



wwPDB EM Validation Summary Report ⓘ

Oct 19, 2026 – 10:06 PM JST

PDB ID : 9X17 / pdb_00009x17
EMDB ID : EMD-66453
Title : Cryo-EM structure of the dITP-bound active form of the KomBC filament
Authors : Li, X.; Liu, M.; Jiang, W.X.; Xing, Q.; Ma, L.X.; Huang, F.T.
Deposited on : 2025-10-01
Resolution : 3.21 Å(reported)

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

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

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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.2
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) : 2.51

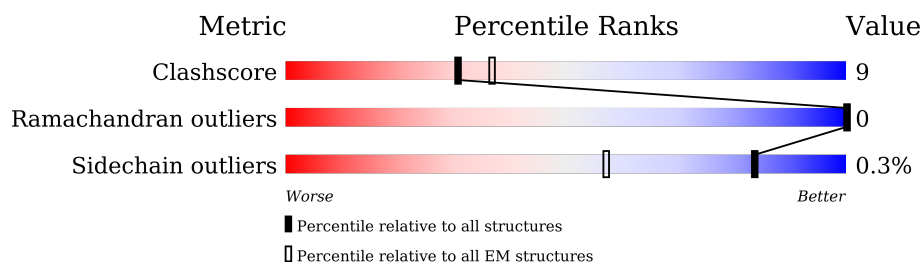
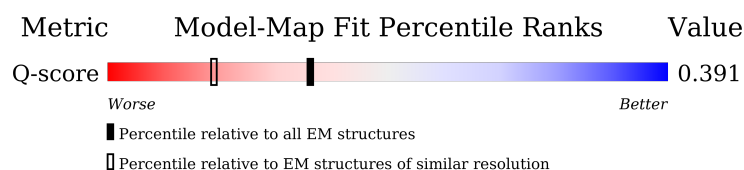
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.21 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	14613 (2.71 - 3.71)

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	AB	197	<div> <div>34%</div> <div>76%</div> <div>19%</div> <div>6%</div> </div>
1	AC	197	<div> <div>44%</div> <div>73%</div> <div>22%</div> <div>6%</div> </div>
1	AG	197	<div> <div>27%</div> <div>77%</div> <div>17%</div> <div>6%</div> </div>
1	AI	197	<div> <div>40%</div> <div>74%</div> <div>20%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	AN	197	
1	AO	197	
1	AS	197	
1	AU	197	
1	BB	197	
1	BC	197	
1	BG	197	
1	BI	197	
1	BN	197	
1	BO	197	
1	BS	197	
1	BU	197	
1	CB	197	
1	CC	197	
1	CG	197	
1	CI	197	
1	CN	197	
1	CO	197	
1	CS	197	
1	CU	197	
1	DB	197	
1	DC	197	
1	DG	197	
1	DI	197	
2	AD	264	

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Mol	Chain	Length	Quality of chain
2	AE	264	
2	AK	264	
2	AL	264	
2	AP	264	
2	AQ	264	
2	AW	264	
2	AX	264	
2	BD	264	
2	BE	264	
2	BK	264	
2	BL	264	
2	BP	264	
2	BQ	264	
2	BW	264	
2	BX	264	
2	CD	264	
2	CE	264	
2	CK	264	
2	CL	264	
2	CP	264	
2	CQ	264	
2	CW	264	
2	CX	264	
2	DD	264	
2	DE	264	

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Mol	Chain	Length	Quality of chain
2	DK	264	
2	DL	264	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	Y43	AB	201	X	-	-	-
3	Y43	AC	201	X	-	-	-
3	Y43	AG	201	X	-	-	-
3	Y43	AI	201	X	-	-	-
3	Y43	AN	201	X	-	-	-
3	Y43	AO	201	X	-	-	-
3	Y43	AS	201	X	-	-	-
3	Y43	AU	201	X	-	-	-
3	Y43	BB	201	X	-	-	-
3	Y43	BC	201	X	-	-	-
3	Y43	BG	201	X	-	-	-
3	Y43	BI	201	X	-	-	-
3	Y43	BN	201	X	-	-	-
3	Y43	BO	201	X	-	-	-
3	Y43	BS	201	X	-	-	-
3	Y43	BU	201	X	-	-	-
3	Y43	CB	201	X	-	-	-
3	Y43	CC	201	X	-	-	-
3	Y43	CG	201	X	-	-	-
3	Y43	CI	201	X	-	-	-
3	Y43	CN	201	X	-	-	-
3	Y43	CO	201	X	-	-	-
3	Y43	CS	201	X	-	-	-
3	Y43	CU	201	X	-	-	-
3	Y43	DB	201	X	-	-	-
3	Y43	DC	201	X	-	-	-
3	Y43	DG	201	X	-	-	-
3	Y43	DI	201	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 103012 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 KomB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BC	186	Total 1483	C 951	N 251	O 275	S 6	0	0
1	BG	186	Total 1483	C 951	N 251	O 275	S 6	0	0
1	BI	186	Total 1483	C 951	N 251	O 275	S 6	0	0
1	BN	186	Total 1483	C 951	N 251	O 275	S 6	0	0
1	BO	186	Total 1483	C 951	N 251	O 275	S 6	0	0
1	BS	186	Total 1483	C 951	N 251	O 275	S 6	0	0
1	BU	186	Total 1483	C 951	N 251	O 275	S 6	0	0
1	CB	186	Total 1483	C 951	N 251	O 275	S 6	0	0
1	CC	186	Total 1483	C 951	N 251	O 275	S 6	0	0
1	AB	186	Total 1483	C 951	N 251	O 275	S 6	0	0
1	CG	186	Total 1483	C 951	N 251	O 275	S 6	0	0
1	CI	186	Total 1483	C 951	N 251	O 275	S 6	0	0
1	CN	186	Total 1483	C 951	N 251	O 275	S 6	0	0
1	CO	186	Total 1483	C 951	N 251	O 275	S 6	0	0
1	CS	186	Total 1483	C 951	N 251	O 275	S 6	0	0
1	CU	186	Total 1483	C 951	N 251	O 275	S 6	0	0
1	DB	186	Total 1483	C 951	N 251	O 275	S 6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	DC	186	Total	C	N	O	S	0	0
			1483	951	251	275	6		
1	AC	186	Total	C	N	O	S	0	0
			1483	951	251	275	6		
1	DG	186	Total	C	N	O	S	0	0
			1483	951	251	275	6		
1	DI	186	Total	C	N	O	S	0	0
			1483	951	251	275	6		
1	AG	186	Total	C	N	O	S	0	0
			1483	951	251	275	6		
1	AI	186	Total	C	N	O	S	0	0
			1483	951	251	275	6		
1	AN	186	Total	C	N	O	S	0	0
			1483	951	251	275	6		
1	AO	186	Total	C	N	O	S	0	0
			1483	951	251	275	6		
1	AS	186	Total	C	N	O	S	0	0
			1483	951	251	275	6		
1	AU	186	Total	C	N	O	S	0	0
			1483	951	251	275	6		
1	BB	186	Total	C	N	O	S	0	0
			1483	951	251	275	6		

- Molecule 2 is a protein called KomC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BD	264	Total	C	N	O	S	0	0
			2166	1403	348	410	5		
2	BE	264	Total	C	N	O	S	0	0
			2166	1403	348	410	5		
2	BK	264	Total	C	N	O	S	0	0
			2166	1403	348	410	5		
2	BL	264	Total	C	N	O	S	0	0
			2166	1403	348	410	5		
2	BP	264	Total	C	N	O	S	0	0
			2166	1403	348	410	5		
2	BQ	264	Total	C	N	O	S	0	0
			2166	1403	348	410	5		
2	BW	264	Total	C	N	O	S	0	0
			2166	1403	348	410	5		
2	BX	264	Total	C	N	O	S	0	0
			2166	1403	348	410	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	CD	264	Total 2166	C 1403	N 348	O 410	S 5	0	0
2	CE	264	Total 2166	C 1403	N 348	O 410	S 5	0	0
2	CK	264	Total 2166	C 1403	N 348	O 410	S 5	0	0
2	CL	264	Total 2166	C 1403	N 348	O 410	S 5	0	0
2	CP	264	Total 2166	C 1403	N 348	O 410	S 5	0	0
2	CQ	264	Total 2166	C 1403	N 348	O 410	S 5	0	0
2	CW	264	Total 2166	C 1403	N 348	O 410	S 5	0	0
2	CX	264	Total 2166	C 1403	N 348	O 410	S 5	0	0
2	DD	264	Total 2166	C 1403	N 348	O 410	S 5	0	0
2	DE	264	Total 2166	C 1403	N 348	O 410	S 5	0	0
2	DK	264	Total 2166	C 1403	N 348	O 410	S 5	0	0
2	DL	264	Total 2166	C 1403	N 348	O 410	S 5	0	0
2	AD	264	Total 2166	C 1403	N 348	O 410	S 5	0	0
2	AE	264	Total 2166	C 1403	N 348	O 410	S 5	0	0
2	AK	264	Total 2166	C 1403	N 348	O 410	S 5	0	0
2	AL	264	Total 2166	C 1403	N 348	O 410	S 5	0	0
2	AP	264	Total 2166	C 1403	N 348	O 410	S 5	0	0
2	AQ	264	Total 2166	C 1403	N 348	O 410	S 5	0	0
2	AW	264	Total 2166	C 1403	N 348	O 410	S 5	0	0
2	AX	264	Total 2166	C 1403	N 348	O 410	S 5	0	0

- Molecule 3 is 2'-deoxyinosine 5'-triphosphate (CCD ID: Y43) (formula: $C_{10}H_{15}N_4O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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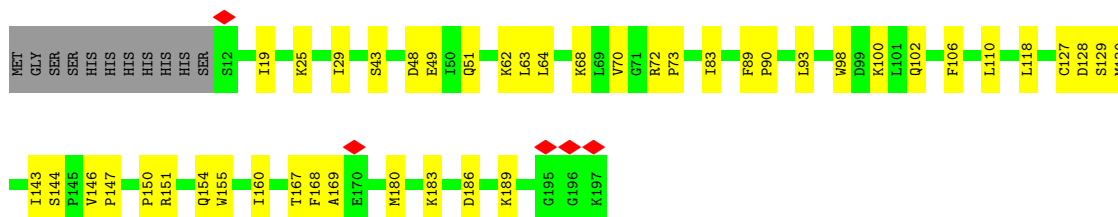
Mol	Chain	Residues	Atoms					AltConf
3	CS	1	Total	C	N	O	P	0
			30	10	4	13	3	
3	CU	1	Total	C	N	O	P	0
			30	10	4	13	3	
3	DB	1	Total	C	N	O	P	0
			30	10	4	13	3	
3	DC	1	Total	C	N	O	P	0
			30	10	4	13	3	
3	AC	1	Total	C	N	O	P	0
			30	10	4	13	3	
3	DG	1	Total	C	N	O	P	0
			30	10	4	13	3	
3	DI	1	Total	C	N	O	P	0
			30	10	4	13	3	
3	AG	1	Total	C	N	O	P	0
			30	10	4	13	3	
3	AI	1	Total	C	N	O	P	0
			30	10	4	13	3	
3	AN	1	Total	C	N	O	P	0
			30	10	4	13	3	
3	AO	1	Total	C	N	O	P	0
			30	10	4	13	3	
3	AS	1	Total	C	N	O	P	0
			30	10	4	13	3	
3	AU	1	Total	C	N	O	P	0
			30	10	4	13	3	
3	BB	1	Total	C	N	O	P	0
			30	10	4	13	3	

3 Residue-property plots [i](#)

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.

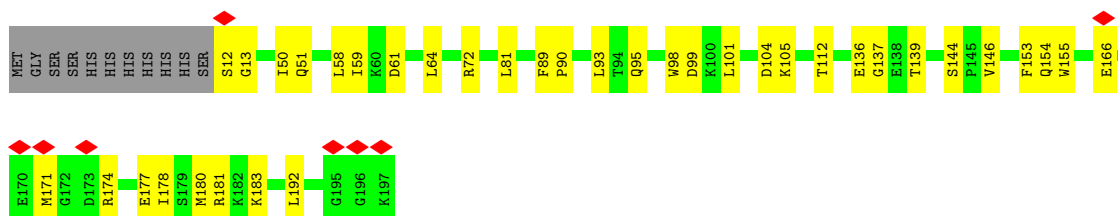
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Chain BC: 



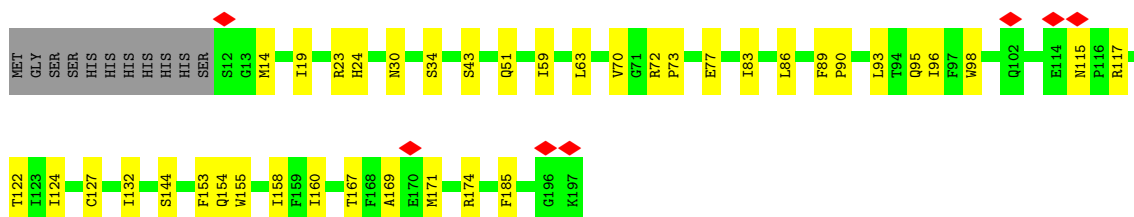
- Molecule 1: KomB

Chain BG: 



- Molecule 1: KomB

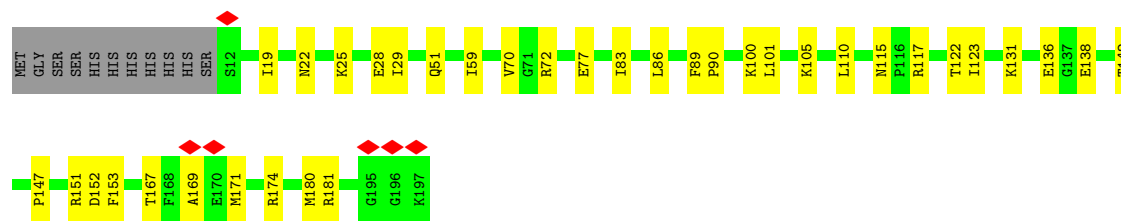
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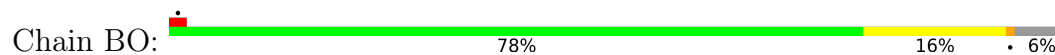
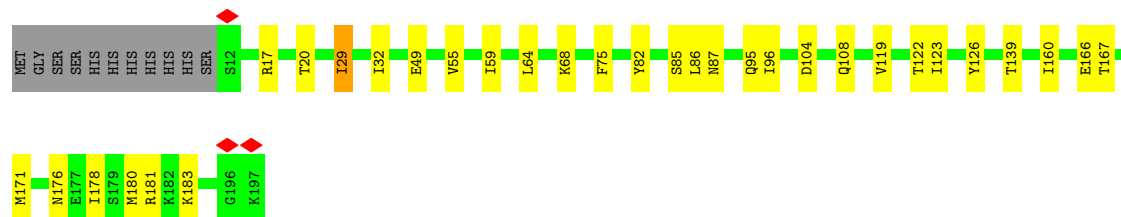
- Molecule 1: KomB

Chain BN: 

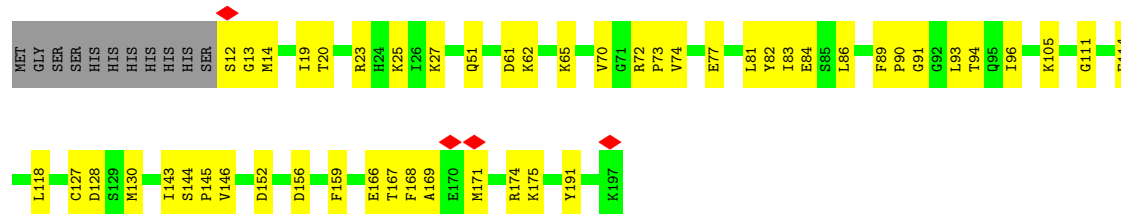




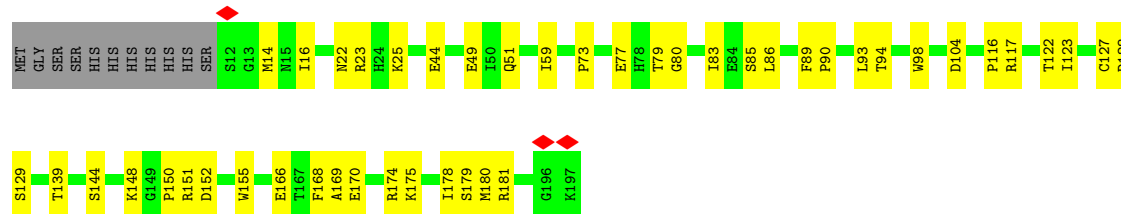
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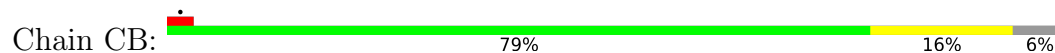
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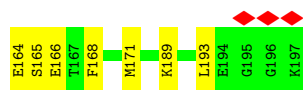


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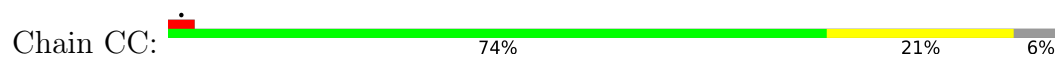
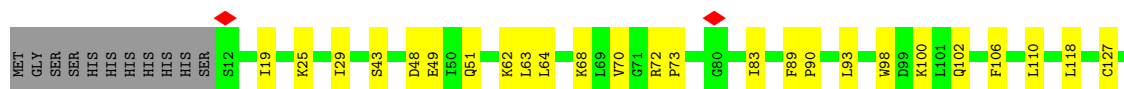


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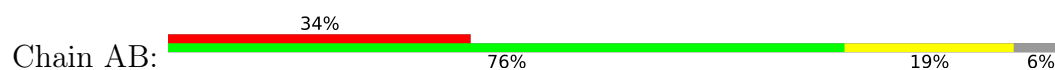
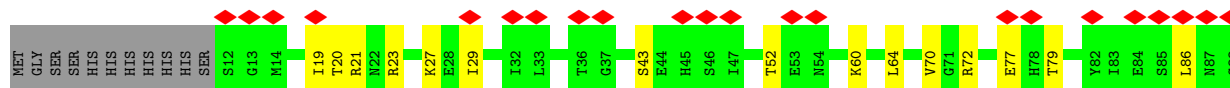
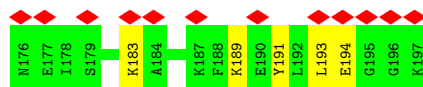




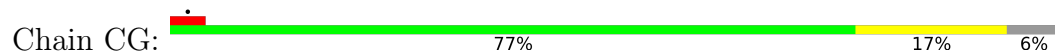
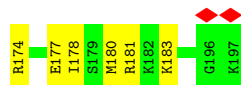
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• Molecule 1: KomB



• Molecule 1: KomB

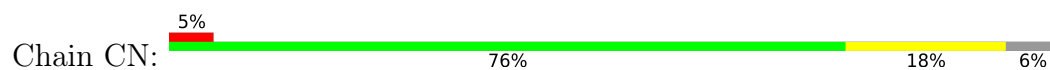


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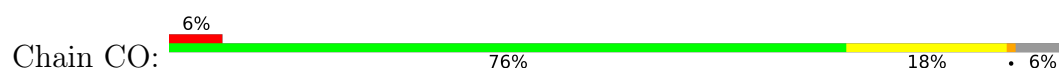
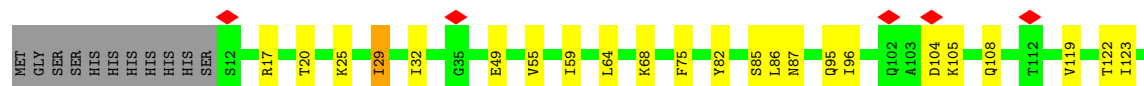




- Molecule 1: KomB



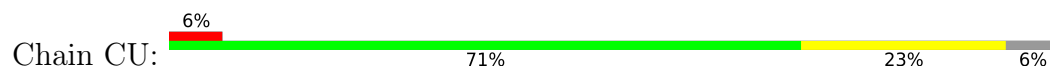
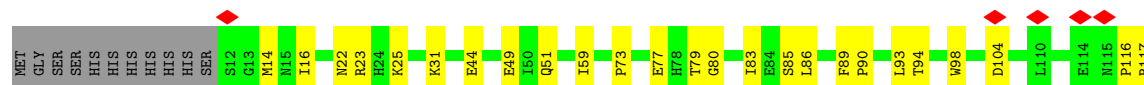
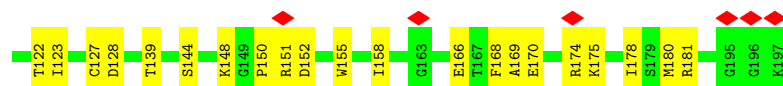
- Molecule 1: KomB



- Molecule 1: KomB

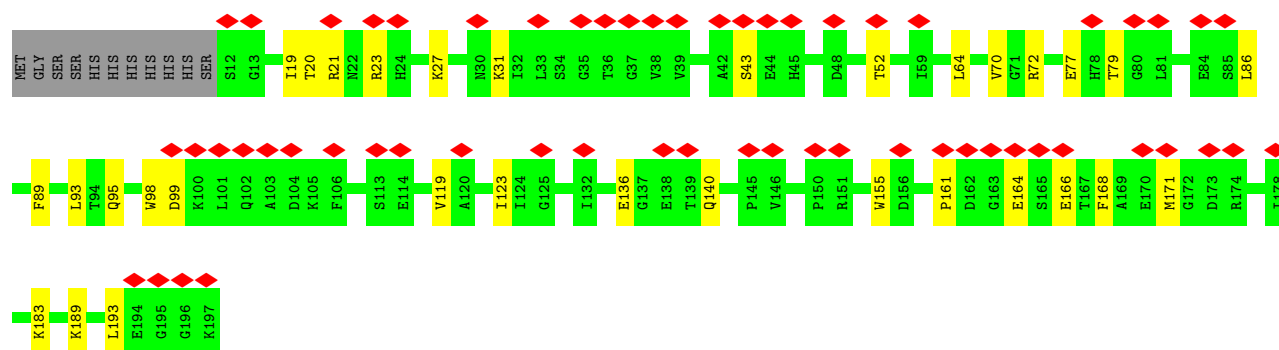


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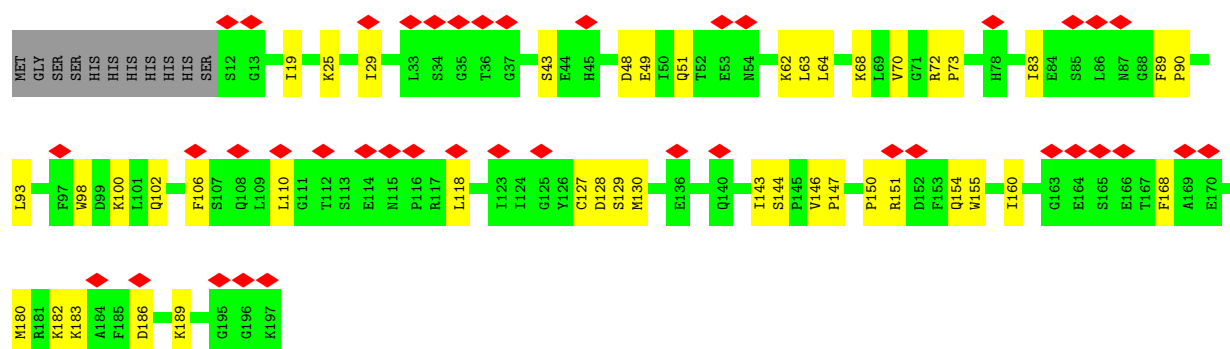
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Chain DB: 



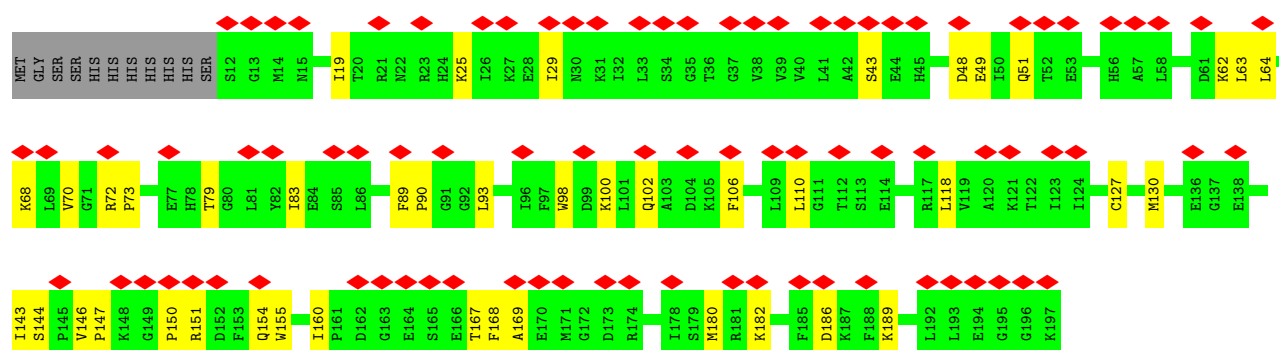
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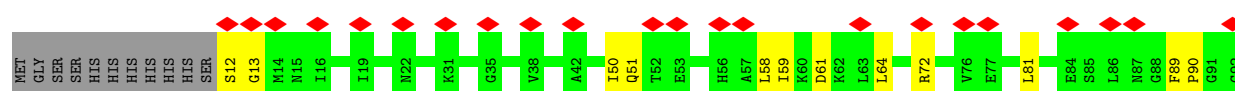
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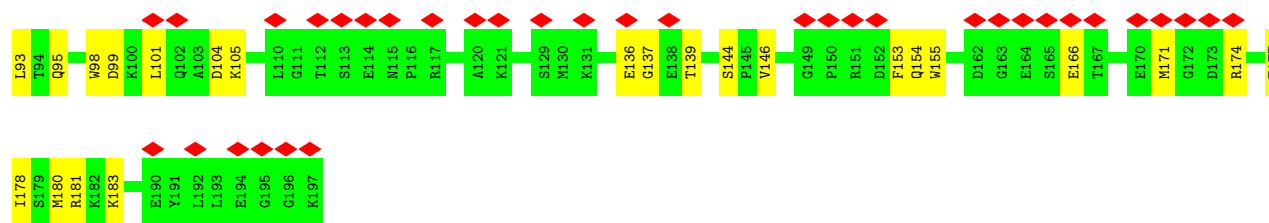
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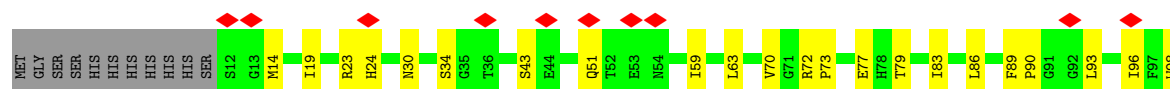
• Molecule 1: KomB

Chain DG: 

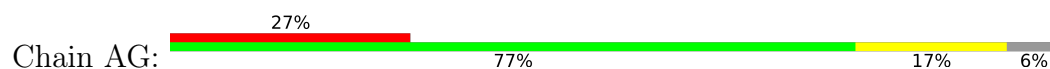
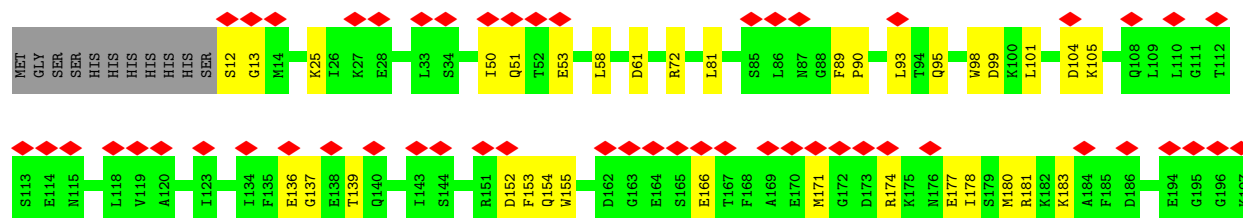




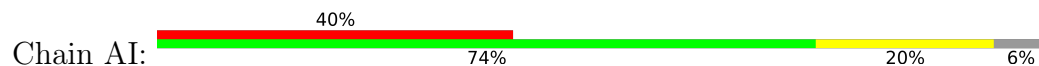
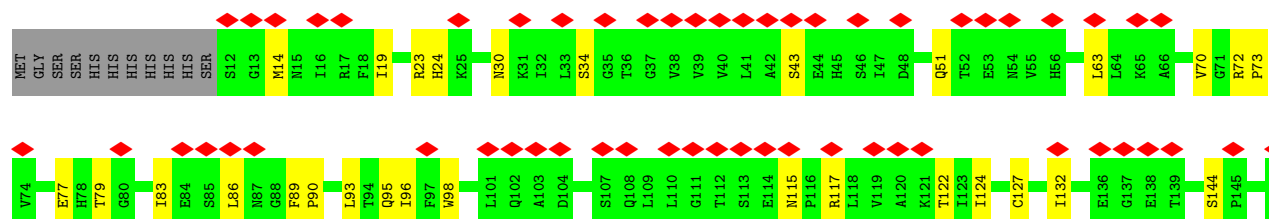
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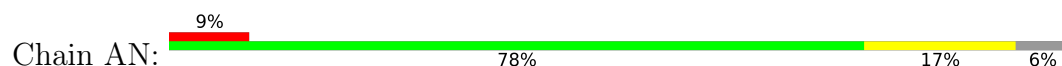
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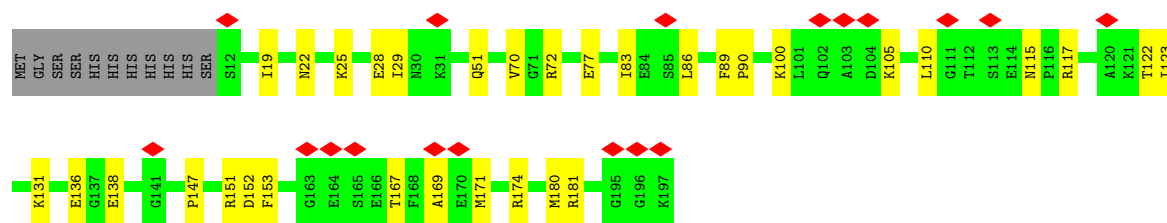


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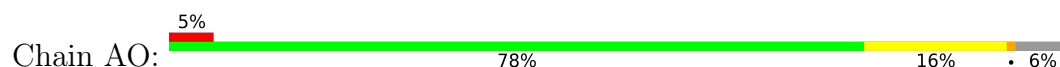
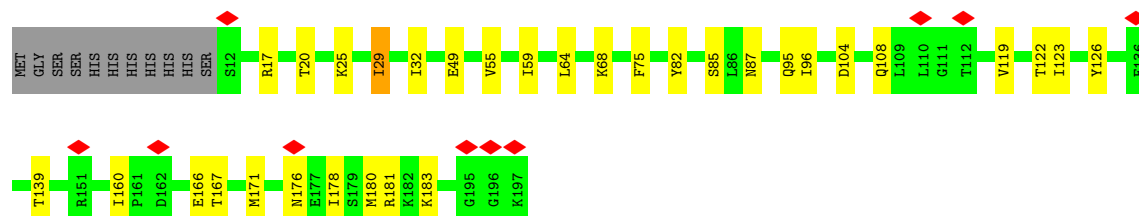


• Molecule 1: KomB

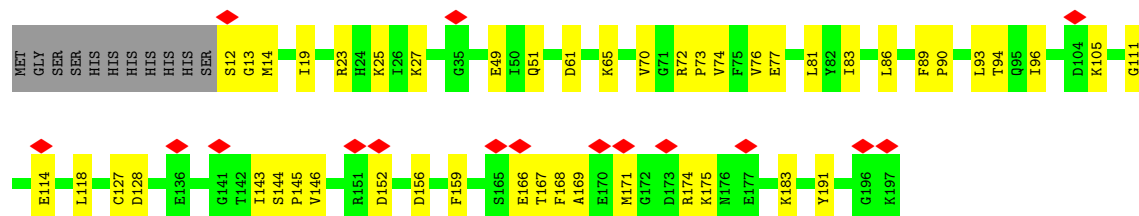




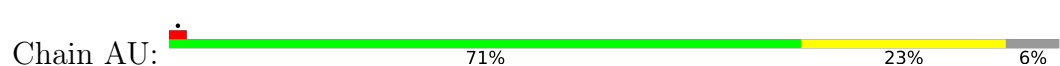
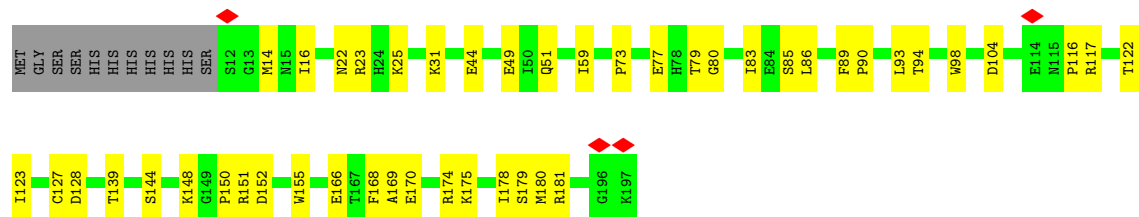
• Molecule 1: KomB



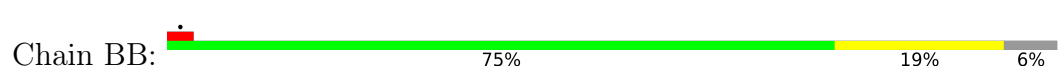
• Molecule 1: KomB



• Molecule 1: KomB

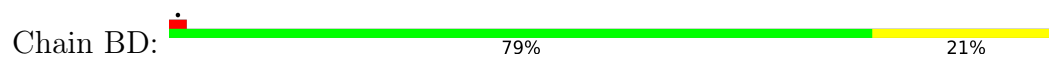


• Molecule 1: KomB

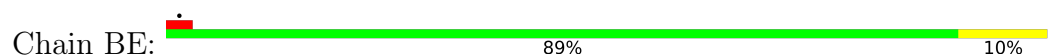




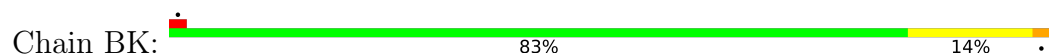
• Molecule 2: KomC



• Molecule 2: KomC



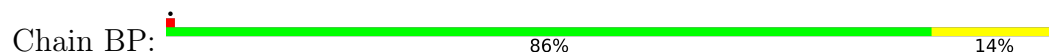
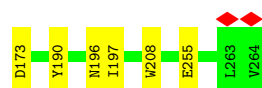
• Molecule 2: KomC



• Molecule 2: KomC

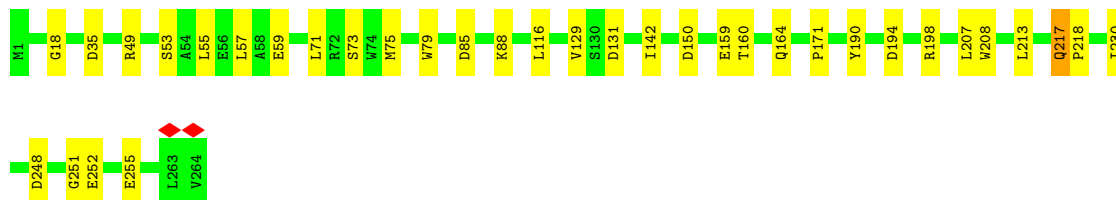


• Molecule 2: KomC



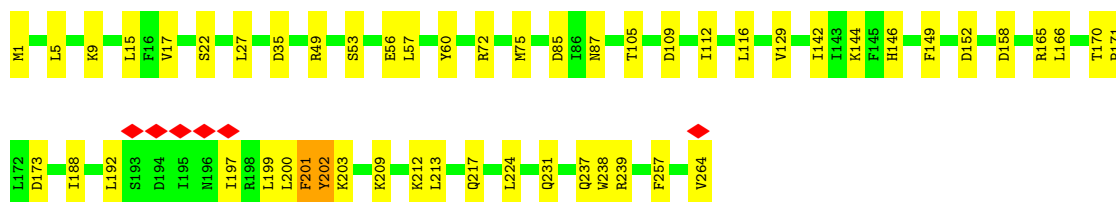
- Molecule 2: KomC

Chain BQ:  87% 13%



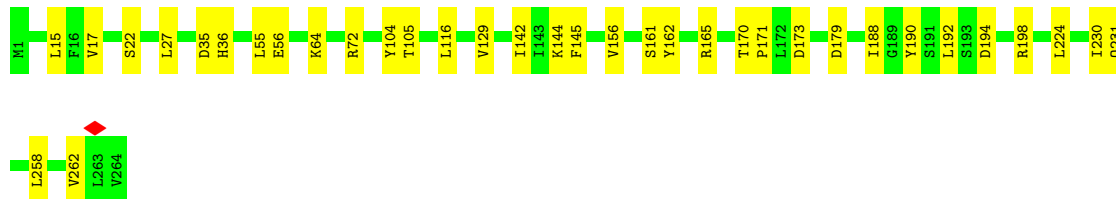
- Molecule 2: KomC

Chain BW:  80% 19%



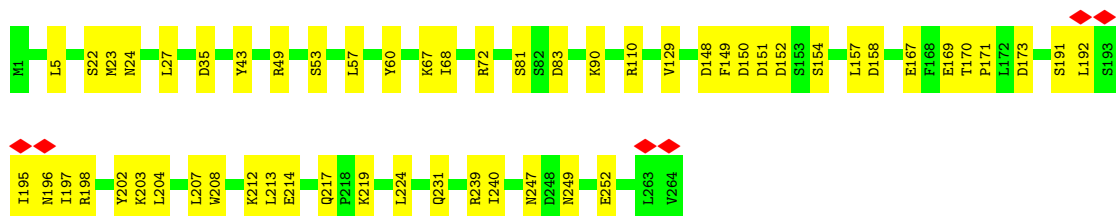
- Molecule 2: KomC

Chain BX:  87% 13%



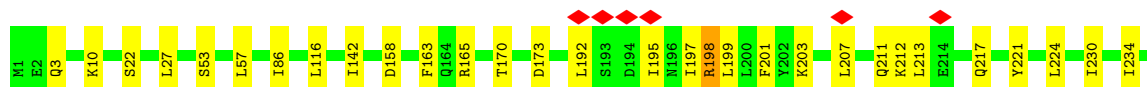
- Molecule 2: KomC

Chain CD:  79% 21%



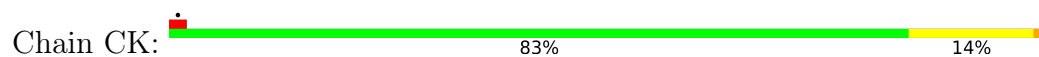
- Molecule 2: KomC

Chain CE:  88% 11%

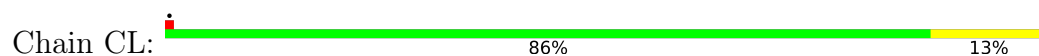




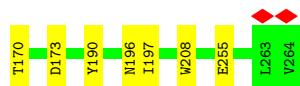
- Molecule 2: KomC



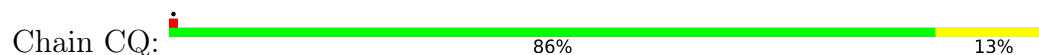
- Molecule 2: KomC



- Molecule 2: KomC

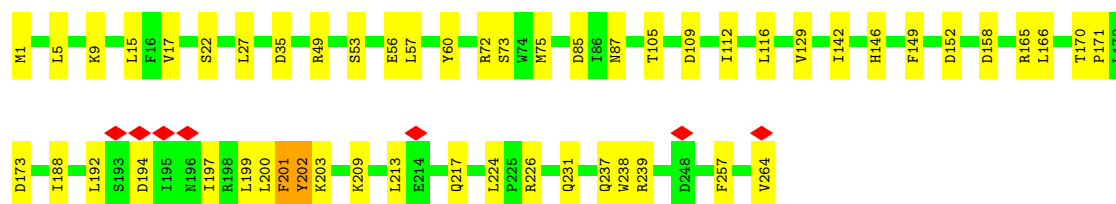


- Molecule 2: KomC



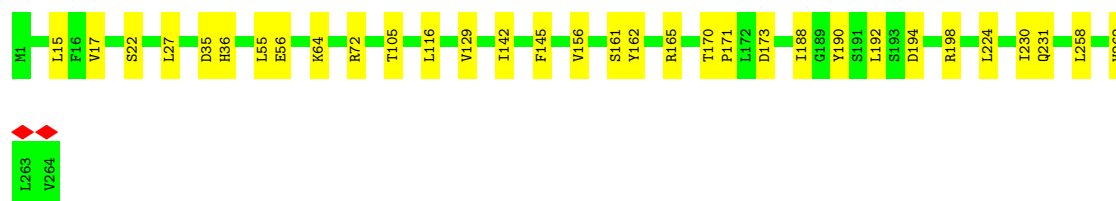
- Molecule 2: KomC

Chain CW:  80% 19%



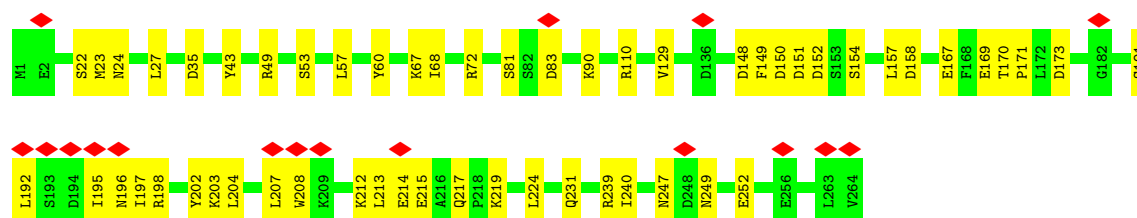
• Molecule 2: KomC

Chain CX:  88% 12%



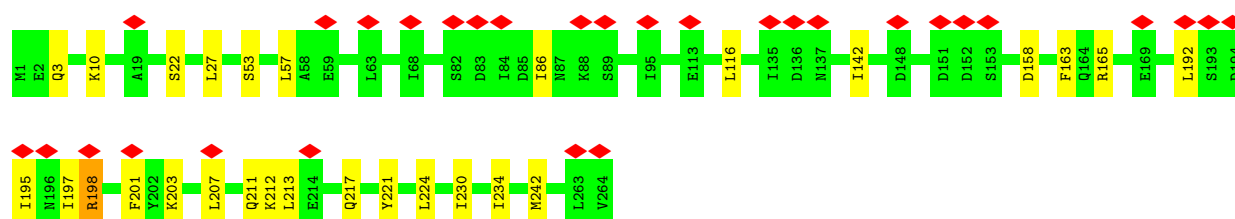
• Molecule 2: KomC

Chain DD:  79% 21%



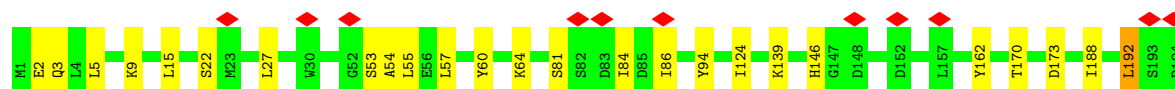
• Molecule 2: KomC

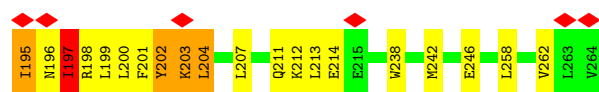
Chain DE:  89% 10%



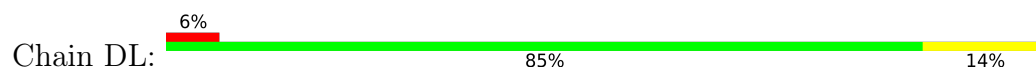
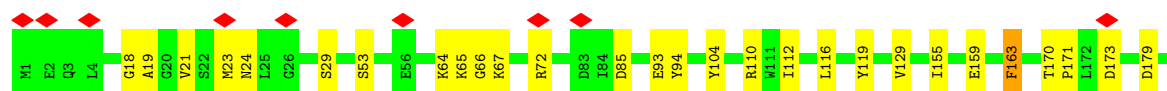
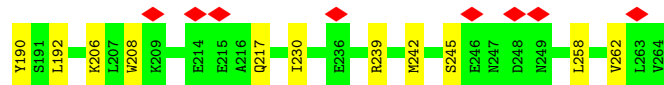
• Molecule 2: KomC

Chain DK:  83% 15%

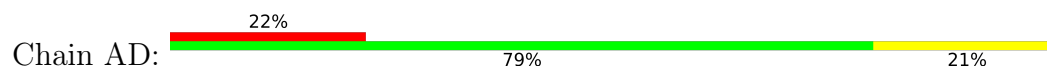
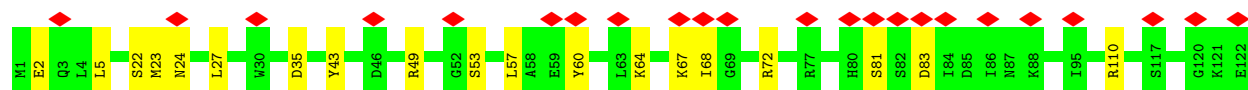




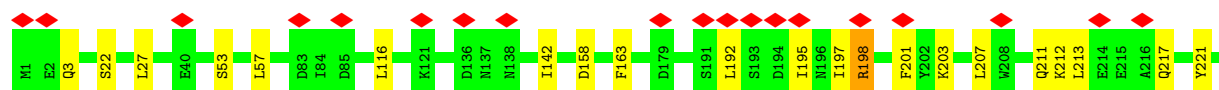
• Molecule 2: KomC



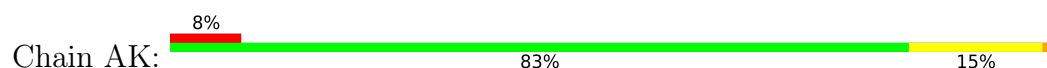
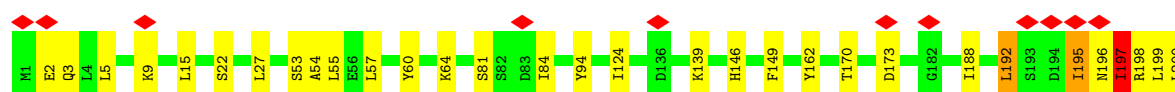
• Molecule 2: KomC

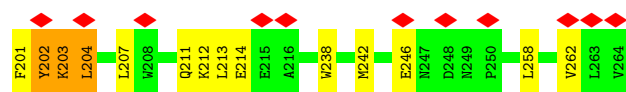


• Molecule 2: KomC

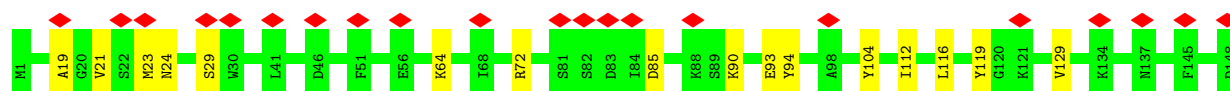
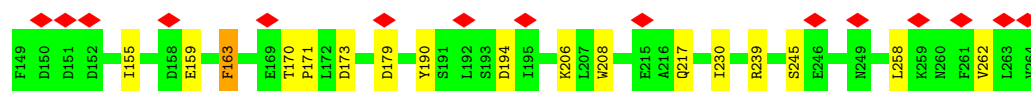


• Molecule 2: KomC

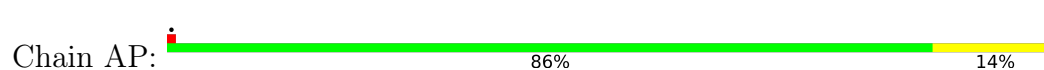
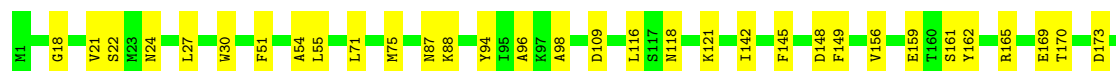




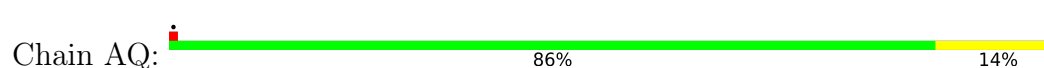
• Molecule 2: KomC



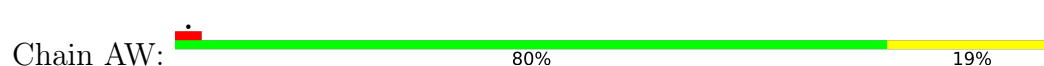
• Molecule 2: KomC



• Molecule 2: KomC

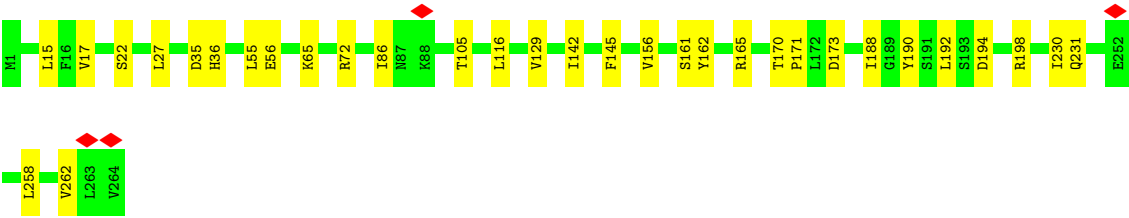


• Molecule 2: KomC



• Molecule 2: KomC





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	240153	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.746	Depositor
Minimum map value	-0.451	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.07	Depositor
Map size ($\text{\AA}$)	453.59998, 453.59998, 453.59998	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.756, 0.756, 0.756	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: Y43

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	AB	0.12	0/1513	0.29	0/2031
1	AC	0.11	0/1513	0.28	0/2031
1	AG	0.12	0/1513	0.32	0/2031
1	AI	0.11	0/1513	0.28	0/2031
1	AN	0.10	0/1513	0.26	0/2031
1	AO	0.14	0/1513	0.34	0/2031
1	AS	0.12	0/1513	0.32	0/2031
1	AU	0.15	0/1513	0.36	0/2031
1	BB	0.11	0/1513	0.29	0/2031
1	BC	0.11	0/1513	0.28	0/2031
1	BG	0.12	0/1513	0.32	0/2031
1	BI	0.11	0/1513	0.28	0/2031
1	BN	0.10	0/1513	0.26	0/2031
1	BO	0.13	0/1513	0.34	0/2031
1	BS	0.12	0/1513	0.32	0/2031
1	BU	0.14	0/1513	0.36	0/2031
1	CB	0.12	0/1513	0.29	0/2031
1	CC	0.11	0/1513	0.28	0/2031
1	CG	0.12	0/1513	0.32	0/2031
1	CI	0.11	0/1513	0.28	0/2031
1	CN	0.10	0/1513	0.26	0/2031
1	CO	0.14	0/1513	0.34	0/2031
1	CS	0.12	0/1513	0.32	0/2031
1	CU	0.15	0/1513	0.36	0/2031
1	DB	0.12	0/1513	0.29	0/2031
1	DC	0.12	0/1513	0.28	0/2031
1	DG	0.12	0/1513	0.32	0/2031
1	DI	0.11	0/1513	0.28	0/2031
2	AD	0.11	0/2218	0.26	0/2997
2	AE	0.10	0/2218	0.29	1/2997 (0.0%)
2	AK	0.40	2/2218 (0.1%)	0.59	6/2997 (0.2%)
2	AL	0.21	0/2218	0.31	1/2997 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	AP	0.09	0/2218	0.21	0/2997
2	AQ	0.18	0/2218	0.29	1/2997 (0.0%)
2	AW	0.20	0/2218	0.34	1/2997 (0.0%)
2	AX	0.09	0/2218	0.22	0/2997
2	BD	0.10	0/2218	0.26	0/2997
2	BE	0.09	0/2218	0.29	1/2997 (0.0%)
2	BK	0.40	2/2218 (0.1%)	0.59	6/2997 (0.2%)
2	BL	0.21	0/2218	0.31	1/2997 (0.0%)
2	BP	0.09	0/2218	0.21	0/2997
2	BQ	0.17	0/2218	0.29	1/2997 (0.0%)
2	BW	0.19	0/2218	0.34	1/2997 (0.0%)
2	BX	0.09	0/2218	0.22	0/2997
2	CD	0.11	0/2218	0.26	0/2997
2	CE	0.10	0/2218	0.29	1/2997 (0.0%)
2	CK	0.40	2/2218 (0.1%)	0.59	6/2997 (0.2%)
2	CL	0.21	0/2218	0.31	1/2997 (0.0%)
2	CP	0.09	0/2218	0.21	0/2997
2	CQ	0.18	0/2218	0.30	1/2997 (0.0%)
2	CW	0.20	0/2218	0.34	1/2997 (0.0%)
2	CX	0.09	0/2218	0.22	0/2997
2	DD	0.11	0/2218	0.26	0/2997
2	DE	0.10	0/2218	0.29	1/2997 (0.0%)
2	DK	0.40	2/2218 (0.1%)	0.59	6/2997 (0.2%)
2	DL	0.21	0/2218	0.31	1/2997 (0.0%)
All	All	0.17	8/104468 (0.0%)	0.33	38/140784 (0.0%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BK	203	LYS	CA-C	-6.44	1.45	1.52
2	DK	203	LYS	CA-C	-6.42	1.46	1.52
2	CK	203	LYS	CA-C	-6.41	1.46	1.52
2	AK	203	LYS	CA-C	-6.41	1.46	1.52
2	BK	211	GLN	CA-C	-5.51	1.47	1.53

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CK	213	LEU	N-CA-C	-10.88	100.31	112.72
2	DK	213	LEU	N-CA-C	-10.88	100.32	112.72
2	BK	213	LEU	N-CA-C	-10.88	100.32	112.72
2	AK	213	LEU	N-CA-C	-10.83	100.38	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AK	202	TYR	N-CA-C	8.53	120.35	111.14

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	AB	1483	0	1499	35	0
1	AC	1483	0	1499	40	0
1	AG	1483	0	1499	36	0
1	AI	1483	0	1499	33	0
1	AN	1483	0	1499	25	0
1	AO	1483	0	1499	31	0
1	AS	1483	0	1499	40	0
1	AU	1483	0	1499	39	0
1	BB	1483	0	1499	35	0
1	BC	1483	0	1499	39	0
1	BG	1483	0	1499	39	0
1	BI	1483	0	1499	32	0
1	BN	1483	0	1499	26	0
1	BO	1483	0	1499	30	0
1	BS	1483	0	1499	43	0
1	BU	1483	0	1499	36	0
1	CB	1483	0	1499	29	0
1	CC	1483	0	1499	37	0
1	CG	1483	0	1499	36	0
1	CI	1483	0	1499	33	0
1	CN	1483	0	1499	27	0
1	CO	1483	0	1499	34	0
1	CS	1483	0	1499	44	0
1	CU	1483	0	1499	34	0
1	DB	1483	0	1499	31	0
1	DC	1483	0	1499	41	0
1	DG	1483	0	1499	37	0
1	DI	1483	0	1499	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AD	2166	0	2150	50	0
2	AE	2166	0	2150	18	0
2	AK	2166	0	2150	53	0
2	AL	2166	0	2150	27	0
2	AP	2166	0	2150	25	0
2	AQ	2166	0	2150	31	0
2	AW	2166	0	2150	48	0
2	AX	2166	0	2150	25	0
2	BD	2166	0	2150	54	0
2	BE	2166	0	2150	20	0
2	BK	2166	0	2150	54	0
2	BL	2166	0	2150	24	0
2	BP	2166	0	2150	27	0
2	BQ	2166	0	2150	27	0
2	BW	2166	0	2150	47	0
2	BX	2166	0	2150	27	0
2	CD	2166	0	2150	52	0
2	CE	2166	0	2150	23	0
2	CK	2166	0	2150	52	0
2	CL	2166	0	2150	30	0
2	CP	2166	0	2150	26	0
2	CQ	2166	0	2150	29	0
2	CW	2166	0	2150	47	0
2	CX	2166	0	2150	25	0
2	DD	2166	0	2150	52	0
2	DE	2166	0	2150	22	0
2	DK	2166	0	2150	54	0
2	DL	2166	0	2150	34	0
3	AB	30	0	0	0	0
3	AC	30	0	0	1	0
3	AG	30	0	0	1	0
3	AI	30	0	0	1	0
3	AN	30	0	0	1	0
3	AO	30	0	0	1	0
3	AS	30	0	0	0	0
3	AU	30	0	0	1	0
3	BB	30	0	0	0	0
3	BC	30	0	0	0	0
3	BG	30	0	0	0	0
3	BI	30	0	0	0	0
3	BN	30	0	0	1	0
3	BO	30	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BS	30	0	0	2	0
3	BU	30	0	0	1	0
3	CB	30	0	0	0	0
3	CC	30	0	0	0	0
3	CG	30	0	0	1	0
3	CI	30	0	0	1	0
3	CN	30	0	0	1	0
3	CO	30	0	0	1	0
3	CS	30	0	0	2	0
3	CU	30	0	0	1	0
3	DB	30	0	0	0	0
3	DC	30	0	0	0	0
3	DG	30	0	0	0	0
3	DI	30	0	0	1	0
All	All	103012	0	102172	1819	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 1819 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)
2:CD:198:ARG:HG3	2:CD:202:TYR:CE2	1.74	1.21
2:DD:198:ARG:HG3	2:DD:202:TYR:CE2	1.74	1.21
2:AD:198:ARG:HG3	2:AD:202:TYR:CE2	1.74	1.21
2:BD:198:ARG:HG3	2:BD:202:TYR:CE2	1.74	1.19
2:DK:192:LEU:O	2:DK:197:ILE:HG12	1.43	1.18

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	AB	184/197 (93%)	178 (97%)	6 (3%)	0	100	100
1	AC	184/197 (93%)	179 (97%)	5 (3%)	0	100	100
1	AG	184/197 (93%)	177 (96%)	7 (4%)	0	100	100
1	AI	184/197 (93%)	181 (98%)	3 (2%)	0	100	100
1	AN	184/197 (93%)	177 (96%)	7 (4%)	0	100	100
1	AO	184/197 (93%)	175 (95%)	9 (5%)	0	100	100
1	AS	184/197 (93%)	178 (97%)	6 (3%)	0	100	100
1	AU	184/197 (93%)	176 (96%)	8 (4%)	0	100	100
1	BB	184/197 (93%)	178 (97%)	6 (3%)	0	100	100
1	BC	184/197 (93%)	179 (97%)	5 (3%)	0	100	100
1	BG	184/197 (93%)	177 (96%)	7 (4%)	0	100	100
1	BI	184/197 (93%)	181 (98%)	3 (2%)	0	100	100
1	BN	184/197 (93%)	177 (96%)	7 (4%)	0	100	100
1	BO	184/197 (93%)	175 (95%)	9 (5%)	0	100	100
1	BS	184/197 (93%)	178 (97%)	6 (3%)	0	100	100
1	BU	184/197 (93%)	175 (95%)	9 (5%)	0	100	100
1	CB	184/197 (93%)	178 (97%)	6 (3%)	0	100	100
1	CC	184/197 (93%)	179 (97%)	5 (3%)	0	100	100
1	CG	184/197 (93%)	177 (96%)	7 (4%)	0	100	100
1	CI	184/197 (93%)	181 (98%)	3 (2%)	0	100	100
1	CN	184/197 (93%)	177 (96%)	7 (4%)	0	100	100
1	CO	184/197 (93%)	175 (95%)	9 (5%)	0	100	100
1	CS	184/197 (93%)	178 (97%)	6 (3%)	0	100	100
1	CU	184/197 (93%)	176 (96%)	8 (4%)	0	100	100
1	DB	184/197 (93%)	178 (97%)	6 (3%)	0	100	100
1	DC	184/197 (93%)	179 (97%)	5 (3%)	0	100	100
1	DG	184/197 (93%)	177 (96%)	7 (4%)	0	100	100
1	DI	184/197 (93%)	181 (98%)	3 (2%)	0	100	100
2	AD	262/264 (99%)	257 (98%)	5 (2%)	0	100	100
2	AE	262/264 (99%)	262 (100%)	0	0	100	100
2	AK	262/264 (99%)	260 (99%)	2 (1%)	0	100	100
2	AL	262/264 (99%)	255 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AP	262/264 (99%)	259 (99%)	3 (1%)	0	100	100
2	AQ	262/264 (99%)	260 (99%)	2 (1%)	0	100	100
2	AW	262/264 (99%)	257 (98%)	5 (2%)	0	100	100
2	AX	262/264 (99%)	258 (98%)	4 (2%)	0	100	100
2	BD	262/264 (99%)	257 (98%)	5 (2%)	0	100	100
2	BE	262/264 (99%)	262 (100%)	0	0	100	100
2	BK	262/264 (99%)	260 (99%)	2 (1%)	0	100	100
2	BL	262/264 (99%)	256 (98%)	6 (2%)	0	100	100
2	BP	262/264 (99%)	259 (99%)	3 (1%)	0	100	100
2	BQ	262/264 (99%)	260 (99%)	2 (1%)	0	100	100
2	BW	262/264 (99%)	257 (98%)	5 (2%)	0	100	100
2	BX	262/264 (99%)	258 (98%)	4 (2%)	0	100	100
2	CD	262/264 (99%)	257 (98%)	5 (2%)	0	100	100
2	CE	262/264 (99%)	262 (100%)	0	0	100	100
2	CK	262/264 (99%)	260 (99%)	2 (1%)	0	100	100
2	CL	262/264 (99%)	256 (98%)	6 (2%)	0	100	100
2	CP	262/264 (99%)	259 (99%)	3 (1%)	0	100	100
2	CQ	262/264 (99%)	259 (99%)	3 (1%)	0	100	100
2	CW	262/264 (99%)	257 (98%)	5 (2%)	0	100	100
2	CX	262/264 (99%)	258 (98%)	4 (2%)	0	100	100
2	DD	262/264 (99%)	257 (98%)	5 (2%)	0	100	100
2	DE	262/264 (99%)	262 (100%)	0	0	100	100
2	DK	262/264 (99%)	260 (99%)	2 (1%)	0	100	100
2	DL	262/264 (99%)	256 (98%)	6 (2%)	0	100	100
All	All	12488/12908 (97%)	12217 (98%)	271 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AB	162/172 (94%)	162 (100%)	0	100	100
1	AC	162/172 (94%)	162 (100%)	0	100	100
1	AG	162/172 (94%)	162 (100%)	0	100	100
1	AI	162/172 (94%)	162 (100%)	0	100	100
1	AN	162/172 (94%)	161 (99%)	1 (1%)	78	83
1	AO	162/172 (94%)	161 (99%)	1 (1%)	78	83
1	AS	162/172 (94%)	161 (99%)	1 (1%)	78	83
1	AU	162/172 (94%)	162 (100%)	0	100	100
1	BB	162/172 (94%)	162 (100%)	0	100	100
1	BC	162/172 (94%)	162 (100%)	0	100	100
1	BG	162/172 (94%)	162 (100%)	0	100	100
1	BI	162/172 (94%)	162 (100%)	0	100	100
1	BN	162/172 (94%)	160 (99%)	2 (1%)	63	77
1	BO	162/172 (94%)	161 (99%)	1 (1%)	78	83
1	BS	162/172 (94%)	162 (100%)	0	100	100
1	BU	162/172 (94%)	162 (100%)	0	100	100
1	CB	162/172 (94%)	162 (100%)	0	100	100
1	CC	162/172 (94%)	162 (100%)	0	100	100
1	CG	162/172 (94%)	162 (100%)	0	100	100
1	CI	162/172 (94%)	162 (100%)	0	100	100
1	CN	162/172 (94%)	162 (100%)	0	100	100
1	CO	162/172 (94%)	161 (99%)	1 (1%)	78	83
1	CS	162/172 (94%)	161 (99%)	1 (1%)	78	83
1	CU	162/172 (94%)	161 (99%)	1 (1%)	78	83
1	DB	162/172 (94%)	162 (100%)	0	100	100
1	DC	162/172 (94%)	162 (100%)	0	100	100
1	DG	162/172 (94%)	162 (100%)	0	100	100
1	DI	162/172 (94%)	162 (100%)	0	100	100
2	AD	240/240 (100%)	239 (100%)	1 (0%)	84	85
2	AE	240/240 (100%)	239 (100%)	1 (0%)	84	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AK	240/240 (100%)	237 (99%)	3 (1%)	61	75
2	AL	240/240 (100%)	240 (100%)	0	100	100
2	AP	240/240 (100%)	240 (100%)	0	100	100
2	AQ	240/240 (100%)	240 (100%)	0	100	100
2	AW	240/240 (100%)	239 (100%)	1 (0%)	84	85
2	AX	240/240 (100%)	240 (100%)	0	100	100
2	BD	240/240 (100%)	239 (100%)	1 (0%)	84	85
2	BE	240/240 (100%)	239 (100%)	1 (0%)	84	85
2	BK	240/240 (100%)	237 (99%)	3 (1%)	61	75
2	BL	240/240 (100%)	240 (100%)	0	100	100
2	BP	240/240 (100%)	240 (100%)	0	100	100
2	BQ	240/240 (100%)	240 (100%)	0	100	100
2	BW	240/240 (100%)	239 (100%)	1 (0%)	84	85
2	BX	240/240 (100%)	240 (100%)	0	100	100
2	CD	240/240 (100%)	239 (100%)	1 (0%)	84	85
2	CE	240/240 (100%)	239 (100%)	1 (0%)	84	85
2	CK	240/240 (100%)	237 (99%)	3 (1%)	61	75
2	CL	240/240 (100%)	240 (100%)	0	100	100
2	CP	240/240 (100%)	239 (100%)	1 (0%)	84	85
2	CQ	240/240 (100%)	239 (100%)	1 (0%)	84	85
2	CW	240/240 (100%)	239 (100%)	1 (0%)	84	85
2	CX	240/240 (100%)	240 (100%)	0	100	100
2	DD	240/240 (100%)	240 (100%)	0	100	100
2	DE	240/240 (100%)	239 (100%)	1 (0%)	84	85
2	DK	240/240 (100%)	237 (99%)	3 (1%)	61	75
2	DL	240/240 (100%)	239 (100%)	1 (0%)	84	85
All	All	11256/11536 (98%)	11222 (100%)	34 (0%)	84	87

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AK	197	ILE
2	AK	242	MET

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Mol	Chain	Res	Type
1	AS	76	VAL
2	CK	197	ILE
2	CK	192	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
1	DB	176	ASN
2	DK	146	HIS
1	AU	30	ASN
1	DC	56	HIS
2	DE	146	HIS

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](#)

28 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	$\# Z > 2$
3	Y43	BS	201	-	28,32,32	2.51	9 (32%)	35,50,50	1.67	6 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	Y43	CC	201	-	28,32,32	2.54	9 (32%)	35,50,50	1.75	6 (17%)
3	Y43	AU	201	-	28,32,32	2.48	9 (32%)	35,50,50	1.69	6 (17%)
3	Y43	AB	201	-	28,32,32	2.56	9 (32%)	35,50,50	1.74	6 (17%)
3	Y43	DC	201	-	28,32,32	2.54	9 (32%)	35,50,50	1.75	6 (17%)
3	Y43	DI	201	-	28,32,32	2.56	9 (32%)	35,50,50	1.69	7 (20%)
3	Y43	BN	201	-	28,32,32	2.55	9 (32%)	35,50,50	1.72	6 (17%)
3	Y43	CI	201	-	28,32,32	2.56	9 (32%)	35,50,50	1.69	7 (20%)
3	Y43	AS	201	-	28,32,32	2.50	9 (32%)	35,50,50	1.67	6 (17%)
3	Y43	DB	201	-	28,32,32	2.57	9 (32%)	35,50,50	1.73	6 (17%)
3	Y43	CU	201	-	28,32,32	2.48	8 (28%)	35,50,50	1.69	6 (17%)
3	Y43	BB	201	-	28,32,32	2.57	9 (32%)	35,50,50	1.74	6 (17%)
3	Y43	BG	201	-	28,32,32	2.55	9 (32%)	35,50,50	1.76	6 (17%)
3	Y43	AG	201	-	28,32,32	2.55	9 (32%)	35,50,50	1.75	6 (17%)
3	Y43	BU	201	-	28,32,32	2.48	8 (28%)	35,50,50	1.69	6 (17%)
3	Y43	CN	201	-	28,32,32	2.55	9 (32%)	35,50,50	1.71	6 (17%)
3	Y43	BC	201	-	28,32,32	2.54	9 (32%)	35,50,50	1.74	6 (17%)
3	Y43	AN	201	-	28,32,32	2.55	9 (32%)	35,50,50	1.72	6 (17%)
3	Y43	CS	201	-	28,32,32	2.51	9 (32%)	35,50,50	1.67	6 (17%)
3	Y43	AO	201	-	28,32,32	2.49	9 (32%)	35,50,50	1.69	6 (17%)
3	Y43	AC	201	-	28,32,32	2.54	9 (32%)	35,50,50	1.74	6 (17%)
3	Y43	CB	201	-	28,32,32	2.56	9 (32%)	35,50,50	1.74	6 (17%)
3	Y43	CG	201	-	28,32,32	2.56	9 (32%)	35,50,50	1.76	6 (17%)
3	Y43	BI	201	-	28,32,32	2.56	9 (32%)	35,50,50	1.69	7 (20%)
3	Y43	CO	201	-	28,32,32	2.49	9 (32%)	35,50,50	1.68	6 (17%)
3	Y43	DG	201	-	28,32,32	2.55	9 (32%)	35,50,50	1.76	6 (17%)
3	Y43	BO	201	-	28,32,32	2.49	9 (32%)	35,50,50	1.68	6 (17%)
3	Y43	AI	201	-	28,32,32	2.57	9 (32%)	35,50,50	1.69	7 (20%)

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	Y43	BS	201	-	2/2/6/6	5/22/34/34	0/3/3/3
3	Y43	CC	201	-	2/2/6/6	5/22/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	Y43	AU	201	-	2/2/6/6	2/22/34/34	0/3/3/3
3	Y43	AB	201	-	2/2/6/6	6/22/34/34	0/3/3/3
3	Y43	DC	201	-	2/2/6/6	5/22/34/34	0/3/3/3
3	Y43	DI	201	-	2/2/6/6	6/22/34/34	0/3/3/3
3	Y43	BN	201	-	2/2/6/6	9/22/34/34	0/3/3/3
3	Y43	CI	201	-	2/2/6/6	6/22/34/34	0/3/3/3
3	Y43	AS	201	-	2/2/6/6	5/22/34/34	0/3/3/3
3	Y43	DB	201	-	2/2/6/6	6/22/34/34	0/3/3/3
3	Y43	CU	201	-	2/2/6/6	2/22/34/34	0/3/3/3
3	Y43	BB	201	-	2/2/6/6	5/22/34/34	0/3/3/3
3	Y43	BG	201	-	2/2/6/6	6/22/34/34	0/3/3/3
3	Y43	AG	201	-	2/2/6/6	6/22/34/34	0/3/3/3
3	Y43	BU	201	-	2/2/6/6	2/22/34/34	0/3/3/3
3	Y43	CN	201	-	2/2/6/6	9/22/34/34	0/3/3/3
3	Y43	BC	201	-	2/2/6/6	5/22/34/34	0/3/3/3
3	Y43	AN	201	-	2/2/6/6	9/22/34/34	0/3/3/3
3	Y43	CS	201	-	2/2/6/6	5/22/34/34	0/3/3/3
3	Y43	AO	201	-	2/2/6/6	6/22/34/34	0/3/3/3
3	Y43	AC	201	-	2/2/6/6	5/22/34/34	0/3/3/3
3	Y43	CB	201	-	2/2/6/6	5/22/34/34	0/3/3/3
3	Y43	CG	201	-	2/2/6/6	6/22/34/34	0/3/3/3
3	Y43	BI	201	-	2/2/6/6	6/22/34/34	0/3/3/3
3	Y43	CO	201	-	2/2/6/6	6/22/34/34	0/3/3/3
3	Y43	DG	201	-	2/2/6/6	6/22/34/34	0/3/3/3
3	Y43	BO	201	-	2/2/6/6	6/22/34/34	0/3/3/3
3	Y43	AI	201	-	2/2/6/6	6/22/34/34	0/3/3/3

The worst 5 of 250 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CB	201	Y43	PAI-OAH	7.77	1.90	1.59
3	BB	201	Y43	PAI-OAH	7.77	1.90	1.59
3	AB	201	Y43	PAI-OAH	7.77	1.90	1.59
3	DB	201	Y43	PAI-OAH	7.75	1.90	1.59
3	BS	201	Y43	PAI-OAH	7.59	1.90	1.59

The worst 5 of 172 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BB	201	Y43	O6-C6-N1	-4.61	114.58	120.52
3	DB	201	Y43	O6-C6-N1	-4.61	114.59	120.52
3	AB	201	Y43	O6-C6-N1	-4.59	114.61	120.52
3	CB	201	Y43	O6-C6-N1	-4.58	114.62	120.52
3	DC	201	Y43	O6-C6-N1	-4.55	114.66	120.52

5 of 56 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	BC	201	Y43	CAF
3	BC	201	Y43	CAD
3	BG	201	Y43	CAF
3	BG	201	Y43	CAD
3	BI	201	Y43	CAF

5 of 156 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BC	201	Y43	CAF-CAG-OAH-PAI
3	BG	201	Y43	CAB-CAF-CAG-OAH
3	BG	201	Y43	PAM-OAL-PAI-OAH
3	BI	201	Y43	CAC-CAD-N9-C4
3	BI	201	Y43	CAC-CAD-N9-C8

There are no ring outliers.

17 monomers are involved in 19 short contacts:

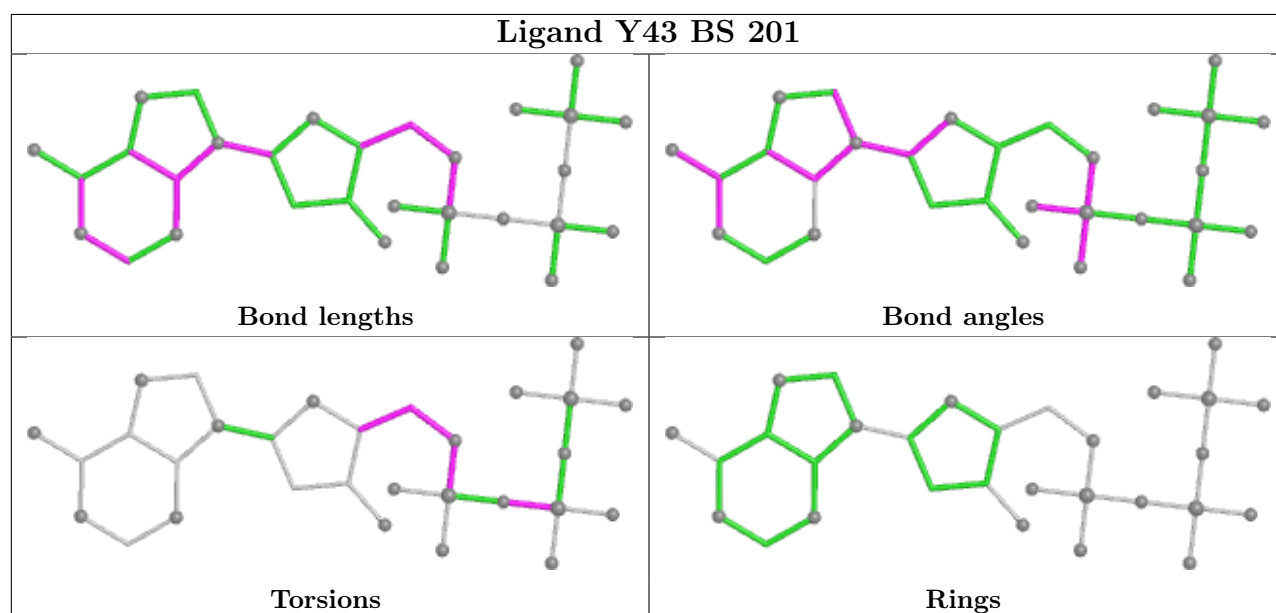
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BS	201	Y43	2	0
3	AU	201	Y43	1	0
3	DI	201	Y43	1	0
3	BN	201	Y43	1	0
3	CI	201	Y43	1	0
3	CU	201	Y43	1	0
3	AG	201	Y43	1	0
3	BU	201	Y43	1	0
3	CN	201	Y43	1	0
3	AN	201	Y43	1	0
3	CS	201	Y43	2	0
3	AO	201	Y43	1	0
3	AC	201	Y43	1	0

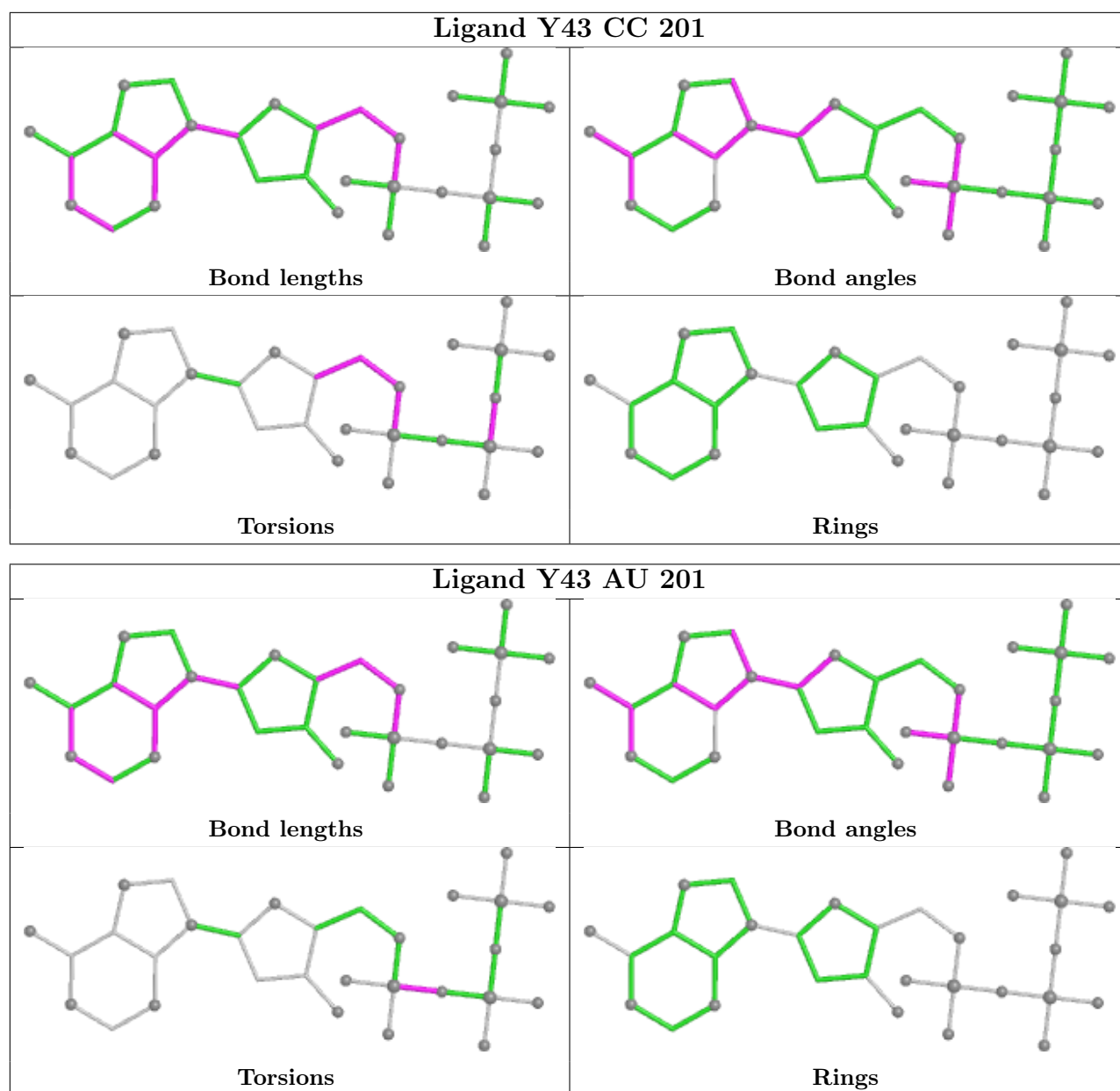
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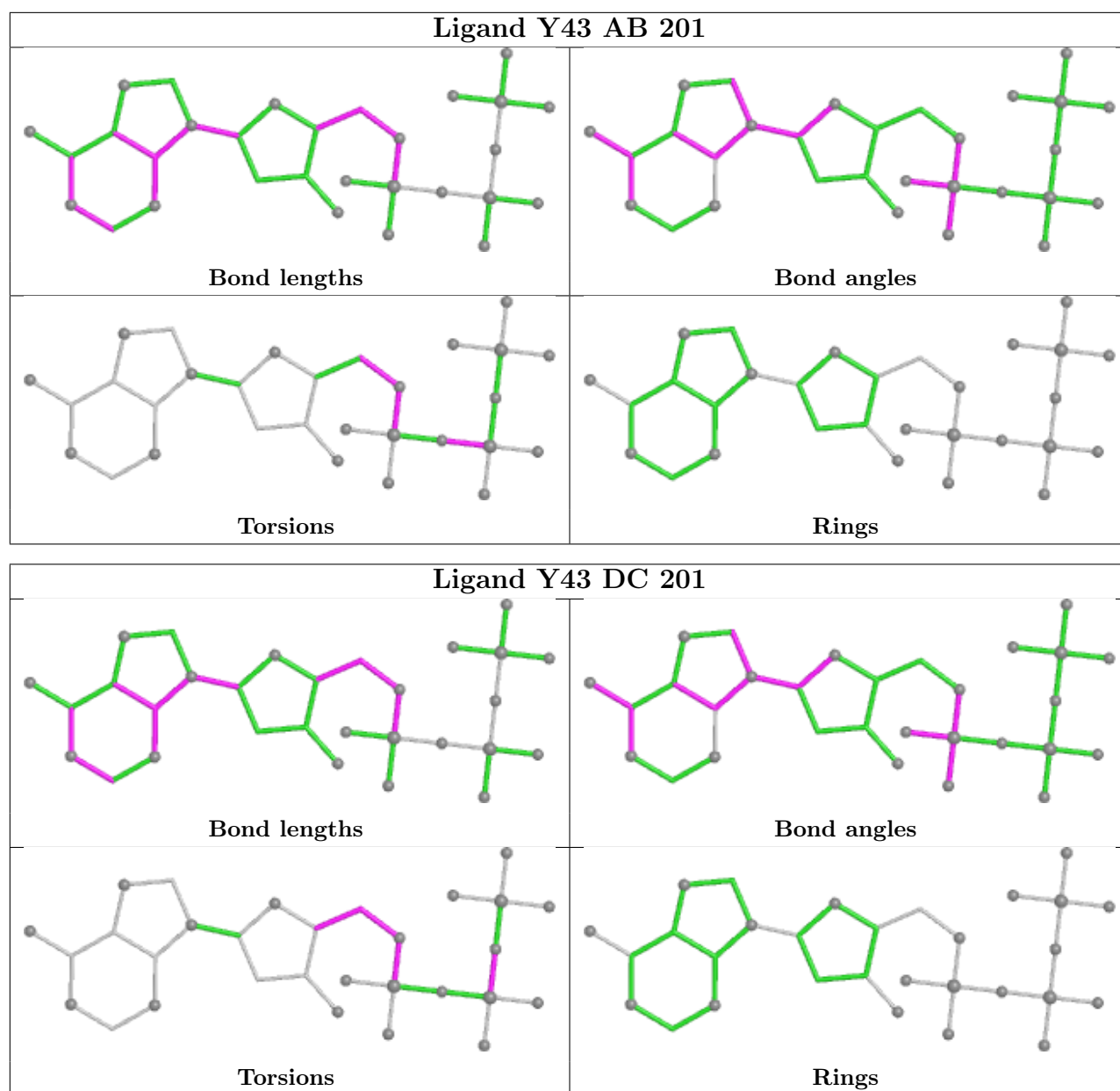
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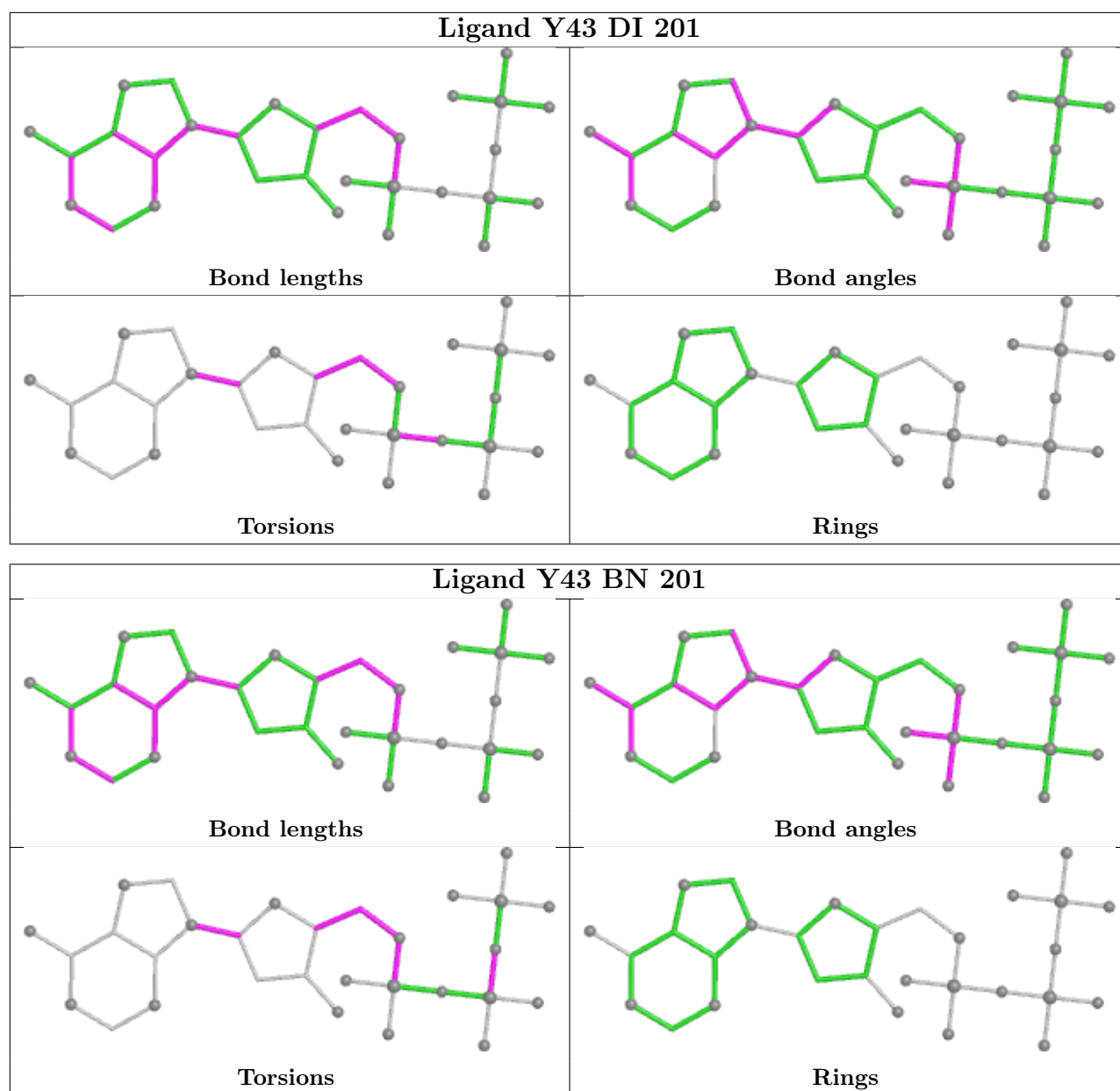
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	CG	201	Y43	1	0
3	CO	201	Y43	1	0
3	BO	201	Y43	1	0
3	AI	201	Y43	1	0

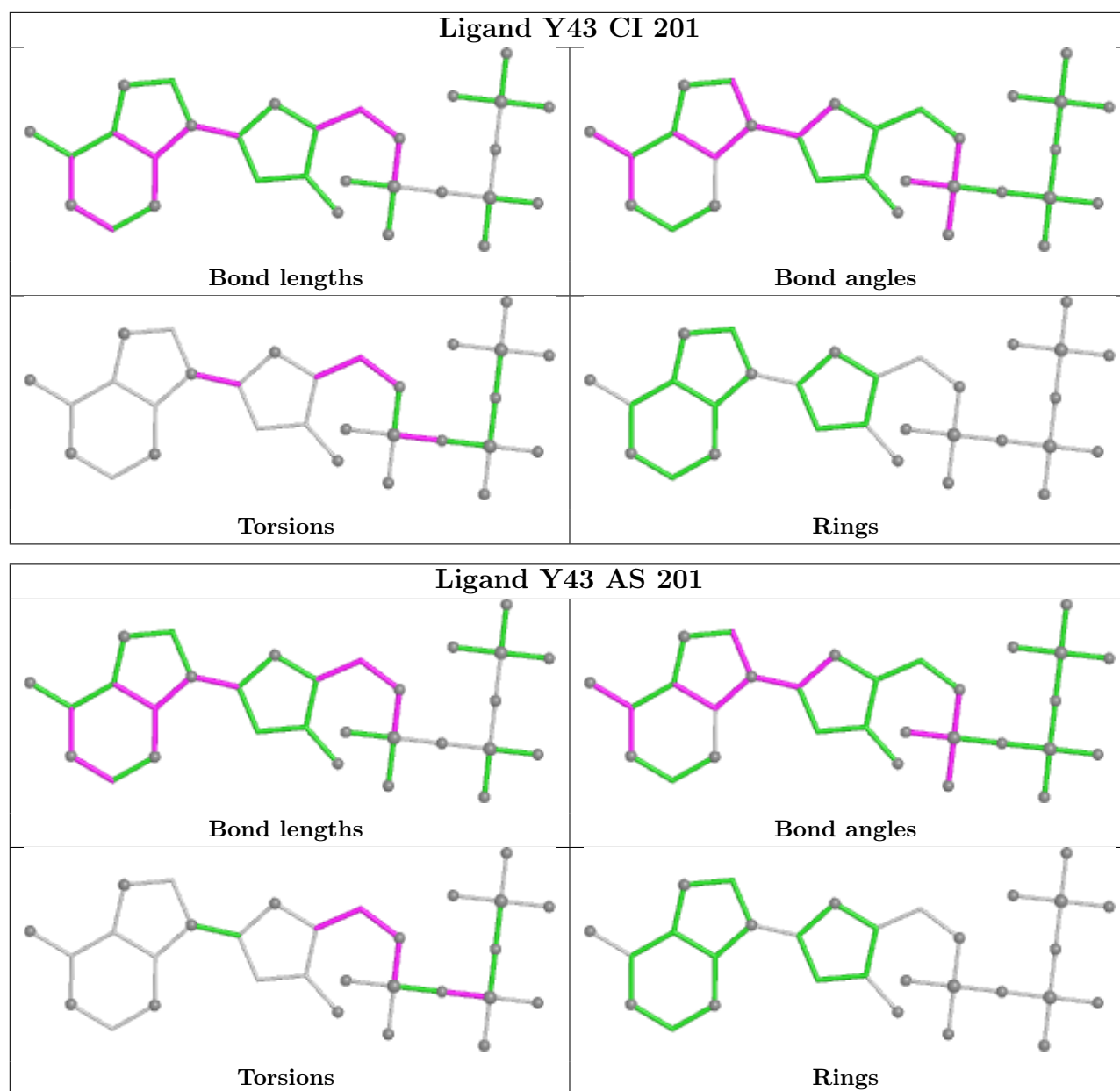
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

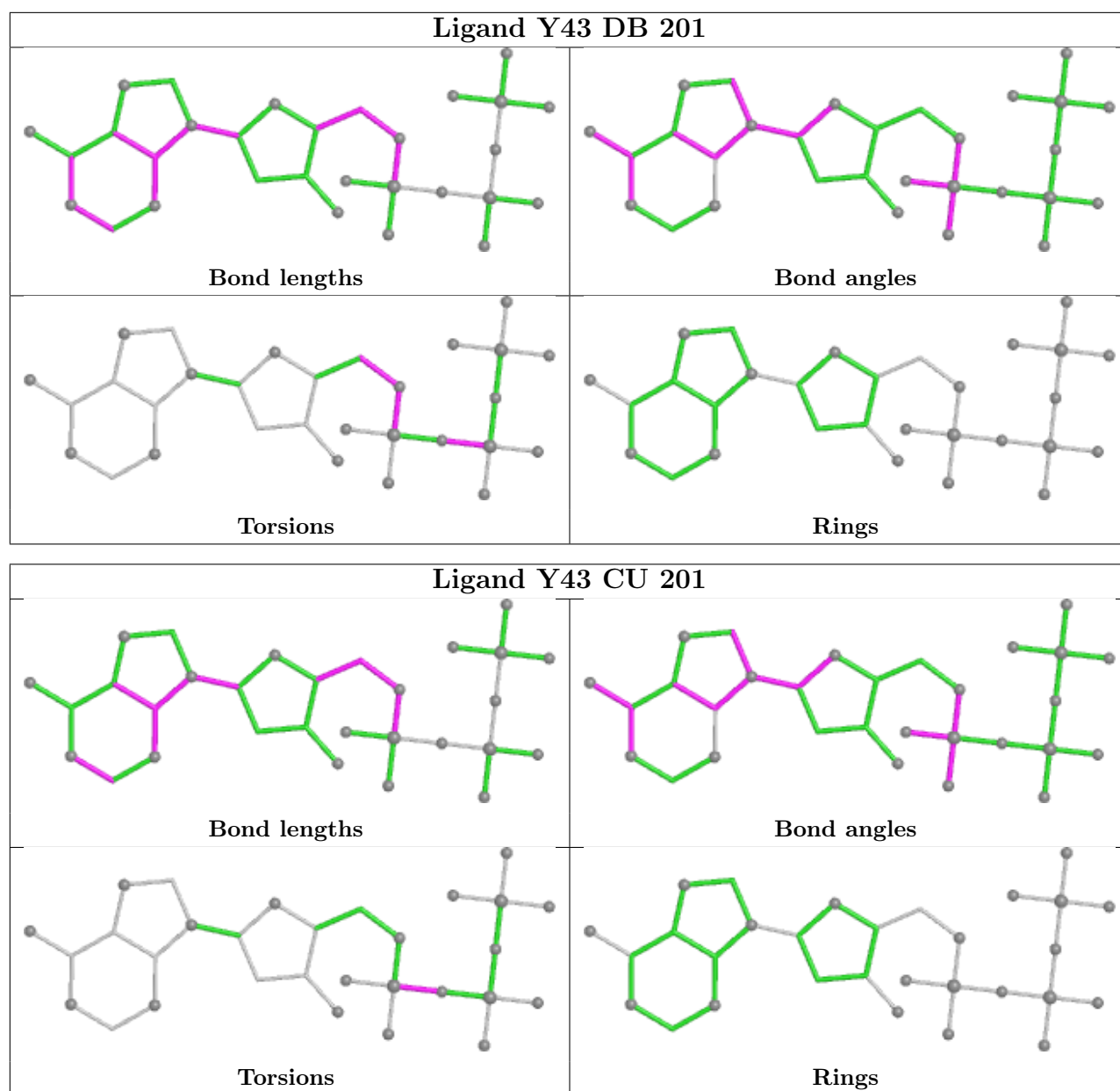


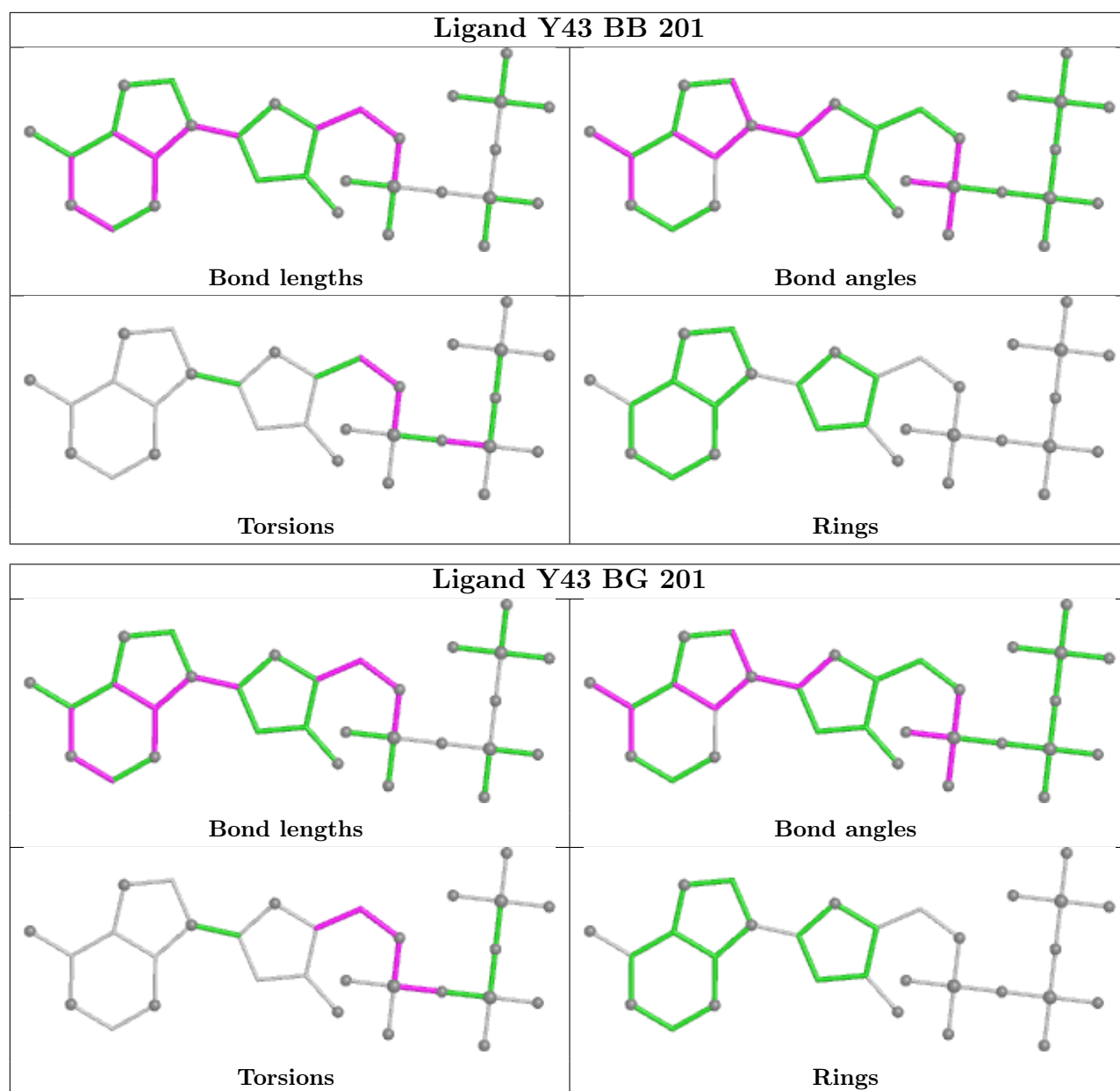




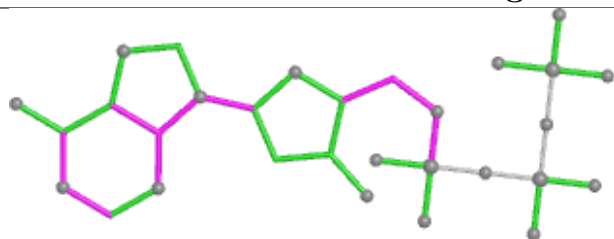




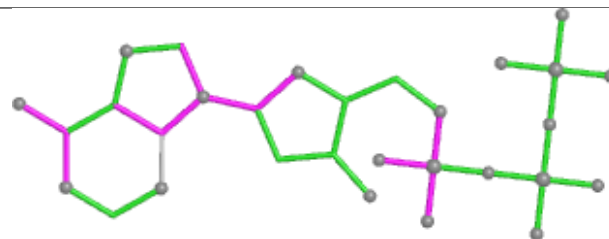




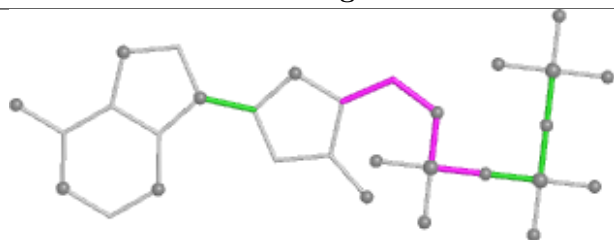
Ligand Y43 AG 201



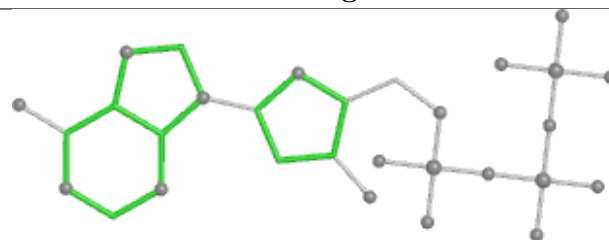
Bond lengths



Bond angles

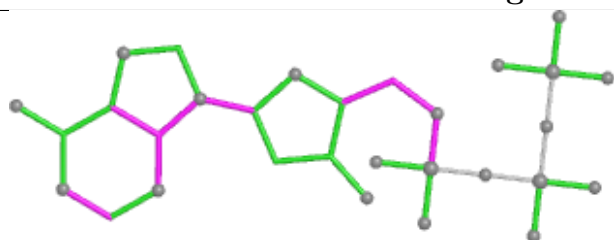


Torsions

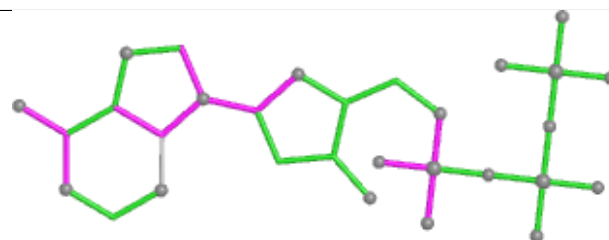


Rings

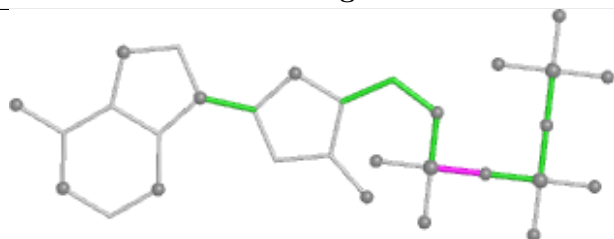
Ligand Y43 BU 201



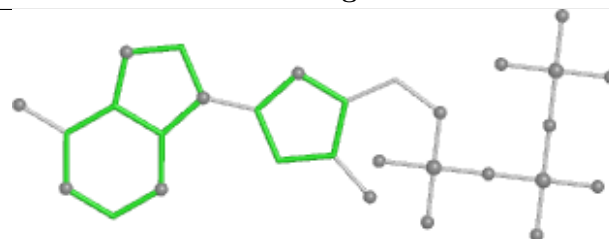
Bond lengths



Bond angles

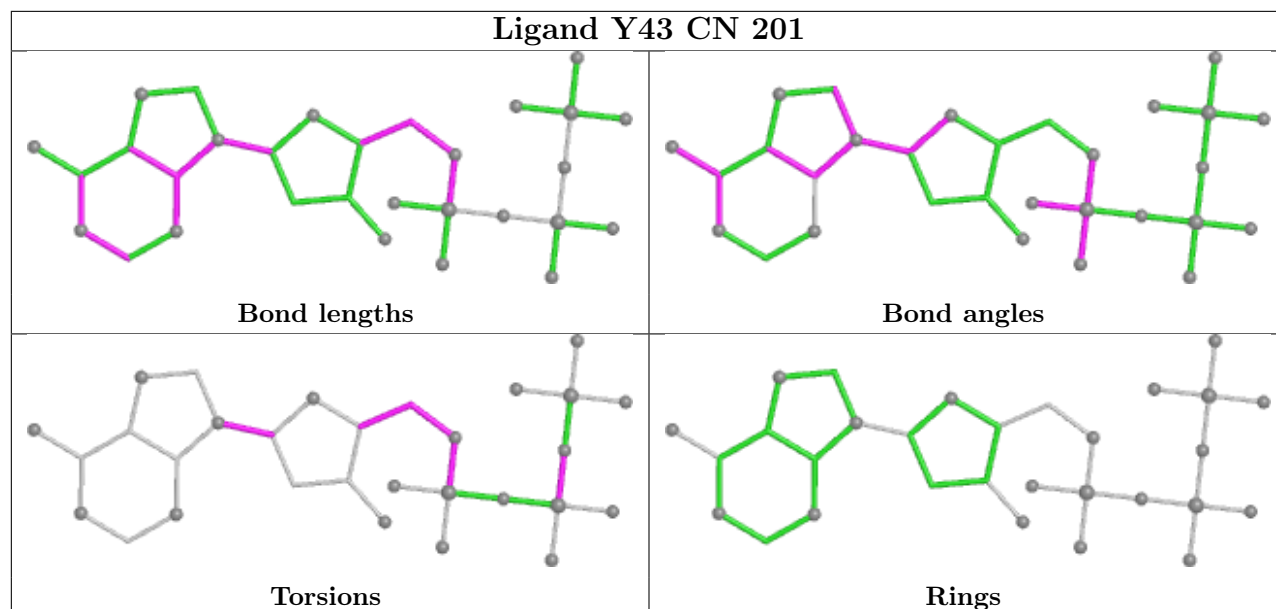


Torsions

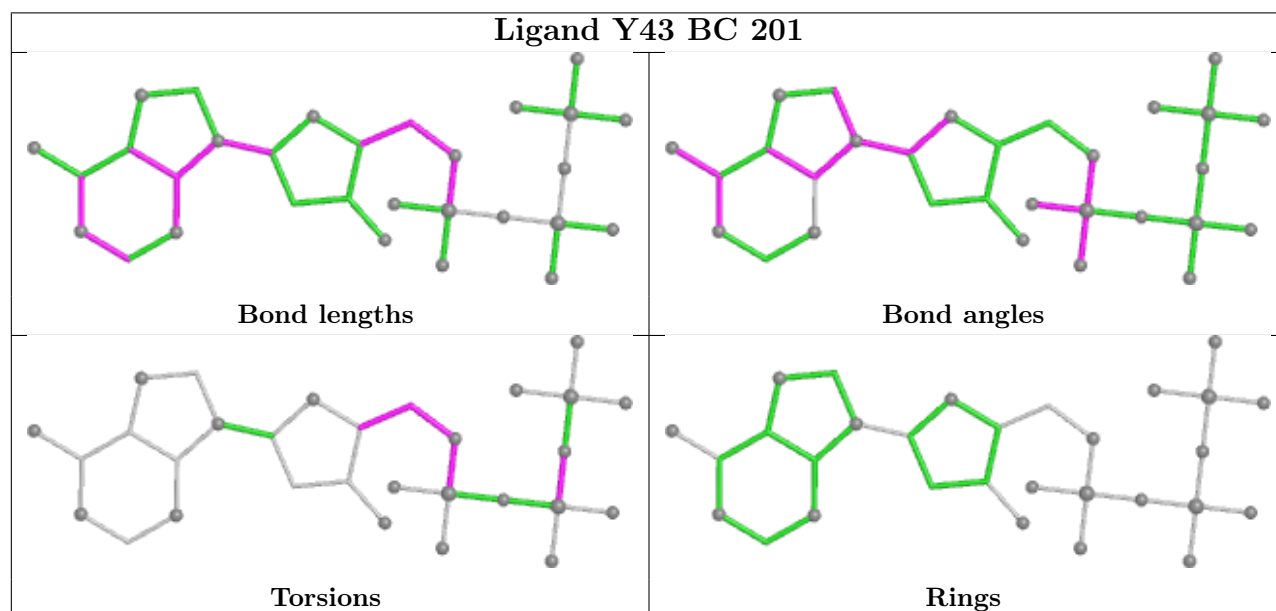


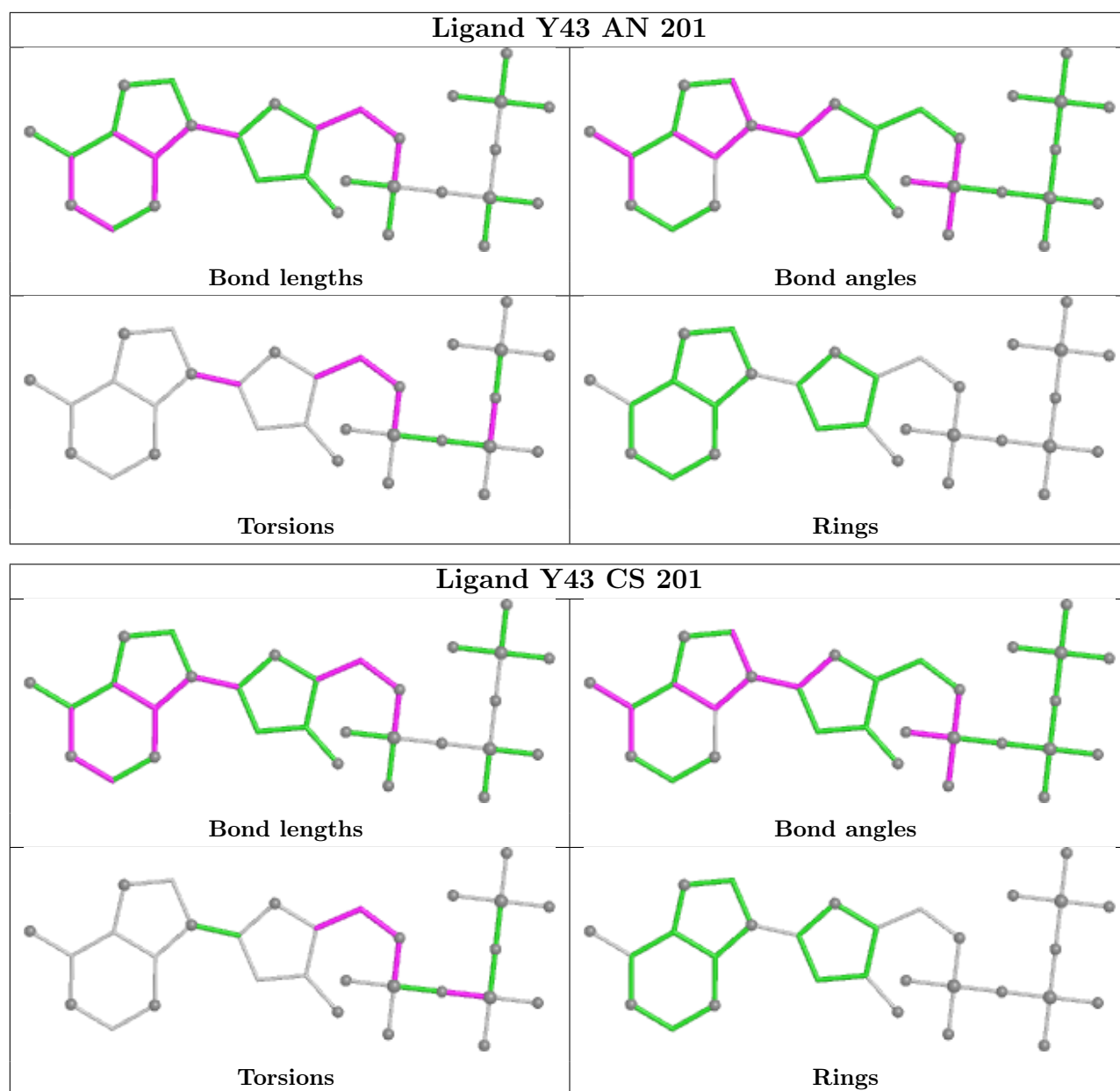
Rings

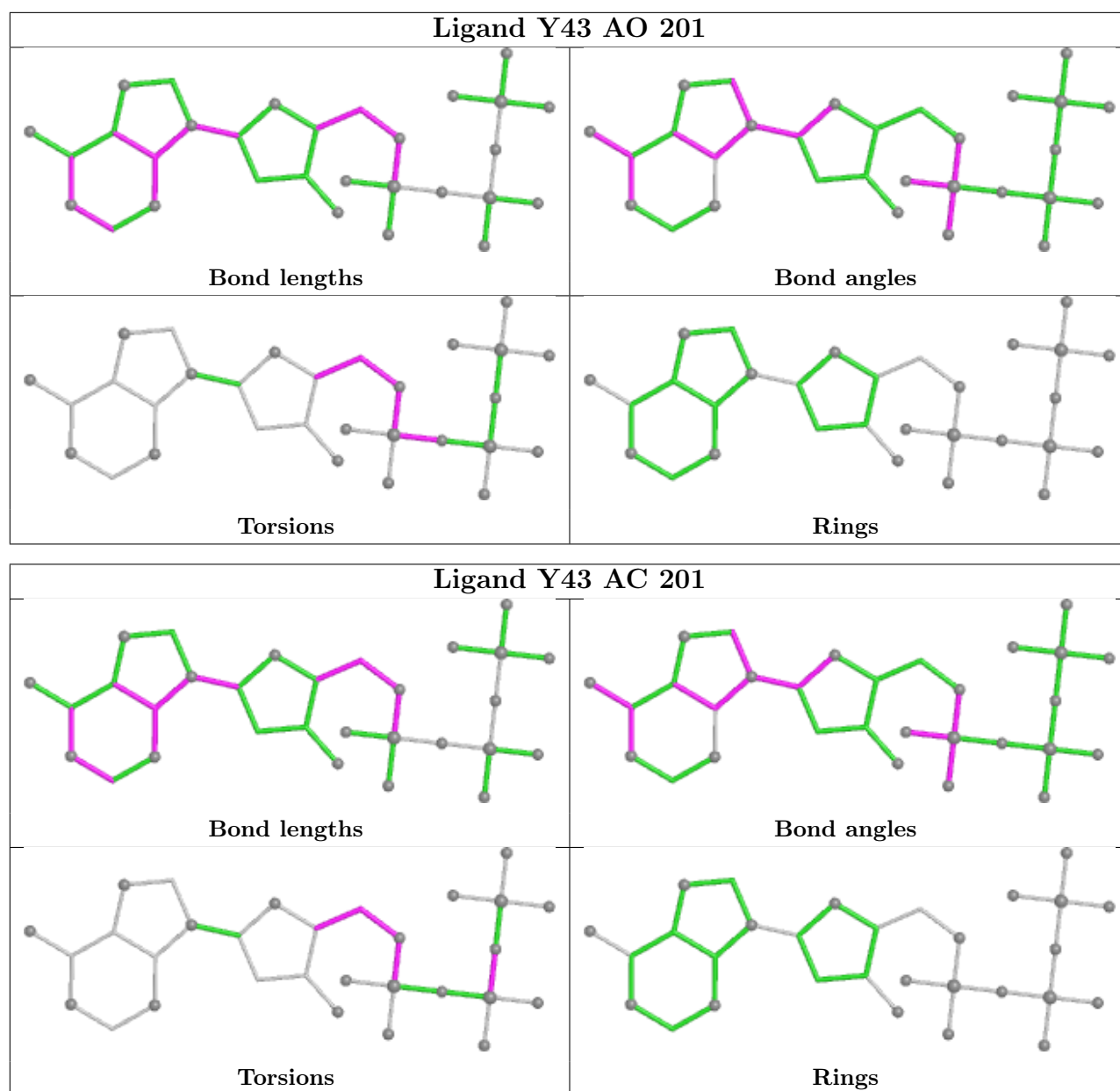
Ligand Y43 CN 201

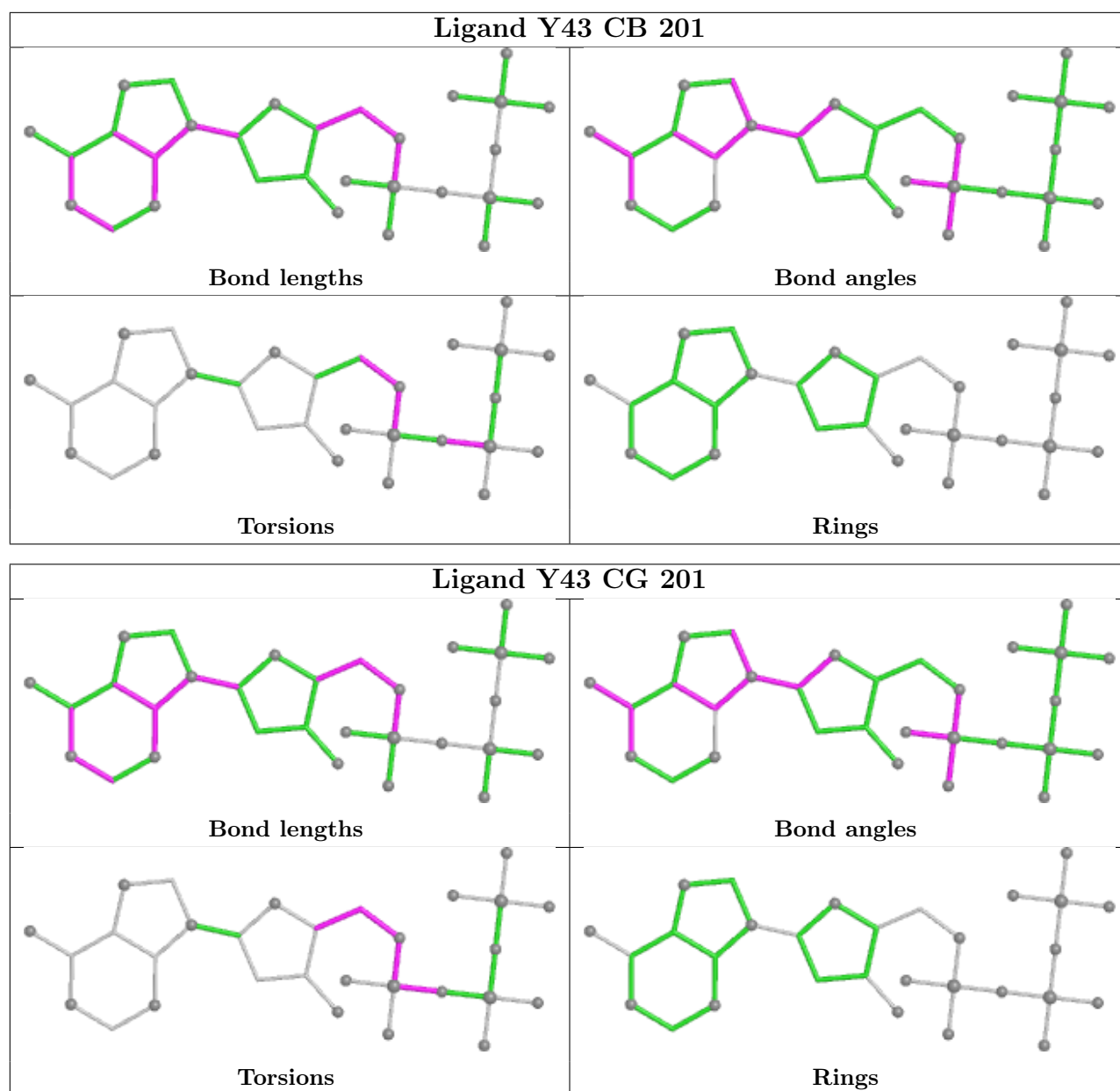


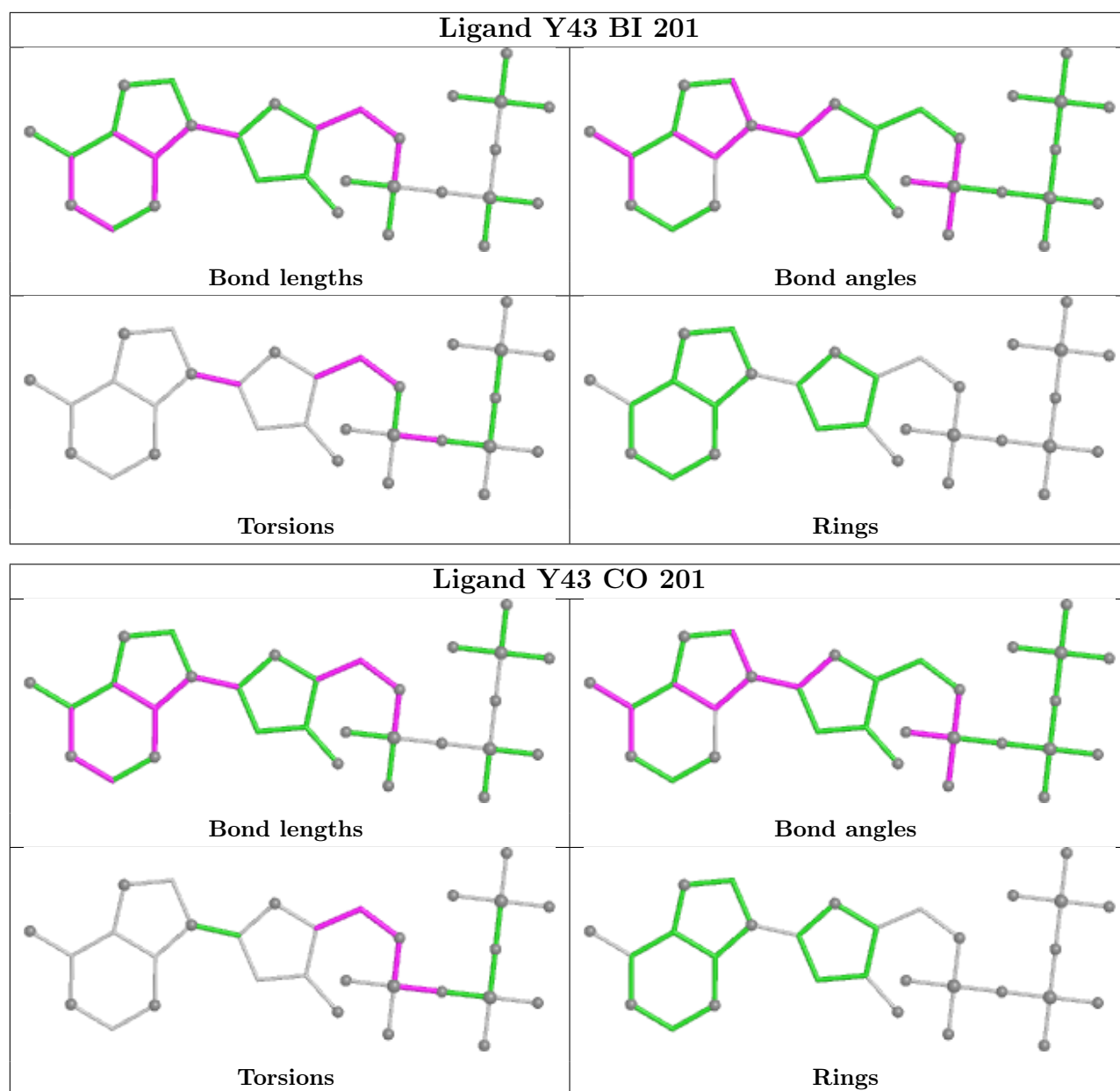
Ligand Y43 BC 201



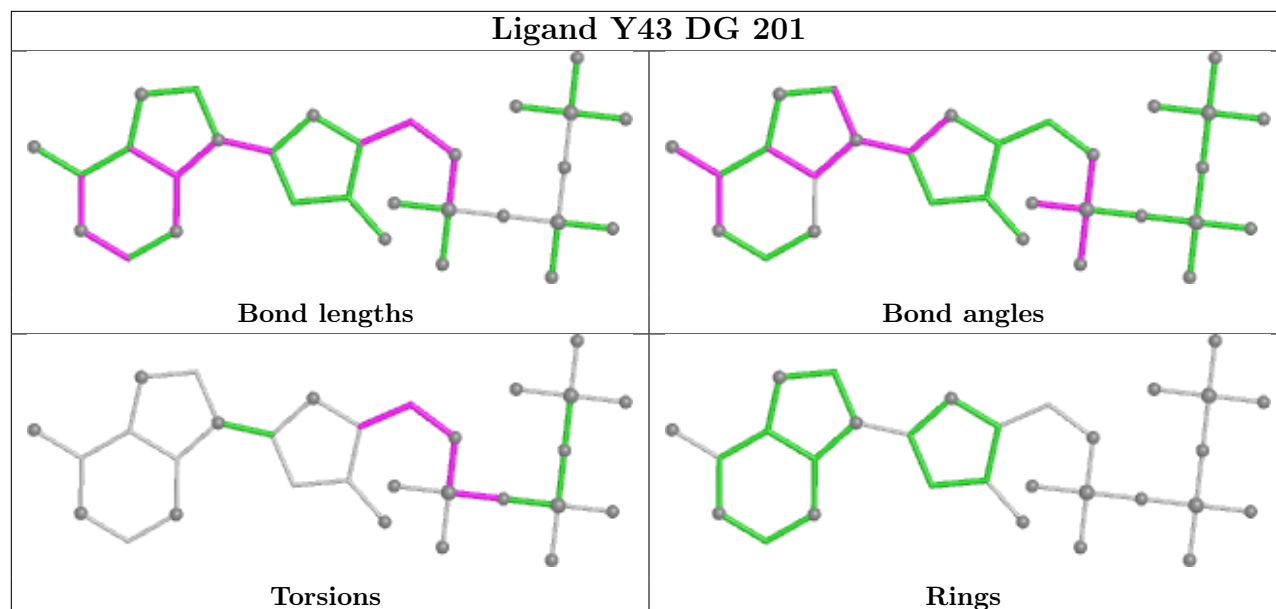




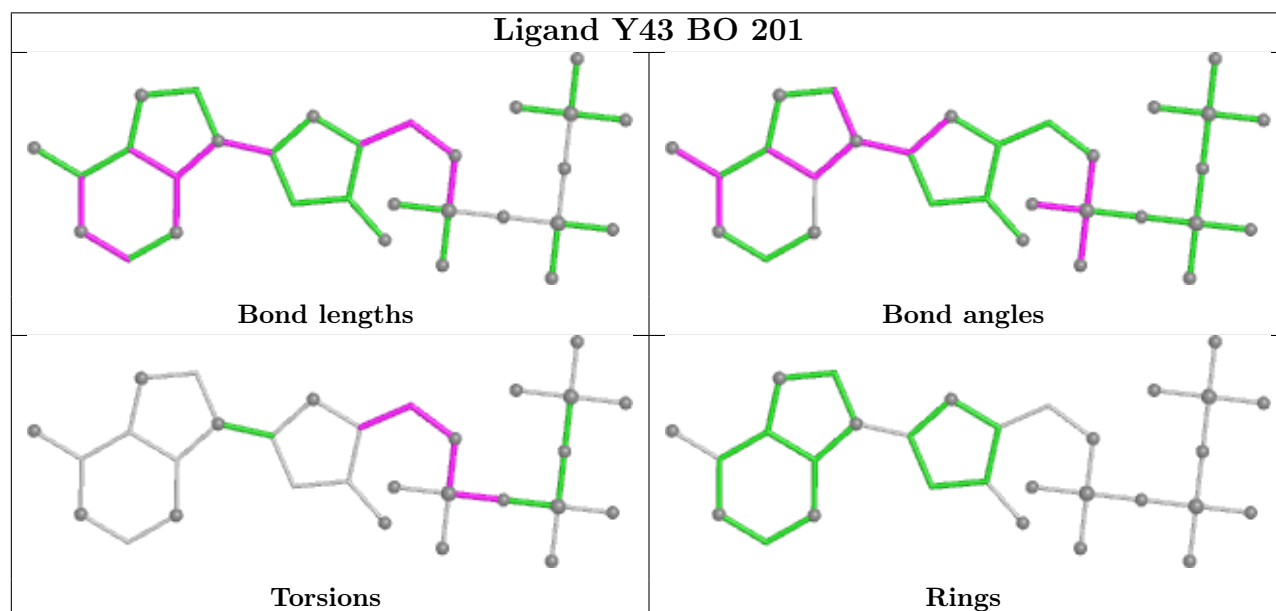


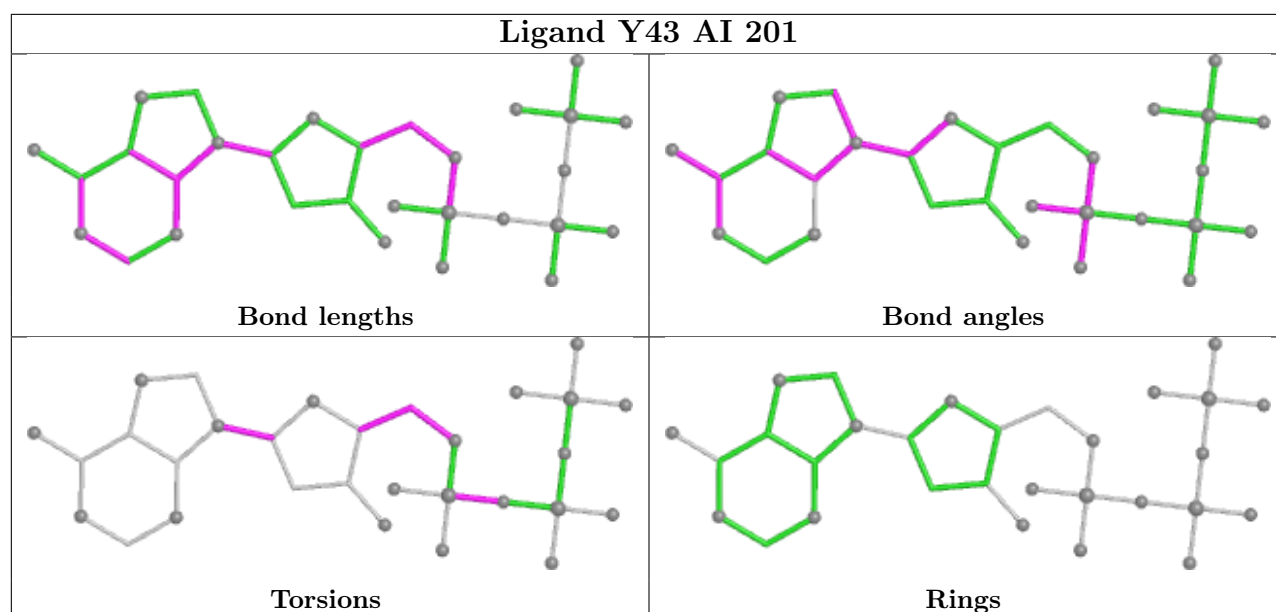


Ligand Y43 DG 201



Ligand Y43 BO 201





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.

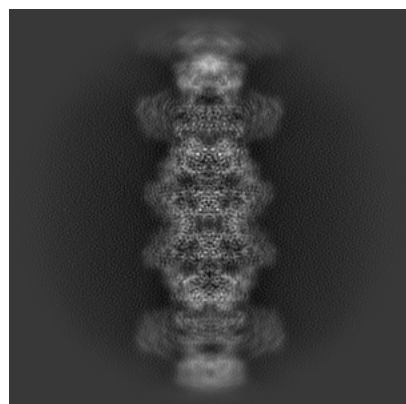
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66453. These allow visual inspection of the internal detail of the map and identification of artifacts.

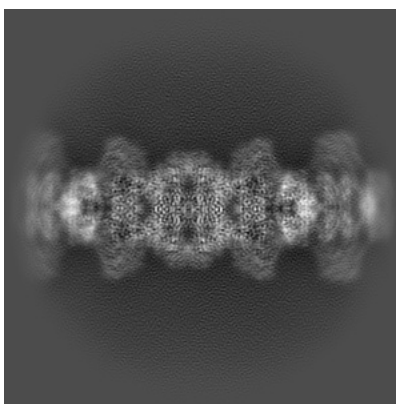
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

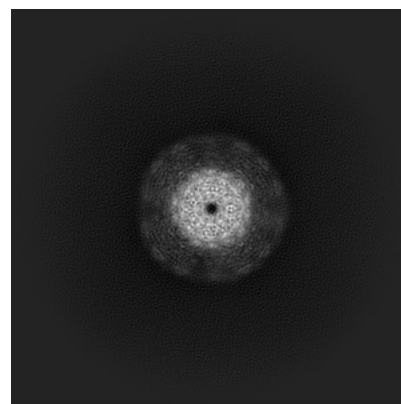
6.1.1 Primary map



X

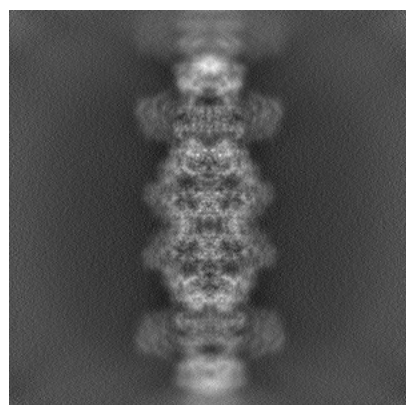


Y

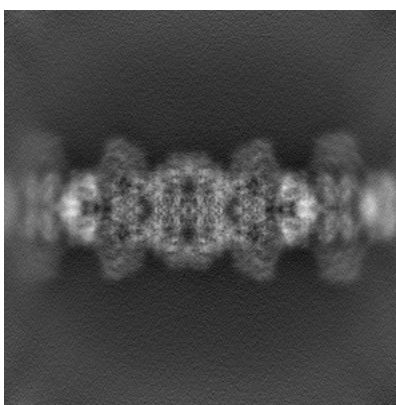


Z

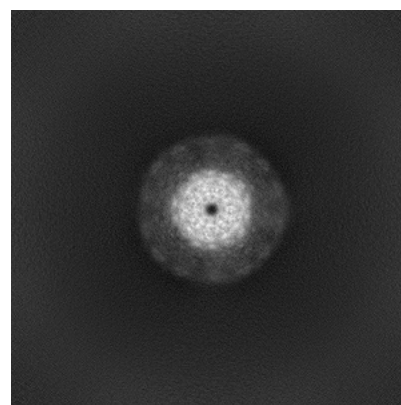
6.1.2 Raw map



X



Y

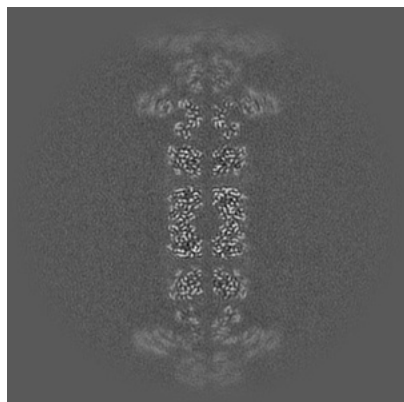


Z

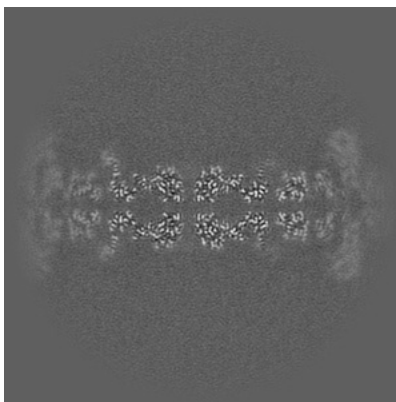
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

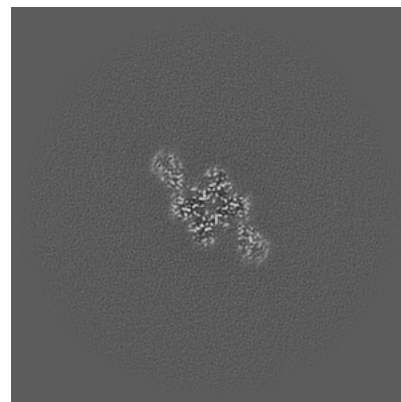
6.2.1 Primary map



X Index: 300

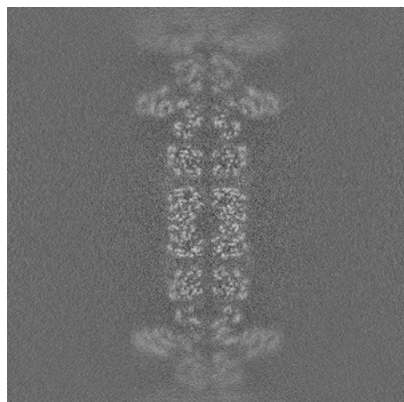


Y Index: 300

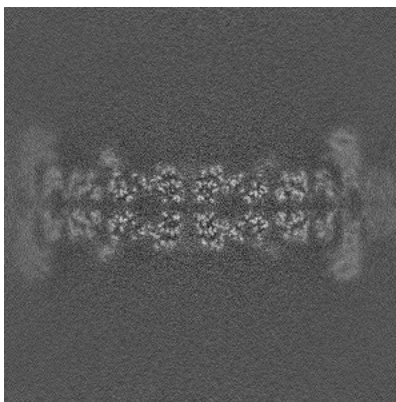


Z Index: 300

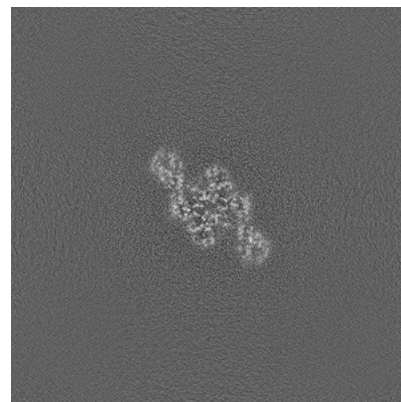
6.2.2 Raw map



X Index: 300



Y Index: 300

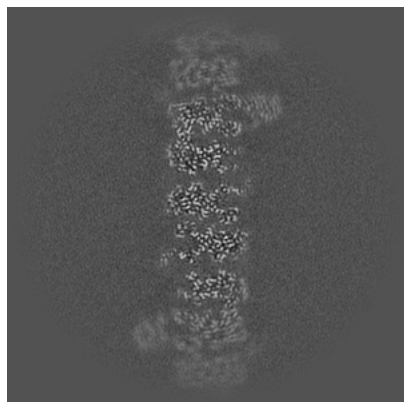


Z Index: 300

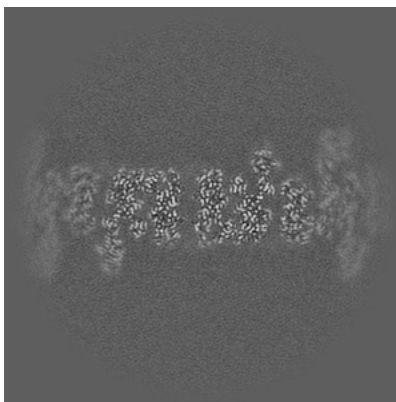
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

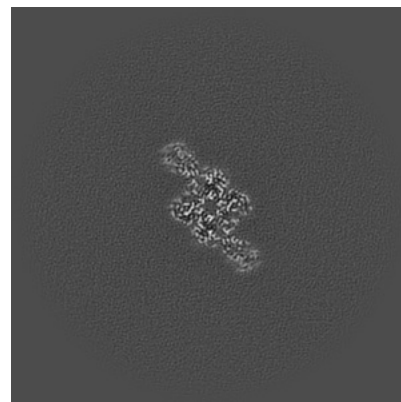
6.3.1 Primary map



X Index: 286

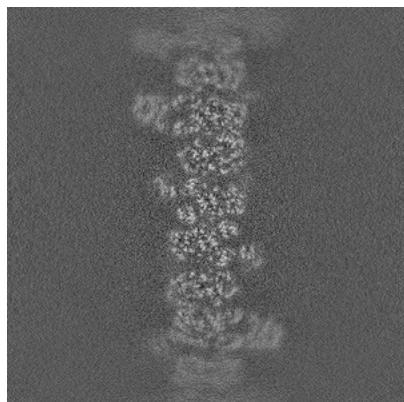


Y Index: 313

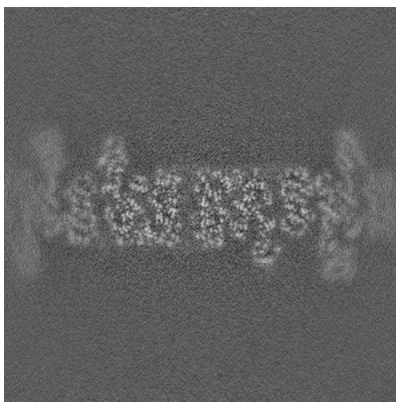


Z Index: 319

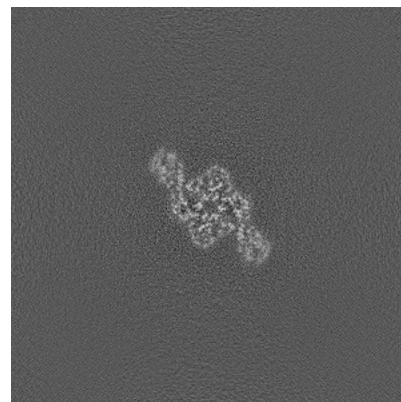
6.3.2 Raw map



X Index: 318



Y Index: 287

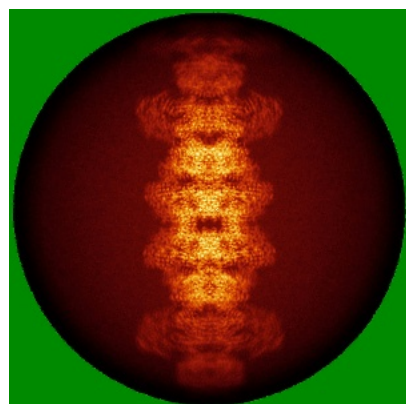


Z Index: 298

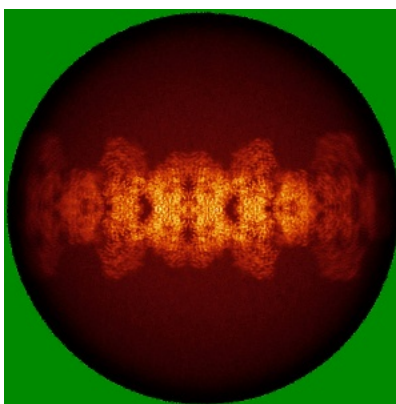
The images above show the largest variance slices of the map in three orthogonal directions.

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

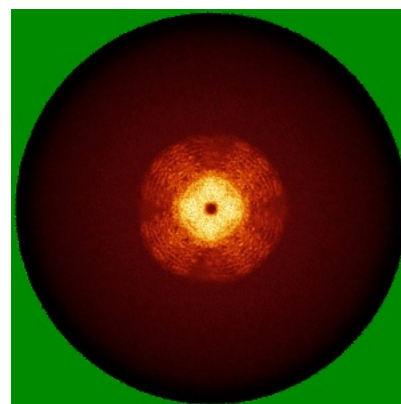
6.4.1 Primary map



X

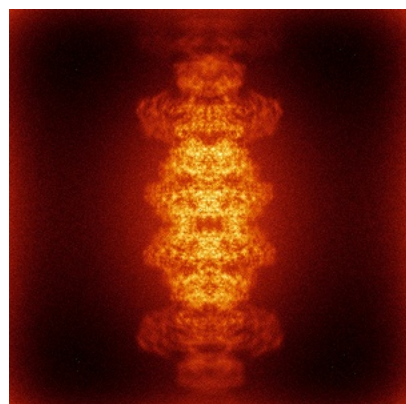


Y

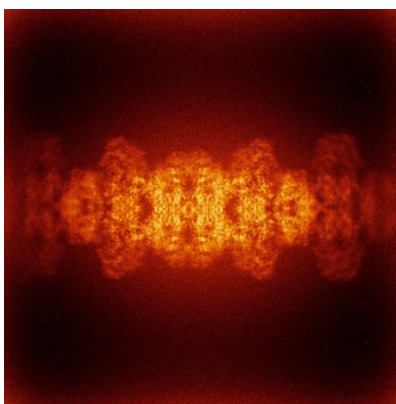


Z

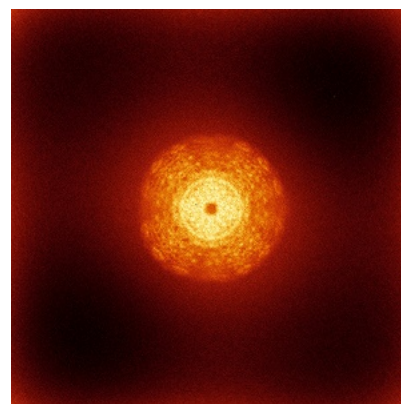
6.4.2 Raw map



X



Y

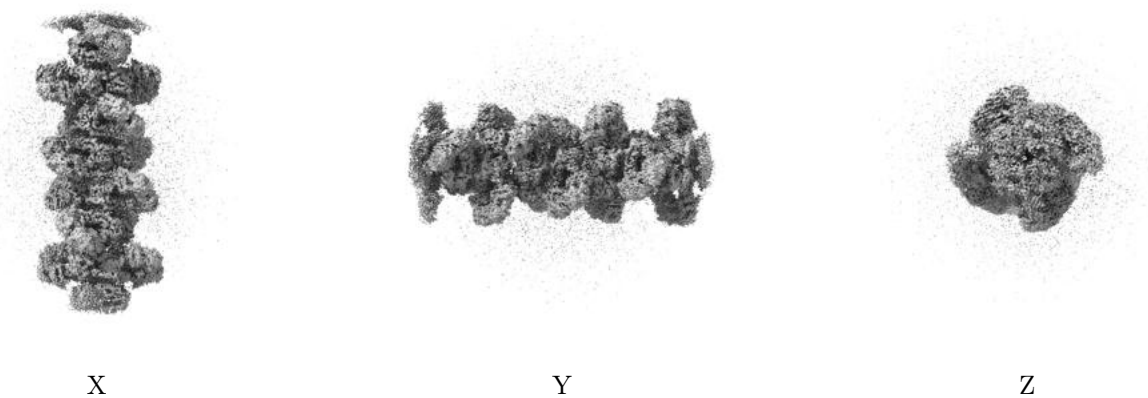


Z

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.

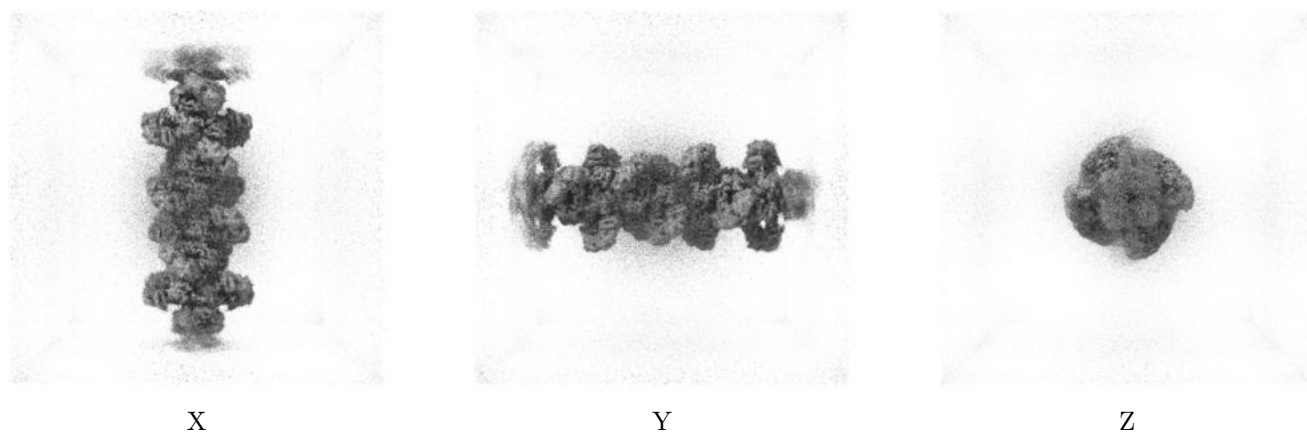
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. 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.

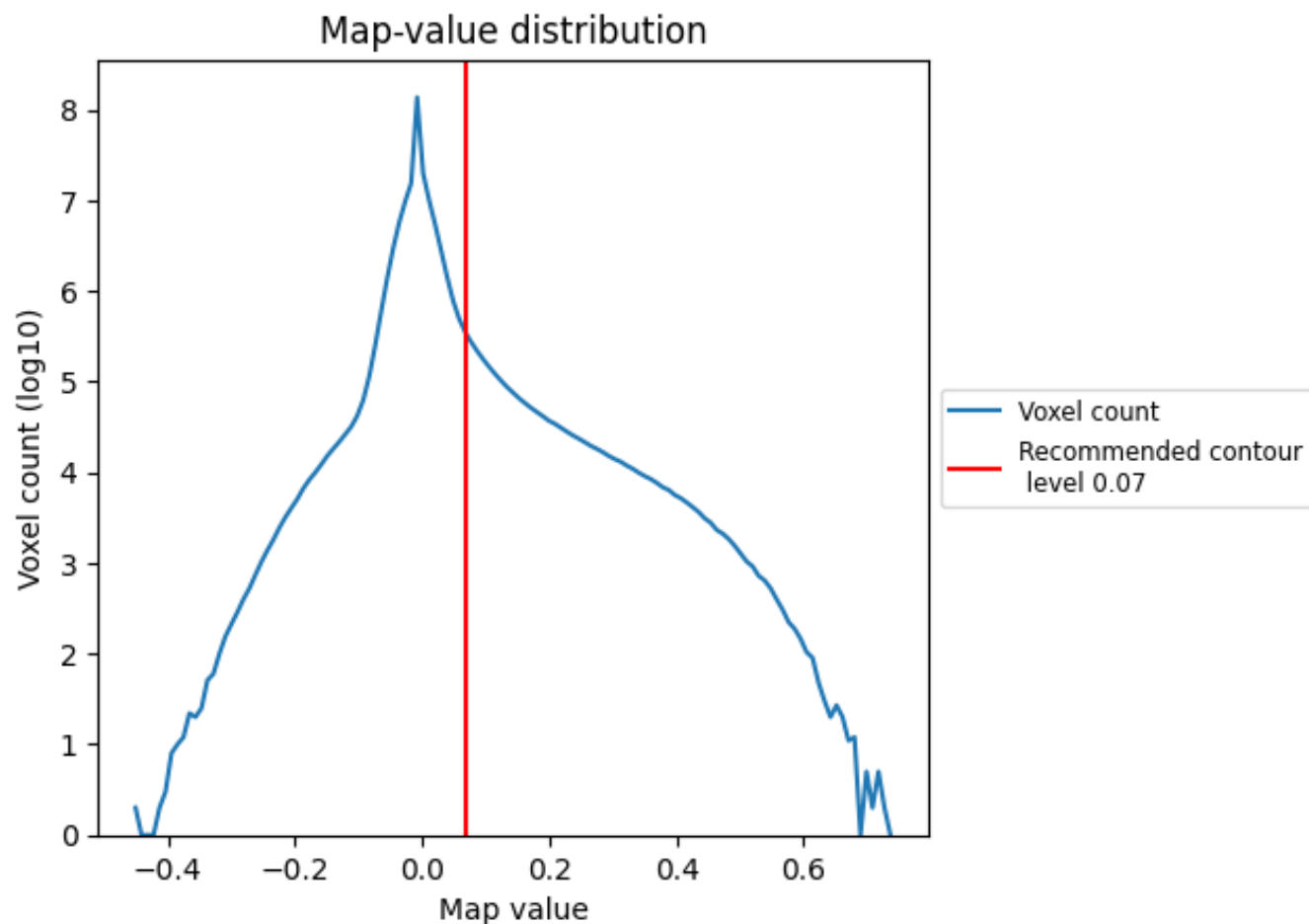
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

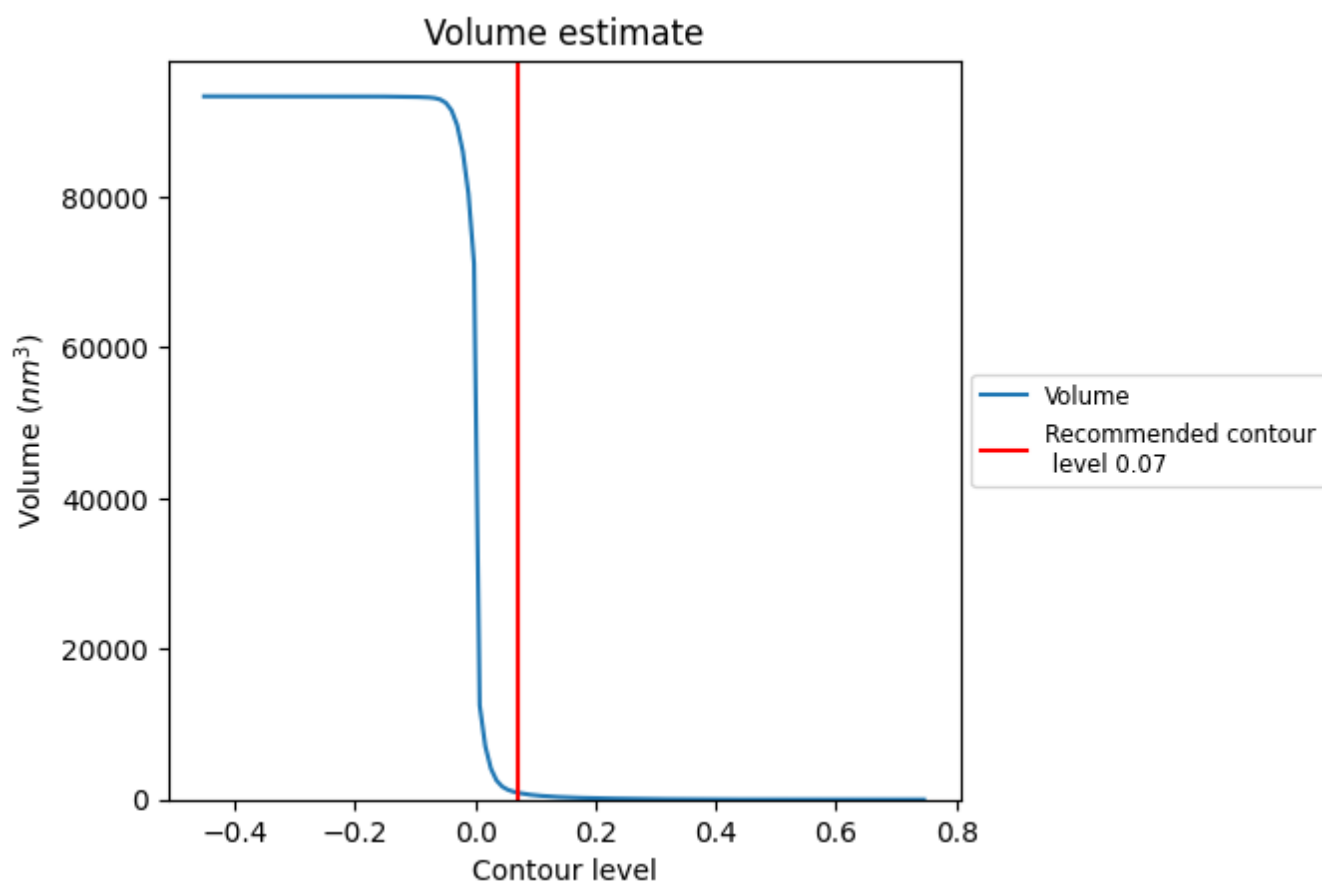
This section contains the results of statistical analysis of the map.

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.

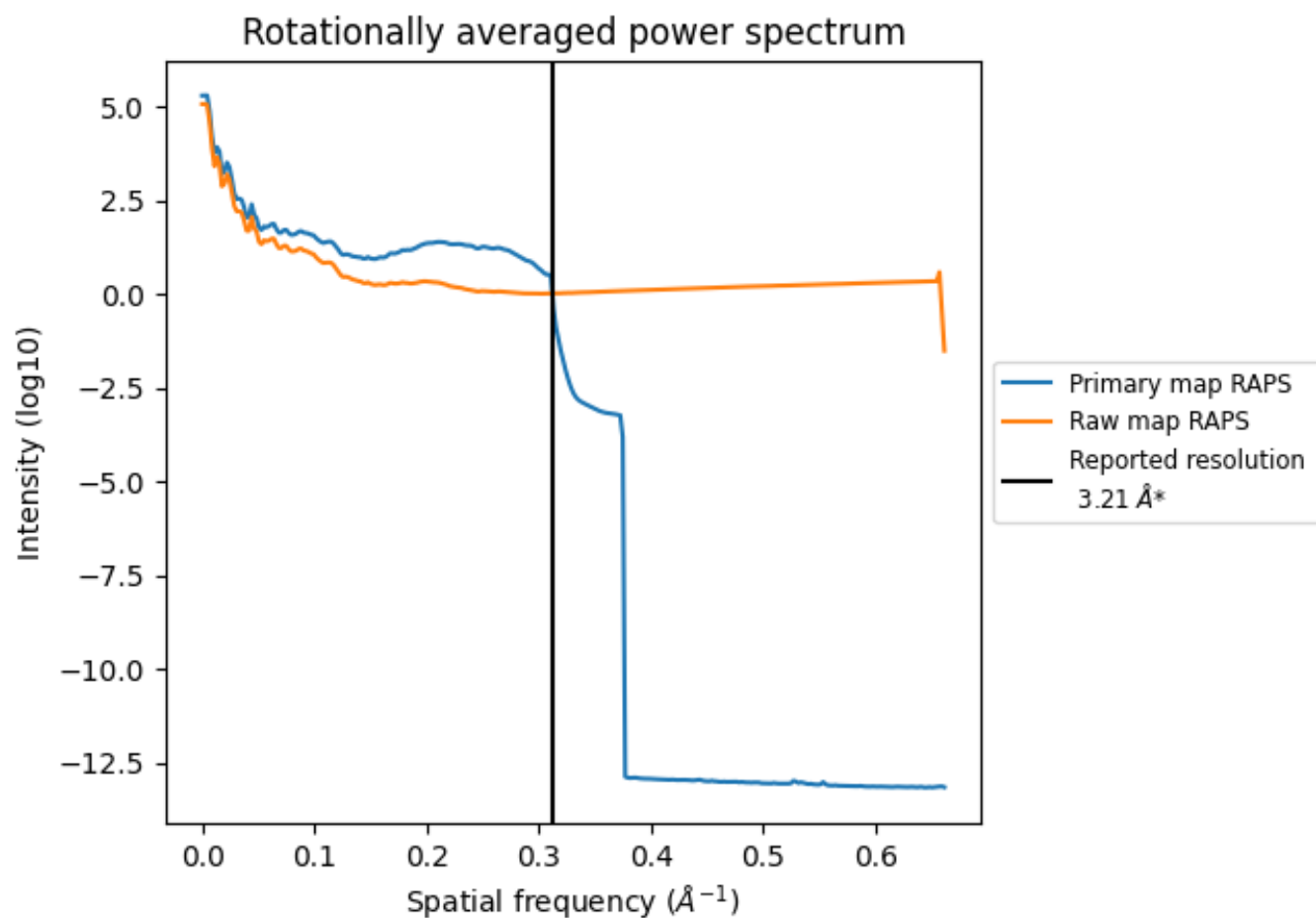
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 927 nm³; this corresponds to an approximate mass of 837 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 ⓘ

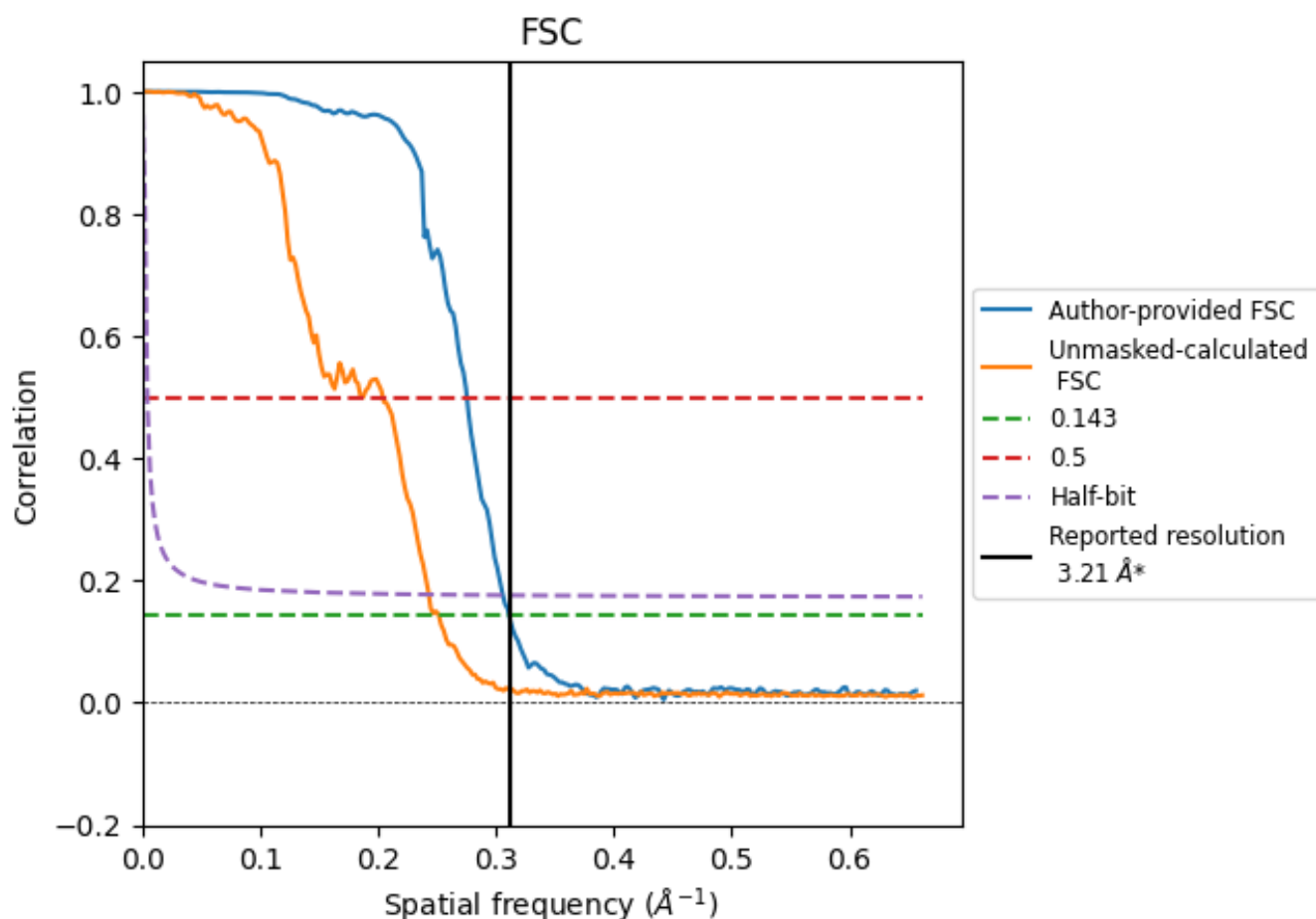


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates

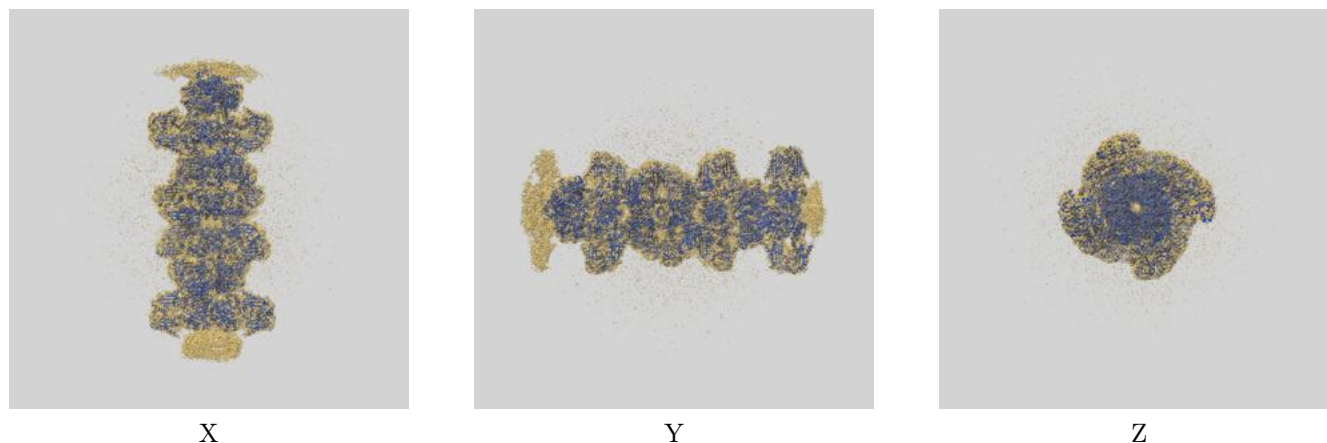
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.21	-	-
Author-provided FSC curve	3.21	3.63	3.27
Unmasked-calculated*	3.98	5.35	4.12

*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 3.98 differs from the reported value 3.21 by more than 10 %

9 Map-model fit [i](#)

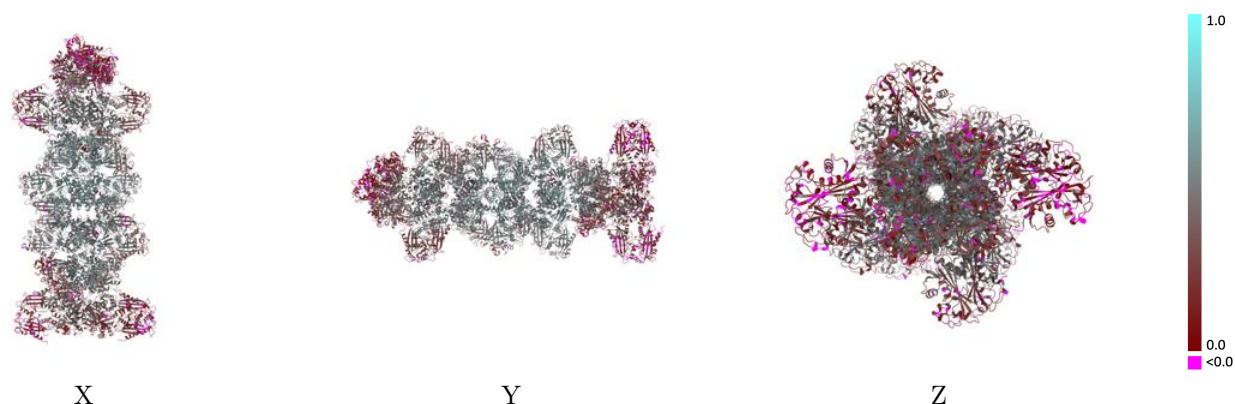
This section contains information regarding the fit between EMDB map EMD-66453 and PDB model 9X17. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



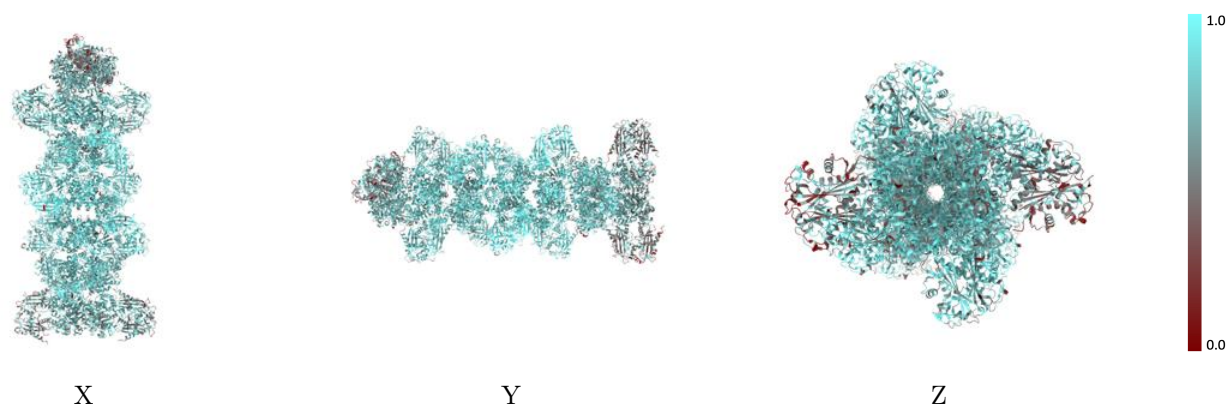
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



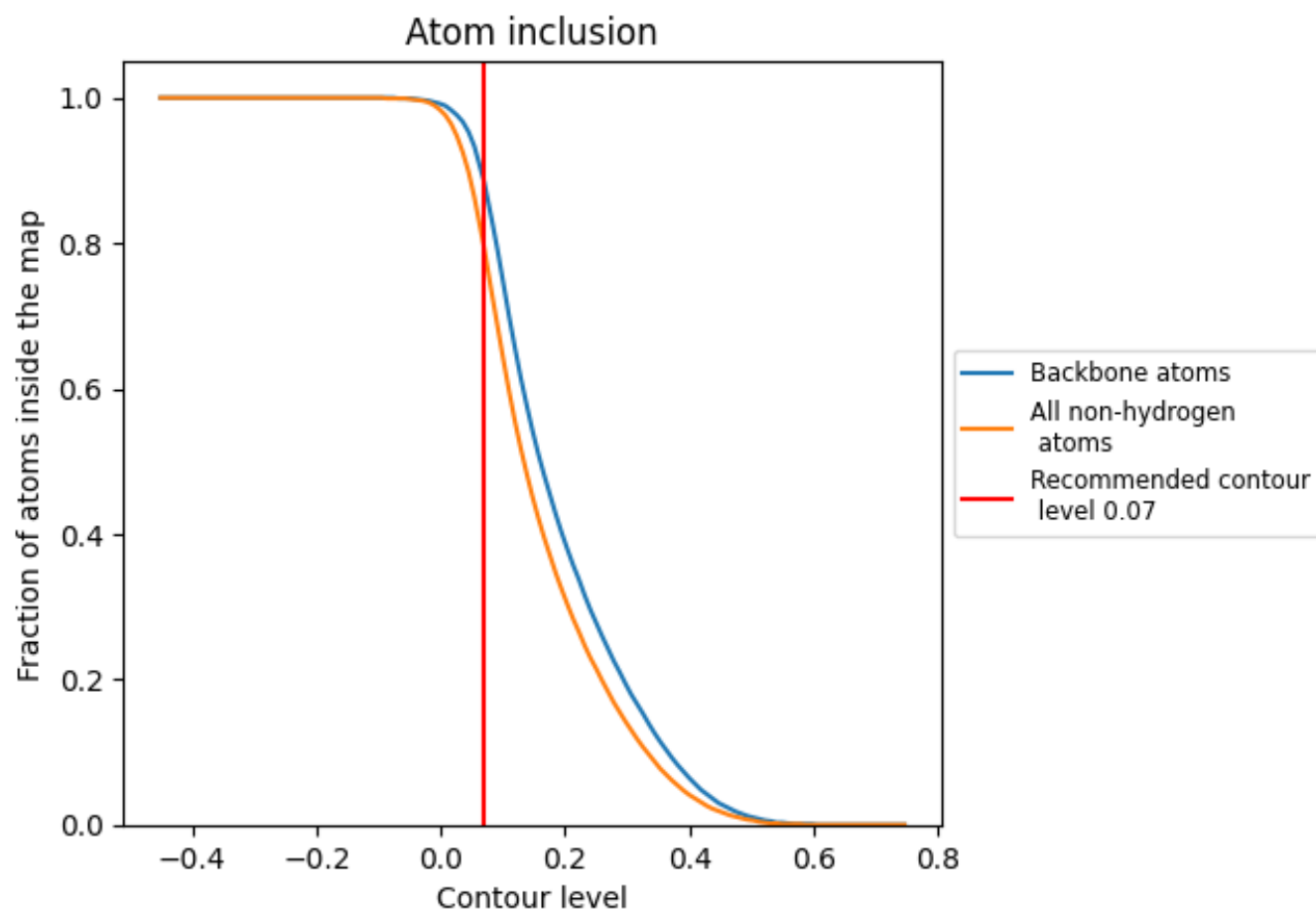
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 79% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7930	 0.3910
AB	 0.5250	 0.1370
AC	 0.4480	 0.0980
AD	 0.6040	 0.2240
AE	 0.6810	 0.3030
AG	 0.5480	 0.1620
AI	 0.4680	 0.1130
AK	 0.6840	 0.3090
AL	 0.6130	 0.2430
AN	 0.7460	 0.2960
AO	 0.7460	 0.2920
AP	 0.8520	 0.4550
AQ	 0.8810	 0.4880
AS	 0.7300	 0.2730
AU	 0.7580	 0.2780
AW	 0.8470	 0.4660
AX	 0.8560	 0.4590
BB	 0.8720	 0.4420
BC	 0.8760	 0.4460
BD	 0.8890	 0.5140
BE	 0.8940	 0.5270
BG	 0.8770	 0.4360
BI	 0.8760	 0.4460
BK	 0.9030	 0.5280
BL	 0.9100	 0.5350
BN	 0.8970	 0.4580
BO	 0.8970	 0.4730
BP	 0.9310	 0.5450
BQ	 0.9250	 0.5440
BS	 0.8990	 0.4490
BU	 0.9100	 0.4620
BW	 0.9110	 0.5300
BX	 0.9210	 0.5410
CB	 0.8380	 0.4080
CC	 0.8420	 0.4110



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Chain	Atom inclusion	Q-score
CD	 0.8670	 0.4890
CE	 0.8650	 0.4910
CG	 0.8390	 0.3880
CI	 0.8480	 0.4030
CK	 0.8810	 0.4990
CL	 0.9000	 0.5180
CN	 0.7840	 0.3220
CO	 0.7540	 0.2950
CP	 0.8770	 0.4890
CQ	 0.8570	 0.4520
CS	 0.7970	 0.3280
CU	 0.7720	 0.3220
CW	 0.8610	 0.4760
CX	 0.8880	 0.5030
DB	 0.5480	 0.1310
DC	 0.6110	 0.1960
DD	 0.7400	 0.3610
DE	 0.6690	 0.2900
DG	 0.5250	 0.1100
DI	 0.6030	 0.1830
DK	 0.6880	 0.3140
DL	 0.7470	 0.3740