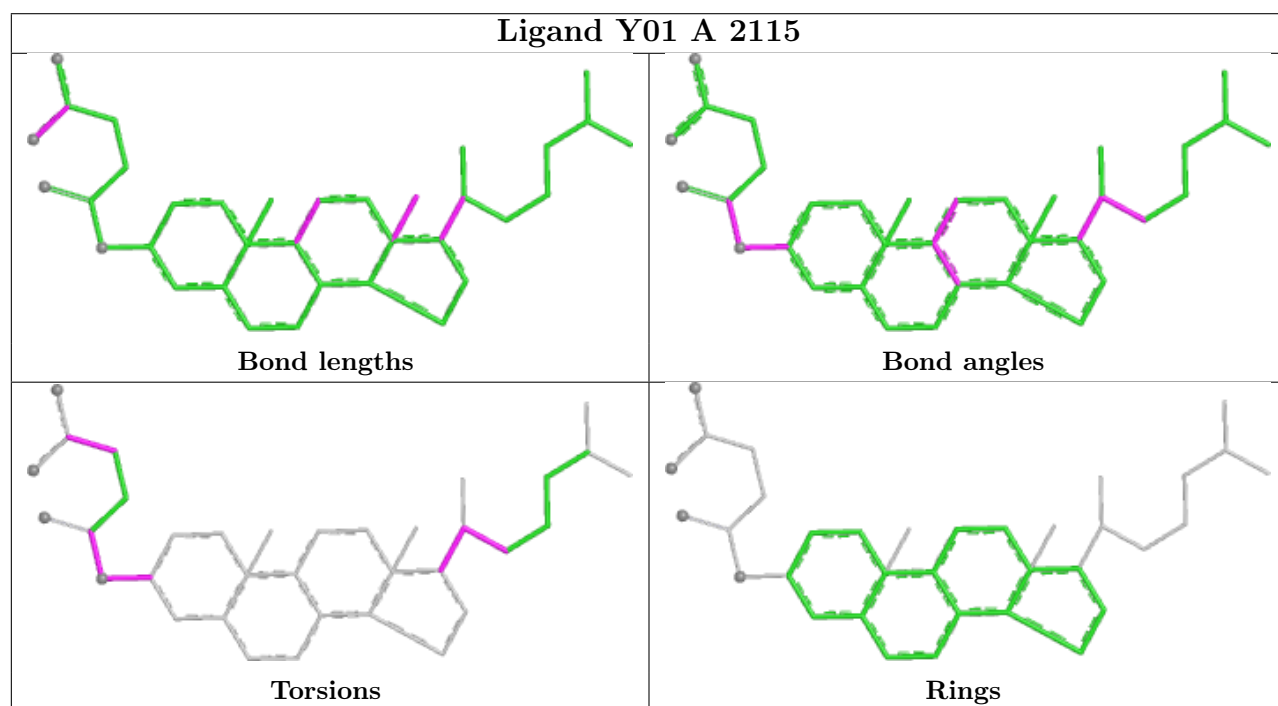
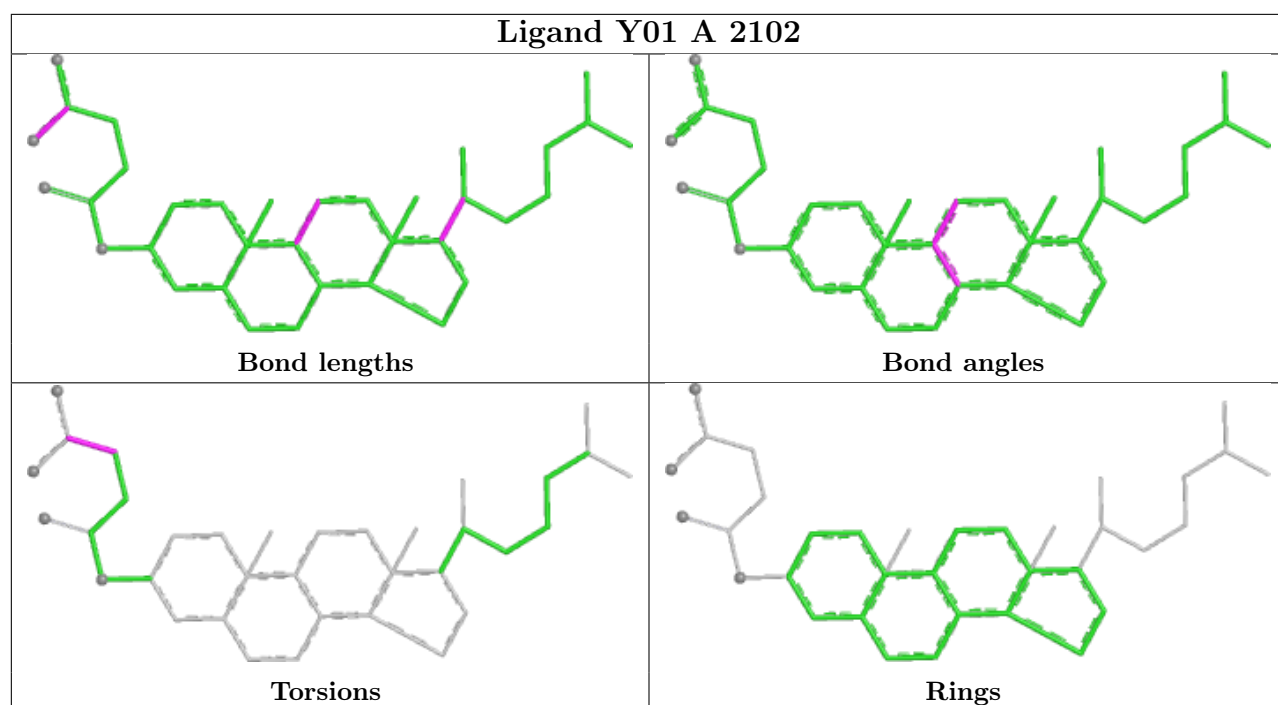
There are no ring outliers.

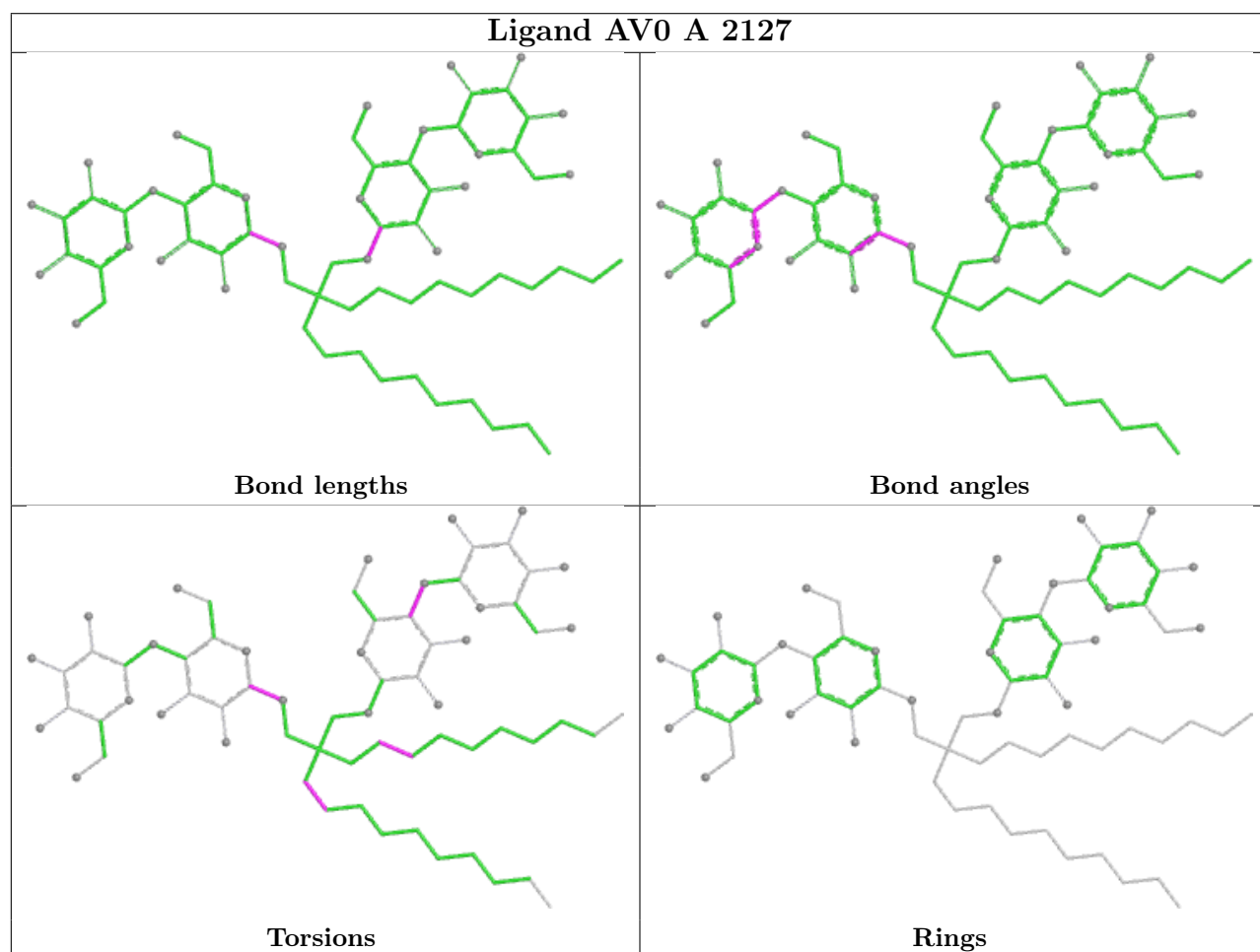
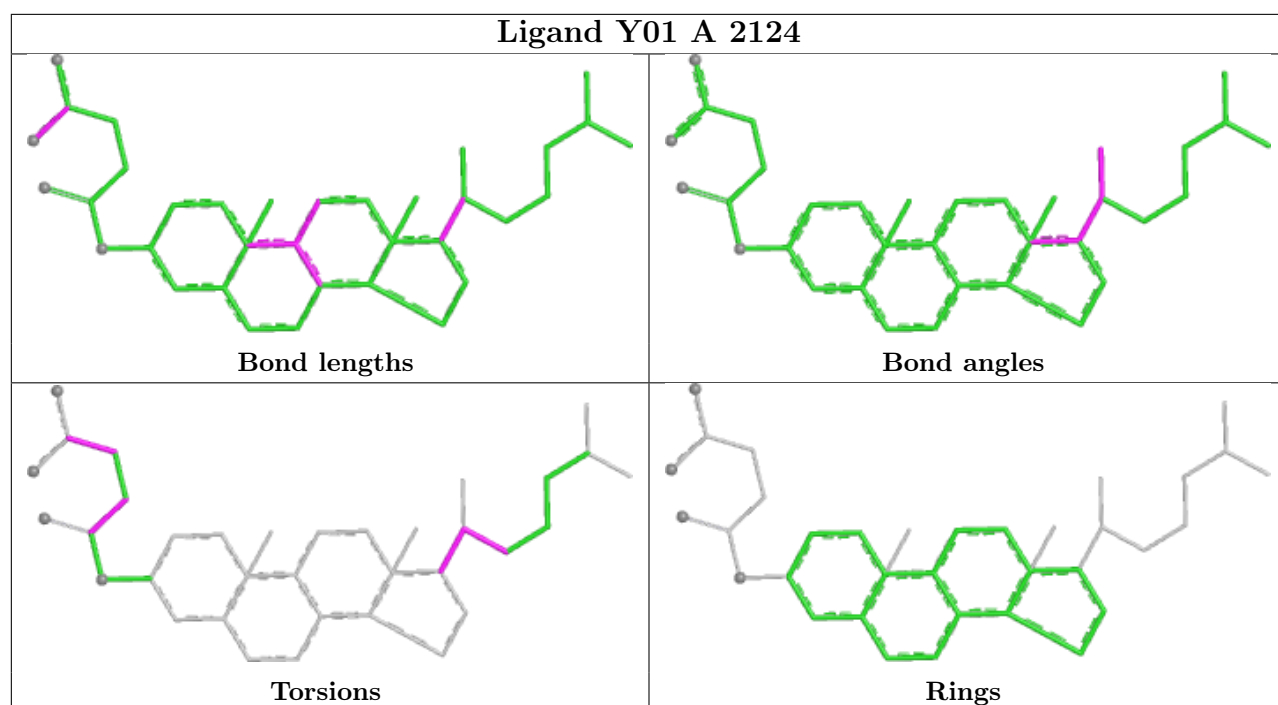
9 monomers are involved in 9 short contacts:

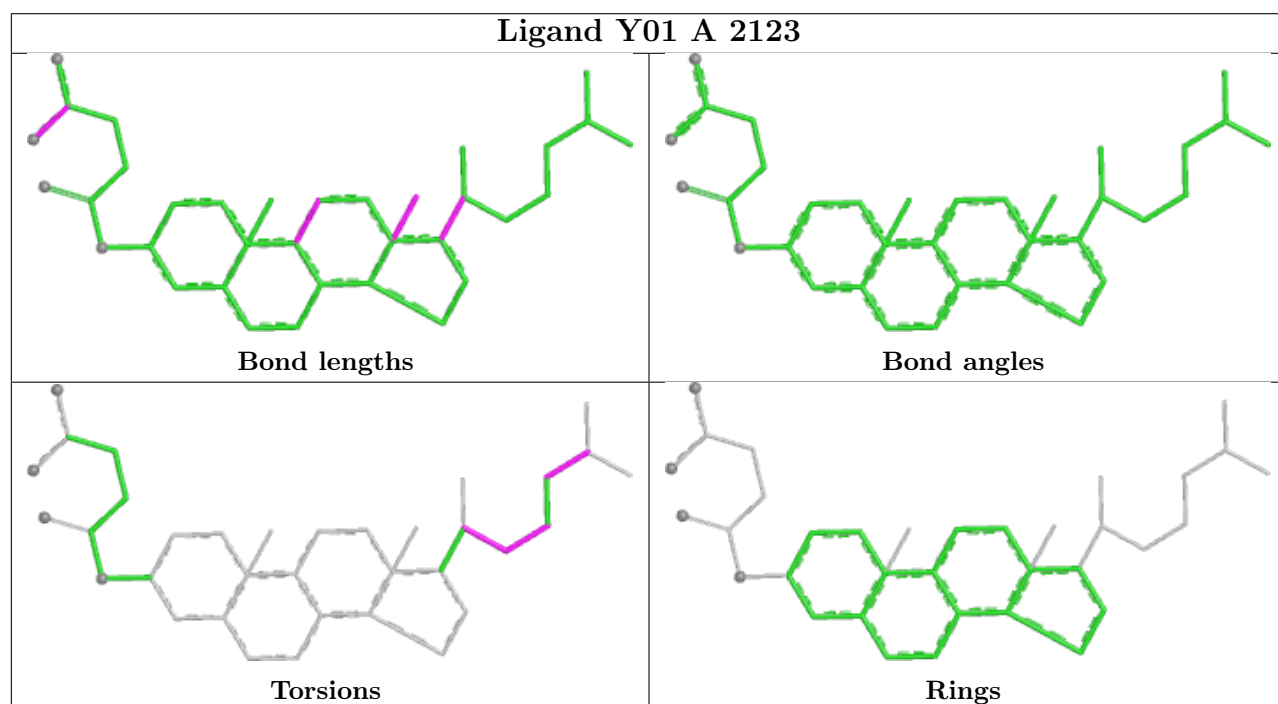
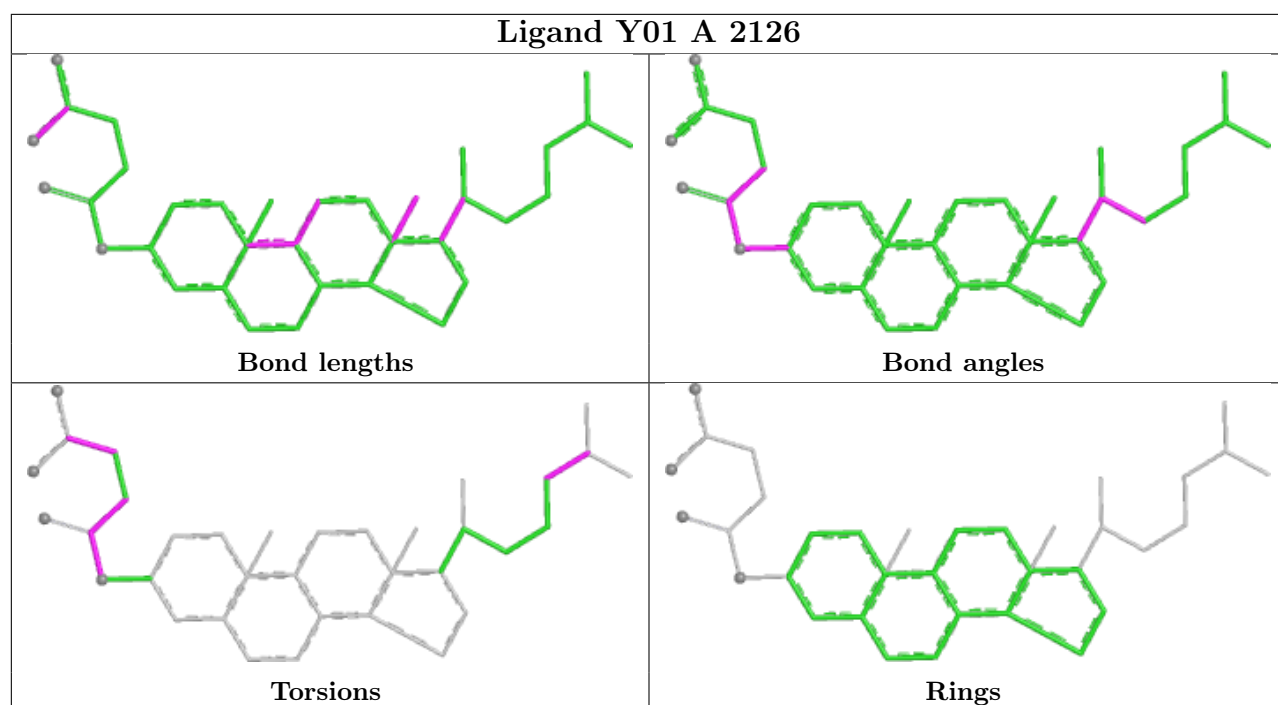
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2102	Y01	1	0
3	A	2124	Y01	1	0
3	A	2126	Y01	1	0
3	A	2107	Y01	1	0
3	A	2116	Y01	1	0
3	A	2118	Y01	1	0
3	A	2112	Y01	1	0
3	A	2106	Y01	1	0
3	A	2114	Y01	1	0

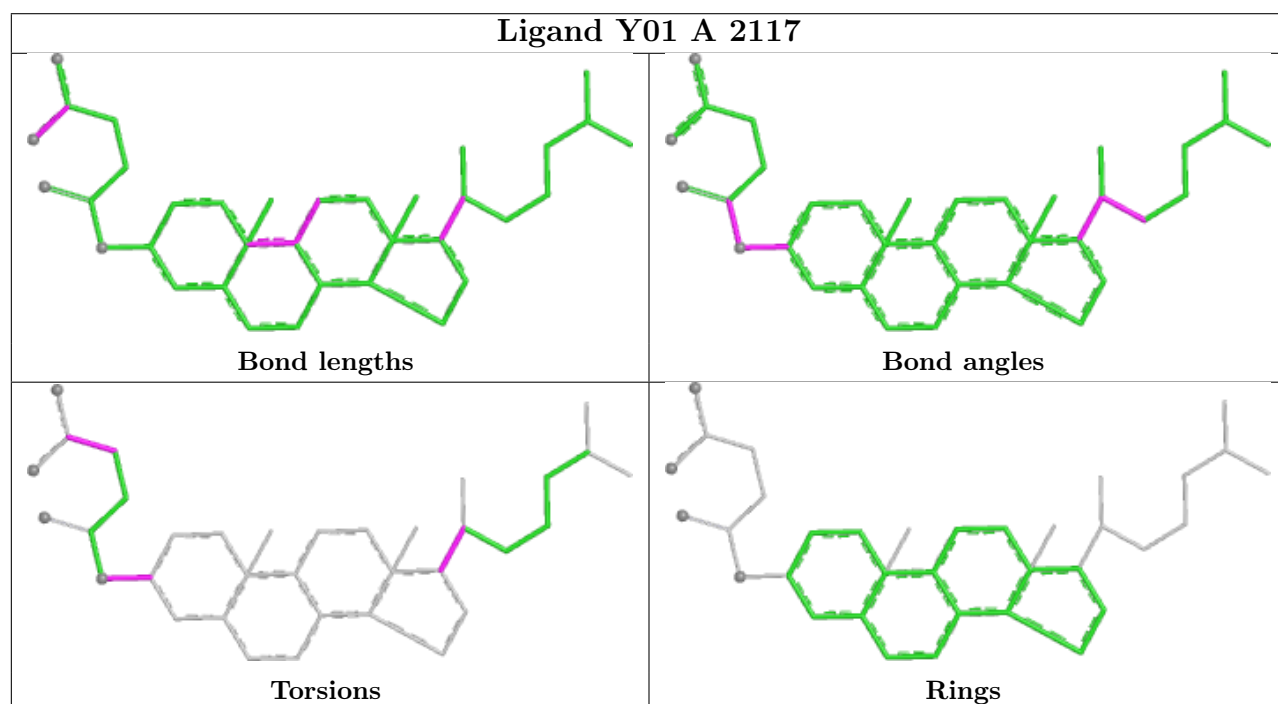
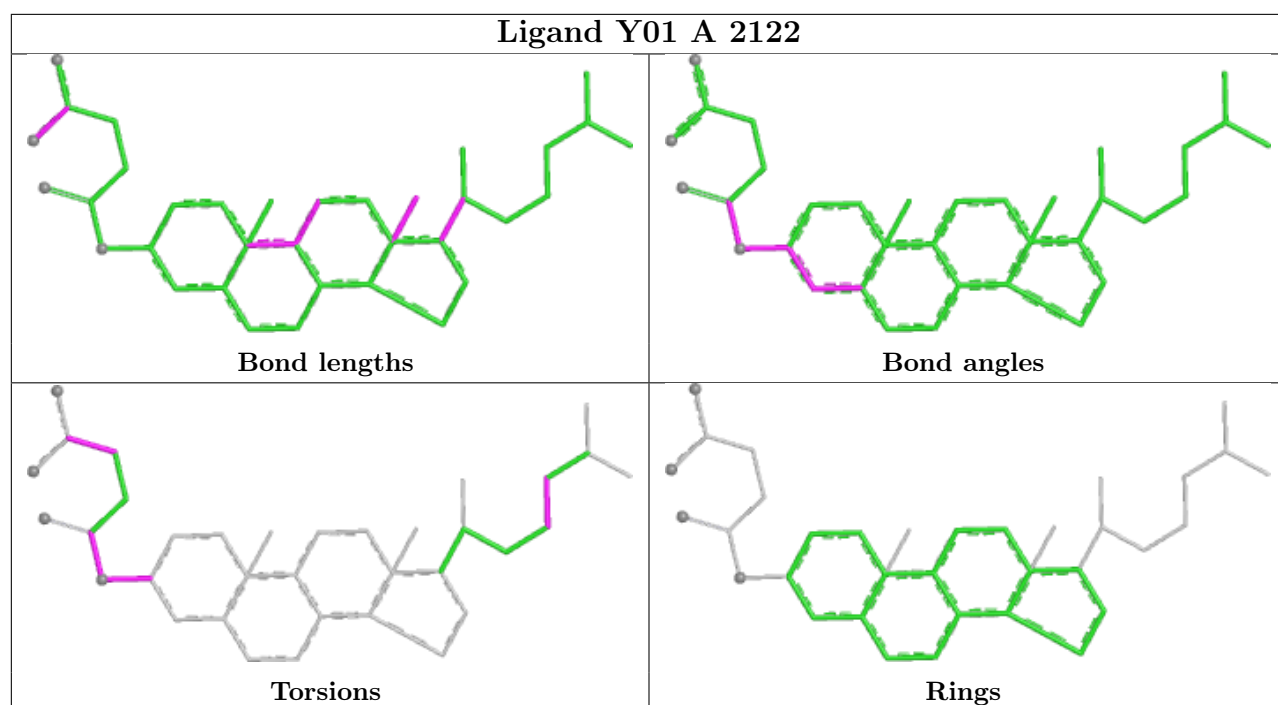
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

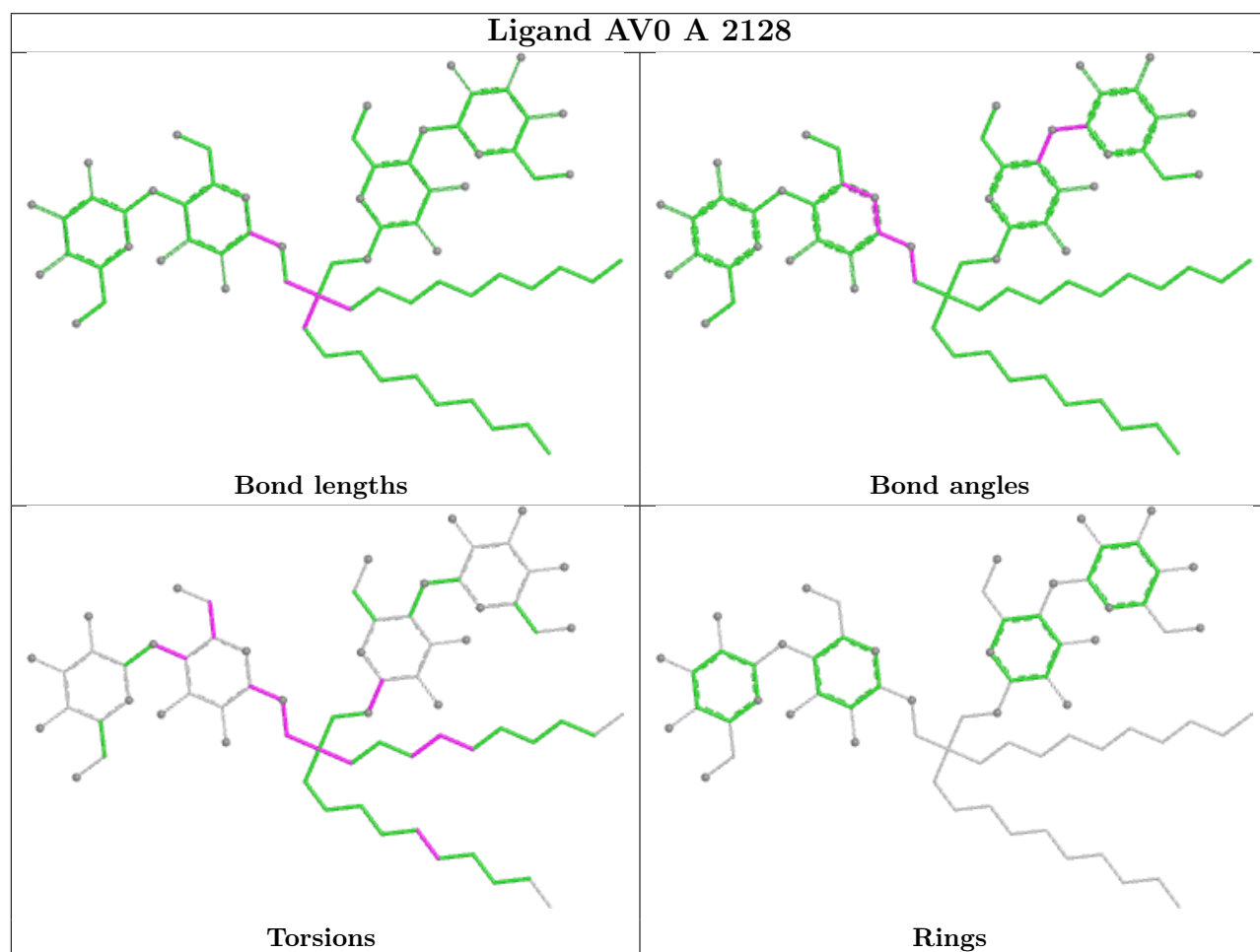
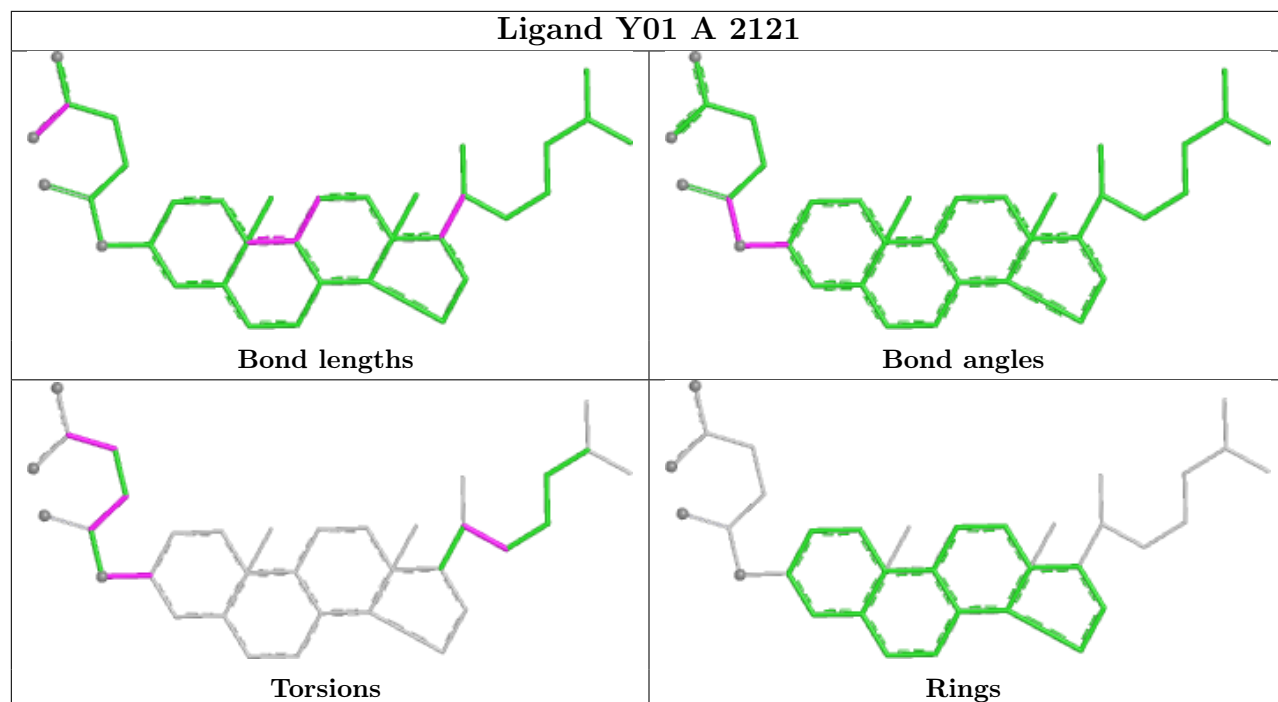


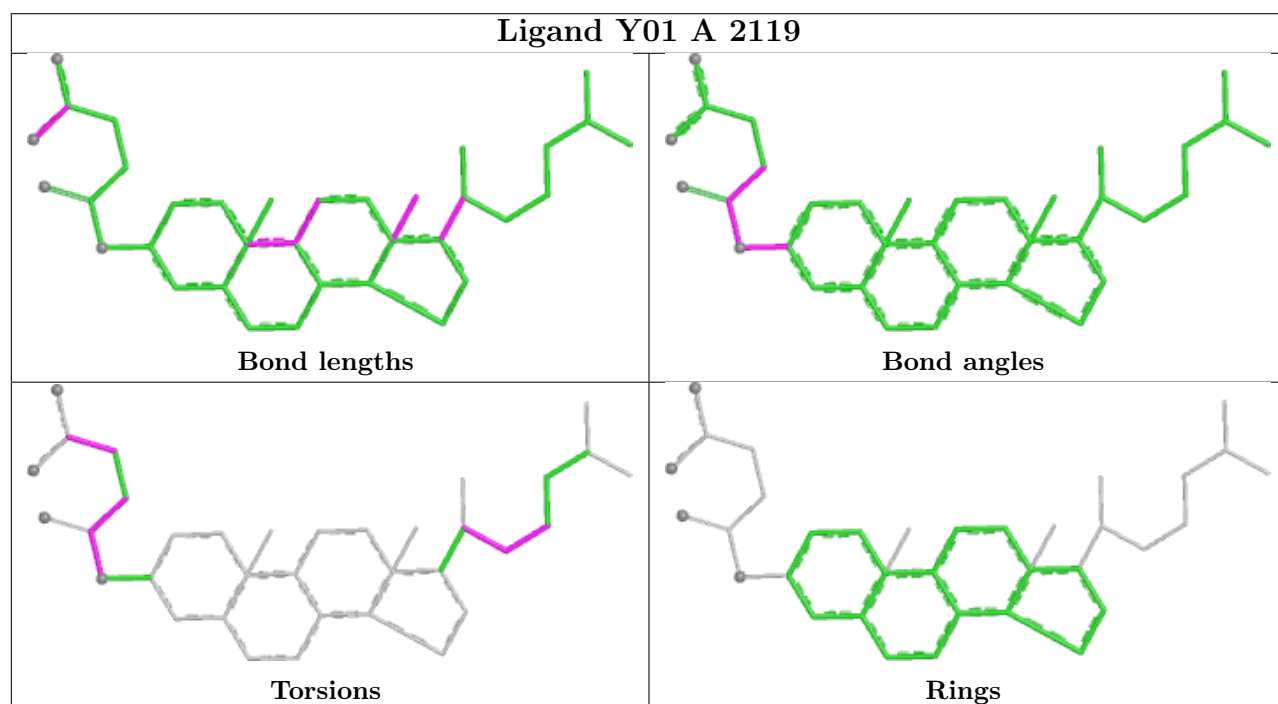
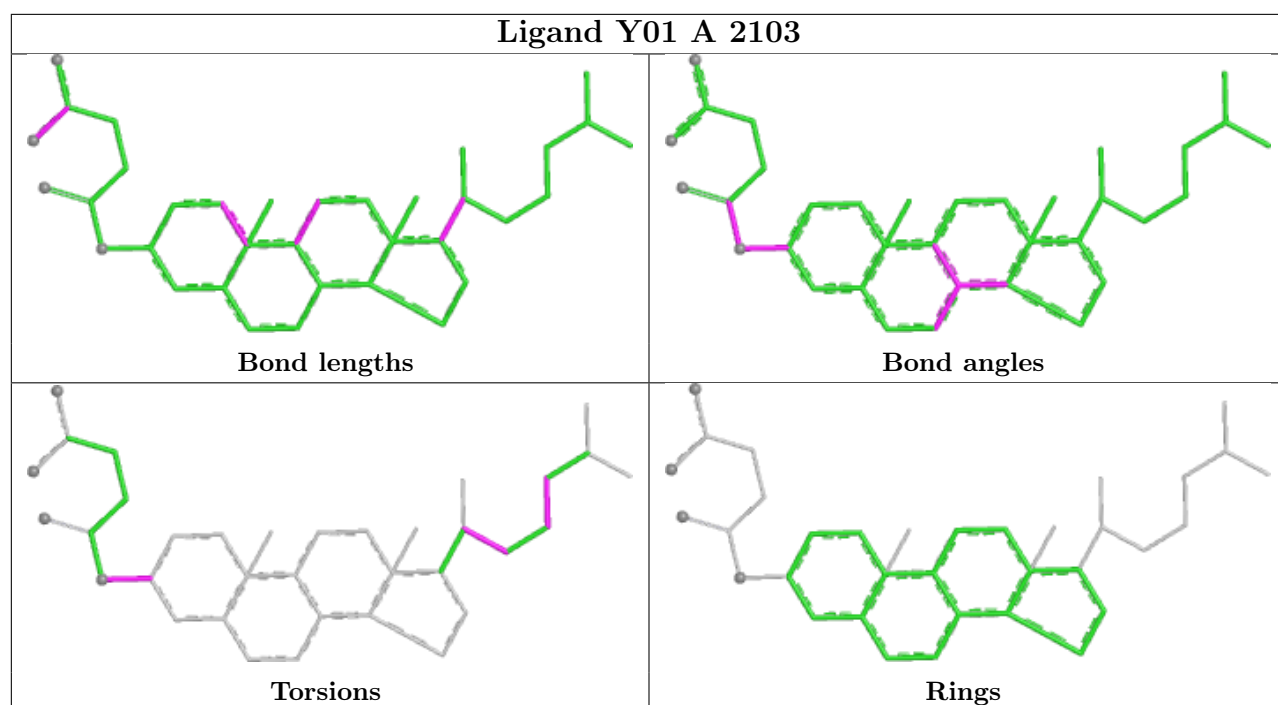


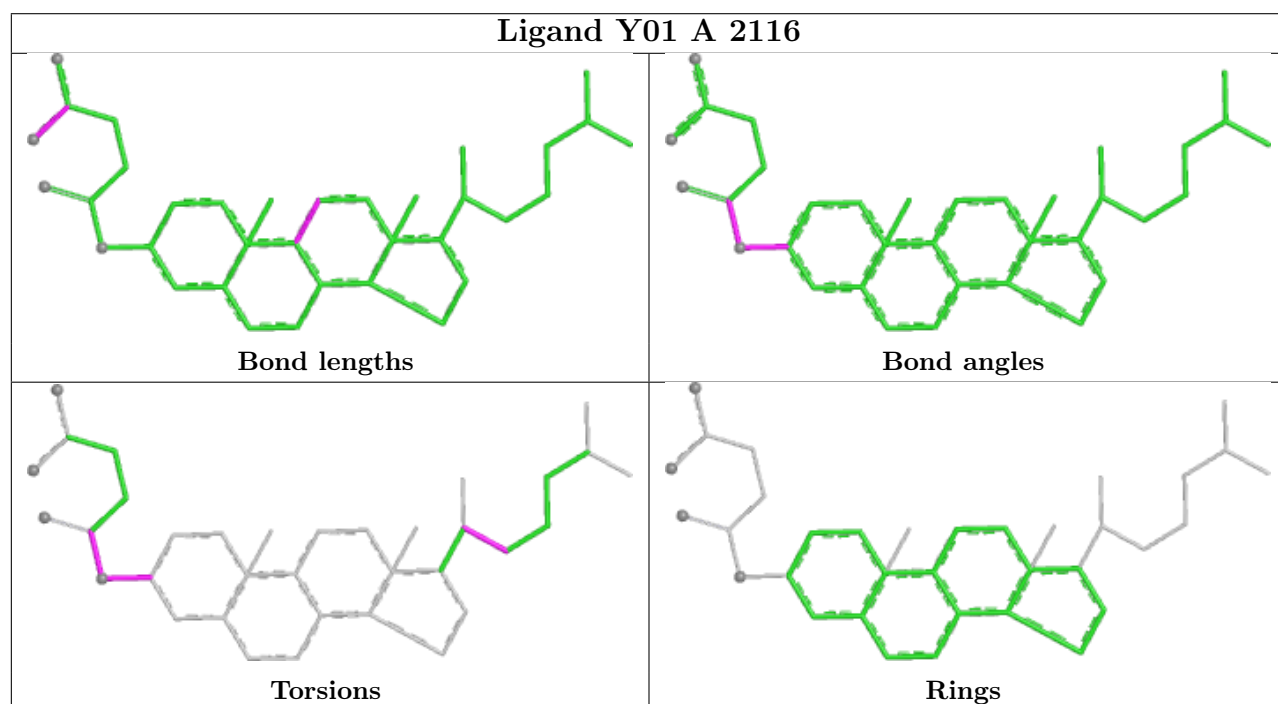
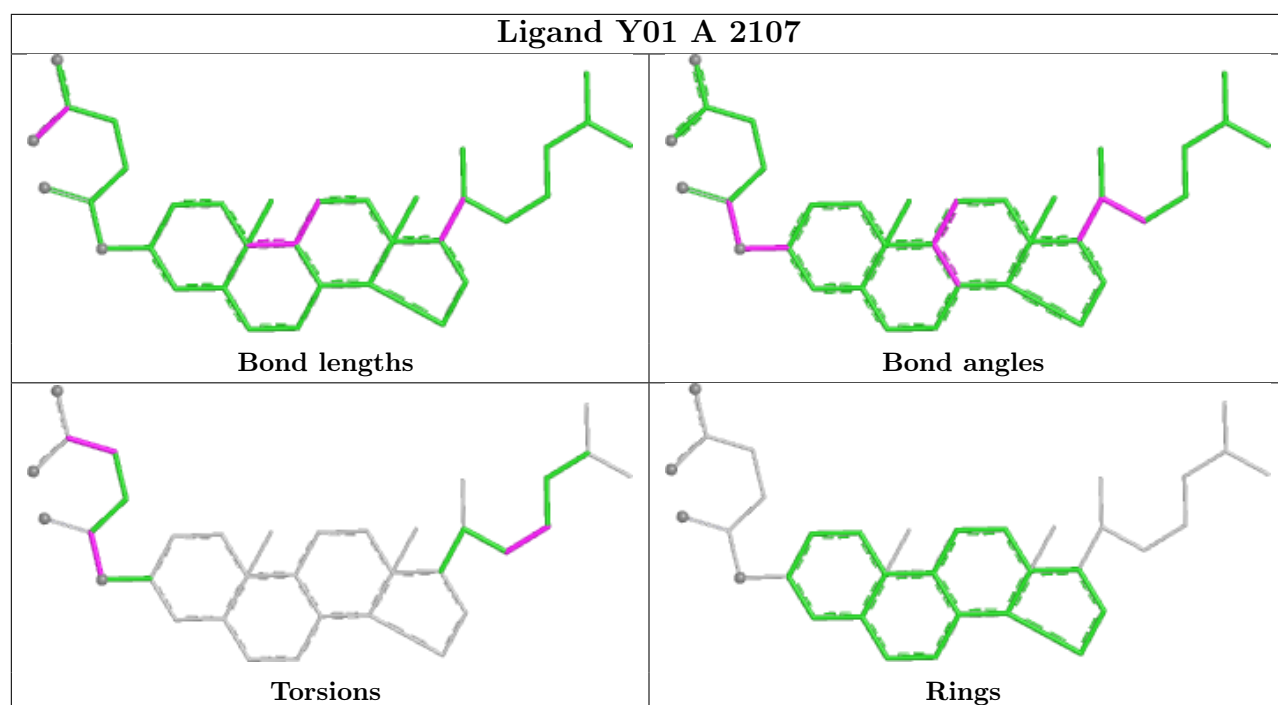


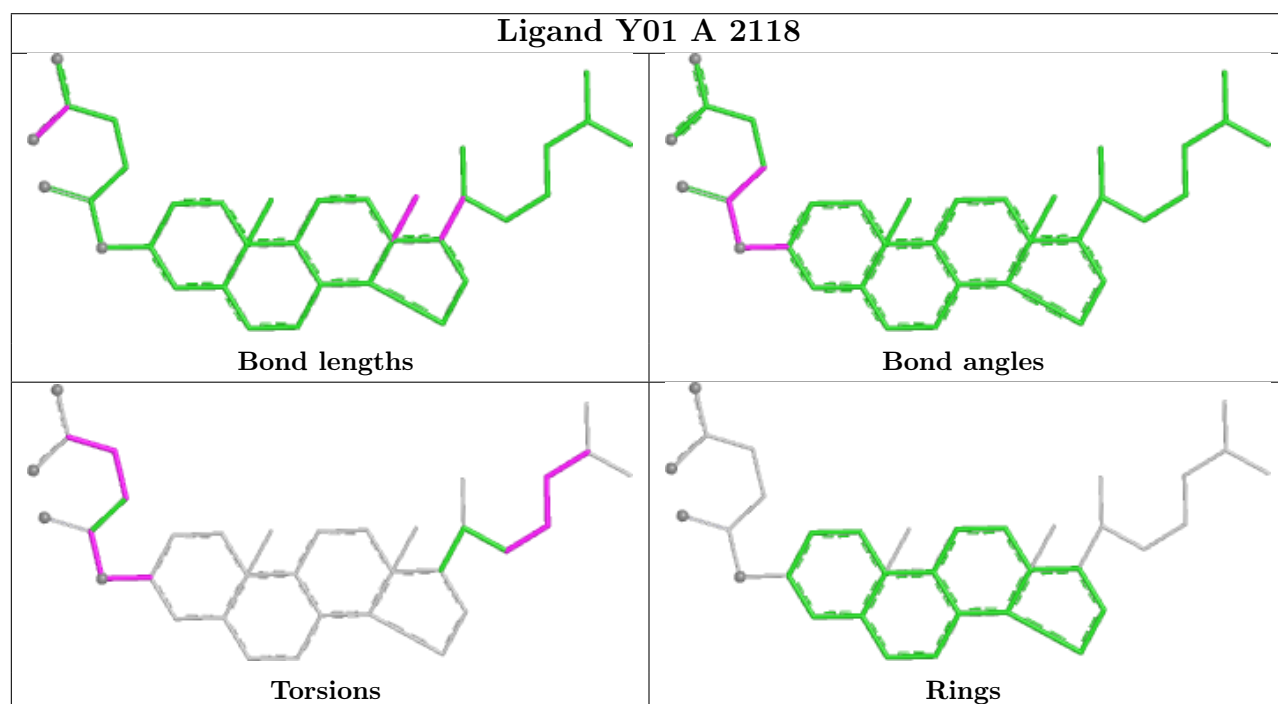
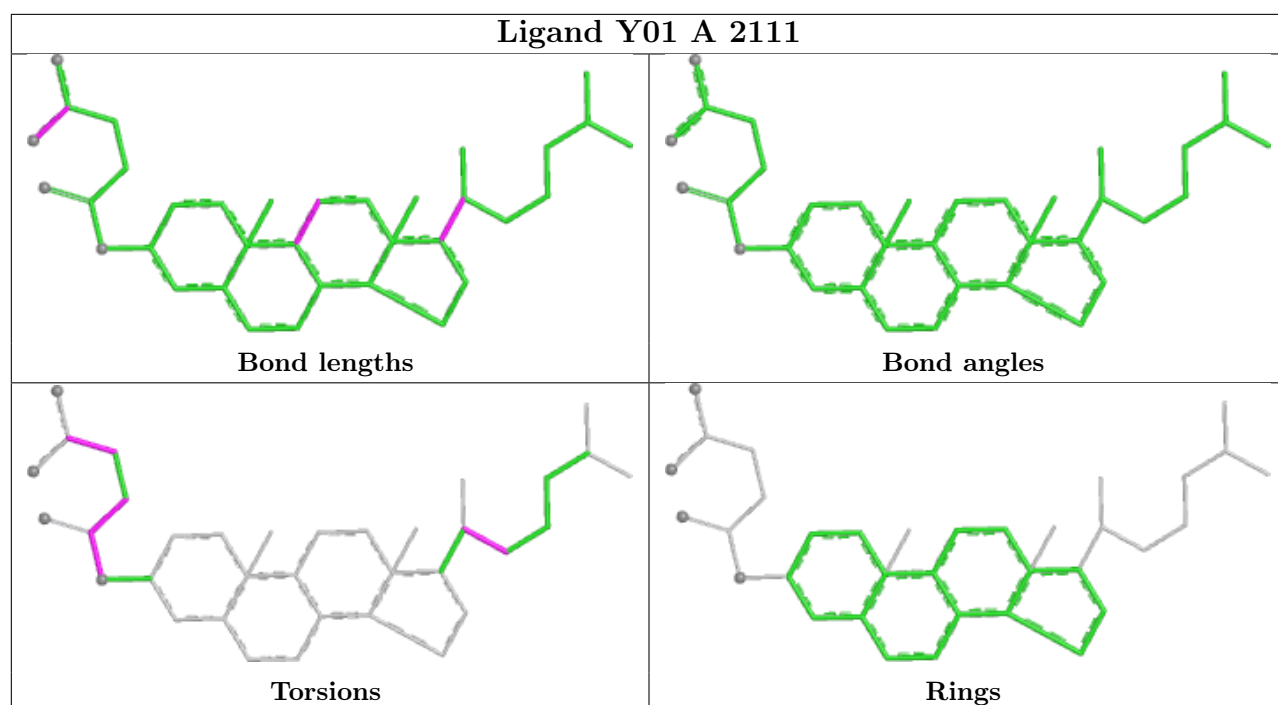


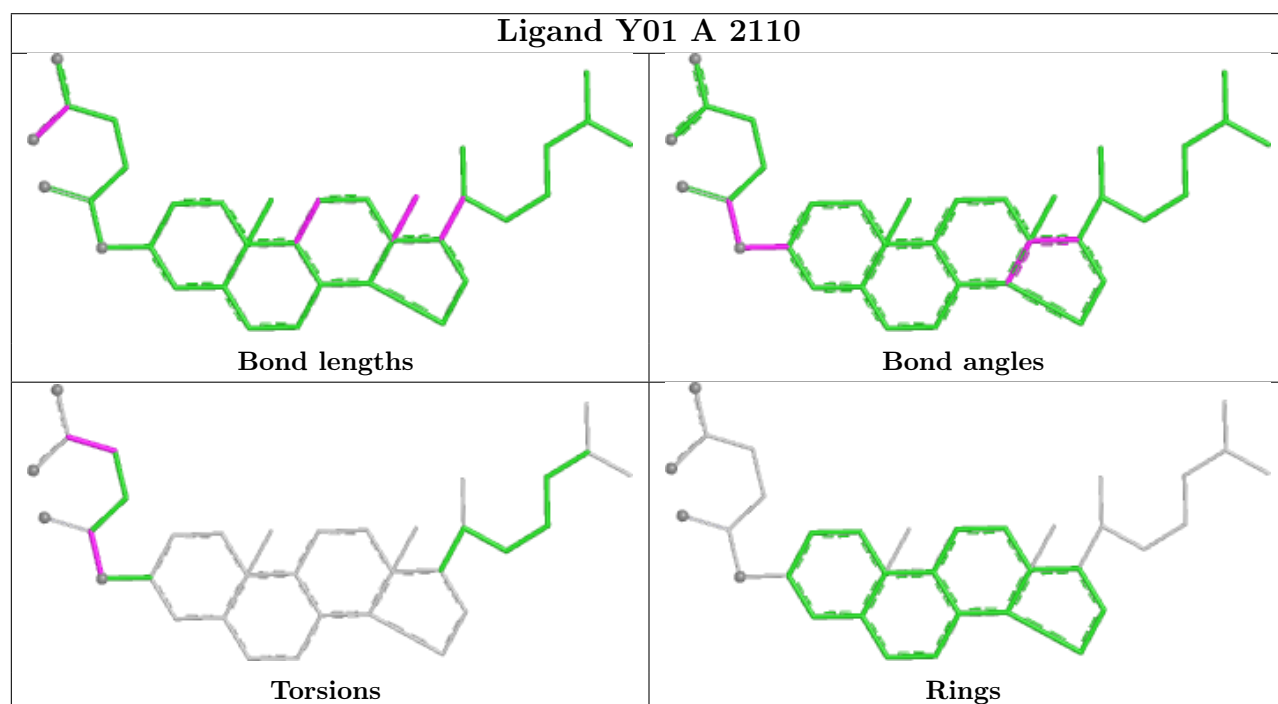
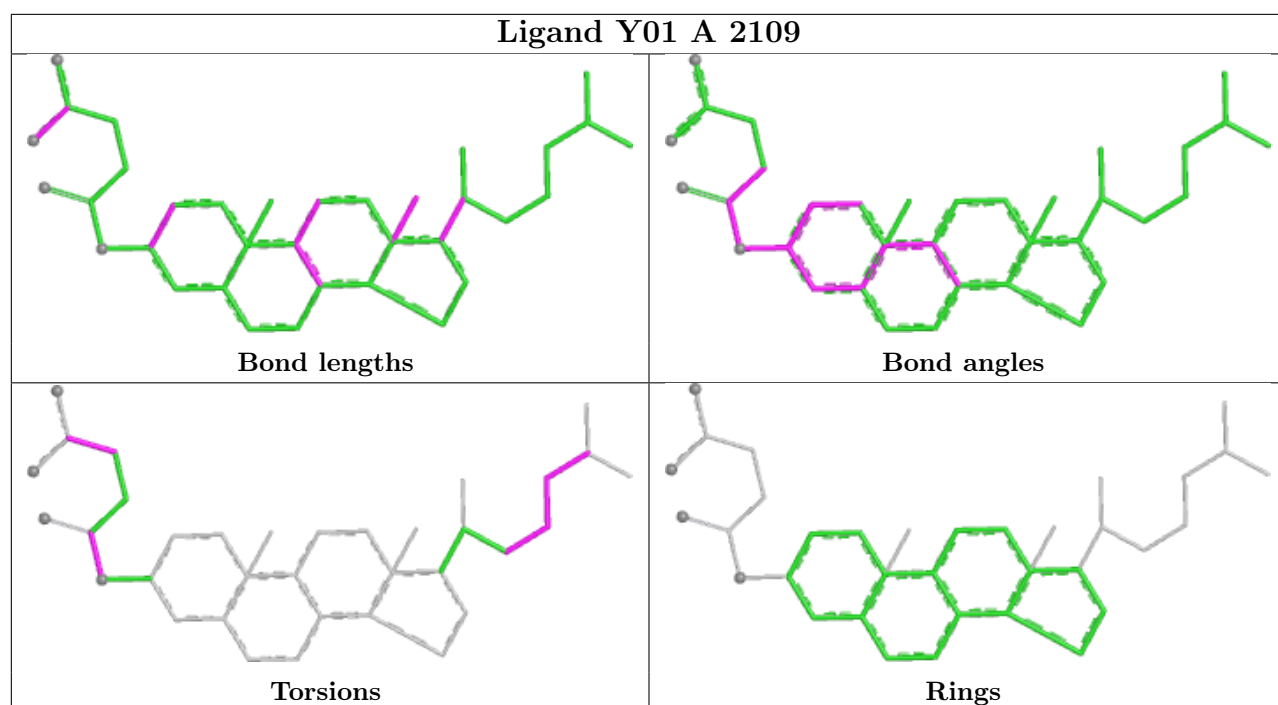


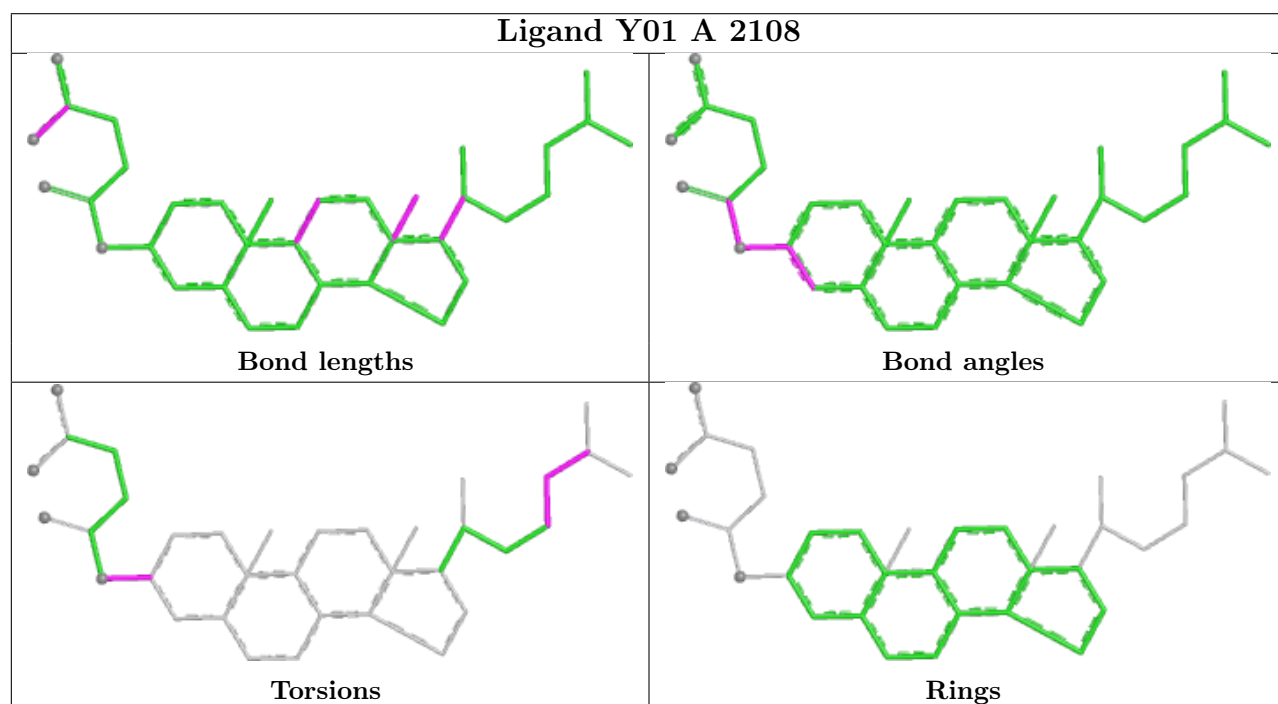
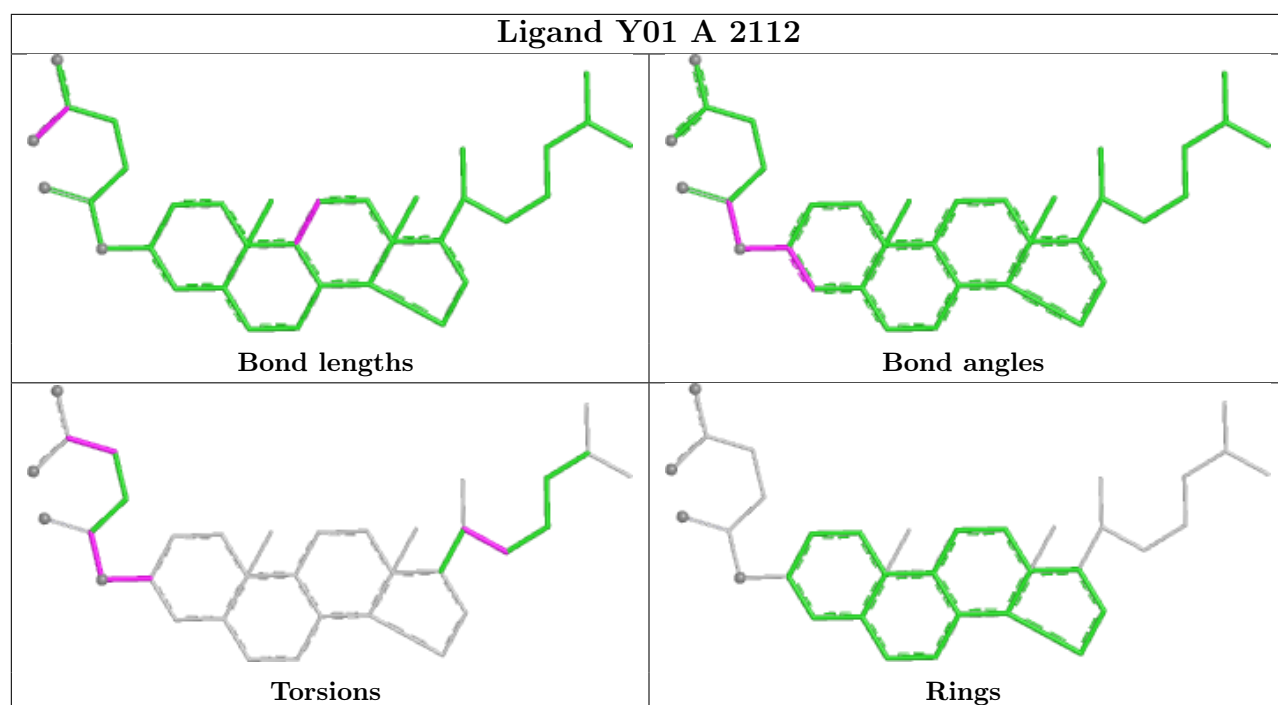


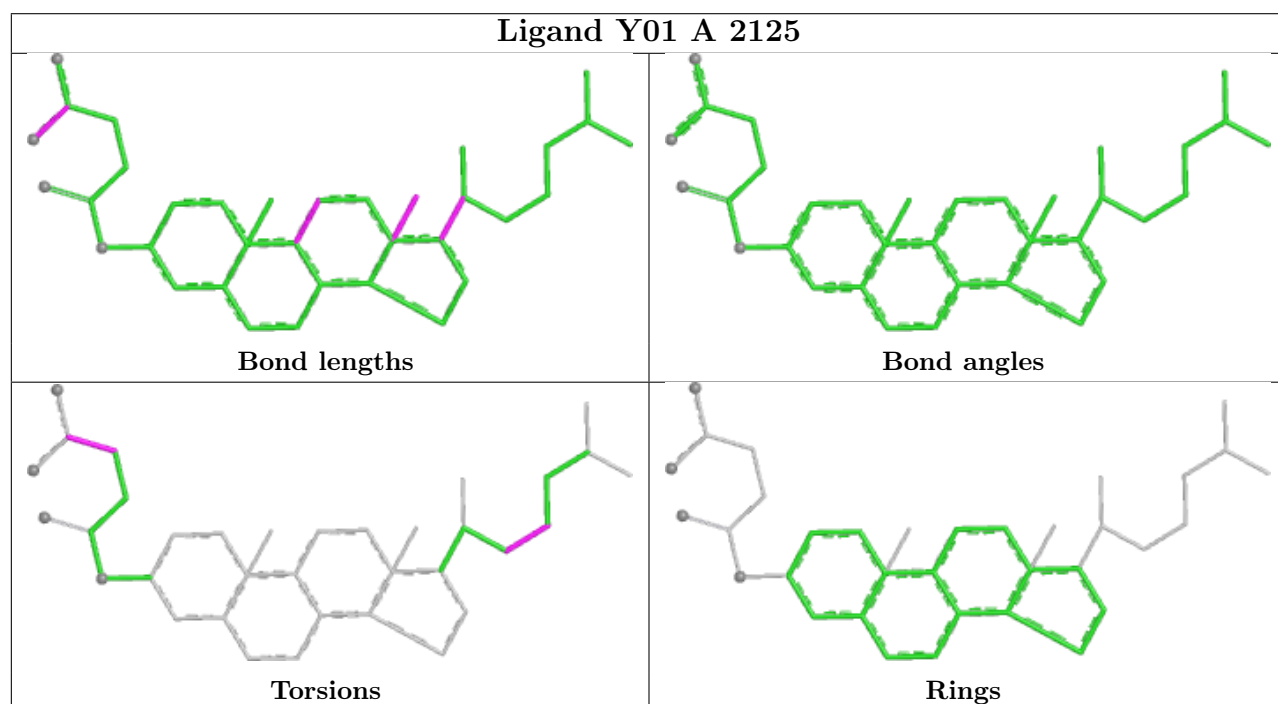
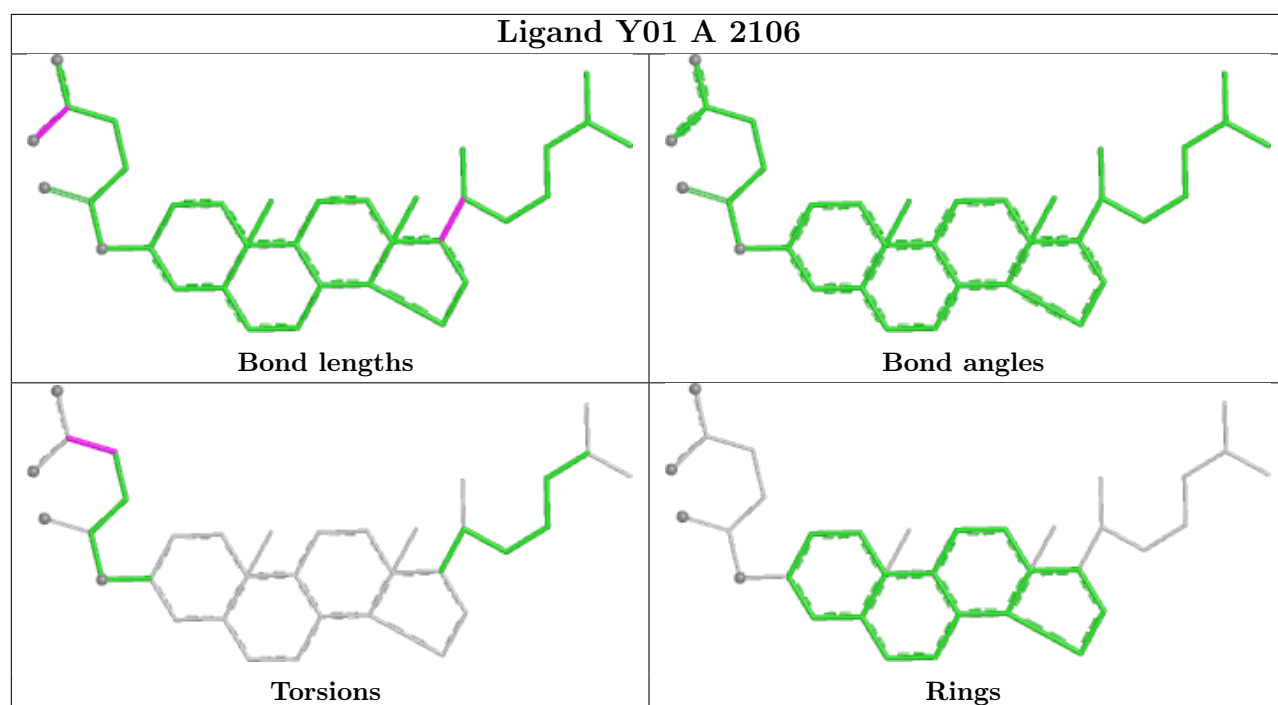


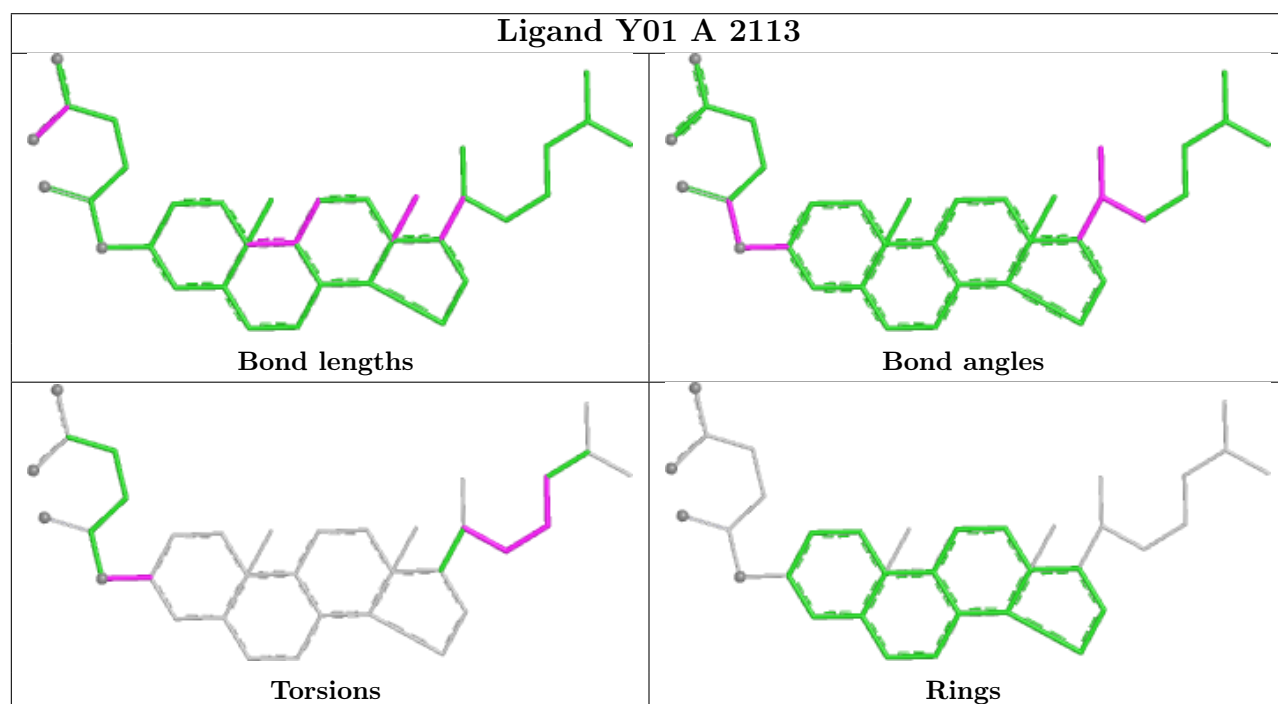
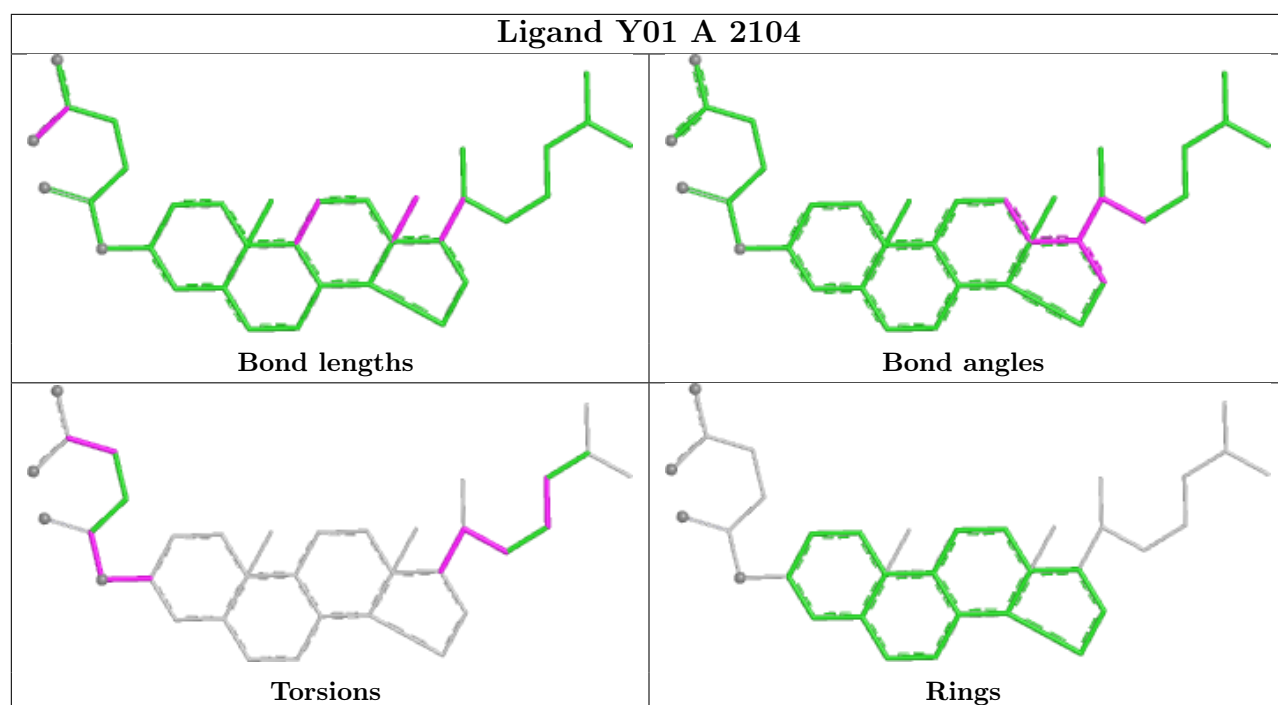


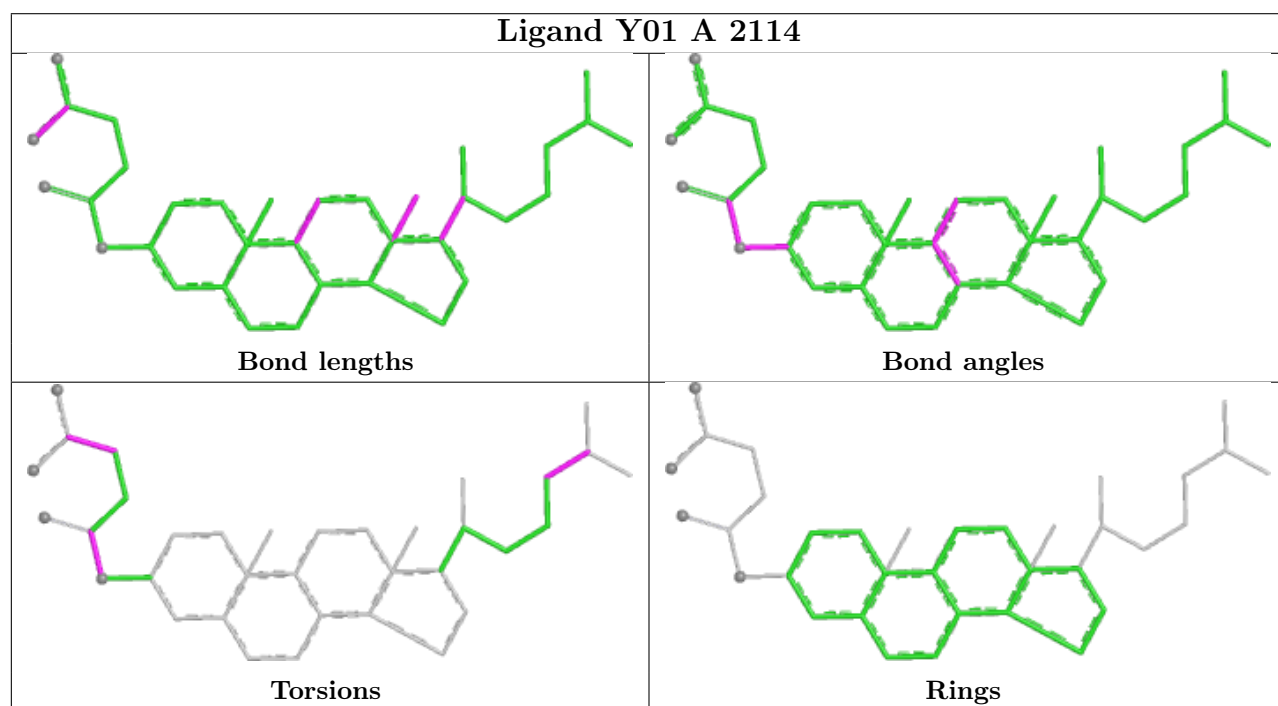
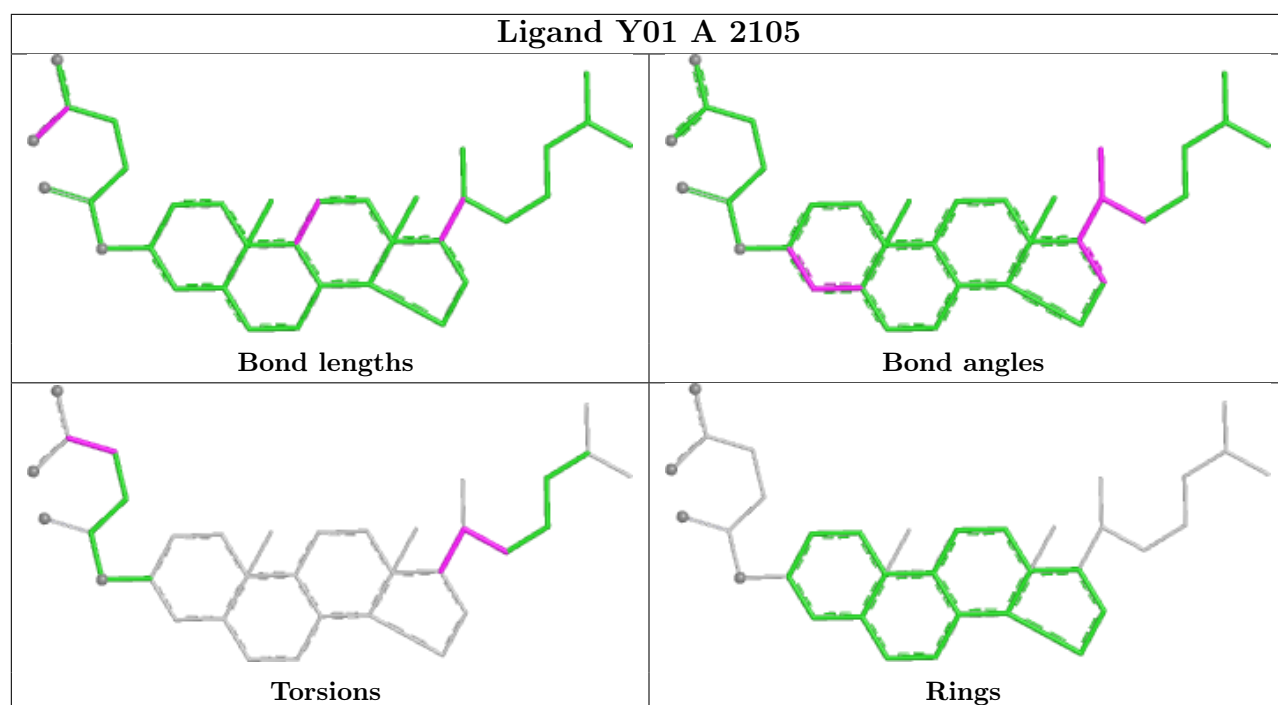


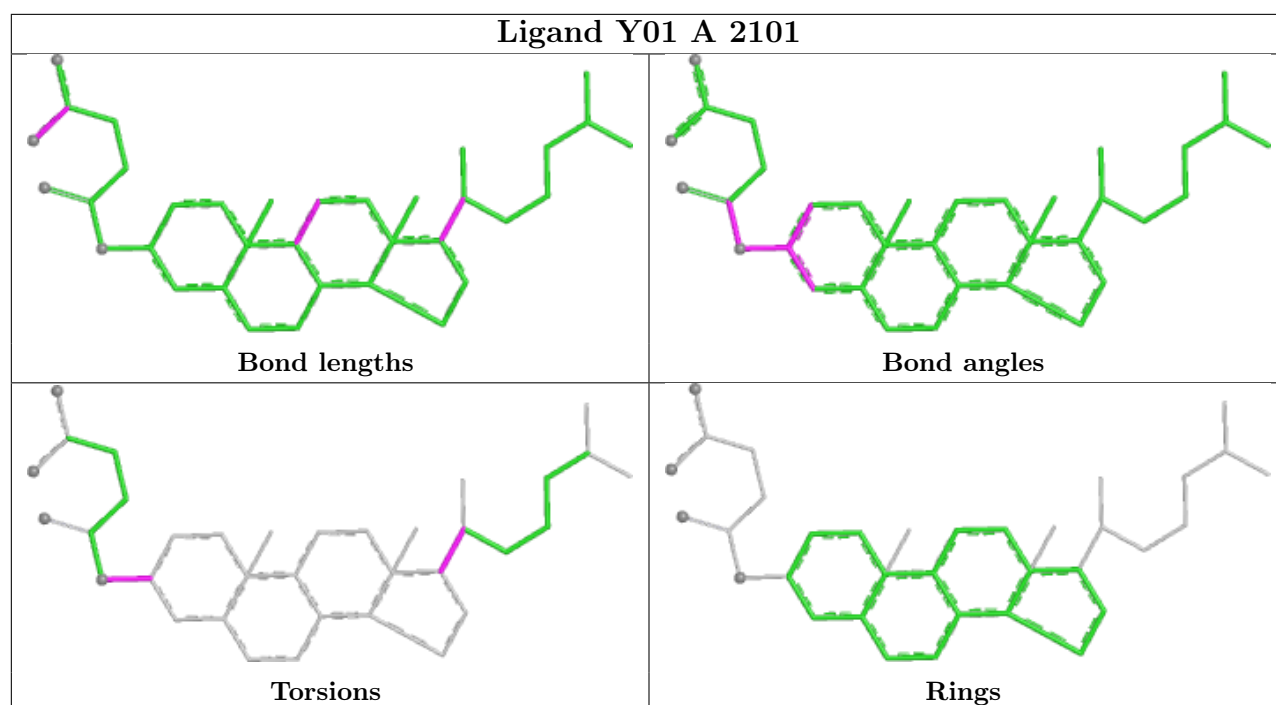












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

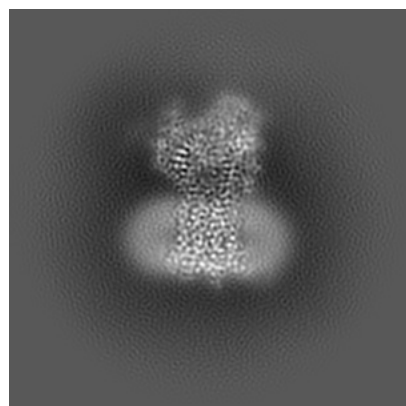
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24617. These allow visual inspection of the internal detail of the map and identification of artifacts.

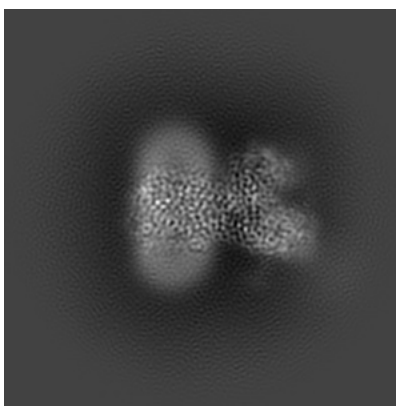
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

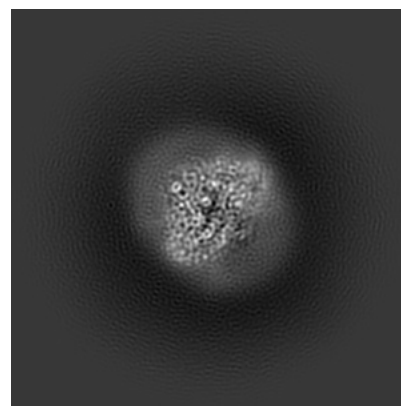
6.1.1 Primary map



X

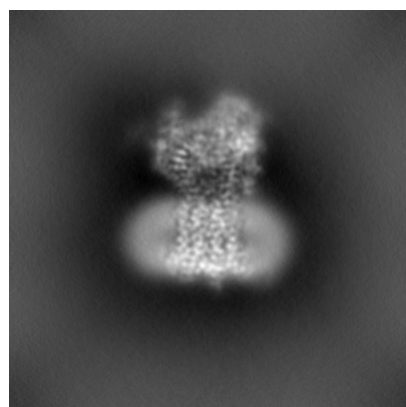


Y

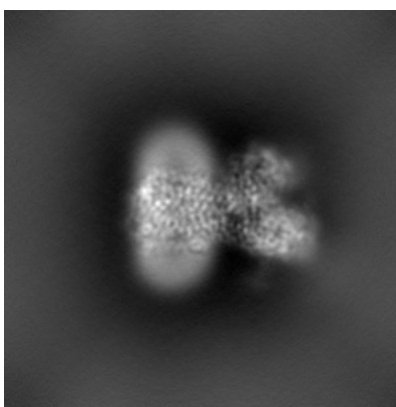


Z

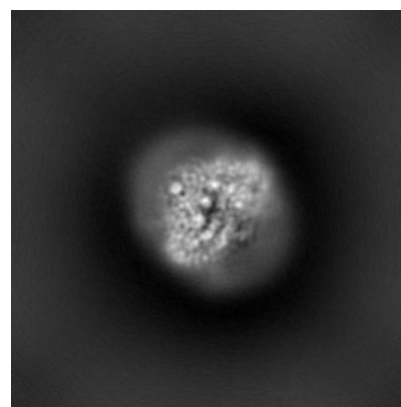
6.1.2 Raw map



X



Y

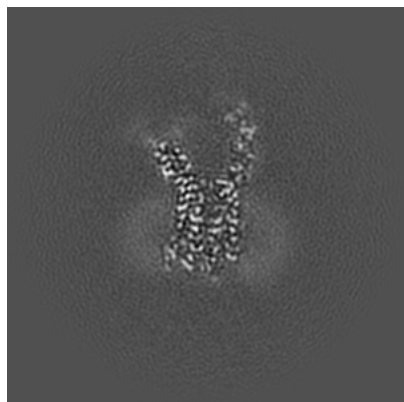


Z

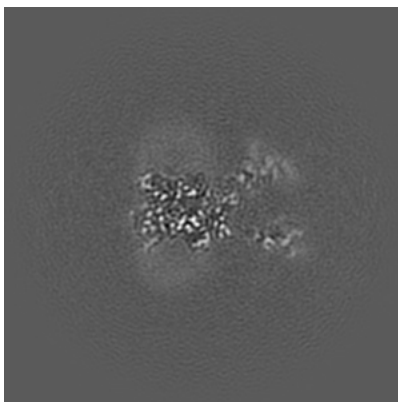
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

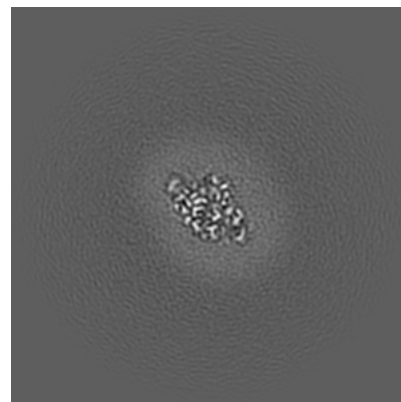
6.2.1 Primary map



X Index: 144

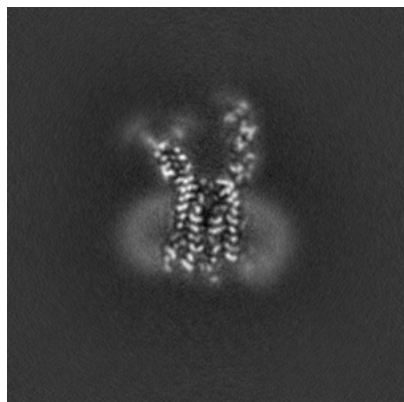


Y Index: 144

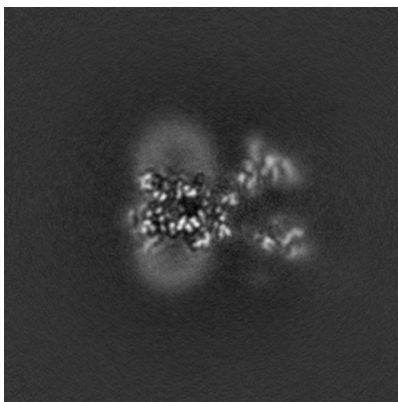


Z Index: 144

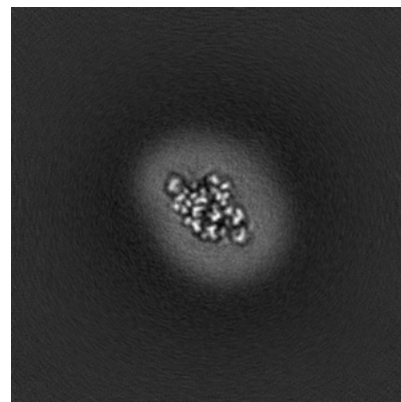
6.2.2 Raw map



X Index: 144



Y Index: 144

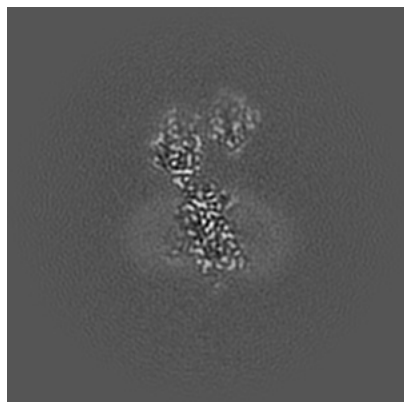


Z Index: 144

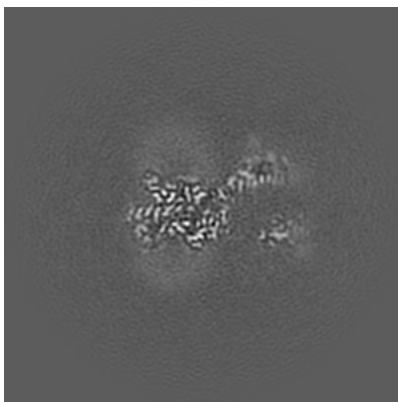
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

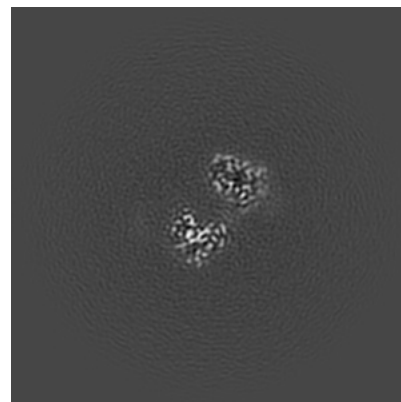
6.3.1 Primary map



X Index: 132

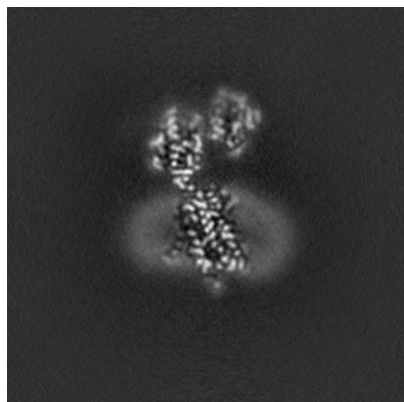


Y Index: 147

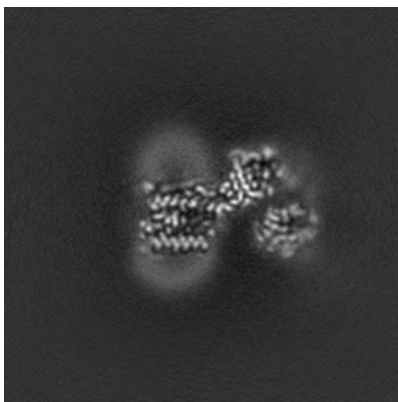


Z Index: 174

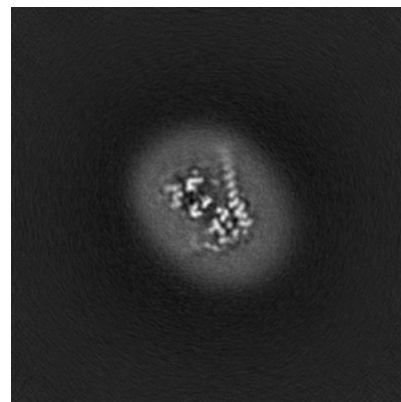
6.3.2 Raw map



X Index: 132



Y Index: 160

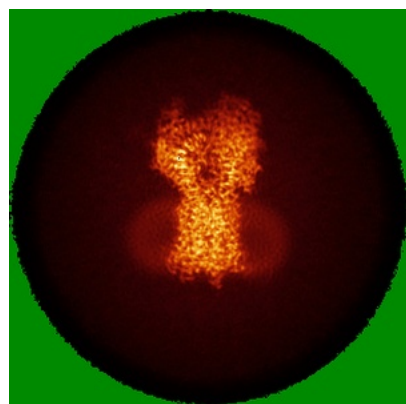


Z Index: 104

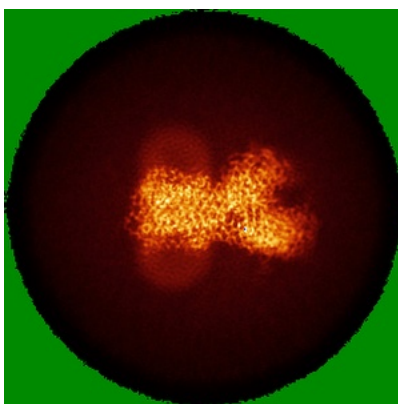
The images above show the largest variance slices of the map in three orthogonal directions.

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

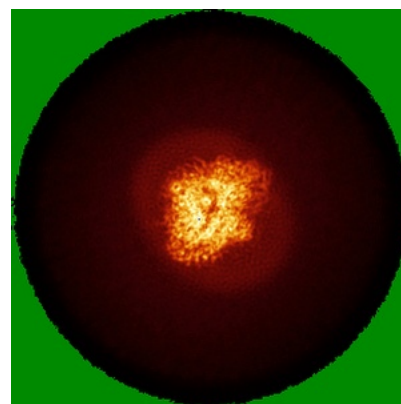
6.4.1 Primary map



X

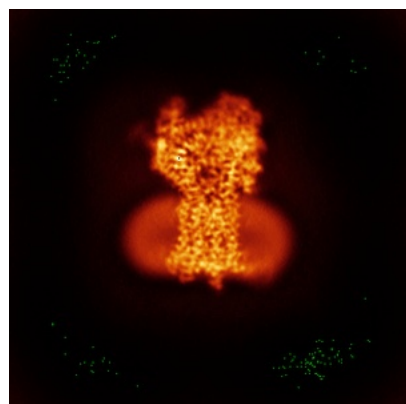


Y

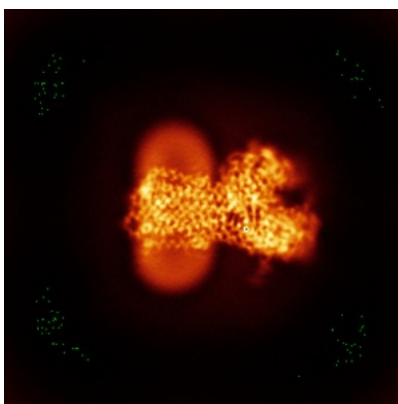


Z

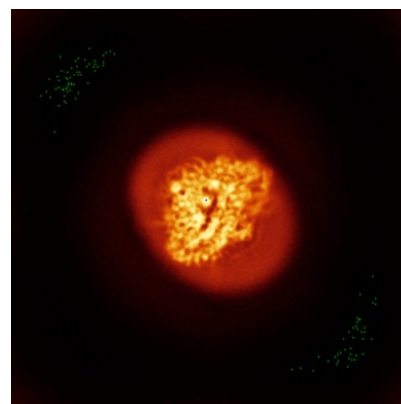
6.4.2 Raw map



X



Y

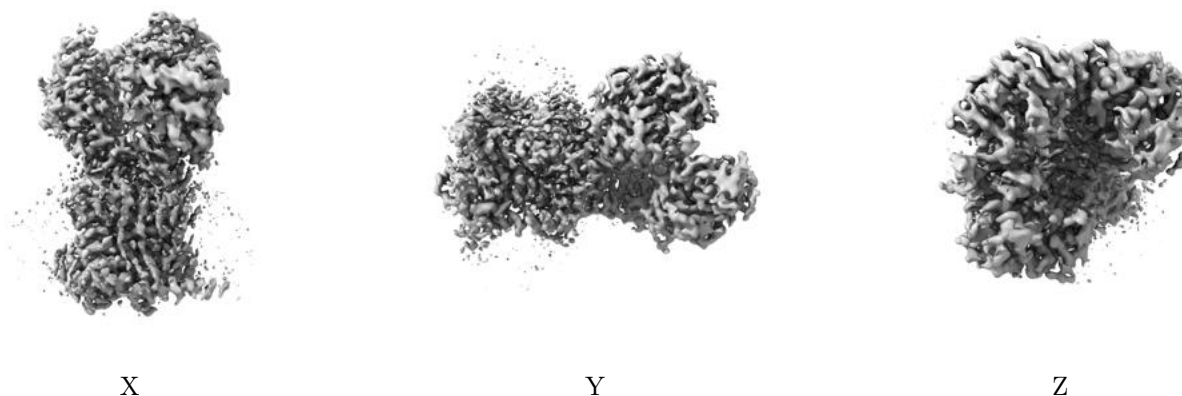


Z

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.

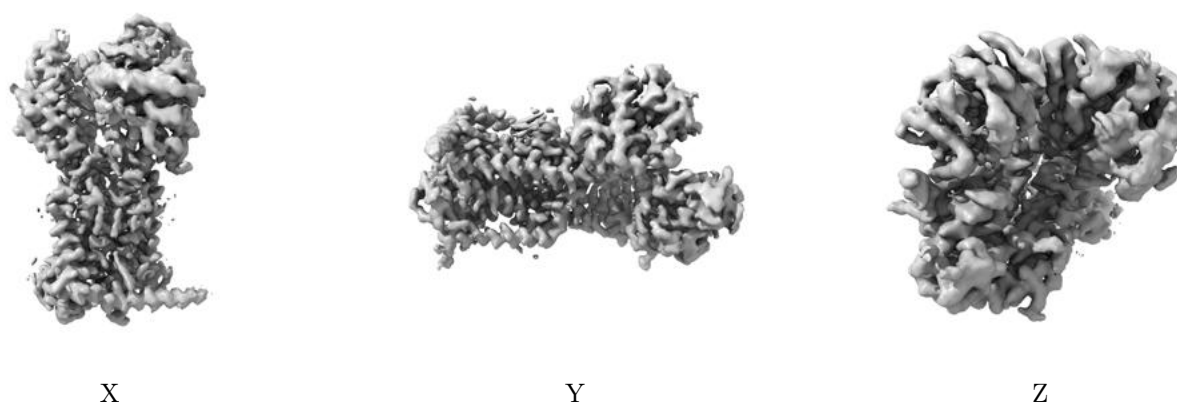
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

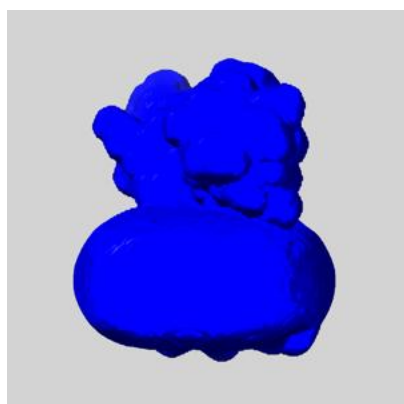
6.6 Mask visualisation [i](#)

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

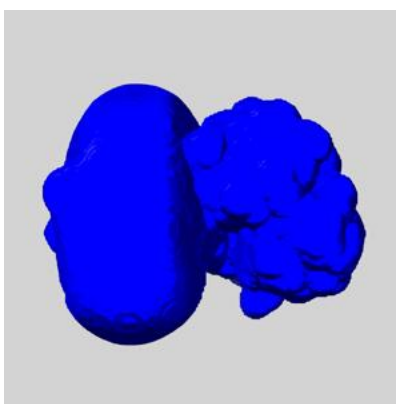
A mask typically either:

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

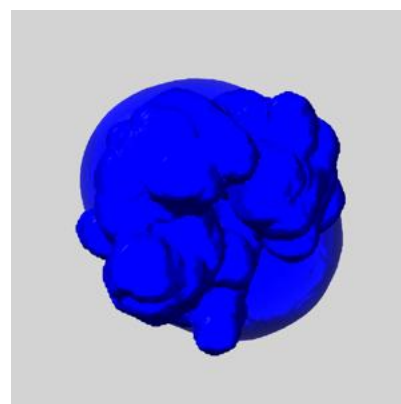
6.6.1 emd_24617_msk_1.map [i](#)



X

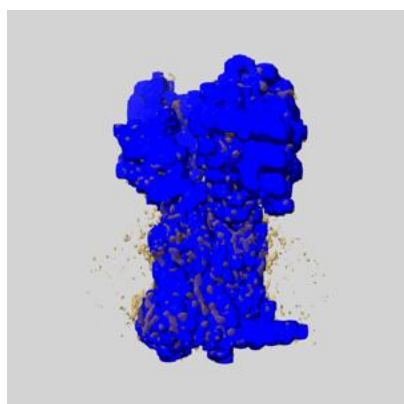


Y

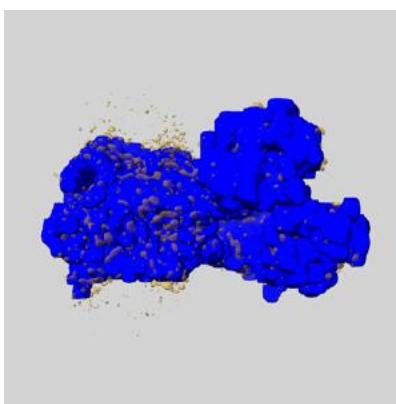


Z

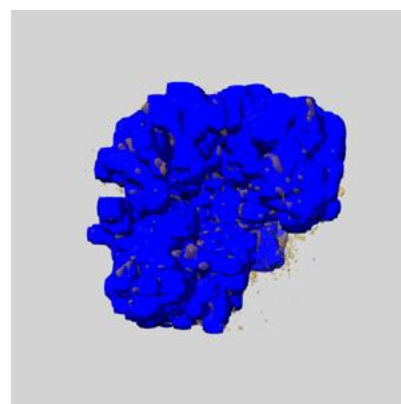
6.6.2 emd_24617_msk_2.map [i](#)



X



Y

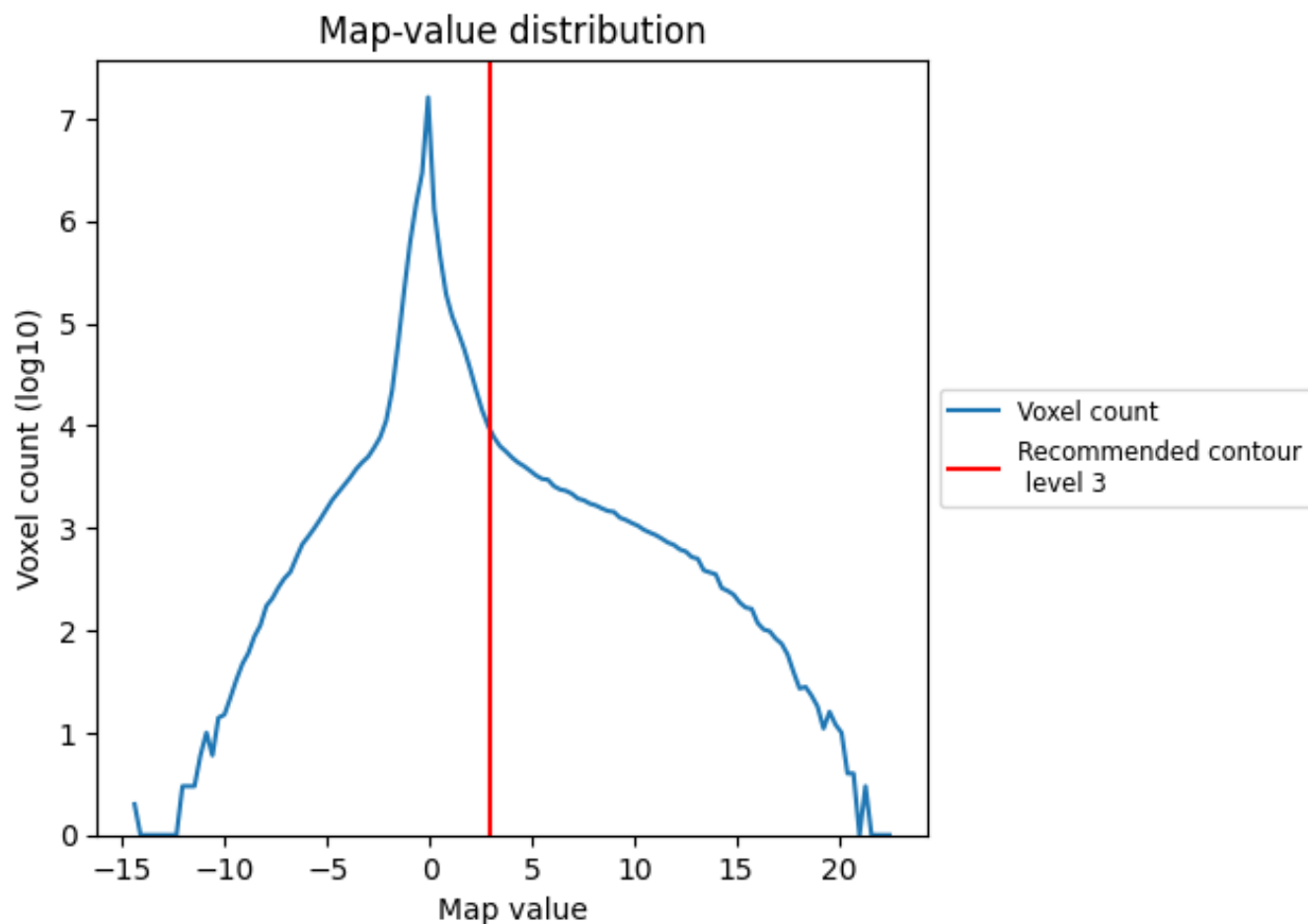


Z

7 Map analysis [i](#)

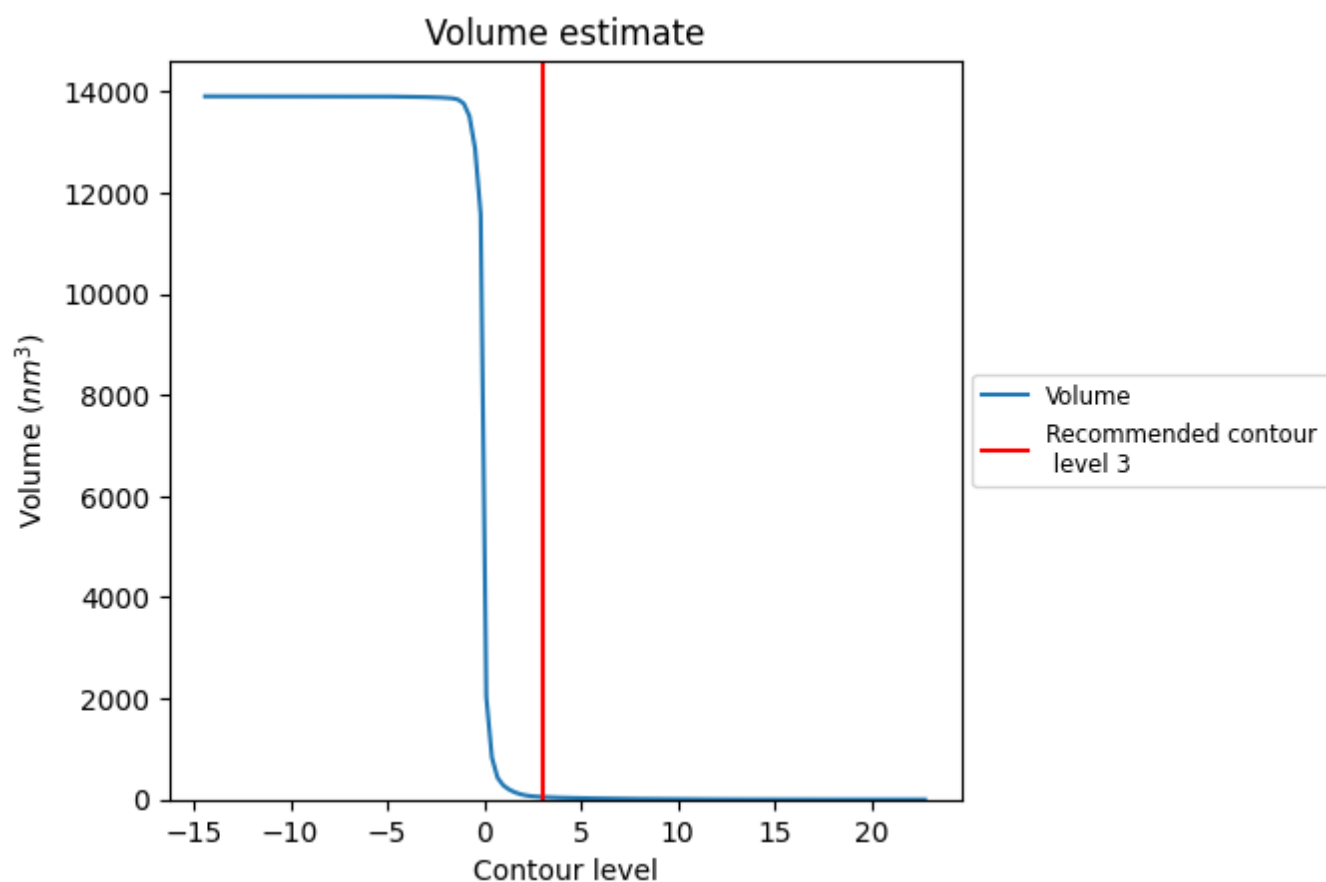
This section contains the results of statistical analysis of the map.

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.

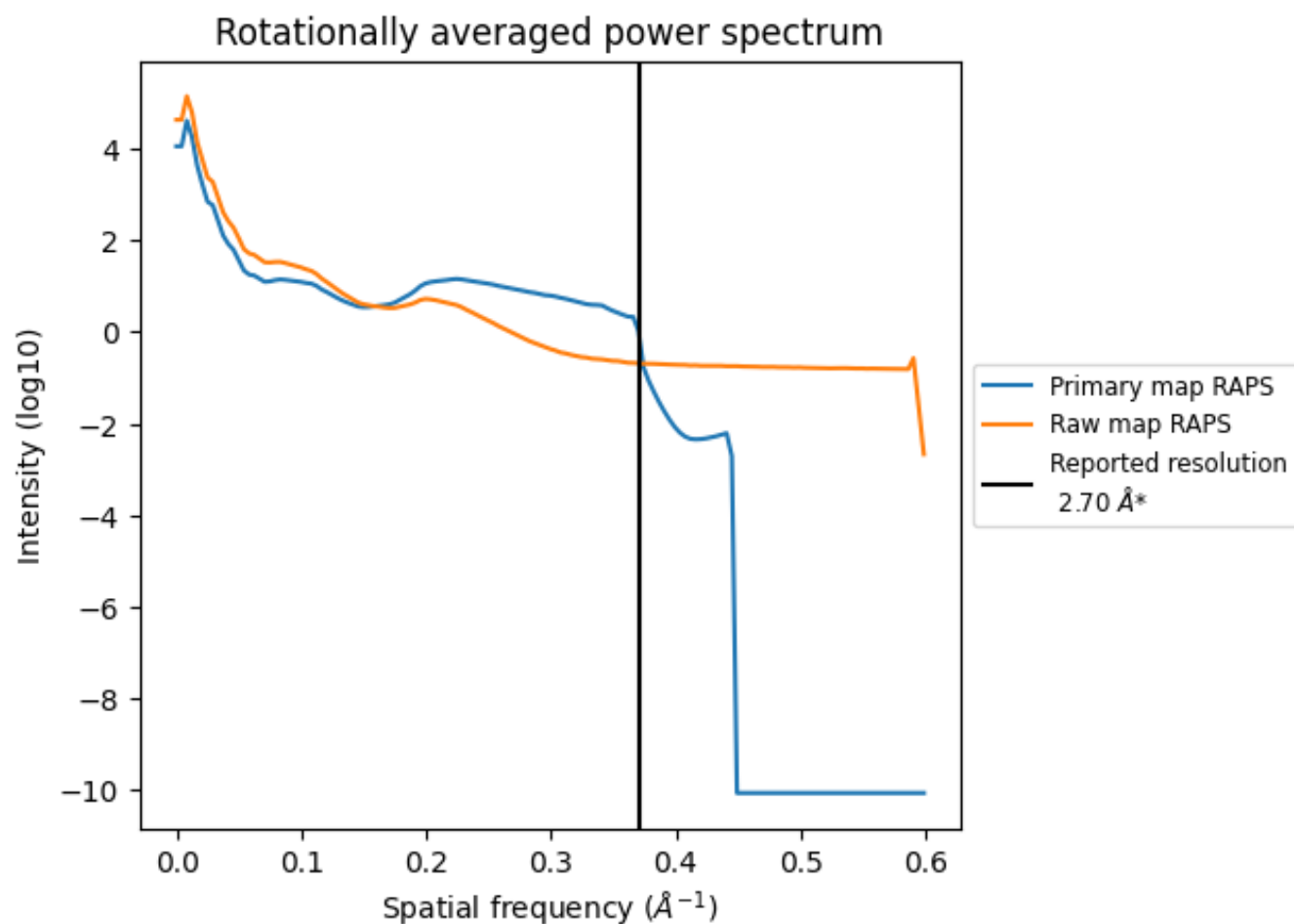
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 50 nm³; this corresponds to an approximate mass of 46 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 ⓘ

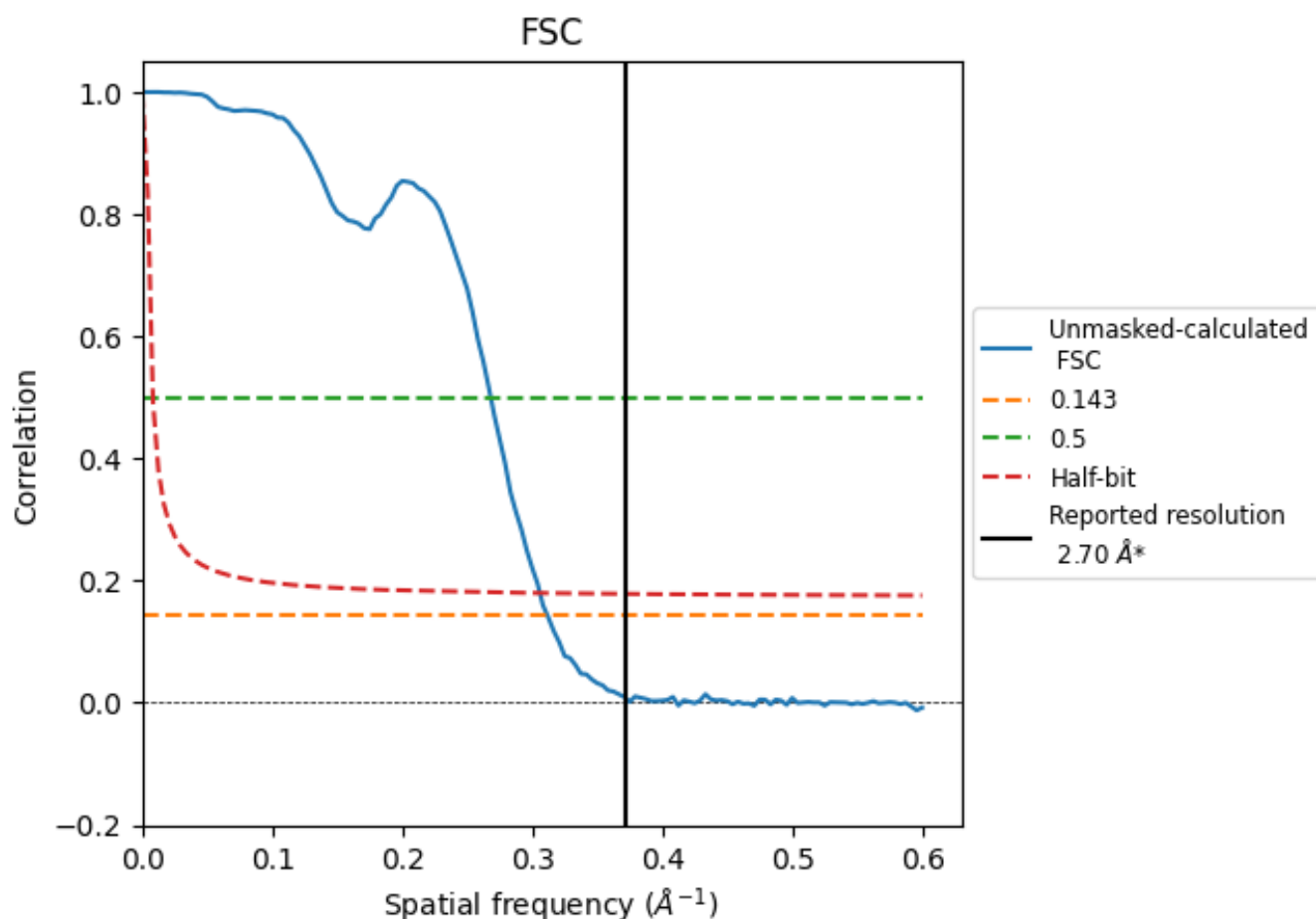


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

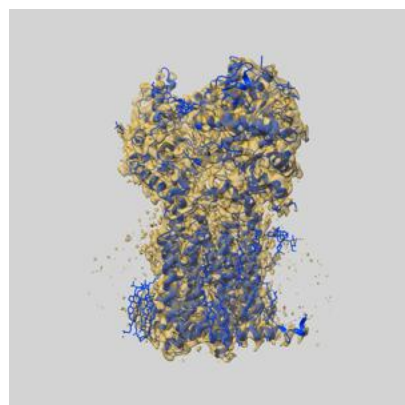
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.22	3.74	3.28

*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 3.22 differs from the reported value 2.7 by more than 10 %

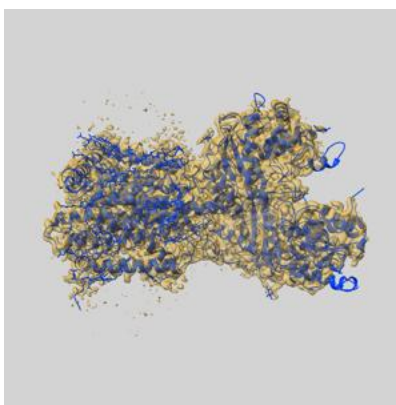
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24617 and PDB model 7RPK. Per-residue inclusion information can be found in section [3](#) on page [9](#).

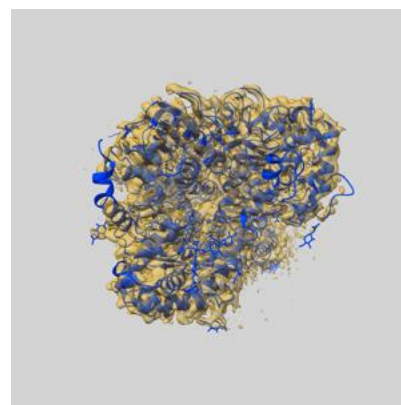
9.1 Map-model overlay [i](#)



X



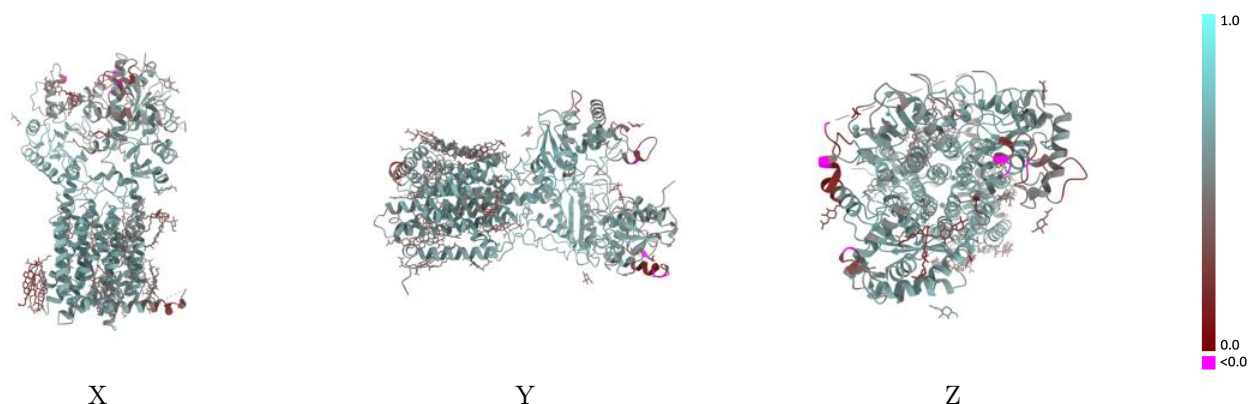
Y



Z

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](#)

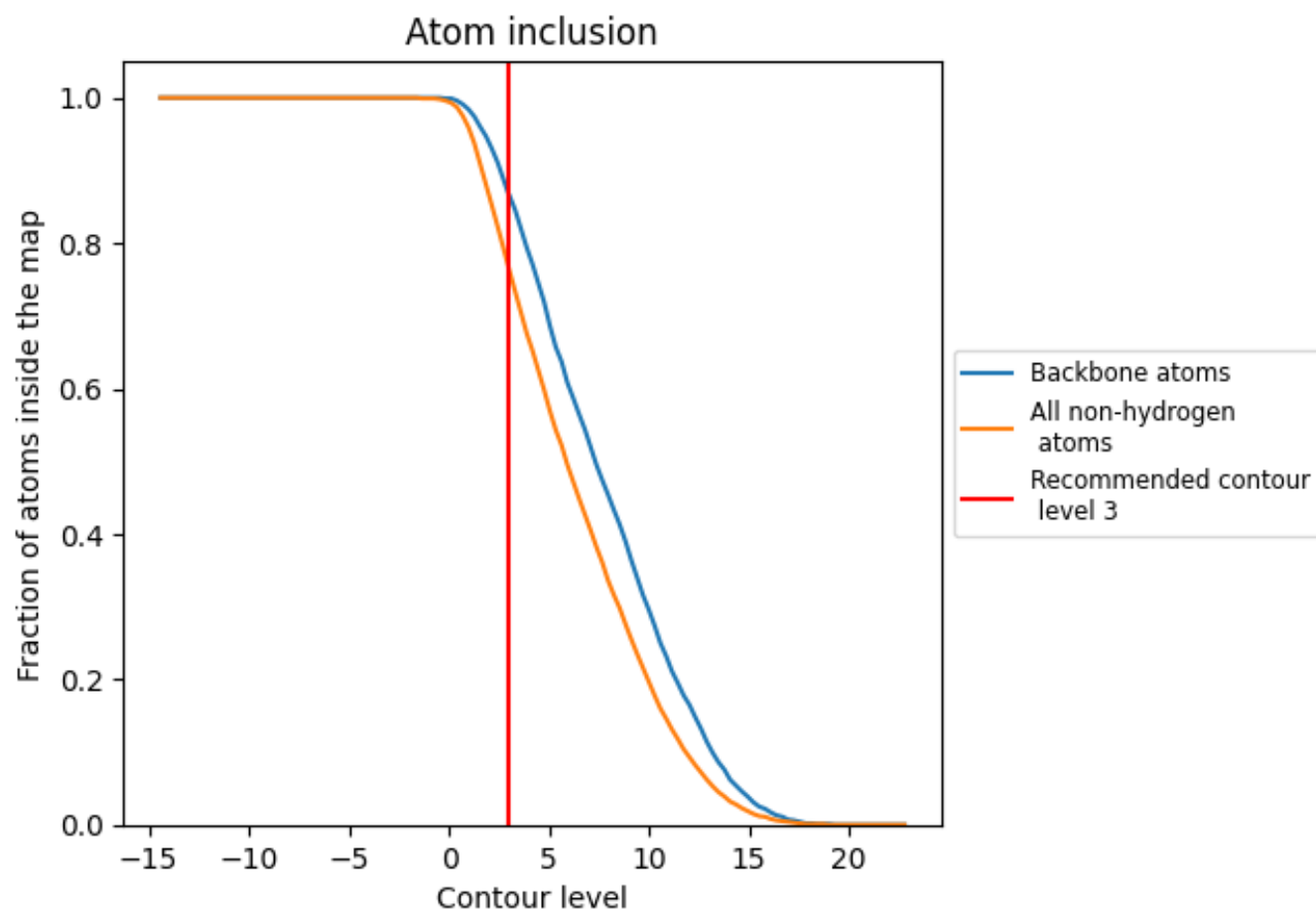


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 76% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7640	0.5470
A	0.7710	0.5480
H	0.7260	0.5360

