



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 06:09 pm BST

PDB ID : 7QA8
EMDB ID : EMD-13880
Title : Structure of the GPCR dimer Ste2 bound to an antagonist
Authors : Velazhahan, V.; Tate, C.G.
Deposited on : 2021-11-16
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

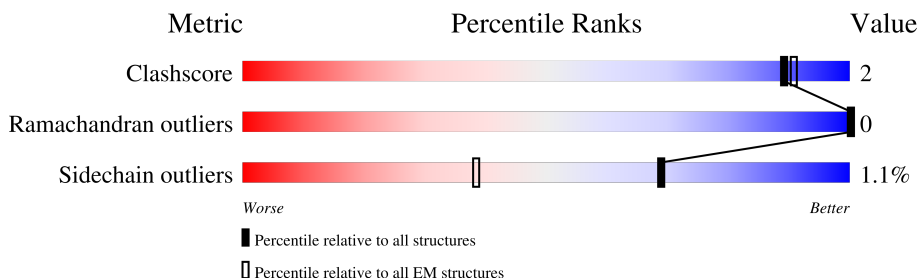
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	431	
1	B	431	
2	I	12	
2	K	12	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6111 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 Pheromone alpha factor receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	299	Total	C	N	O	S	0	0
			2299	1510	365	414	10		
1	B	299	Total	C	N	O	S	0	0
			2302	1511	366	415	10		

- Molecule 2 is a protein called HIS-ALA-LEU-GLN-LEU-LYS-PRO-GLY-GLN-PRO-NLE-TYR.

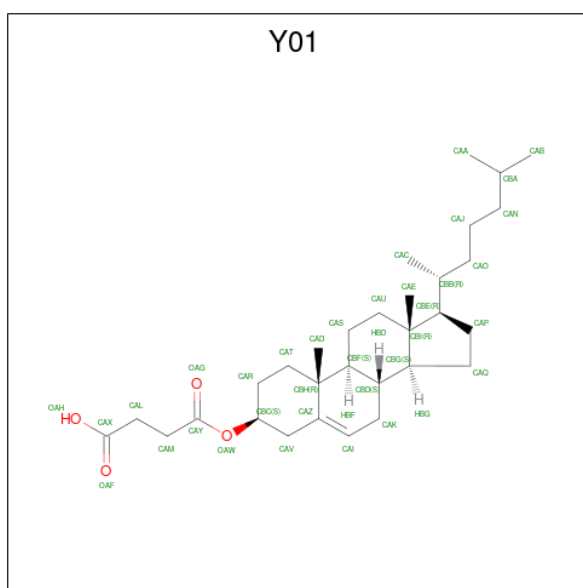
Mol	Chain	Residues	Atoms				AltConf	Trace
2	K	12	Total	C	N	O	0	0
			97	64	17	16		
2	I	12	Total	C	N	O	0	0
			97	64	17	16		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	32	Total	O	0
			32	32	
5	K	4	Total	O	0
			4	4	
5	I	4	Total	O	0
			4	4	
5	B	30	Total	O	0
			30	30	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	136877	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.213	Depositor
Minimum map value	-0.143	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0233	Depositor
Map size (\AA)	211.56, 211.56, 211.56	wwPDB
Map dimensions	246, 246, 246	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.86, 0.86, 0.86	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: Y01, NLE, 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	0.36	0/2346	0.61	0/3197
1	B	0.36	0/2349	0.61	0/3201
2	I	0.27	0/91	0.50	0/120
2	K	0.27	0/91	0.50	0/120
All	All	0.36	0/4877	0.61	0/6638

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2299	0	2377	9	0
1	B	2302	0	2381	7	0
2	I	97	0	98	0	0
2	K	97	0	98	0	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
4	A	560	0	784	8	0
4	B	595	0	833	6	0
4	I	35	0	49	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	32	0	0	0	0
5	B	30	0	0	0	0
5	I	4	0	0	0	0
5	K	4	0	0	0	0
All	All	6111	0	6672	22	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (22) 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)
4:B:509:Y01:HAQ1	4:B:516:Y01:HAQ2	1.88	0.55
4:B:509:Y01:HAO1	4:B:516:Y01:HAP2	1.87	0.55
4:A:508:Y01:HAN2	4:A:517:Y01:HAB2	1.93	0.49
4:A:503:Y01:HAK2	4:A:518:Y01:HAK2	1.95	0.48
1:A:64:LEU:HB3	1:B:64:LEU:HD23	1.96	0.48
1:B:277:LEU:HD21	4:B:517:Y01:HAT2	1.96	0.48
1:A:266:TYR:HE1	4:A:511:Y01:HAD2	1.77	0.48
1:A:64:LEU:HD23	1:B:64:LEU:HB3	1.95	0.47
1:A:257:VAL:HG11	4:A:507:Y01:HAB1	1.97	0.47
1:B:48:THR:HA	1:B:51:GLN:HG2	1.98	0.46
4:A:504:Y01:HAR1	4:A:505:Y01:HAD3	1.99	0.45
1:A:48:THR:HA	1:A:51:GLN:HG2	1.98	0.44
1:B:266:TYR:HE1	4:B:516:Y01:HAS1	1.81	0.44
1:B:58:ARG:HG2	1:B:283:LEU:HD13	2.00	0.43
1:A:111:TYR:HH	1:A:197:SER:HG	1.65	0.43
1:A:58:ARG:HG2	1:A:283:LEU:HD13	2.00	0.42
1:B:89:PHE:HE2	4:B:514:Y01:HAB1	1.83	0.42
4:A:510:Y01:HAE2	4:A:510:Y01:HBB	1.98	0.41
4:B:511:Y01:HAQ2	4:B:519:Y01:HAU1	2.03	0.41
4:A:510:Y01:HAO2	4:A:510:Y01:HAP1	1.45	0.41
1:A:67:ILE:HG12	4:A:508:Y01:HAQ2	2.03	0.40
1:A:225:LYS:NZ	1:A:296:ALA:O	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	297/431 (69%)	288 (97%)	9 (3%)	0	100	100
1	B	297/431 (69%)	288 (97%)	9 (3%)	0	100	100
2	I	9/12 (75%)	8 (89%)	1 (11%)	0	100	100
2	K	9/12 (75%)	8 (89%)	1 (11%)	0	100	100
All	All	612/886 (69%)	592 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/383 (67%)	255 (99%)	3 (1%)	67	86
1	B	259/383 (68%)	256 (99%)	3 (1%)	67	86
2	I	9/9 (100%)	9 (100%)	0	100	100
2	K	9/9 (100%)	9 (100%)	0	100	100
All	All	535/784 (68%)	529 (99%)	6 (1%)	69	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	TYR
1	A	106	TYR

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Mol	Chain	Res	Type
1	A	274	THR
1	B	98	TYR
1	B	106	TYR
1	B	274	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	B	51	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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
2	NLE	K	12	2	6,7,8	0.91	1 (16%)	2,7,9	0.33	0
2	NLE	I	12	2	6,7,8	0.91	1 (16%)	2,7,9	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NLE	K	12	2	-	0/5/6/8	-
2	NLE	I	12	2	-	0/5/6/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	12	NLE	O-C	2.10	1.28	1.19
2	I	12	NLE	O-C	2.09	1.28	1.19

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

38 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	$\# Z > 2$
4	Y01	A	518	-	38,38,38	0.51	0	57,57,57	0.68	1 (1%)
3	NAG	B	501	1	14,14,15	2.02	4 (28%)	17,19,21	1.36	4 (23%)
4	Y01	B	505	-	38,38,38	0.47	0	57,57,57	0.53	0
4	Y01	B	518	-	38,38,38	0.47	0	57,57,57	0.44	0
4	Y01	B	511	-	38,38,38	0.48	0	57,57,57	0.53	0
4	Y01	A	506	-	38,38,38	0.44	0	57,57,57	0.51	0
4	Y01	A	512	-	38,38,38	0.49	0	57,57,57	0.66	2 (3%)
4	Y01	B	508	-	38,38,38	0.50	0	57,57,57	0.53	0
4	Y01	A	504	-	38,38,38	0.49	0	57,57,57	0.48	0
4	Y01	A	510	-	38,38,38	0.48	0	57,57,57	0.52	0
4	Y01	B	509	-	38,38,38	0.44	0	57,57,57	0.49	0
4	Y01	I	101	-	38,38,38	0.46	0	57,57,57	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	Y01	B	512	-	38,38,38	0.50	0	57,57,57	0.52	0
4	Y01	A	513	-	38,38,38	0.49	0	57,57,57	0.52	0
4	Y01	A	503	-	38,38,38	0.47	0	57,57,57	0.53	0
4	Y01	B	519	-	38,38,38	0.47	0	57,57,57	0.46	0
3	NAG	B	502	1	14,14,15	2.02	4 (28%)	17,19,21	1.29	3 (17%)
4	Y01	A	509	-	38,38,38	0.49	0	57,57,57	0.46	0
4	Y01	A	507	-	38,38,38	0.47	0	57,57,57	0.52	0
4	Y01	A	508	-	38,38,38	0.50	0	57,57,57	0.49	0
4	Y01	A	517	-	38,38,38	0.49	0	57,57,57	0.56	0
4	Y01	B	506	-	38,38,38	0.48	0	57,57,57	0.48	0
4	Y01	B	516	-	38,38,38	0.47	0	57,57,57	0.57	0
4	Y01	B	517	-	38,38,38	0.47	0	57,57,57	0.47	0
4	Y01	A	514	-	38,38,38	0.50	0	57,57,57	0.65	1 (1%)
4	Y01	B	513	-	38,38,38	0.49	0	57,57,57	0.51	0
4	Y01	A	511	-	38,38,38	0.48	0	57,57,57	0.52	0
3	NAG	A	501	1	14,14,15	2.10	4 (28%)	17,19,21	1.53	2 (11%)
4	Y01	B	515	-	38,38,38	0.48	0	57,57,57	0.47	0
4	Y01	B	514	-	38,38,38	0.48	0	57,57,57	0.46	0
4	Y01	B	507	-	38,38,38	0.52	0	57,57,57	0.59	1 (1%)
3	NAG	A	502	1	14,14,15	2.03	4 (28%)	17,19,21	1.28	3 (17%)
4	Y01	A	515	-	38,38,38	0.48	0	57,57,57	0.53	0
4	Y01	B	504	-	38,38,38	0.48	0	57,57,57	0.51	0
4	Y01	A	516	-	38,38,38	0.48	0	57,57,57	0.50	0
4	Y01	A	505	-	38,38,38	0.48	0	57,57,57	0.53	0
4	Y01	B	510	-	38,38,38	0.48	0	57,57,57	0.50	0
4	Y01	B	503	-	38,38,38	0.49	0	57,57,57	0.57	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	Y01	A	518	-	-	7/19/77/77	0/4/4/4
3	NAG	B	501	1	-	1/6/23/26	0/1/1/1
4	Y01	B	505	-	-	2/19/77/77	0/4/4/4
4	Y01	B	518	-	-	6/19/77/77	0/4/4/4
4	Y01	B	511	-	-	6/19/77/77	0/4/4/4
4	Y01	A	506	-	-	11/19/77/77	0/4/4/4
4	Y01	A	512	-	-	5/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	Y01	B	508	-	-	10/19/77/77	0/4/4/4
4	Y01	A	504	-	-	4/19/77/77	0/4/4/4
4	Y01	A	510	-	-	8/19/77/77	0/4/4/4
4	Y01	B	509	-	-	9/19/77/77	0/4/4/4
4	Y01	I	101	-	-	11/19/77/77	0/4/4/4
4	Y01	B	512	-	-	9/19/77/77	0/4/4/4
4	Y01	A	513	-	-	4/19/77/77	0/4/4/4
4	Y01	A	503	-	-	6/19/77/77	0/4/4/4
4	Y01	B	519	-	-	8/19/77/77	0/4/4/4
3	NAG	B	502	1	-	2/6/23/26	0/1/1/1
4	Y01	A	509	-	-	8/19/77/77	0/4/4/4
4	Y01	A	507	-	-	7/19/77/77	0/4/4/4
4	Y01	A	508	-	-	8/19/77/77	0/4/4/4
4	Y01	A	517	-	-	4/19/77/77	0/4/4/4
4	Y01	B	506	-	-	8/19/77/77	0/4/4/4
4	Y01	B	516	-	-	8/19/77/77	0/4/4/4
4	Y01	B	517	-	-	5/19/77/77	0/4/4/4
4	Y01	A	514	-	-	3/19/77/77	0/4/4/4
4	Y01	B	513	-	-	6/19/77/77	0/4/4/4
4	Y01	A	511	-	-	7/19/77/77	0/4/4/4
3	NAG	A	501	1	-	2/6/23/26	0/1/1/1
4	Y01	B	515	-	-	2/19/77/77	0/4/4/4
4	Y01	B	514	-	-	8/19/77/77	0/4/4/4
4	Y01	B	507	-	-	6/19/77/77	0/4/4/4
3	NAG	A	502	1	-	1/6/23/26	0/1/1/1
4	Y01	A	515	-	-	3/19/77/77	0/4/4/4
4	Y01	B	504	-	-	6/19/77/77	0/4/4/4
4	Y01	A	516	-	-	6/19/77/77	0/4/4/4
4	Y01	A	505	-	-	9/19/77/77	0/4/4/4
4	Y01	B	510	-	-	6/19/77/77	0/4/4/4
4	Y01	B	503	-	-	6/19/77/77	0/4/4/4

All (16) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	NAG	O5-C1	5.24	1.52	1.43
3	B	501	NAG	O5-C1	4.80	1.51	1.43
3	A	502	NAG	O5-C1	4.79	1.51	1.43
3	B	502	NAG	O5-C1	4.59	1.51	1.43
3	B	501	NAG	C7-N2	3.55	1.46	1.34
3	A	502	NAG	C7-N2	3.54	1.46	1.34
3	B	502	NAG	C7-N2	3.51	1.46	1.34
3	A	501	NAG	C7-N2	3.45	1.46	1.34
3	A	502	NAG	C2-N2	2.80	1.51	1.46
3	B	501	NAG	C2-N2	2.73	1.51	1.46
3	B	502	NAG	C2-N2	2.64	1.50	1.46
3	A	501	NAG	O5-C5	2.41	1.48	1.43
3	B	502	NAG	O5-C5	2.31	1.48	1.43
3	A	501	NAG	C2-N2	2.24	1.50	1.46
3	A	502	NAG	O5-C5	2.07	1.47	1.43
3	B	501	NAG	O5-C5	2.03	1.47	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NAG	C1-O5-C5	3.90	117.48	112.19
4	A	518	Y01	OAW-CBC-CAR	2.96	115.47	108.33
3	A	501	NAG	C8-C7-N2	2.92	121.04	116.10
4	A	514	Y01	OAW-CBC-CAR	2.67	114.78	108.33
3	B	501	NAG	C2-N2-C7	2.59	126.59	122.90
3	A	502	NAG	C2-N2-C7	2.57	126.57	122.90
3	B	501	NAG	C4-C3-C2	2.44	114.59	111.02
3	B	501	NAG	C1-O5-C5	2.43	115.49	112.19
3	B	502	NAG	C2-N2-C7	2.37	126.28	122.90
3	A	502	NAG	C1-O5-C5	2.23	115.22	112.19
4	A	512	Y01	OAW-CBC-CAV	2.19	112.60	108.12
4	A	512	Y01	OAW-CBC-CAR	2.16	113.54	108.33
3	A	502	NAG	C4-C3-C2	2.07	114.05	111.02
3	B	502	NAG	O7-C7-C8	-2.06	118.24	122.06
4	B	507	Y01	OAW-CBC-CAR	2.04	113.25	108.33
3	B	502	NAG	C4-C3-C2	2.00	113.95	111.02
3	B	501	NAG	O7-C7-C8	-2.00	118.34	122.06

There are no chirality outliers.

All (228) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	Y01	CAM-CAY-OAW-CBC
4	A	504	Y01	OAG-CAY-OAW-CBC
4	A	504	Y01	CAM-CAY-OAW-CBC
4	A	505	Y01	CAM-CAY-OAW-CBC
4	A	509	Y01	OAG-CAY-OAW-CBC
4	A	509	Y01	CAM-CAY-OAW-CBC
4	A	510	Y01	CAO-CBB-CBE-CAP
4	A	510	Y01	CAC-CBB-CBE-CBI
4	A	511	Y01	CAV-CBC-OAW-CAY
4	A	512	Y01	CAR-CBC-OAW-CAY
4	A	513	Y01	OAG-CAY-OAW-CBC
4	A	516	Y01	OAG-CAY-OAW-CBC
4	A	518	Y01	CAR-CBC-OAW-CAY
4	I	101	Y01	CAR-CBC-OAW-CAY
4	I	101	Y01	CAM-CAY-OAW-CBC
4	B	504	Y01	OAG-CAY-OAW-CBC
4	B	506	Y01	CAM-CAY-OAW-CBC
4	B	509	Y01	CAR-CBC-OAW-CAY
4	B	509	Y01	OAG-CAY-OAW-CBC
4	B	509	Y01	CAM-CAY-OAW-CBC
4	B	510	Y01	OAG-CAY-OAW-CBC
4	B	511	Y01	CAM-CAY-OAW-CBC
4	B	512	Y01	OAG-CAY-OAW-CBC
4	B	514	Y01	OAG-CAY-OAW-CBC
4	B	514	Y01	CAM-CAY-OAW-CBC
4	B	516	Y01	CAV-CBC-OAW-CAY
4	B	516	Y01	CAM-CAY-OAW-CBC
4	B	517	Y01	CAM-CAY-OAW-CBC
4	B	518	Y01	OAG-CAY-OAW-CBC
4	B	518	Y01	CAM-CAY-OAW-CBC
4	B	519	Y01	OAG-CAY-OAW-CBC
4	A	514	Y01	CAV-CBC-OAW-CAY
4	A	510	Y01	CAC-CBB-CBE-CAP
4	B	509	Y01	CAC-CBB-CBE-CBI
4	A	510	Y01	CAO-CBB-CBE-CBI
4	A	503	Y01	OAG-CAY-OAW-CBC
4	A	505	Y01	OAG-CAY-OAW-CBC
4	I	101	Y01	OAG-CAY-OAW-CBC
4	B	506	Y01	OAG-CAY-OAW-CBC
4	B	507	Y01	OAG-CAY-OAW-CBC
4	B	516	Y01	OAG-CAY-OAW-CBC
4	B	517	Y01	OAG-CAY-OAW-CBC
4	A	513	Y01	CAM-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
4	A	516	Y01	CAM-CAY-OAW-CBC
4	A	517	Y01	CAM-CAY-OAW-CBC
4	B	504	Y01	CAM-CAY-OAW-CBC
4	B	507	Y01	CAM-CAY-OAW-CBC
4	B	510	Y01	CAM-CAY-OAW-CBC
4	B	512	Y01	CAM-CAY-OAW-CBC
4	B	519	Y01	CAM-CAY-OAW-CBC
4	B	509	Y01	CAC-CBB-CBE-CAP
4	B	509	Y01	CAO-CBB-CBE-CBI
4	B	511	Y01	OAG-CAY-OAW-CBC
4	B	509	Y01	CAO-CBB-CBE-CAP
3	A	501	NAG	O5-C5-C6-O6
4	B	518	Y01	CAR-CBC-OAW-CAY
4	A	506	Y01	CAJ-CAO-CBB-CBE
4	A	508	Y01	CAJ-CAO-CBB-CBE
4	B	512	Y01	CAJ-CAO-CBB-CBE
4	B	514	Y01	CAJ-CAO-CBB-CBE
3	A	501	NAG	C4-C5-C6-O6
4	A	509	Y01	CAJ-CAO-CBB-CAC
4	A	510	Y01	CAJ-CAO-CBB-CAC
4	A	518	Y01	CAJ-CAO-CBB-CAC
4	B	512	Y01	CAJ-CAO-CBB-CAC
4	B	514	Y01	CAJ-CAO-CBB-CAC
4	A	509	Y01	CAJ-CAO-CBB-CBE
4	A	510	Y01	CAJ-CAO-CBB-CBE
4	A	518	Y01	CAJ-CAO-CBB-CBE
4	B	507	Y01	CAJ-CAO-CBB-CBE
4	B	508	Y01	CAJ-CAO-CBB-CBE
4	B	503	Y01	CAM-CAY-OAW-CBC
4	B	504	Y01	CAV-CBC-OAW-CAY
4	B	519	Y01	CAV-CBC-OAW-CAY
4	A	517	Y01	OAG-CAY-OAW-CBC
4	B	507	Y01	CAJ-CAO-CBB-CAC
4	I	101	Y01	CAN-CAJ-CAO-CBB
4	A	508	Y01	CAJ-CAO-CBB-CAC
4	B	508	Y01	CAJ-CAO-CBB-CAC
4	A	506	Y01	CAM-CAY-OAW-CBC
4	A	511	Y01	CAM-CAY-OAW-CBC
4	B	513	Y01	CAJ-CAO-CBB-CBE
4	A	506	Y01	CAJ-CAO-CBB-CAC
4	A	507	Y01	CAN-CAJ-CAO-CBB
4	B	512	Y01	CAO-CAJ-CAN-CBA

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Mol	Chain	Res	Type	Atoms
4	B	504	Y01	CAR-CBC-OAW-CAY
4	A	511	Y01	OAG-CAY-OAW-CBC
4	B	519	Y01	CAR-CBC-OAW-CAY
4	A	505	Y01	CAX-CAL-CAM-CAY
4	A	512	Y01	CAM-CAY-OAW-CBC
4	A	506	Y01	OAG-CAY-OAW-CBC
4	A	512	Y01	OAG-CAY-OAW-CBC
4	B	503	Y01	OAG-CAY-OAW-CBC
4	B	512	Y01	CAV-CBC-OAW-CAY
4	B	518	Y01	CAV-CBC-OAW-CAY
4	A	506	Y01	CAX-CAL-CAM-CAY
4	B	513	Y01	CAM-CAY-OAW-CBC
4	B	513	Y01	OAG-CAY-OAW-CBC
4	B	513	Y01	CAJ-CAO-CBB-CAC
4	A	508	Y01	CAN-CAJ-CAO-CBB
4	B	510	Y01	CAV-CBC-OAW-CAY
4	A	506	Y01	CAO-CBB-CBE-CBI
4	B	512	Y01	CAR-CBC-OAW-CAY
4	B	517	Y01	CAN-CAJ-CAO-CBB
4	B	510	Y01	CAR-CBC-OAW-CAY
4	A	506	Y01	CAC-CBB-CBE-CAP
4	A	506	Y01	CAC-CBB-CBE-CBI
4	A	508	Y01	CAM-CAY-OAW-CBC
4	A	506	Y01	CAO-CBB-CBE-CAP
4	B	507	Y01	CAL-CAM-CAY-OAW
4	A	508	Y01	OAG-CAY-OAW-CBC
4	A	518	Y01	CAM-CAY-OAW-CBC
4	A	515	Y01	CAL-CAM-CAY-OAW
4	A	516	Y01	CAV-CBC-OAW-CAY
4	A	518	Y01	OAG-CAY-OAW-CBC
3	B	502	NAG	C4-C5-C6-O6
4	A	505	Y01	CAO-CAJ-CAN-CBA
4	B	515	Y01	CAM-CAY-OAW-CBC
4	A	505	Y01	CAO-CBB-CBE-CBI
4	A	509	Y01	CAV-CBC-OAW-CAY
4	A	505	Y01	CAO-CBB-CBE-CAP
4	I	101	Y01	CAO-CBB-CBE-CAP
4	A	505	Y01	CAC-CBB-CBE-CBI
4	B	506	Y01	CAO-CBB-CBE-CAP
4	A	517	Y01	CAN-CAJ-CAO-CBB
4	A	507	Y01	CAO-CBB-CBE-CAP
4	B	503	Y01	CAN-CAJ-CAO-CBB

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Mol	Chain	Res	Type	Atoms
4	I	101	Y01	CAO-CBB-CBE-CBI
4	B	513	Y01	CAM-CAL-CAX-OAF
4	A	516	Y01	CAR-CBC-OAW-CAY
4	A	505	Y01	CAM-CAL-CAX-OAF
4	B	514	Y01	CAM-CAL-CAX-OAF
4	B	506	Y01	CAC-CBB-CBE-CBI
4	A	516	Y01	CAM-CAL-CAX-OAF
4	B	512	Y01	CAM-CAL-CAX-OAF
4	B	516	Y01	CAM-CAL-CAX-OAH
4	B	518	Y01	CAM-CAL-CAX-OAF
4	A	510	Y01	CAM-CAL-CAX-OAF
4	B	506	Y01	CAM-CAL-CAX-OAF
4	I	101	Y01	CAC-CBB-CBE-CBI
4	A	508	Y01	CAM-CAL-CAX-OAF
4	A	514	Y01	CAM-CAL-CAX-OAH
4	B	505	Y01	CAM-CAL-CAX-OAF
4	B	510	Y01	CAM-CAL-CAX-OAF
4	A	503	Y01	CAM-CAL-CAX-OAH
4	A	515	Y01	CAM-CAL-CAX-OAF
4	B	511	Y01	CAM-CAL-CAX-OAF
4	B	516	Y01	CAM-CAL-CAX-OAF
4	B	509	Y01	CAM-CAL-CAX-OAF
4	B	519	Y01	CAM-CAL-CAX-OAF
4	B	515	Y01	OAG-CAY-OAW-CBC
4	A	503	Y01	CAM-CAL-CAX-OAF
4	A	506	Y01	CAM-CAL-CAX-OAF
4	A	507	Y01	CAM-CAL-CAX-OAF
4	A	510	Y01	CAM-CAL-CAX-OAH
4	A	506	Y01	CAM-CAL-CAX-OAH
4	A	509	Y01	CAM-CAL-CAX-OAF
4	A	507	Y01	CAC-CBB-CBE-CBI
4	B	514	Y01	CAV-CBC-OAW-CAY
4	B	506	Y01	CAM-CAL-CAX-OAH
4	B	513	Y01	CAM-CAL-CAX-OAH
4	A	507	Y01	CAO-CBB-CBE-CBI
4	A	514	Y01	CAM-CAL-CAX-OAF
4	B	508	Y01	CAM-CAL-CAX-OAH
4	A	511	Y01	CAM-CAL-CAX-OAH
4	B	505	Y01	CAM-CAL-CAX-OAH
4	B	511	Y01	CAM-CAL-CAX-OAH
4	B	514	Y01	CAM-CAL-CAX-OAH
4	A	507	Y01	CAM-CAL-CAX-OAH

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Mol	Chain	Res	Type	Atoms
4	B	510	Y01	CAM-CAL-CAX-OAH
4	A	511	Y01	CAM-CAL-CAX-OAF
4	B	503	Y01	CAM-CAL-CAX-OAF
4	A	505	Y01	CAM-CAL-CAX-OAH
4	B	518	Y01	CAM-CAL-CAX-OAH
4	A	509	Y01	CAM-CAL-CAX-OAH
4	B	509	Y01	CAM-CAL-CAX-OAH
4	B	506	Y01	CAO-CBB-CBE-CBI
4	A	508	Y01	CAM-CAL-CAX-OAH
4	A	516	Y01	CAM-CAL-CAX-OAH
4	B	512	Y01	CAM-CAL-CAX-OAH
4	B	503	Y01	CAM-CAL-CAX-OAH
4	A	515	Y01	CAM-CAL-CAX-OAH
4	B	508	Y01	CAM-CAL-CAX-OAF
4	B	516	Y01	CAC-CBB-CBE-CBI
4	B	519	Y01	CAM-CAL-CAX-OAH
4	A	512	Y01	CAM-CAL-CAX-OAH
4	B	517	Y01	CAM-CAL-CAX-OAH
4	B	508	Y01	CAM-CAY-OAW-CBC
4	A	518	Y01	CAM-CAL-CAX-OAH
4	B	507	Y01	CAL-CAM-CAY-OAG
4	A	504	Y01	CAJ-CAO-CBB-CBE
4	A	518	Y01	CAM-CAL-CAX-OAF
4	A	509	Y01	CAR-CBC-OAW-CAY
4	B	504	Y01	CAM-CAL-CAX-OAH
4	B	517	Y01	CAM-CAL-CAX-OAF
4	B	506	Y01	CAC-CBB-CBE-CAP
4	B	508	Y01	OAG-CAY-OAW-CBC
4	A	513	Y01	CAM-CAL-CAX-OAH
4	I	101	Y01	CAM-CAL-CAX-OAH
4	I	101	Y01	CAM-CAL-CAX-OAF
4	B	516	Y01	CAN-CAJ-CAO-CBB
4	A	513	Y01	CAM-CAL-CAX-OAF
4	B	504	Y01	CAM-CAL-CAX-OAF
4	A	512	Y01	CAM-CAL-CAX-OAF
4	B	508	Y01	CAL-CAM-CAY-OAW
4	B	508	Y01	CAO-CBB-CBE-CAP
4	A	508	Y01	CAR-CBC-OAW-CAY
4	A	507	Y01	CAM-CAY-OAW-CBC
3	A	502	NAG	C3-C2-N2-C7
3	B	501	NAG	C3-C2-N2-C7
3	B	502	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	B	508	Y01	CAC-CBB-CBE-CBI
4	A	517	Y01	CAJ-CAN-CBA-CAB
4	B	508	Y01	CAL-CAM-CAY-OAG
4	B	503	Y01	CAJ-CAO-CBB-CBE
4	B	519	Y01	CAC-CBB-CBE-CBI
4	B	511	Y01	CAL-CAM-CAY-OAW
4	I	101	Y01	CAC-CBB-CBE-CAP
4	A	511	Y01	CAX-CAL-CAM-CAY
4	I	101	Y01	CAL-CAM-CAY-OAW
4	A	511	Y01	CAN-CAJ-CAO-CBB
4	B	516	Y01	CAO-CBB-CBE-CAP
4	B	519	Y01	CAO-CBB-CBE-CAP
4	A	503	Y01	CAL-CAM-CAY-OAW
4	B	514	Y01	CAR-CBC-OAW-CAY
4	A	503	Y01	CAL-CAM-CAY-OAG
4	B	511	Y01	CAL-CAM-CAY-OAG
4	A	504	Y01	CAL-CAM-CAY-OAW

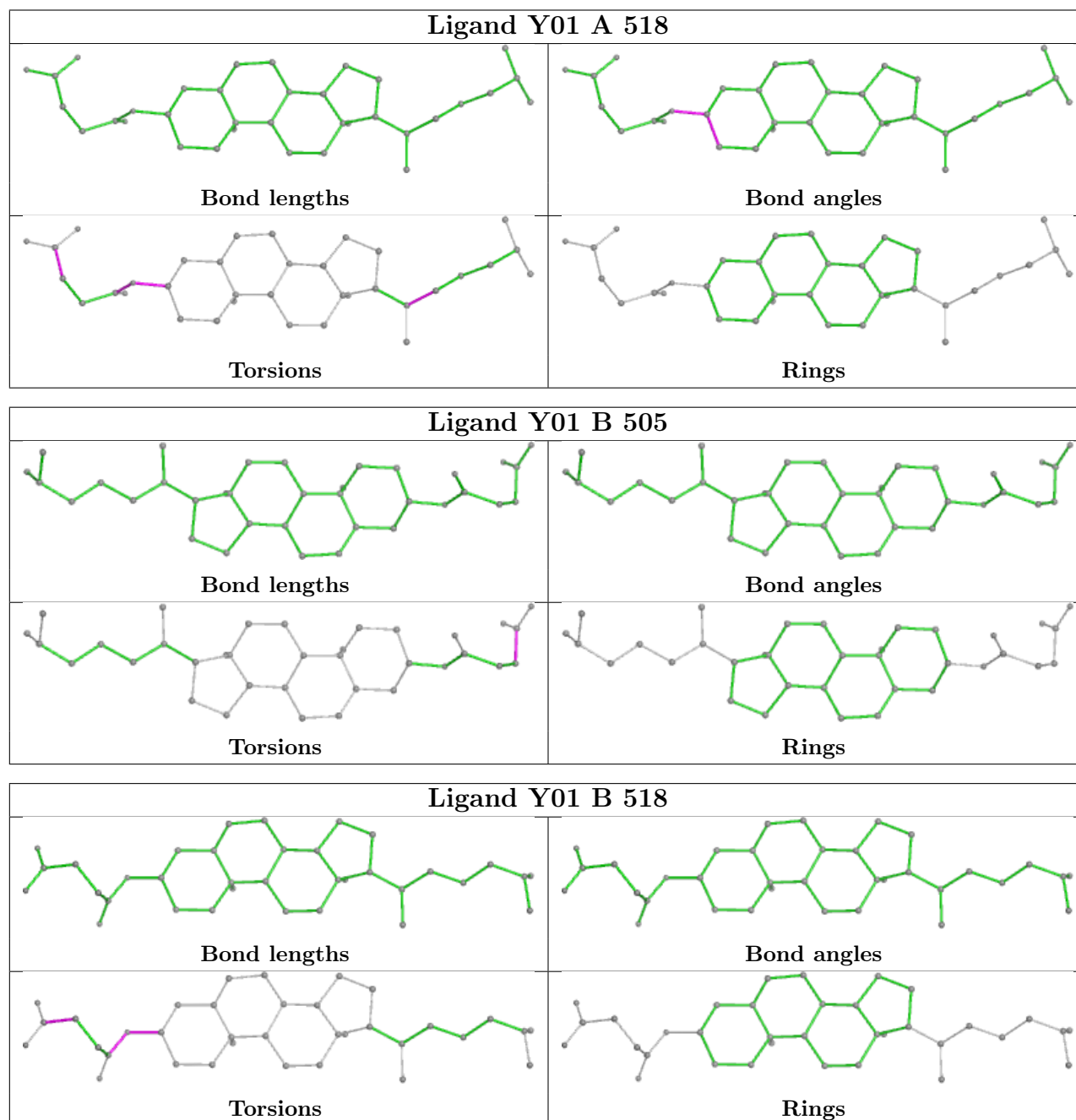
There are no ring outliers.

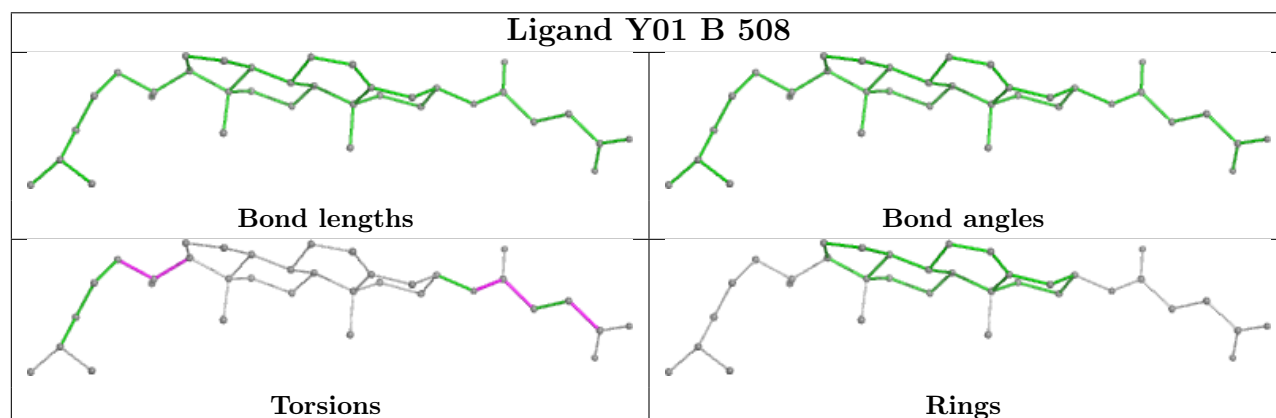
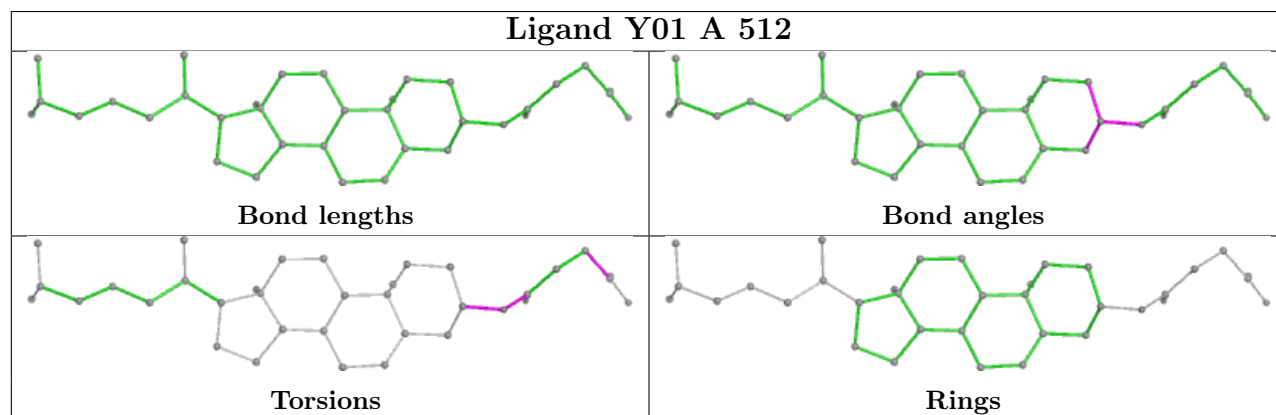
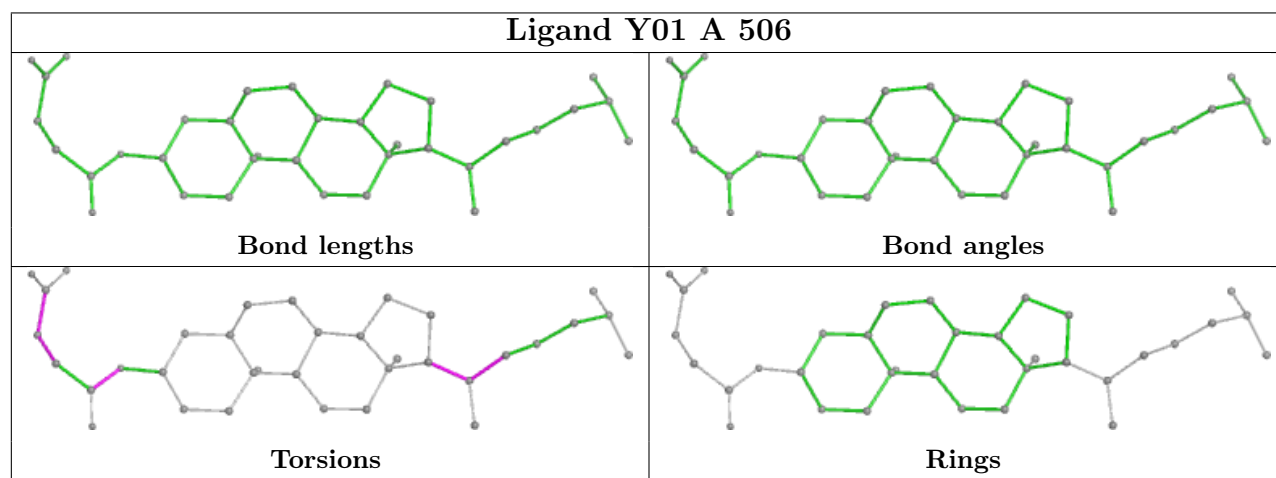
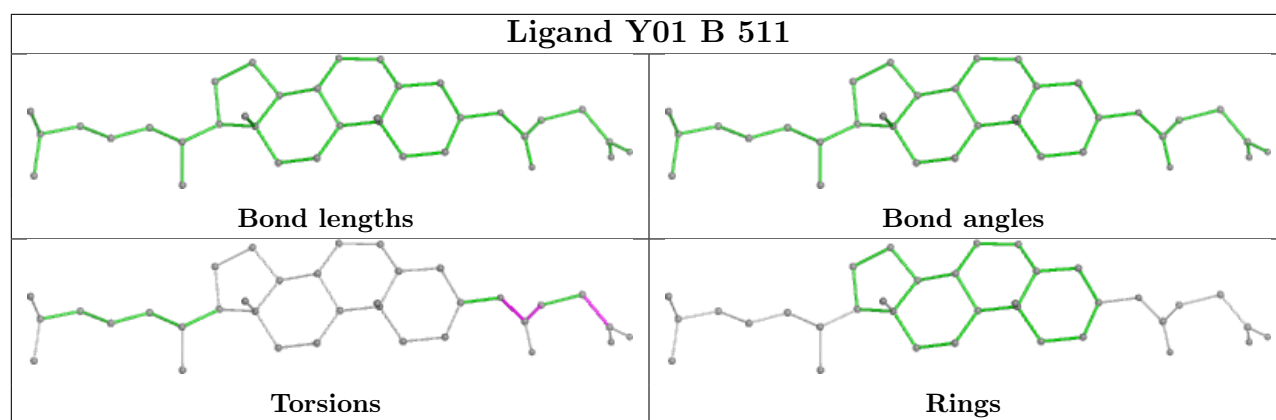
15 monomers are involved in 14 short contacts:

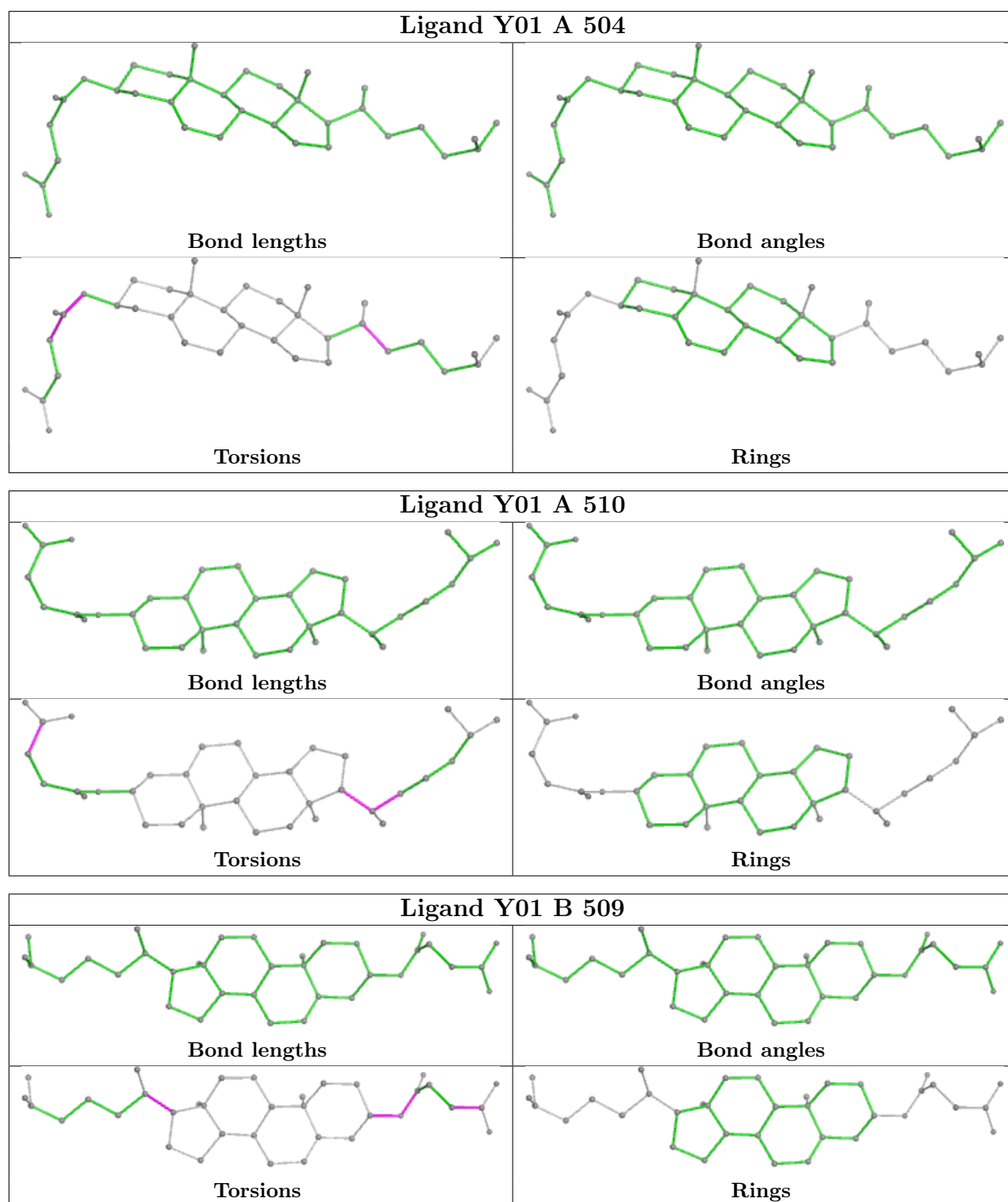
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	518	Y01	1	0
4	B	511	Y01	1	0
4	A	504	Y01	1	0
4	A	510	Y01	2	0
4	B	509	Y01	2	0
4	A	503	Y01	1	0
4	B	519	Y01	1	0
4	A	507	Y01	1	0
4	A	508	Y01	2	0
4	A	517	Y01	1	0
4	B	516	Y01	3	0
4	B	517	Y01	1	0
4	A	511	Y01	1	0
4	B	514	Y01	1	0
4	A	505	Y01	1	0

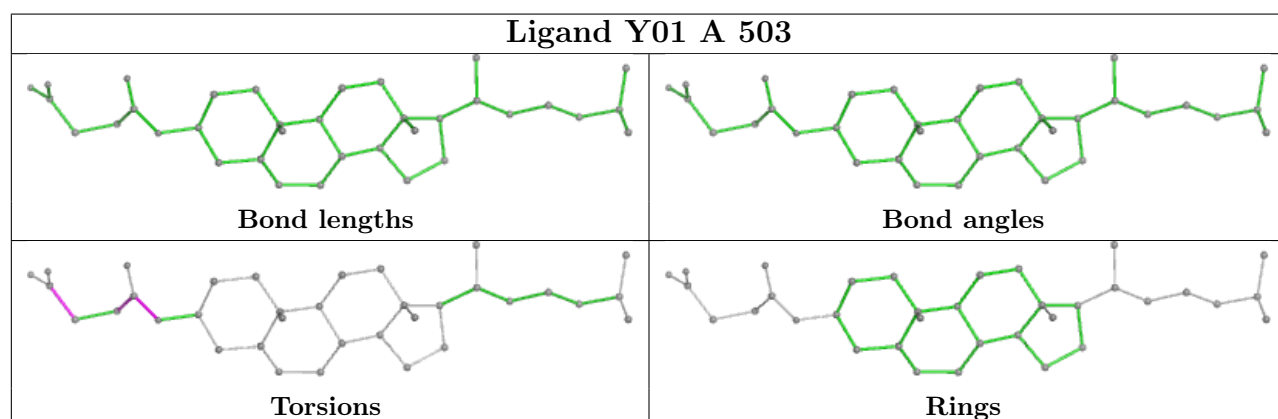
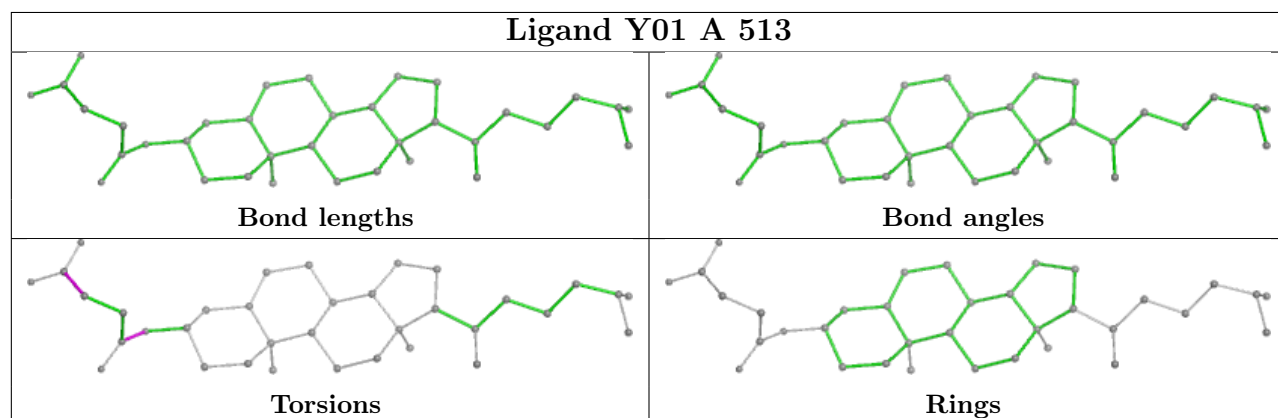
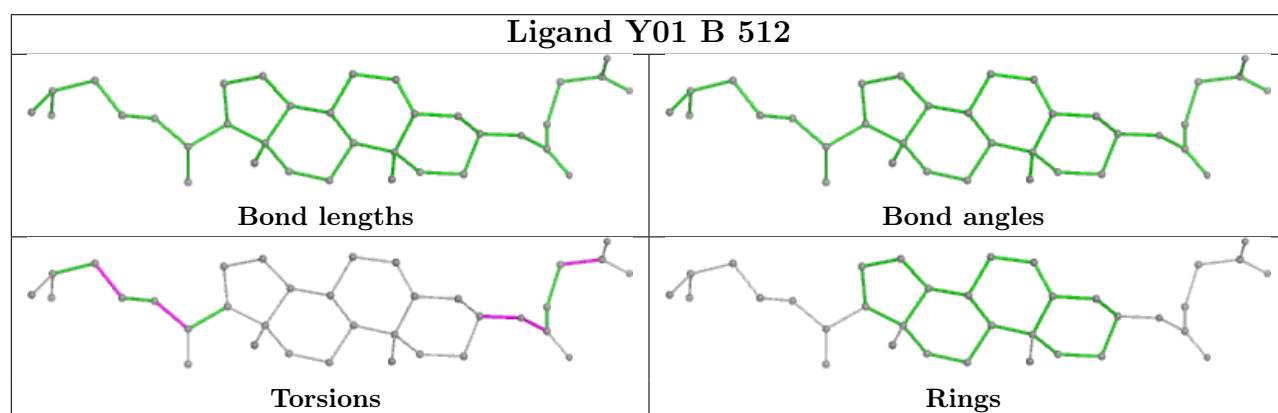
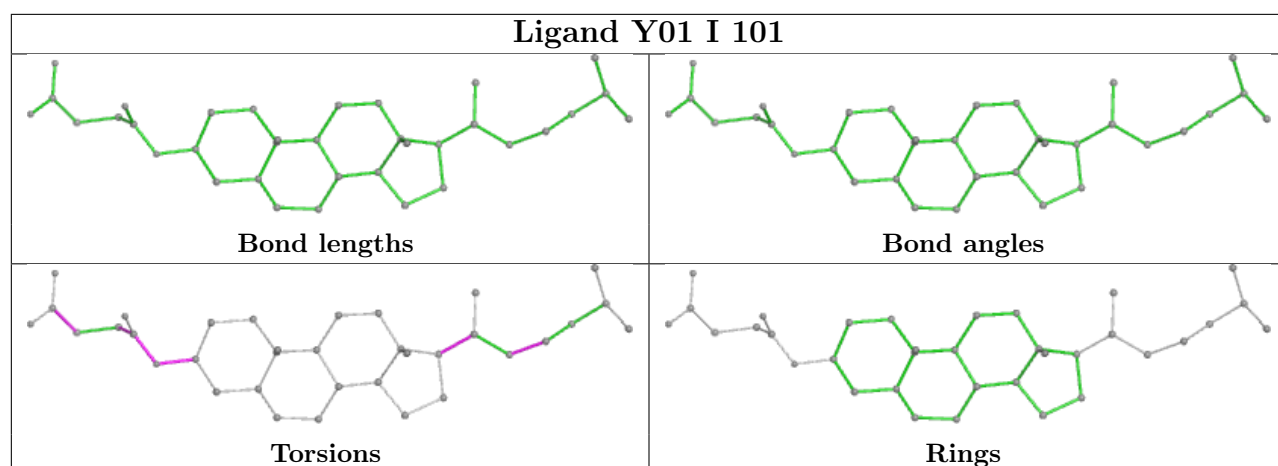
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

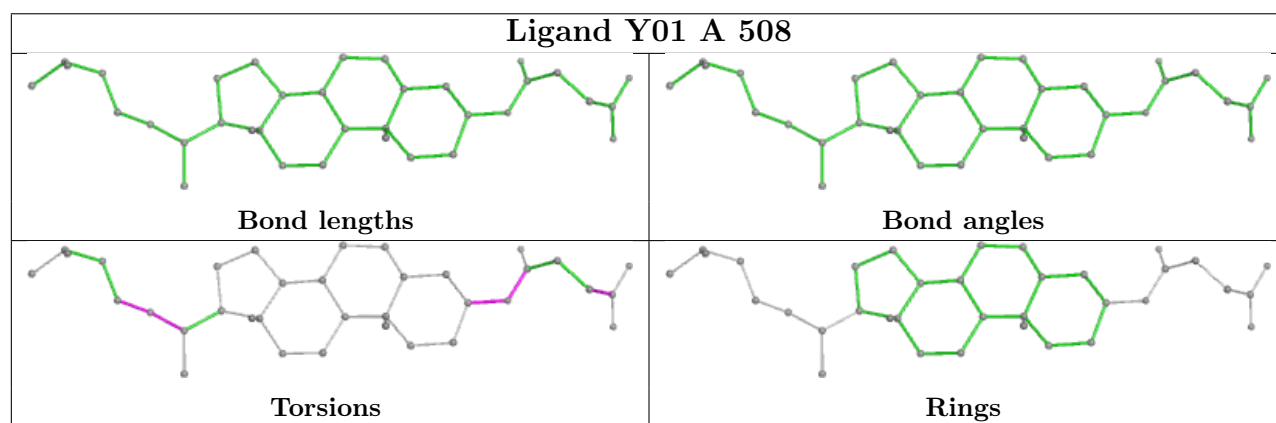
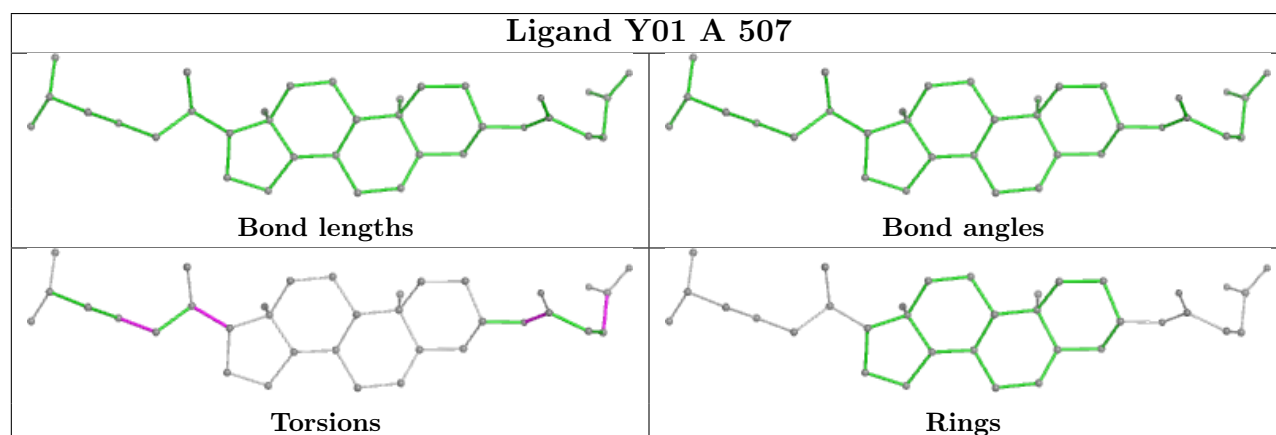
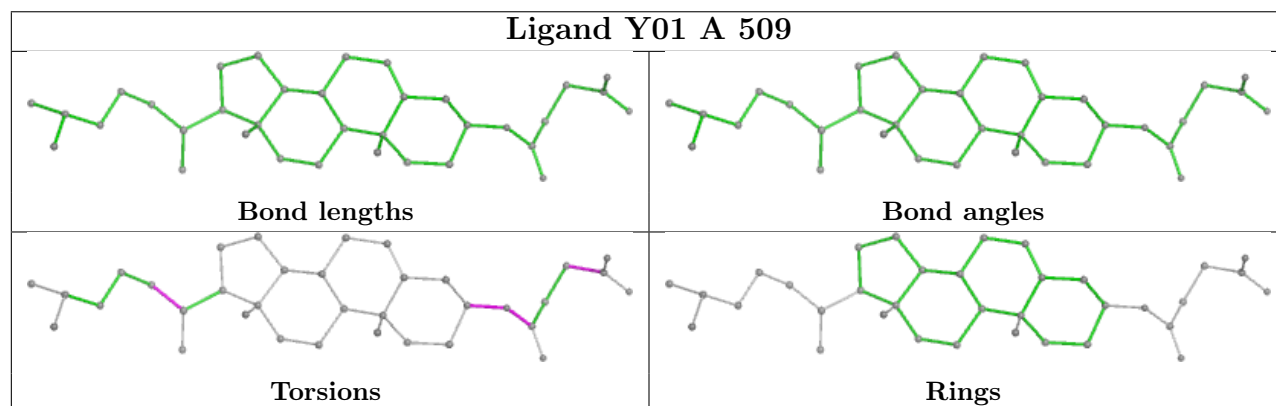
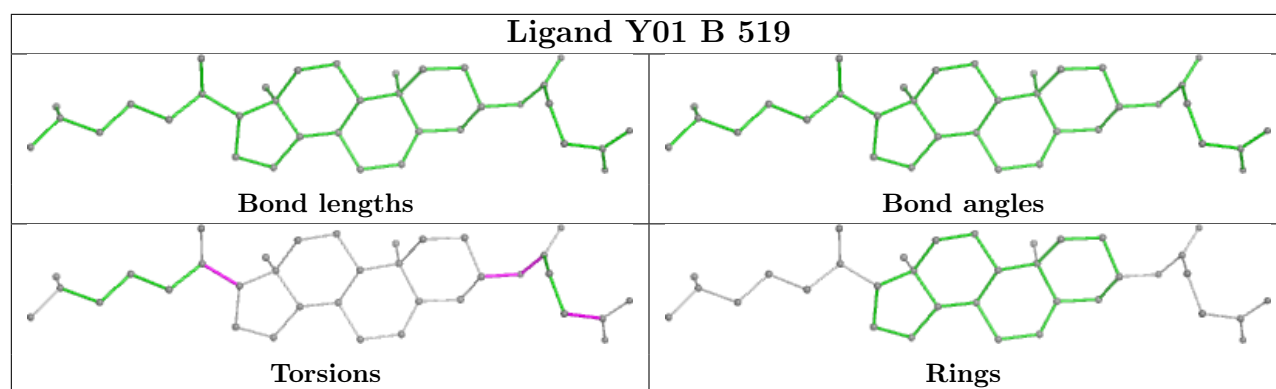
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



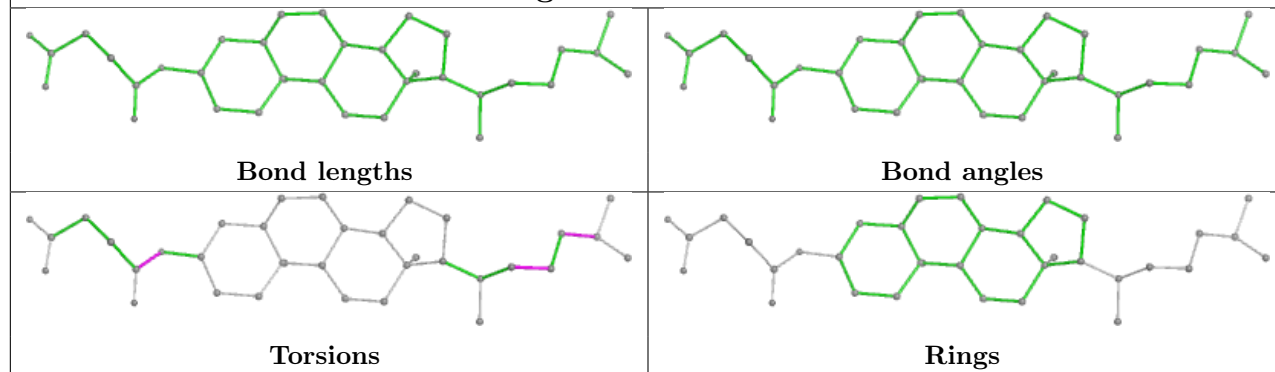




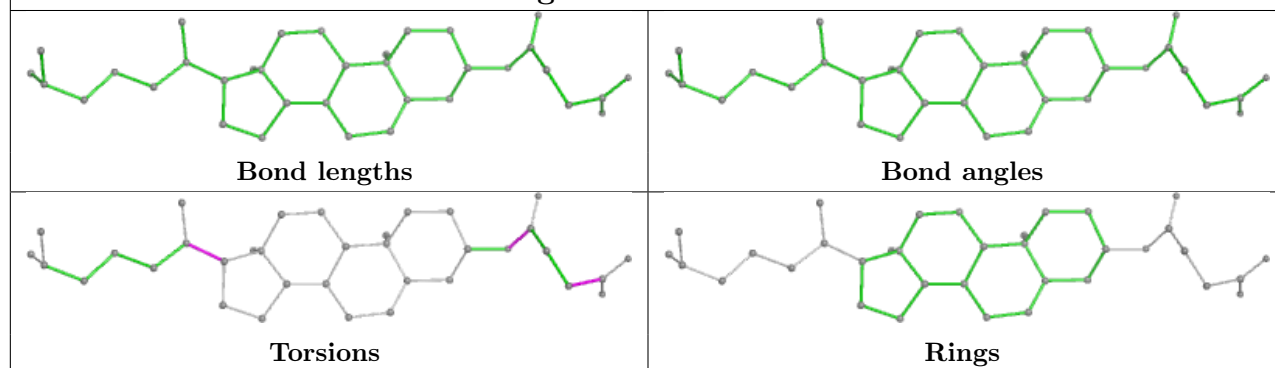




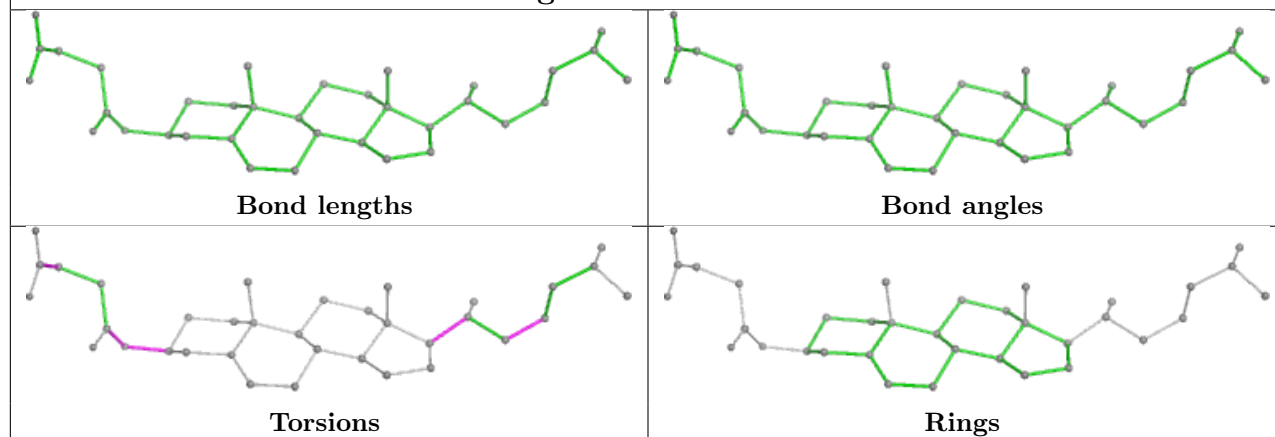
Ligand Y01 A 517



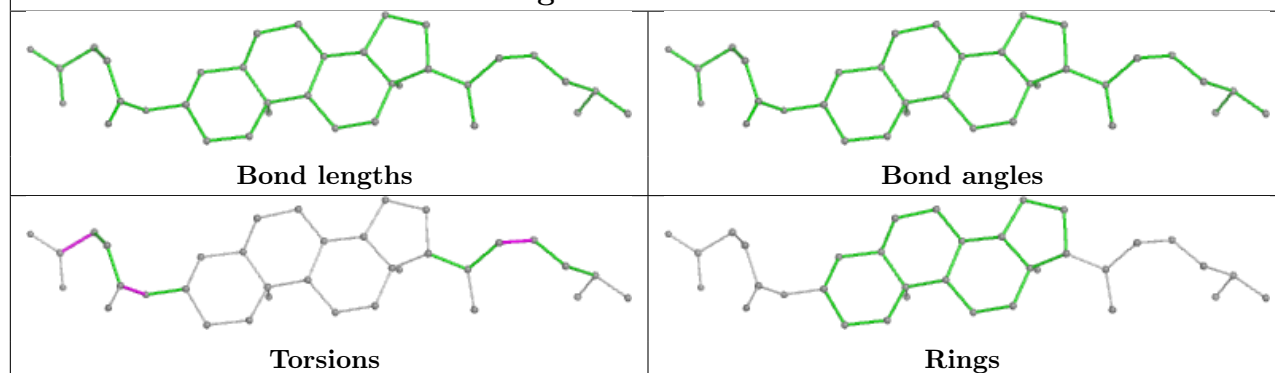
Ligand Y01 B 506

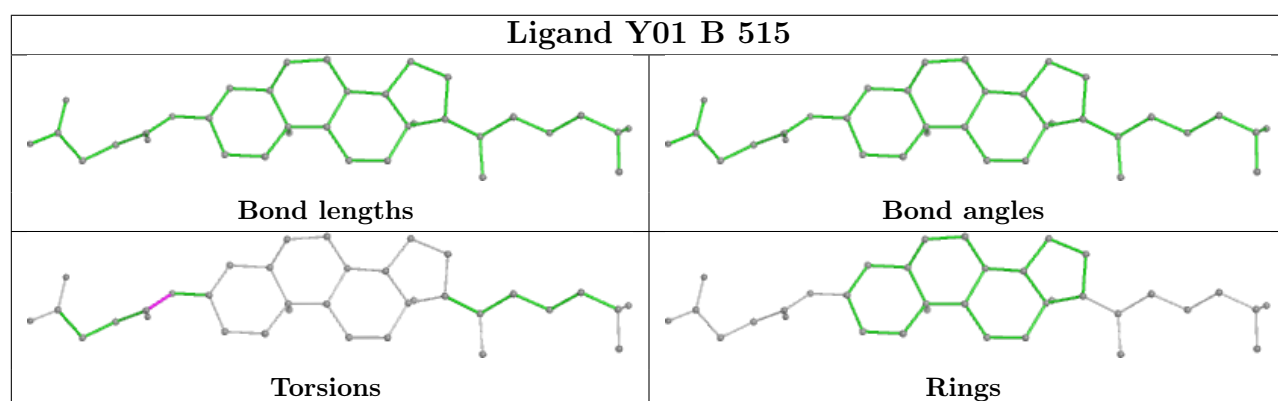
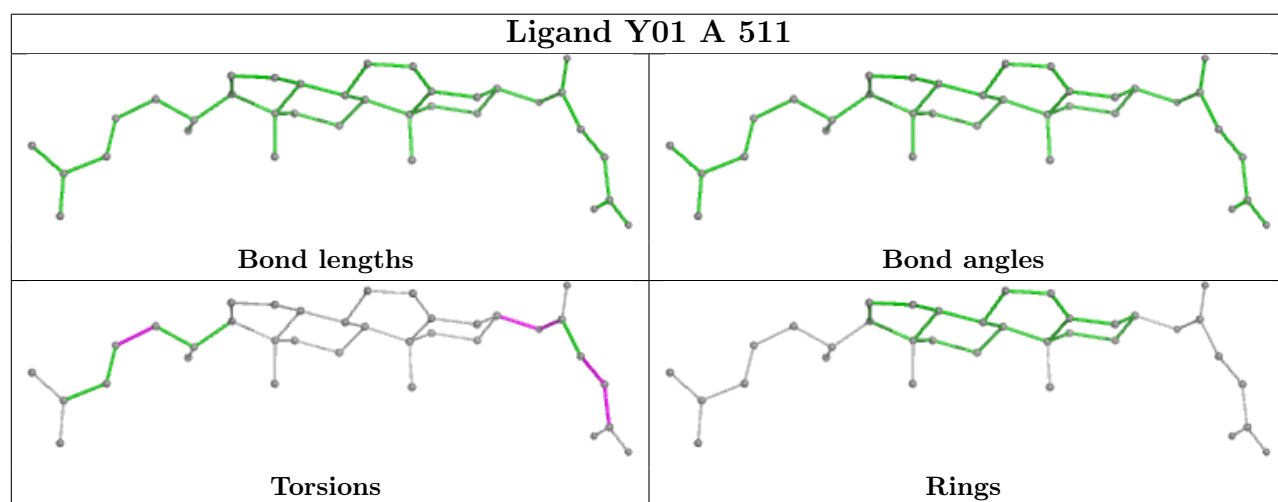
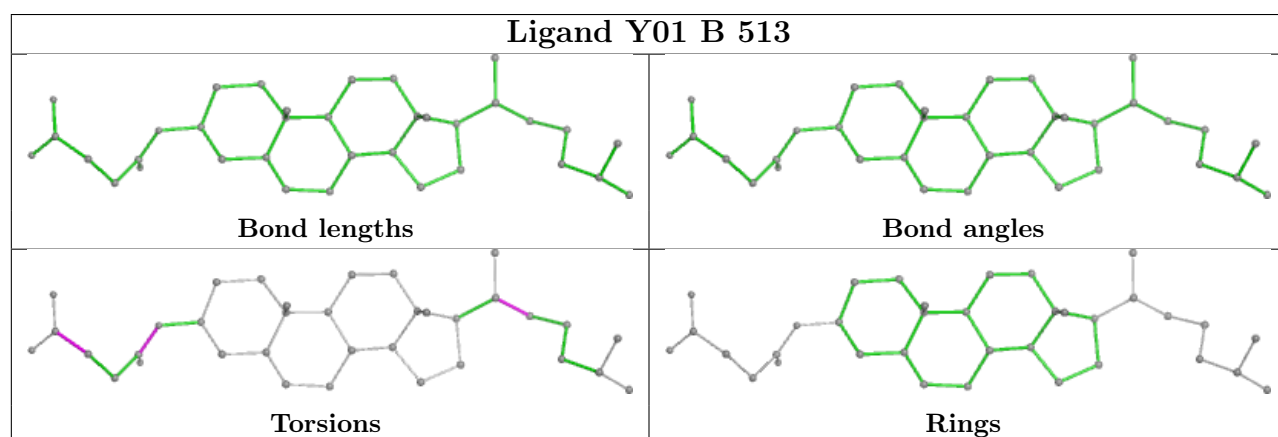
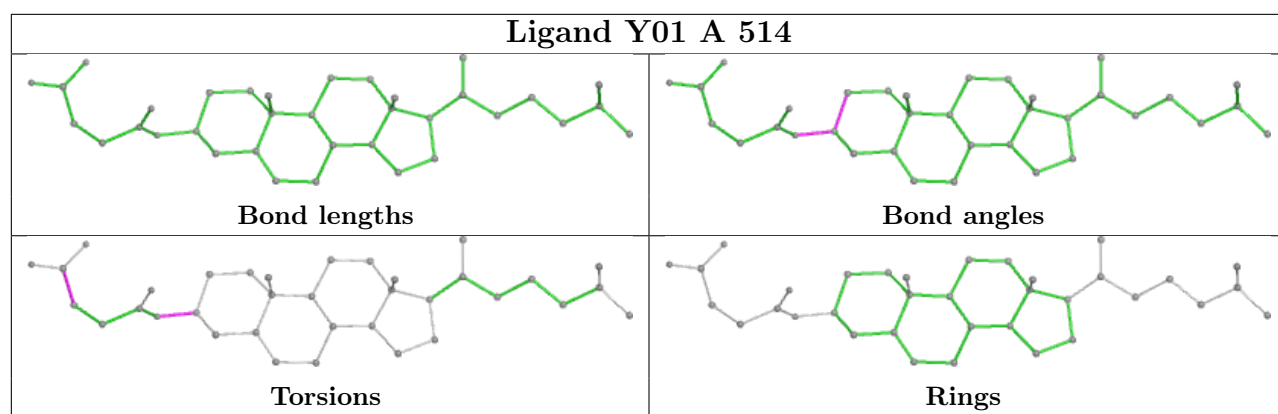


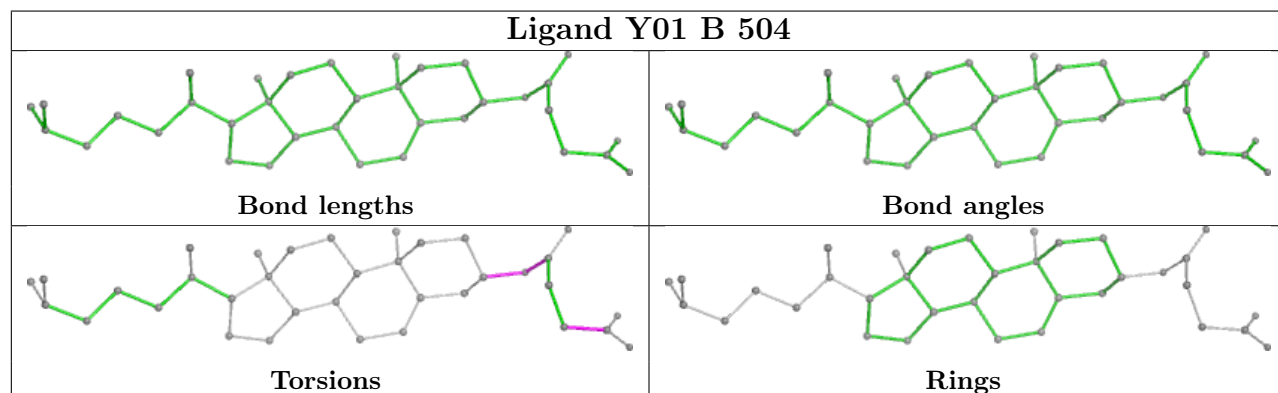
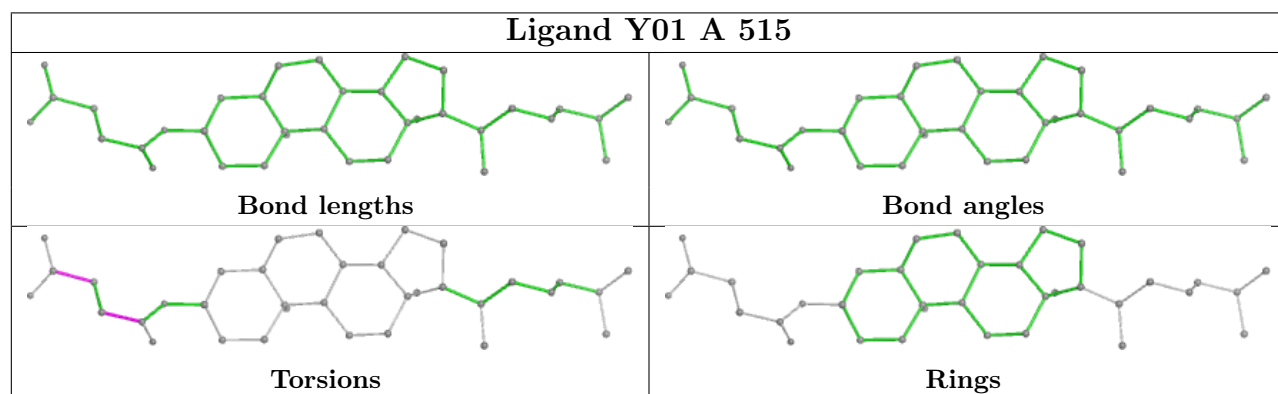
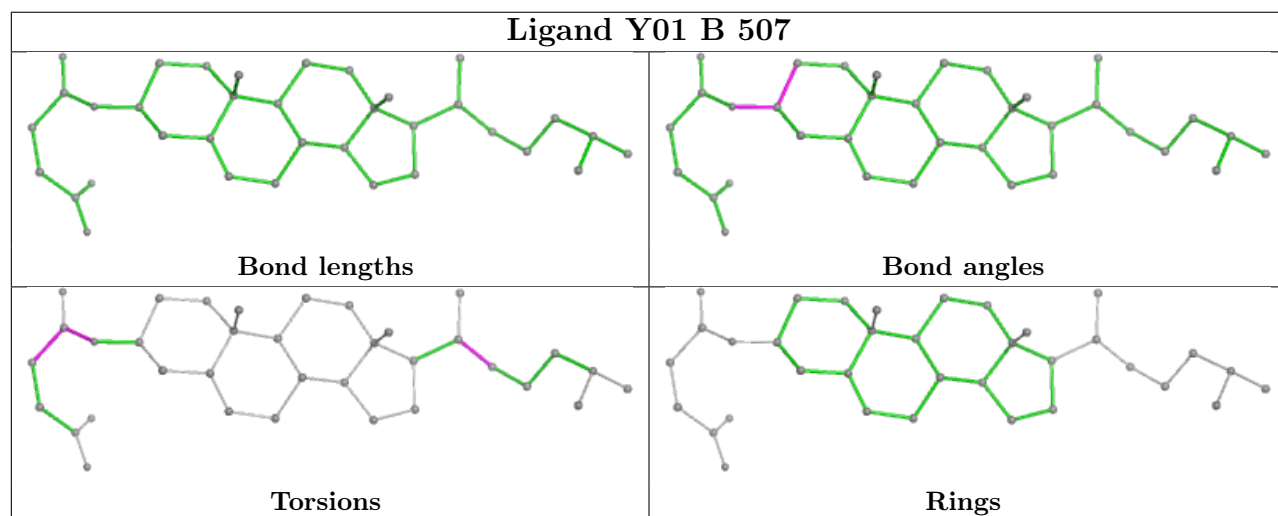
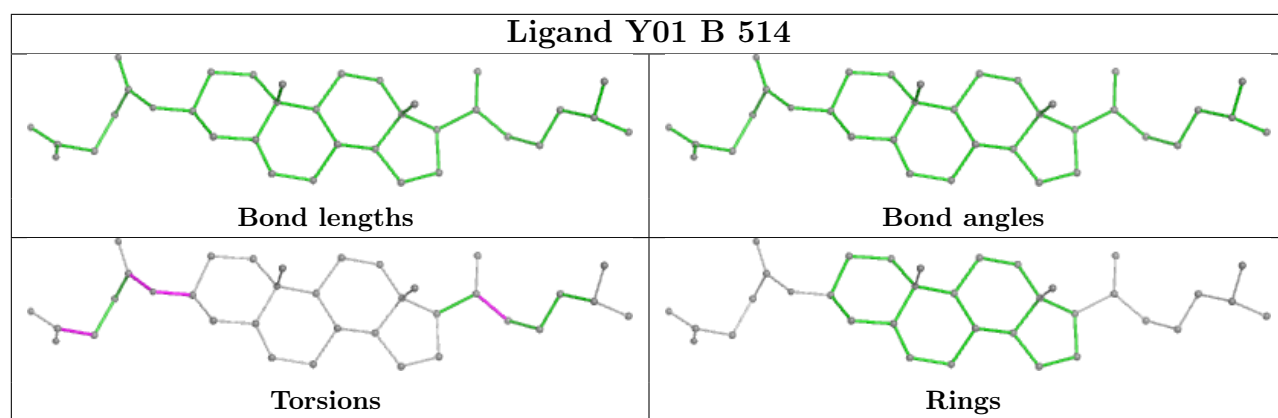
Ligand Y01 B 516

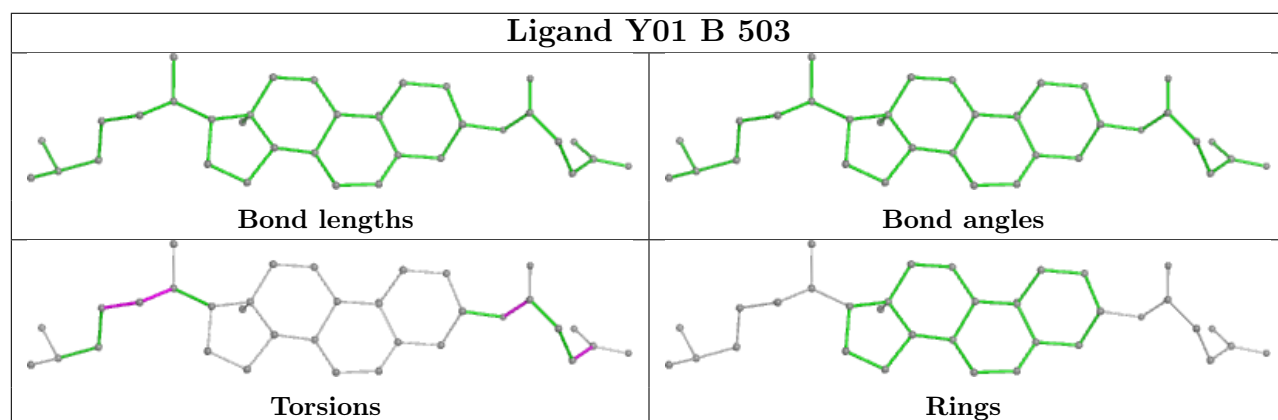
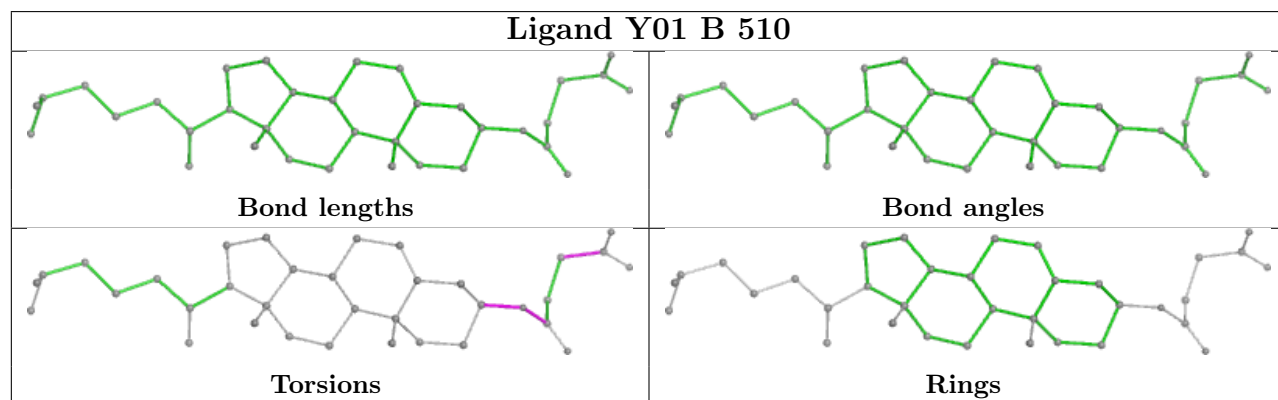
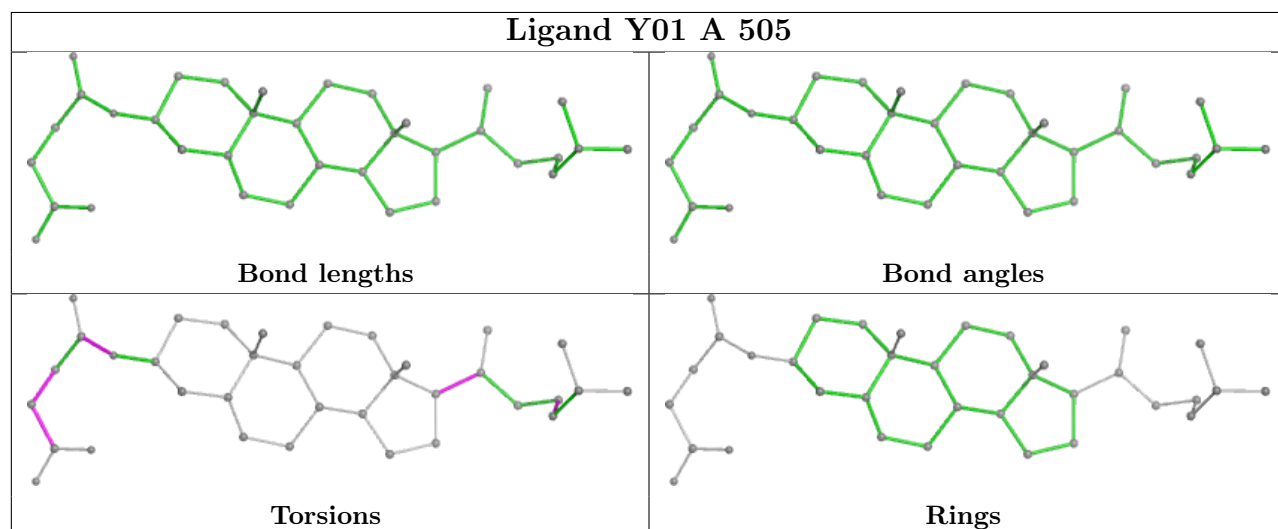
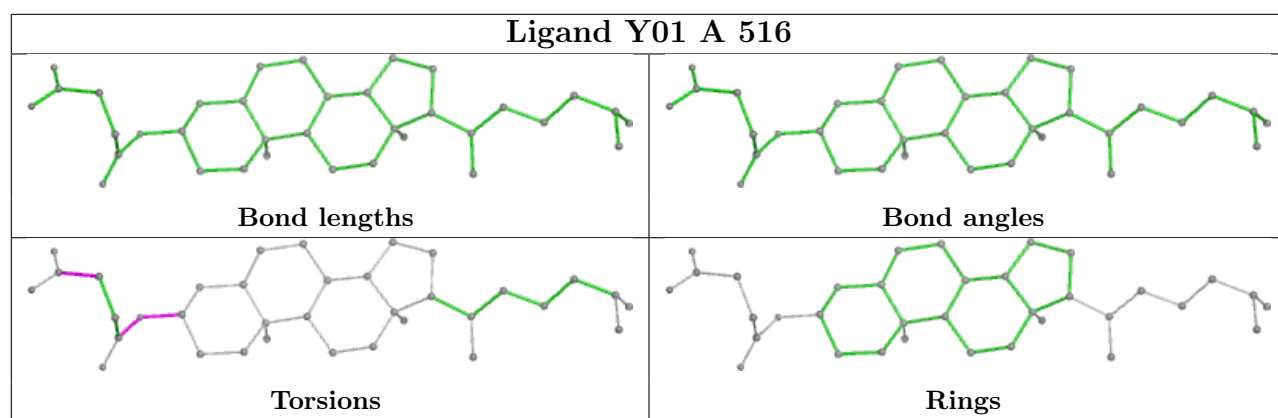


Ligand Y01 B 517









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.

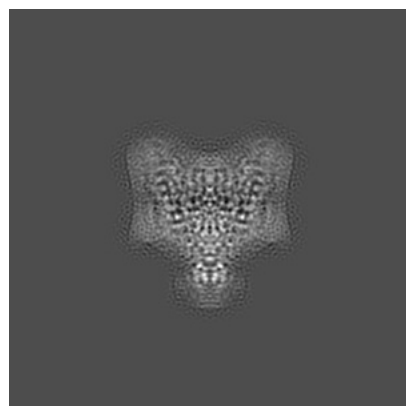
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13880. These allow visual inspection of the internal detail of the map and identification of artifacts.

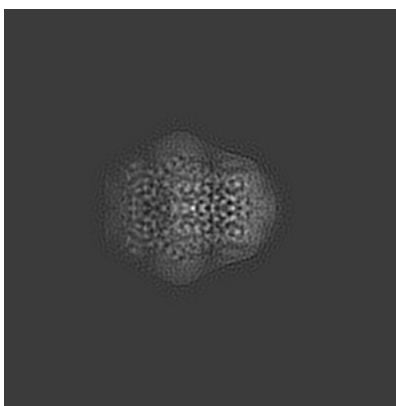
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

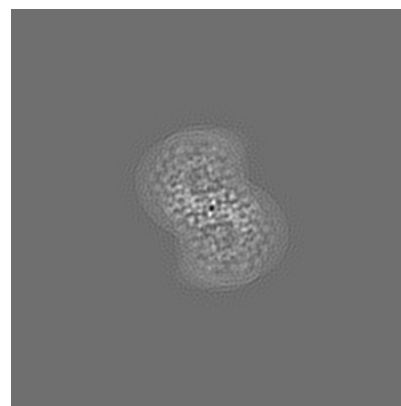
6.1.1 Primary map



X

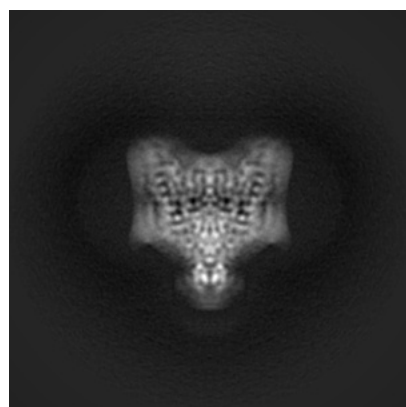


Y

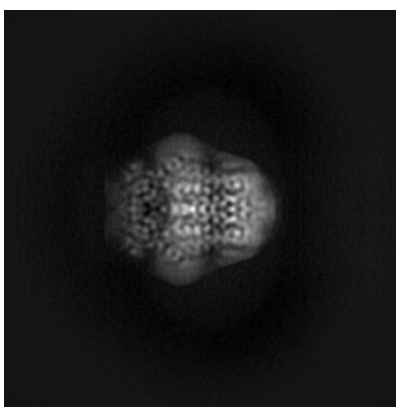


Z

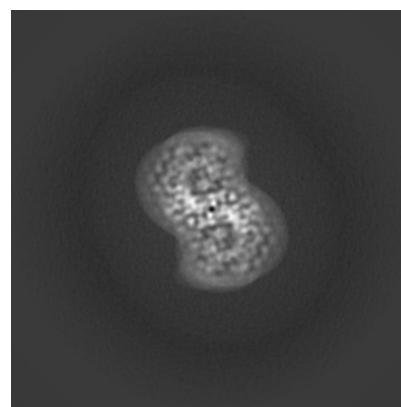
6.1.2 Raw map



X



Y

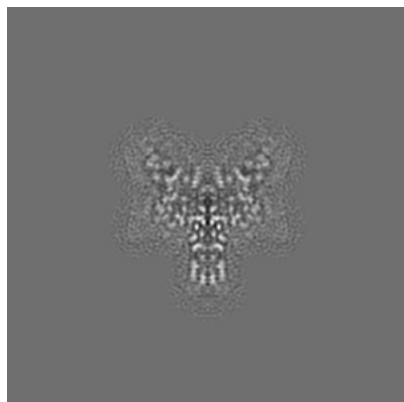


Z

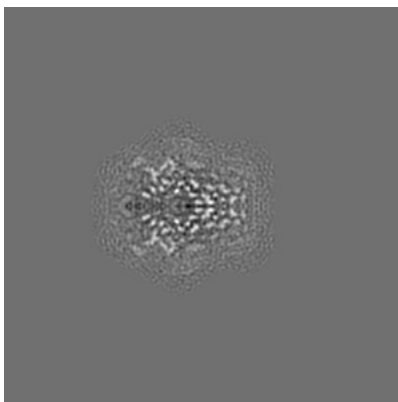
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

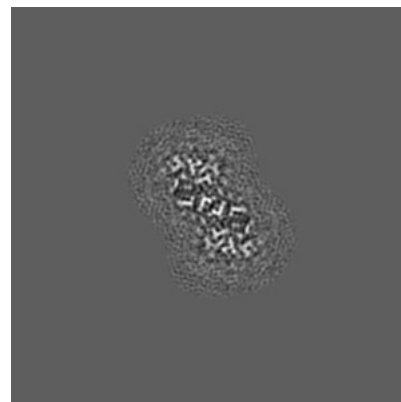
6.2.1 Primary map



X Index: 123

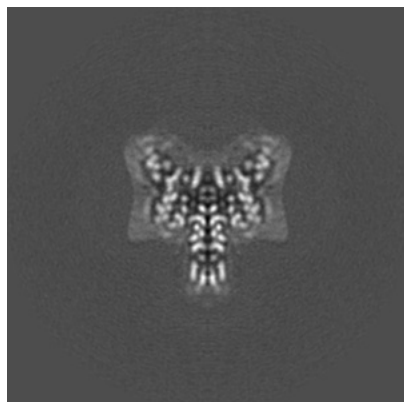


Y Index: 123

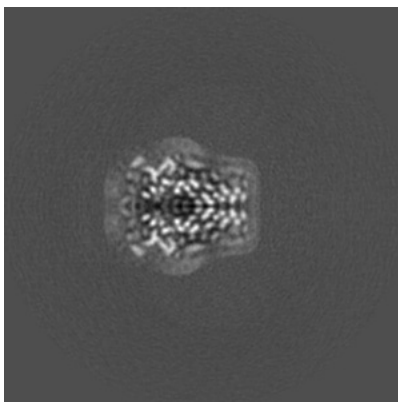


Z Index: 123

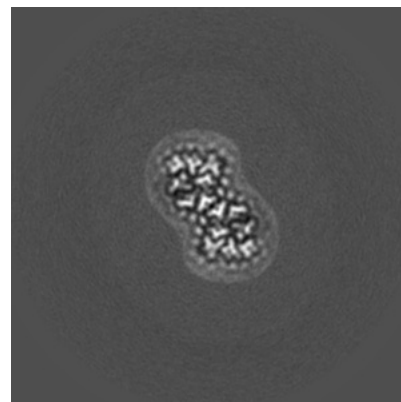
6.2.2 Raw map



X Index: 123



Y Index: 123

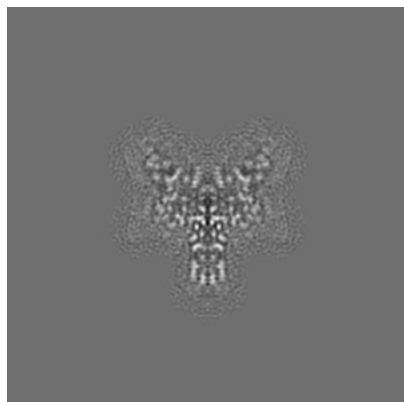


Z Index: 123

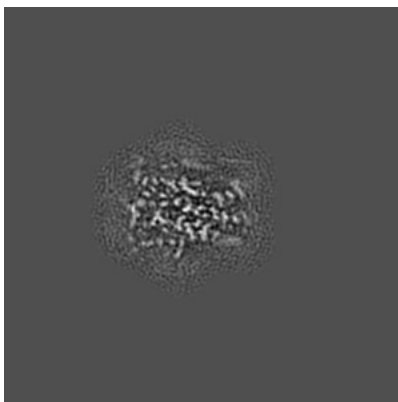
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

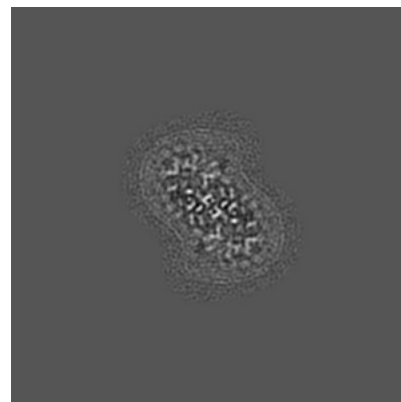
6.3.1 Primary map



X Index: 123

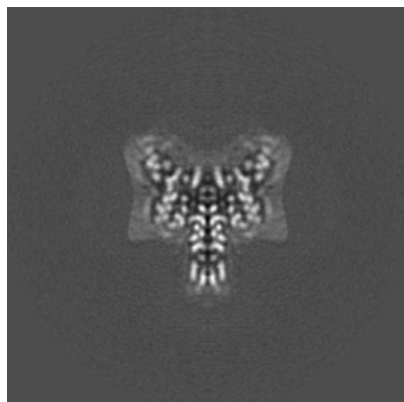


Y Index: 125

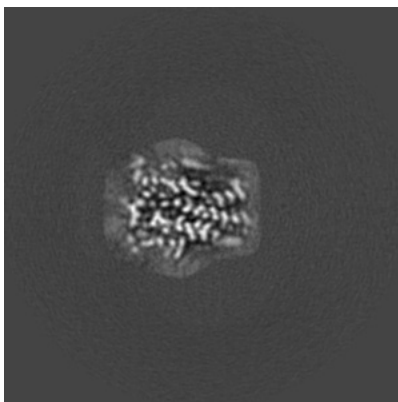


Z Index: 117

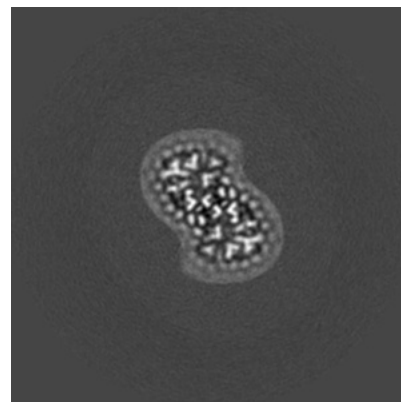
6.3.2 Raw map



X Index: 123



Y Index: 125

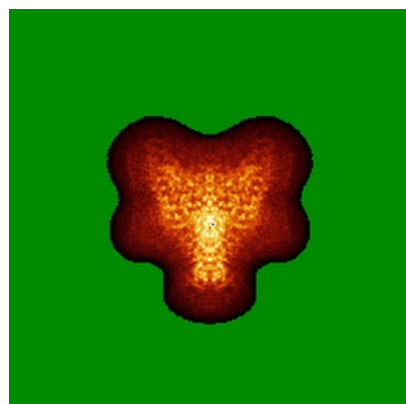


Z Index: 118

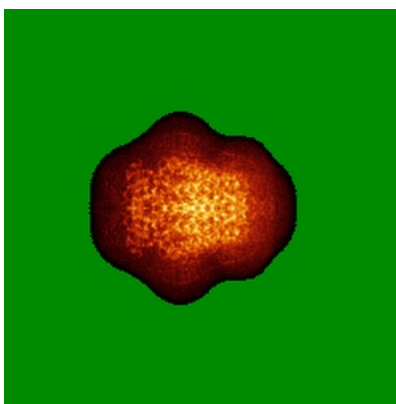
The images above show the largest variance slices of the map in three orthogonal directions.

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

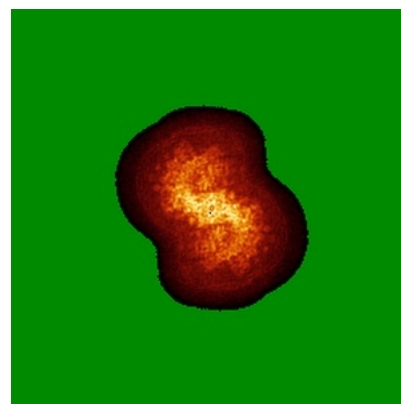
6.4.1 Primary map



X



Y

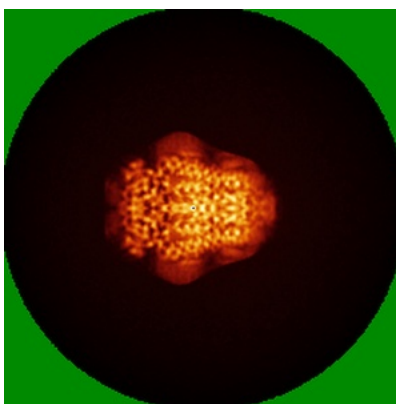


Z

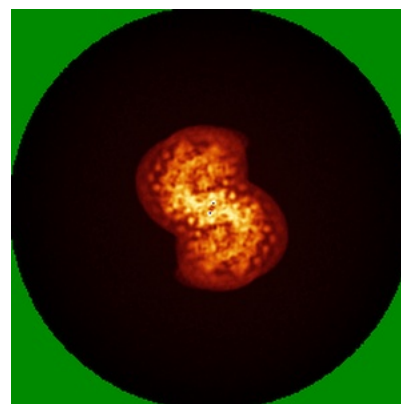
6.4.2 Raw map



X



Y

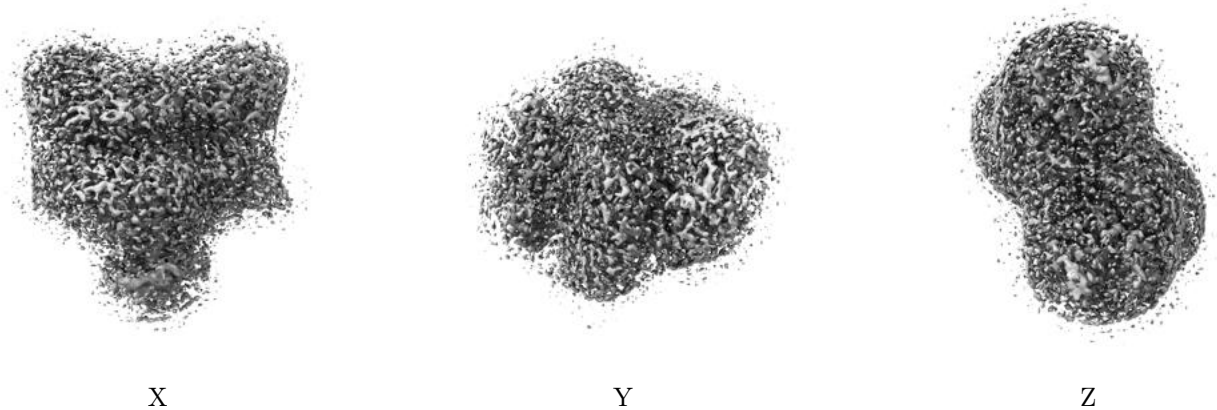


Z

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.

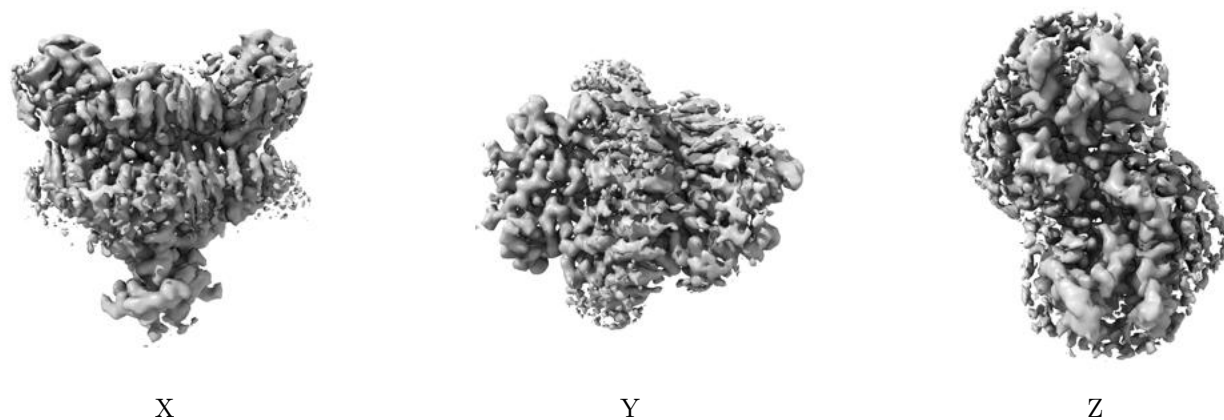
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0233. 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.

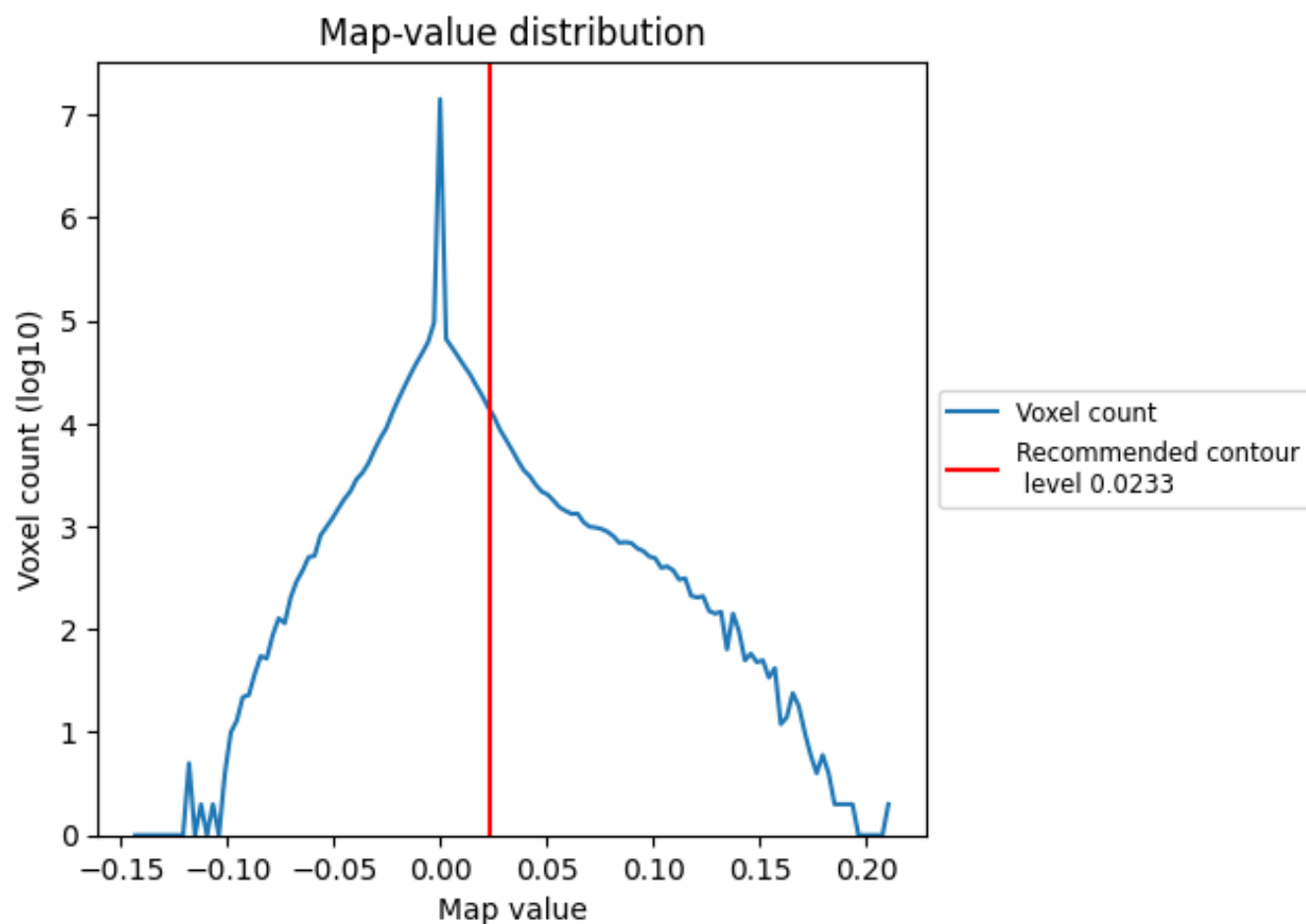
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

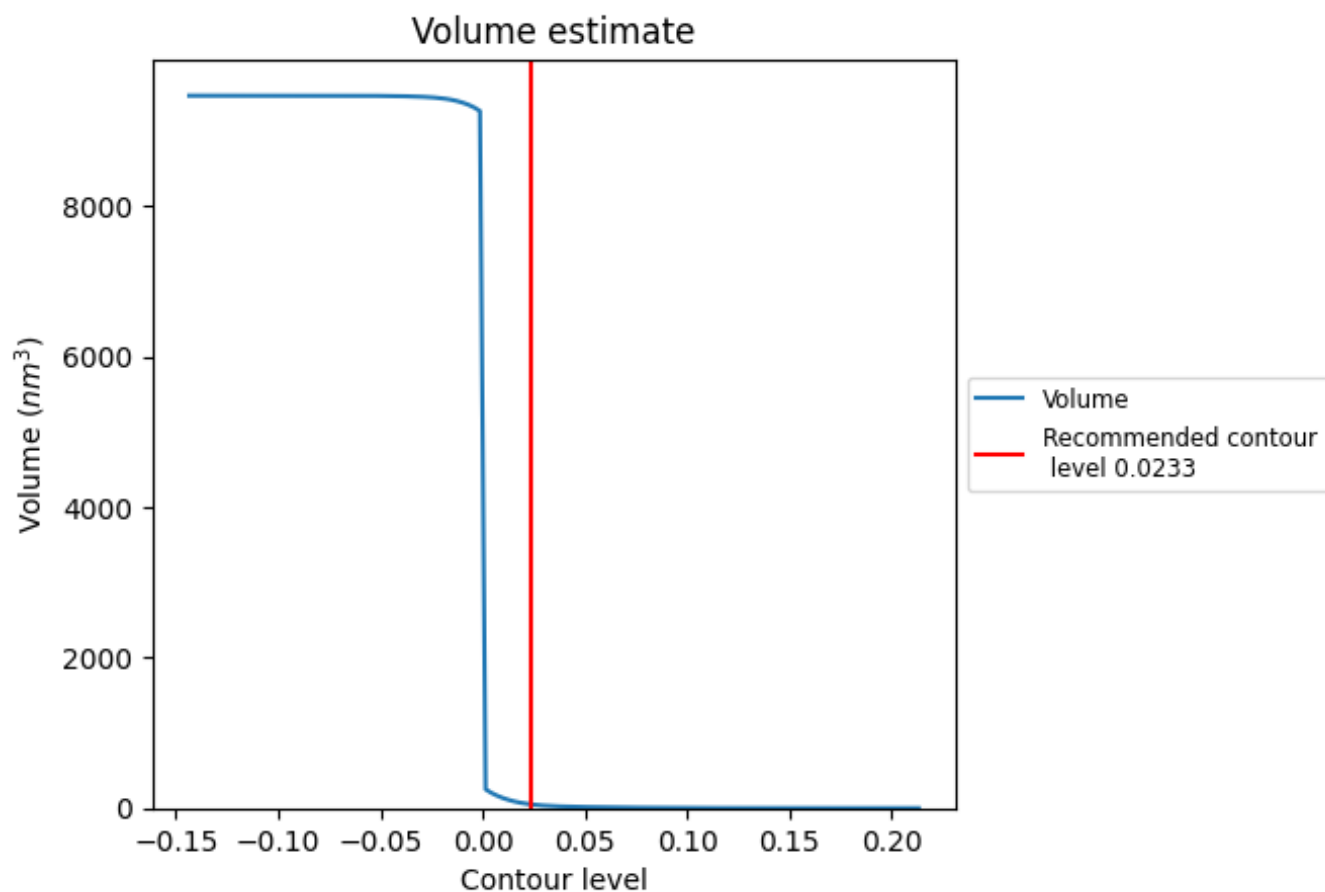
This section contains the results of statistical analysis of the map.

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.

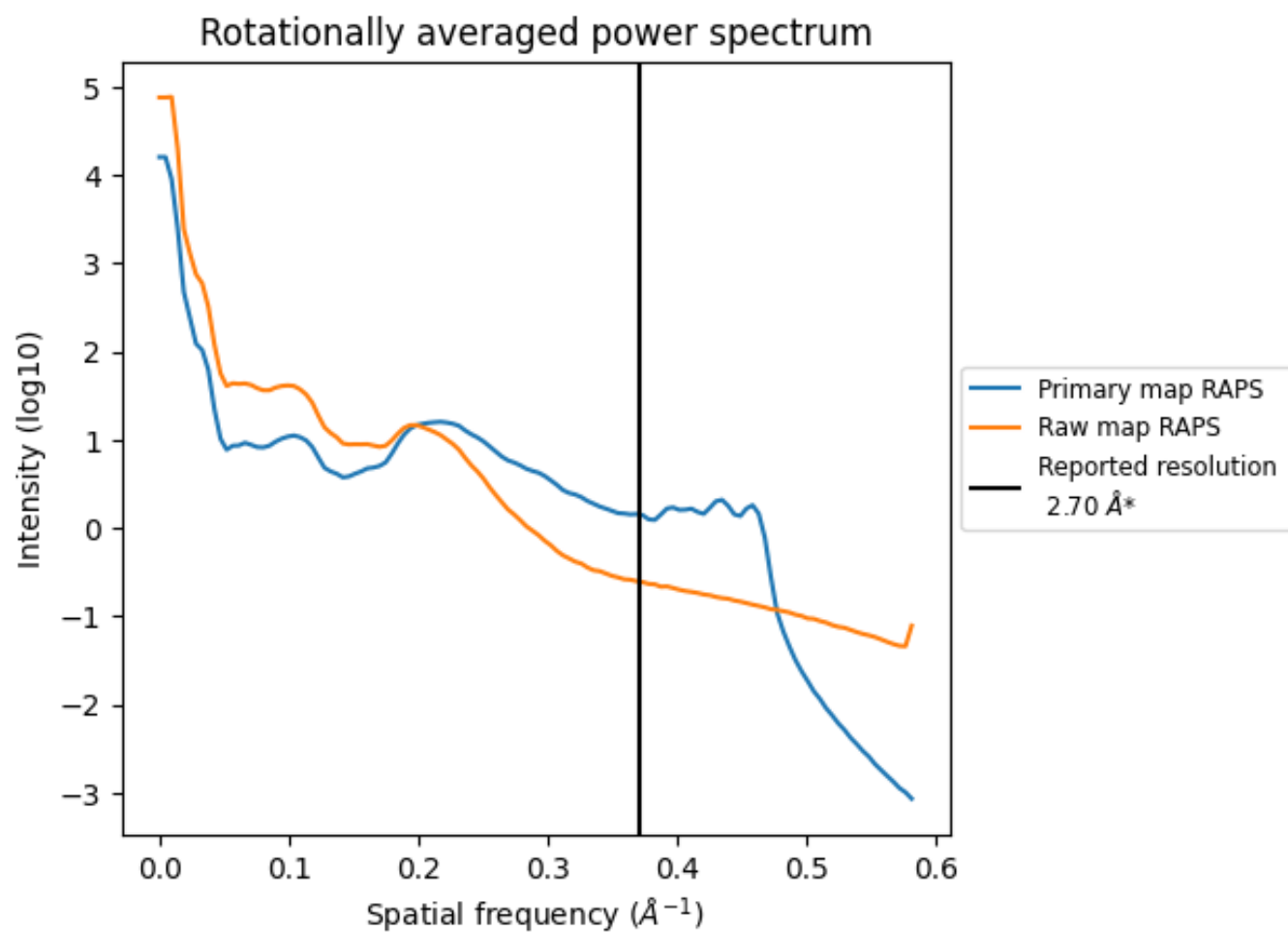
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 51 nm^3 ; 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 ⓘ

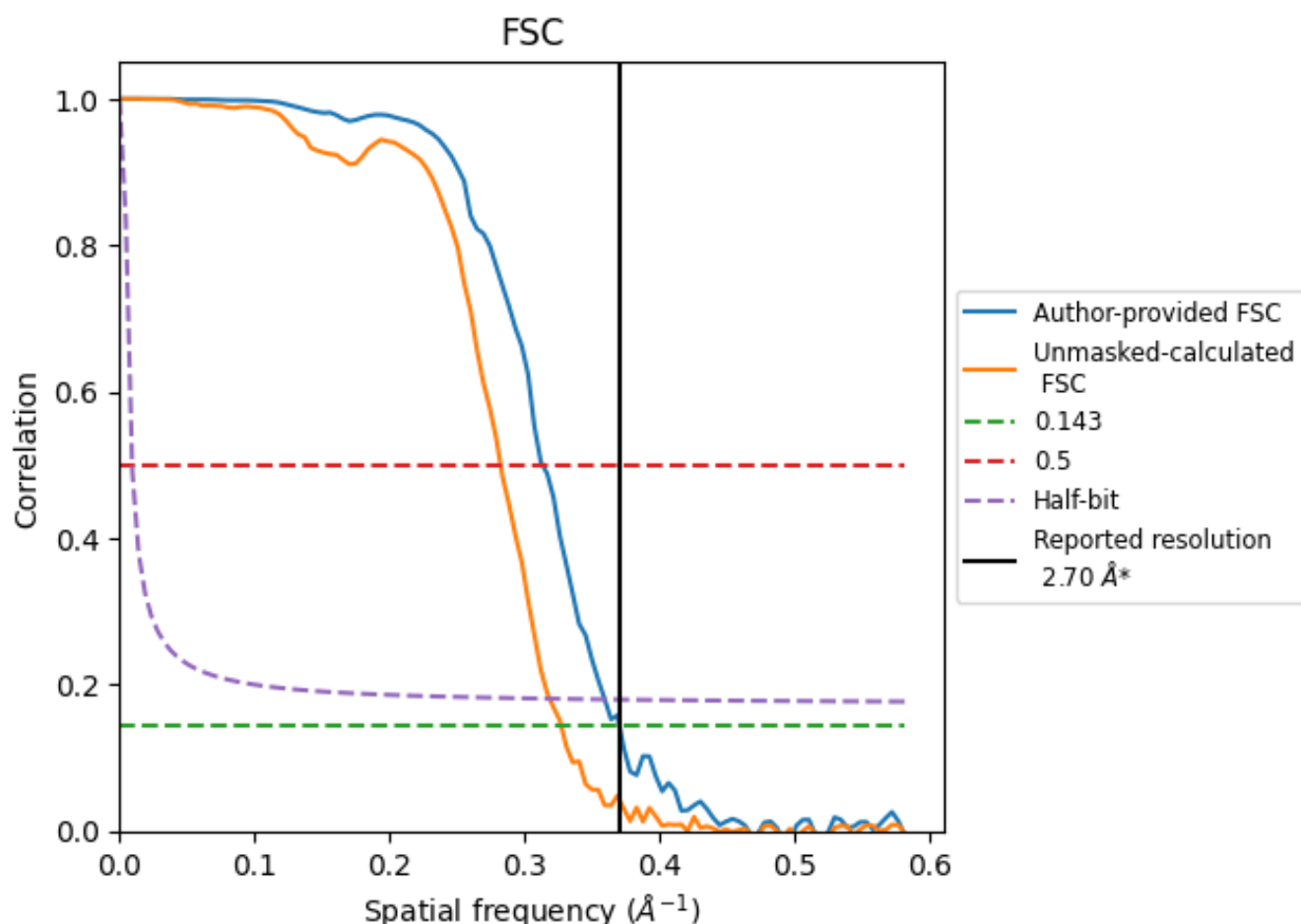


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

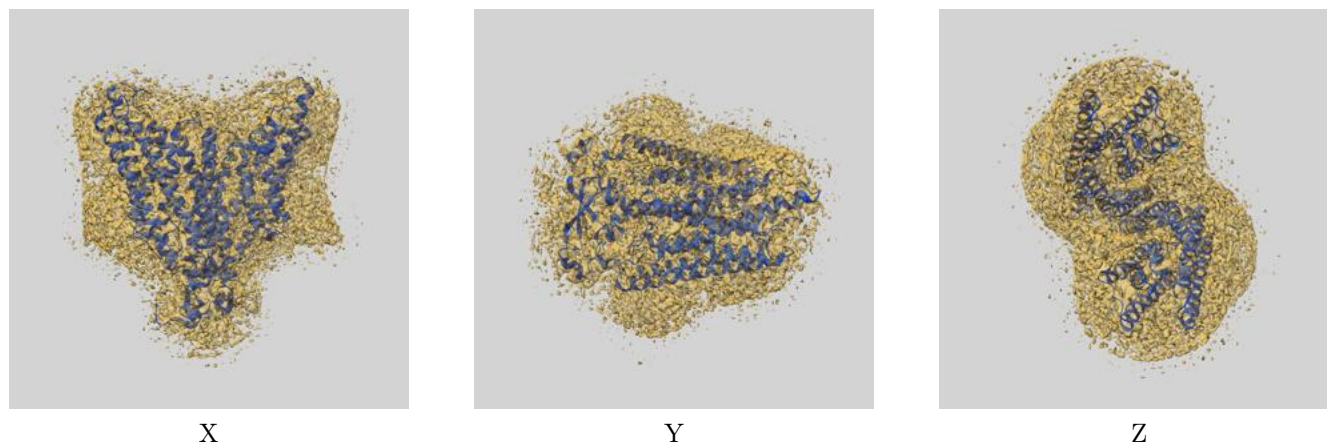
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.19	2.78
Unmasked-calculated*	3.06	3.54	3.14

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

9 Map-model fit [i](#)

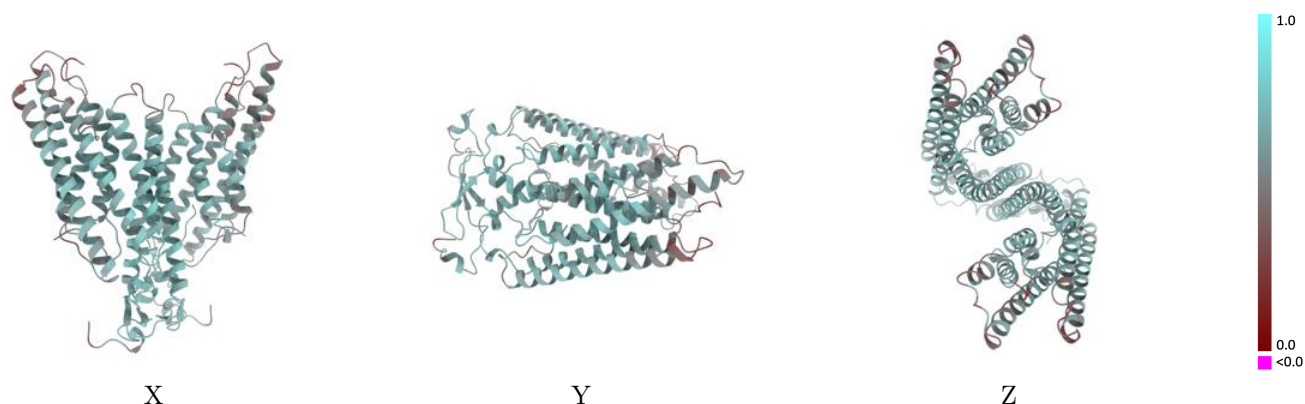
This section contains information regarding the fit between EMDB map EMD-13880 and PDB model 7QA8. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



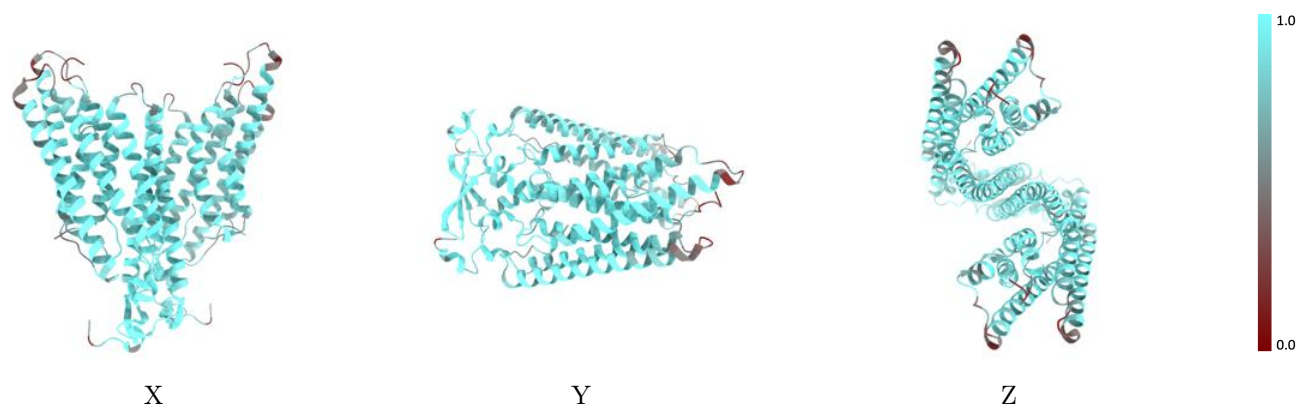
The images above show the 3D surface view of the map at the recommended contour level 0.0233 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



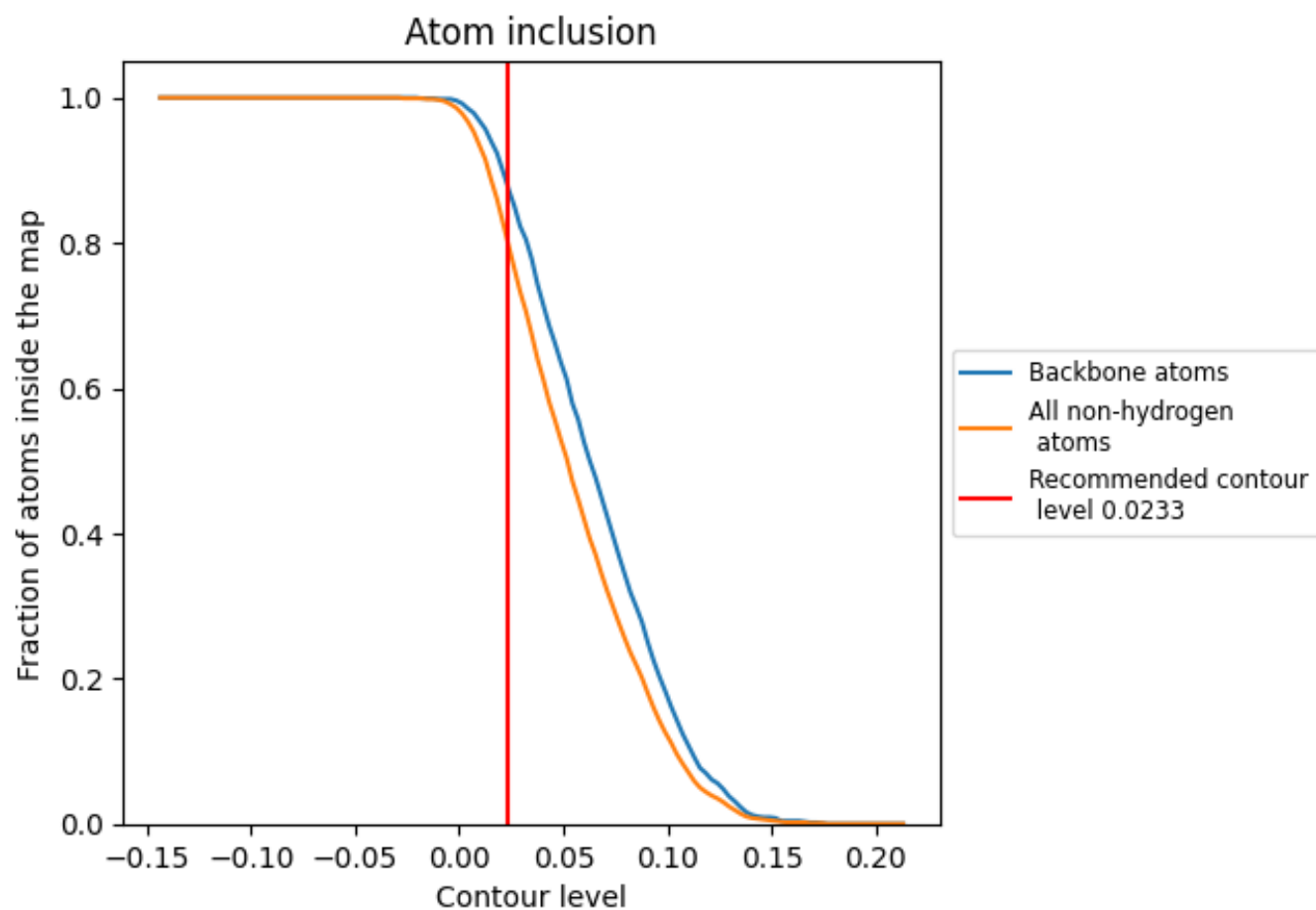
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0233).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 80% 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 (0.0233) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8020	<div></div> 0.5380
A	<div></div> 0.8070	<div></div> 0.5400
B	<div></div> 0.7990	<div></div> 0.5340
I	<div></div> 0.7050	<div></div> 0.5150
K	<div></div> 0.8330	<div></div> 0.5990

