



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 05:13 AM UTC

PDB ID : 8Q54 / pdb_00008q54
EMDB ID : EMD-18162
Title : N5-methyl-H4MPT:CoM methyltransferase -coenzyme M complex + CoM
Authors : Aziz, I.; Vonck, J.; Ermler, U.
Deposited on : 2023-08-08
Resolution : 2.39 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:

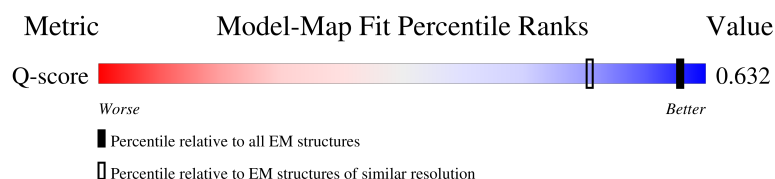
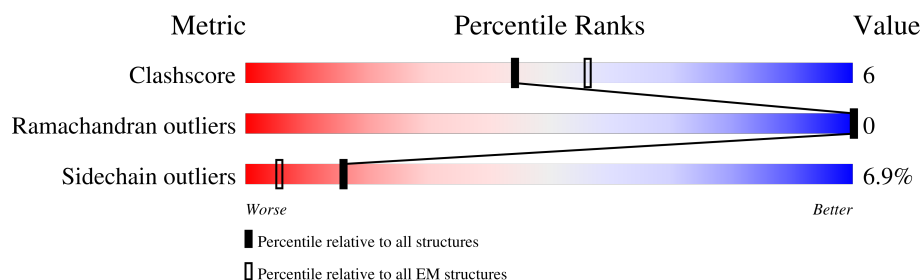
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.39 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.



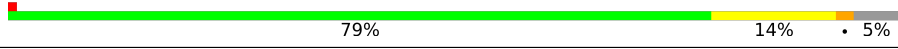
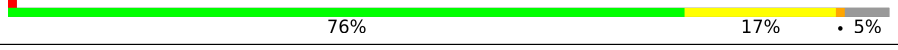
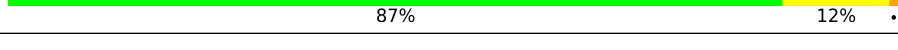
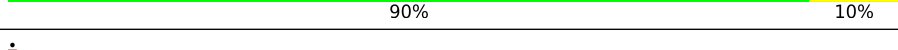
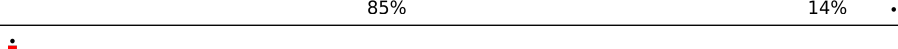
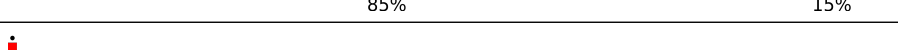
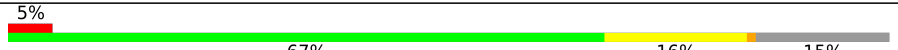
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4884 (1.90 - 2.89)

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	238	
1	Q	238	
1	a	238	
2	B	100	

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Mol	Chain	Length	Quality of chain
2	R	100	
2	b	100	
3	C	267	
3	S	267	
3	c	267	
4	D	233	
4	T	233	
4	d	233	
5	E	295	
5	U	295	
5	e	295	
6	F	68	
6	V	68	
6	f	68	
7	G	86	
7	W	86	
7	g	86	

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
11	COM	E	303[A]	-	X	-	-
11	COM	U	303[A]	-	X	-	-
11	COM	U	303[C]	-	X	-	-
11	COM	e	303[A]	-	X	-	-
9	JCV	E	304	X	-	-	-
9	JCV	E	306	X	-	-	-
9	JCV	S	301	X	-	-	-
9	JCV	U	305	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	JCV	W	101	X	-	-	-
9	JCV	c	301	X	-	-	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 48734 atoms, of which 24135 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 Tetrahydromethanopterin S-methyltransferase subunit A 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	61	Total	C	H	N	O	S	0	0
			962	297	499	78	83	5		
1	a	61	Total	C	H	N	O	S	0	0
			962	297	499	78	83	5		
1	Q	61	Total	C	H	N	O	S	0	0
			962	297	499	78	83	5		

- Molecule 2 is a protein called Tetrahydromethanopterin S-methyltransferase subunit B.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	70	Total	C	H	N	O	S	0	0
			1076	346	545	78	106	1		
2	b	70	Total	C	H	N	O	S	0	0
			1076	346	545	78	106	1		
2	R	70	Total	C	H	N	O	S	0	0
			1076	346	545	78	106	1		

- Molecule 3 is a protein called Tetrahydromethanopterin S-methyltransferase subunit C.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	254	Total	C	H	N	O	S	2	0
			3786	1207	1955	296	317	11		
3	c	254	Total	C	H	N	O	S	4	0
			3806	1213	1964	300	318	11		
3	S	254	Total	C	H	N	O	S	2	0
			3786	1207	1955	296	317	11		

- Molecule 4 is a protein called Tetrahydromethanopterin S-methyltransferase subunit D.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	233	Total	C	H	N	O	S	0	0
			3264	1038	1668	257	288	13		

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Mol	Chain	Residues	Atoms						AltConf	Trace
4	d	233	Total	C	H	N	O	S	0	0
			3264	1038	1668	257	288	13		
4	T	233	Total	C	H	N	O	S	0	0
			3264	1038	1668	257	288	13		

- Molecule 5 is a protein called Tetrahydromethanopterin S-methyltransferase subunit E.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	294	Total	C	H	N	O	S	0	0
			4390	1420	2203	363	388	16		
5	e	294	Total	C	H	N	O	S	0	0
			4390	1420	2203	363	388	16		
5	U	294	Total	C	H	N	O	S	0	0
			4390	1420	2203	363	388	16		

- Molecule 6 is a protein called Tetrahydromethanopterin S-methyltransferase subunit F.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	67	Total	C	H	N	O	S	0	0
			1069	329	564	90	84	2		
6	f	67	Total	C	H	N	O	S	0	0
			1069	329	564	90	84	2		
6	V	67	Total	C	H	N	O	S	0	0
			1069	329	564	90	84	2		

- Molecule 7 is a protein called Tetrahydromethanopterin S-methyltransferase subunit G.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	73	Total	C	H	N	O		0	0
			1164	368	598	92	106			
7	g	73	Total	C	H	N	O		0	0
			1164	368	598	92	106			
7	W	73	Total	C	H	N	O		0	0
			1164	368	598	92	106			

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

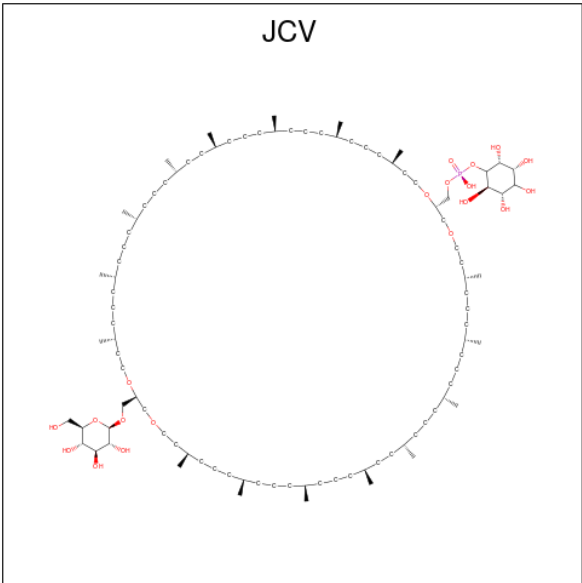
Mol	Chain	Residues	Atoms		AltConf
8	B	1	Total	Mg	0
			1	1	
8	b	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
8	R	1	1	1	0

- Molecule 9 is [(2 {S},7 {R},11 {R},15 {S},19 {S},22 {S},26 {S},30 {R},34 {R},39 {S},43 {R},47 {R},51 {S},55 {S},58 {S},62 {S},66 {R},70 {R})-39-[(2 {R},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxymethyl]-7,11,15,19,22,26,30,34,43,47,51,55,58,62,66,70-hexadecamethyl-1,4,37,40-tetraoxacyclodoheptacont-2-yl]methyl [(2 {R},3 {S},5 {R},6 {R})-2,3,4,5,6-pentakis(oxidanyl)cyclohexyl] hydrogen phosphate (CCD ID: JCV) (formula: C₉₈H₁₉₃O₁₉P).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
9	C	1	118	98	19	1	0
9	E	1	118	98	19	1	0
9	E	1	118	98	19	1	0
9	E	1	118	98	19	1	0
9	c	1	118	98	19	1	0
9	e	1	118	98	19	1	0
9	e	1	118	98	19	1	0
9	g	1	118	98	19	1	0

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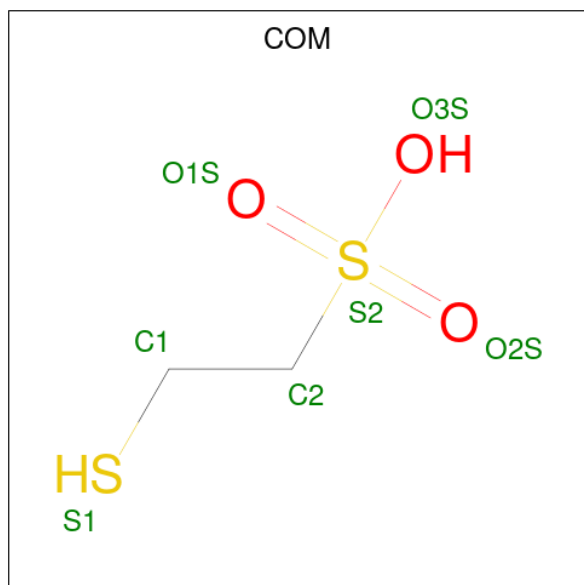
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Mol	Chain	Residues	Atoms				AltConf
9	S	1	Total	C	O	P	0
			118	98	19	1	
9	U	1	Total	C	O	P	0
			114	94	19	1	
9	U	1	Total	C	O	P	0
			118	98	19	1	
9	W	1	Total	C	O	P	0
			118	98	19	1	

- Molecule 10 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
10	E	2	Total	Na	0
			2	2	
10	e	2	Total	Na	0
			2	2	
10	U	2	Total	Na	0
			2	2	

- Molecule 11 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: C₂H₆O₃S₂).



Mol	Chain	Residues	Atoms					AltConf
11	E	1	Total	C	H	O	S	1
			24	4	10	6	4	
11	e	1	Total	C	H	O	S	1
			24	4	10	6	4	

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Mol	Chain	Residues	Atoms					AltConf
11	U	1	Total	C	H	O	S	1
			24	4	10	6	4	

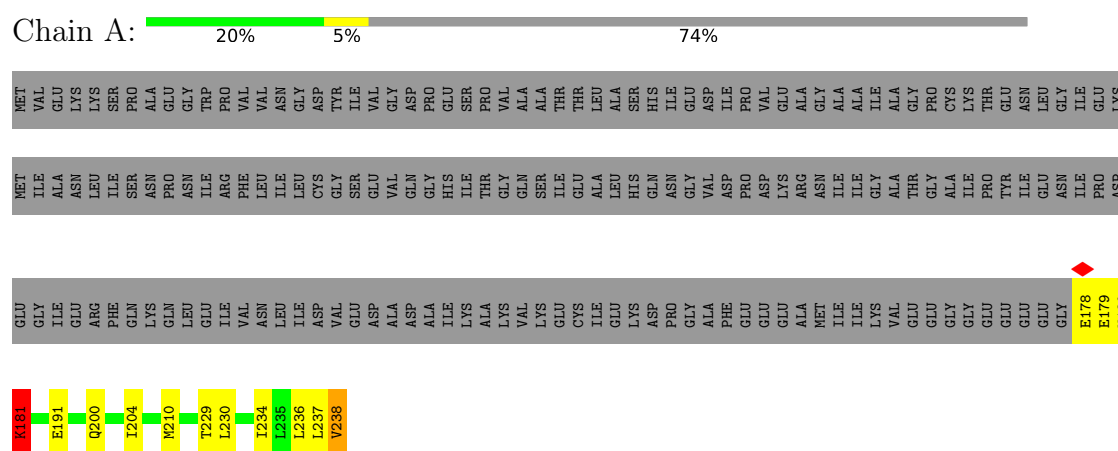
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	A	2	Total	O	0
			2	2	
12	B	2	Total	O	0
			2	2	
12	C	2	Total	O	0
			2	2	
12	D	2	Total	O	0
			2	2	
12	E	18	Total	O	0
			18	18	
12	F	3	Total	O	0
			3	3	
12	a	1	Total	O	0
			1	1	
12	b	2	Total	O	0
			2	2	
12	c	1	Total	O	0
			1	1	
12	d	4	Total	O	0
			4	4	
12	e	20	Total	O	0
			20	20	
12	f	1	Total	O	0
			1	1	
12	Q	1	Total	O	0
			1	1	
12	R	2	Total	O	0
			2	2	
12	S	1	Total	O	0
			1	1	
12	T	3	Total	O	0
			3	3	
12	U	21	Total	O	0
			21	21	
12	V	2	Total	O	0
			2	2	

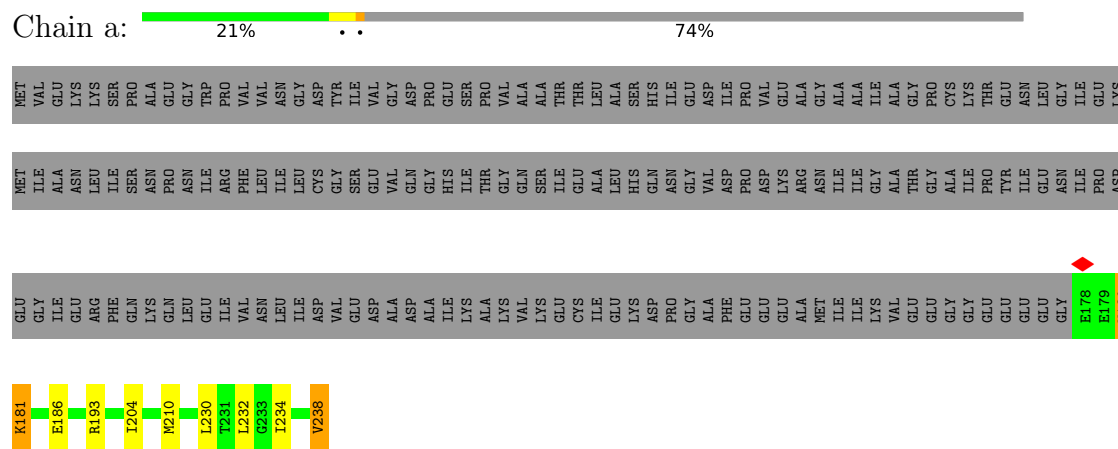
3 Residue-property plots

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

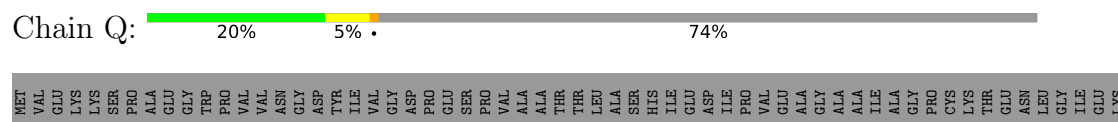
• Molecule 1: Tetrahydromethanopterin S-methyltransferase subunit A 1



• Molecule 1: Tetrahydromethanopterin S-methyltransferase subunit A 1



• Molecule 1: Tetrahydromethanopterin S-methyltransferase subunit A 1



MET ILE ALA ASN LEU ILE SER ASN PRO ASN ILE ARG PHE LEU ILE LEU CYS GLY SER GLU VAL GLN GLY HIS ILE THR GLN LEU SER ILE GLU ALA LEU HIS GLN ASN GLY VAL ASP PRO LYS ASP ARG ASN ILE GLY THR ALA ILE GLU PRO THR ILE GLU ASN ILE PRO ASP

GLU GLY ILE ALA ARG PHE GLN LYS GLN LEU ILE LEU VAL ASN LEU ILE ASP VAL ASP GLU ALA ASP ALA ASP ILE ILE VAL GLU GLY THR ALA ILE GLU PRO THR ILE GLU ASN ILE PRO ASP

K181 P182 E186 L189 M194 Q198 G205 S206 T207 M209 V219 V238

• Molecule 2: Tetrahydromethanopterin S-methyltransferase subunit B

Chain B:  52% 14% 30%

MET GLU MET LEU PRO LEU VAL LYS ILE ALA PRO GLU TYR ASN THR LEU ASP PRO SER THR MET ILE ALA LEU LEU GLY ARG E31 V32 I33 I34 I35 S36 E39 I40 Q43 I44 P64 E65 P69 G70 R71 V74 V75 L76 L81 V85 L100

• Molecule 2: Tetrahydromethanopterin S-methyltransferase subunit B

Chain b:  55% 12% 30%

MET GLU MET LEU PRO LEU VAL LYS ILE ALA PRO GLU TYR ASN THR LEU ASP PRO SER THR MET ILE ALA LEU LEU GLY ARG E31 V32 I33 I34 I35 S36 E39 I40 Q43 I44 P64 E65 P69 G70 R71 V74 V75 L76 L81 V85 L100

• Molecule 2: Tetrahydromethanopterin S-methyltransferase subunit B

Chain R:  53% 14% 30%

MET GLU MET LEU PRO LEU VAL LYS ILE ALA PRO GLU TYR ASN THR LEU ASP PRO SER THR MET ILE ALA LEU LEU GLY ARG E31 V32 I33 I34 I35 S36 E39 I40 Q43 E48 P64 E65 G66 S67 Y68 P69 E72 I94 I95 P96 A97 L98 L99 L100

• Molecule 3: Tetrahydromethanopterin S-methyltransferase subunit C

Chain C:  79% 14% 5%

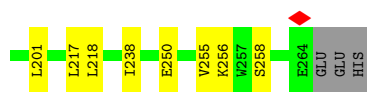
MET SER VAL ALA ALA GLY PRO GLY ALA GLY A11 A12 I13 L18 M19 G25 I39 S45 D57 A58 I59 R60 S64 V65 G70 I74 G75 Y76 Y84 Q85 Y86 Y87 M110 K121 I122 I123 V124 K125 M126 I127 I128 I129 I130 I131 E132 L131 L175 M179

T180 M181 Q184 L201 W212 L217 L218 S225 W226 W227 L228 I238 R242 E250 S254 V255 K256 W257 F264 GLU HIS

• Molecule 3: Tetrahydromethanopterin S-methyltransferase subunit C

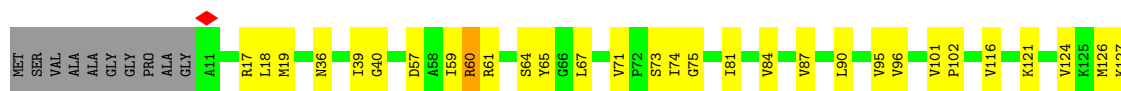
Chain c:  82% 13% 5%

MET SER VAL ALA ALA GLY PRO GLY ALA GLY A11 R17 L18 M19 A20 L21 I39 R60 R61 V65 V71 I74 P102 V103 V118 K121 K122 I123 V124 I128 P129 I130 L131 E132 T158 M162 L174 M179 I180 M181 M182 I183 L191 Q197



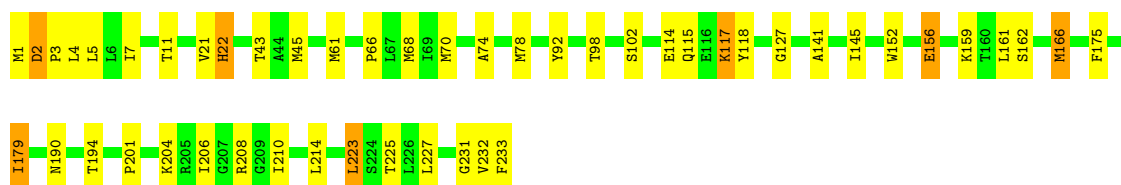
• Molecule 3: Tetrahydromethanopterin S-methyltransferase subunit C

Chain S: 76% 17% 5%



• Molecule 4: Tetrahydromethanopterin S-methyltransferase subunit D

Chain D: 79% 18% 3%



• Molecule 4: Tetrahydromethanopterin S-methyltransferase subunit D

Chain d: 90% 10% 0%



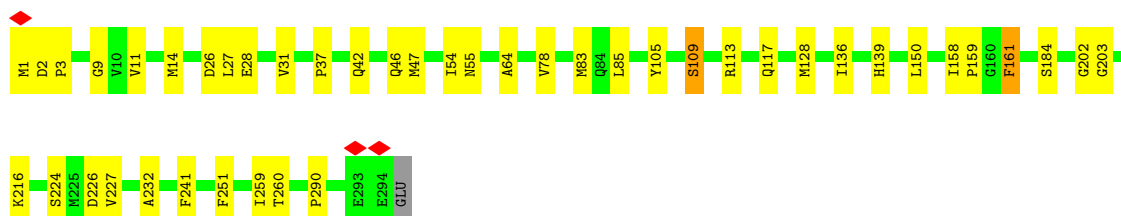
• Molecule 4: Tetrahydromethanopterin S-methyltransferase subunit D

Chain T: 87% 12% 1%

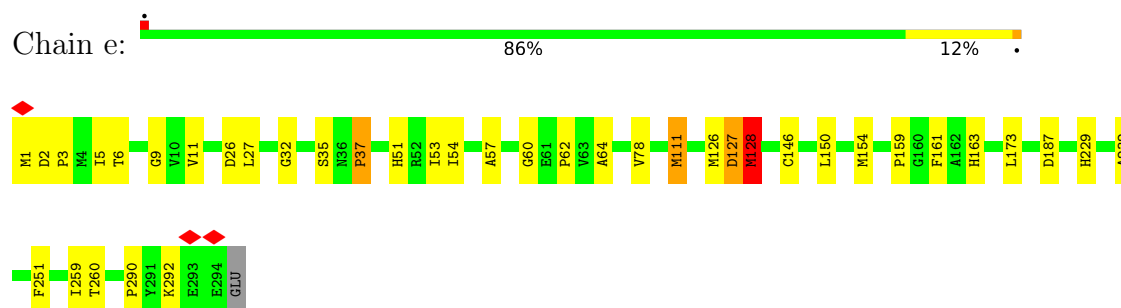


• Molecule 5: Tetrahydromethanopterin S-methyltransferase subunit E

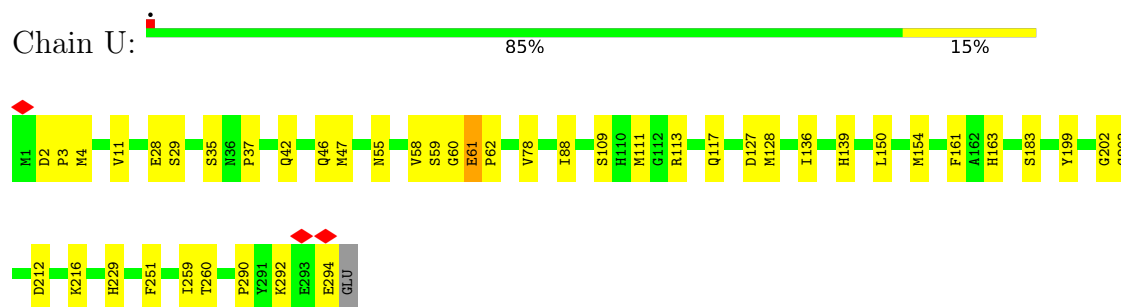
Chain E: 85% 14% 1%



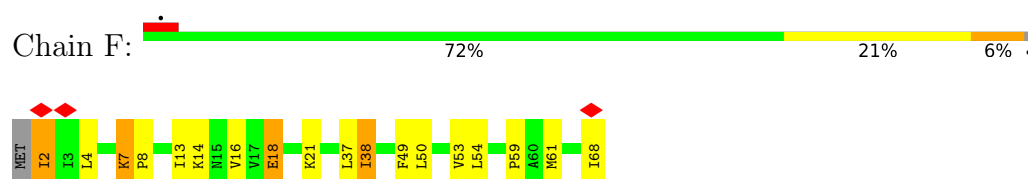
- Molecule 5: Tetrahydromethanopterin S-methyltransferase subunit E



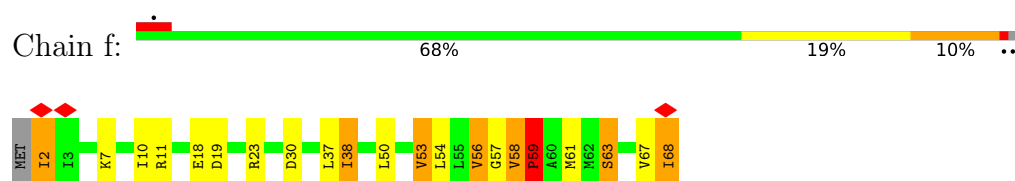
- Molecule 5: Tetrahydromethanopterin S-methyltransferase subunit E



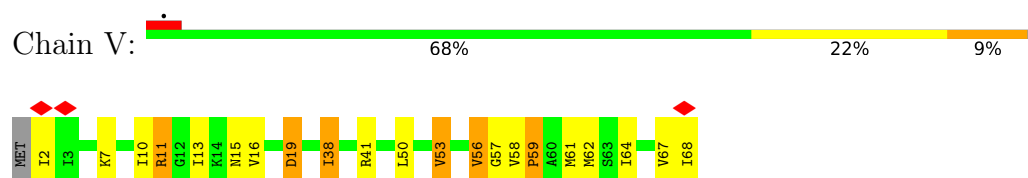
- Molecule 6: Tetrahydromethanopterin S-methyltransferase subunit F



- Molecule 6: Tetrahydromethanopterin S-methyltransferase subunit F



- Molecule 6: Tetrahydromethanopterin S-methyltransferase subunit F



- Molecule 7: Tetrahydromethanopterin S-methyltransferase subunit G





• Molecule 7: Tetrahydromethanopterin S-methyltransferase subunit G



• Molecule 7: Tetrahydromethanopterin S-methyltransferase subunit G



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87173	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	73.9	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.061	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	267.84, 267.84, 267.84	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: JCV, COM, MG, NA

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	1.06	3/467 (0.6%)	0.88	2/626 (0.3%)
1	Q	0.90	6/467 (1.3%)	0.87	0/626
1	a	1.02	2/467 (0.4%)	1.04	3/626 (0.5%)
2	B	0.97	4/538 (0.7%)	1.01	1/733 (0.1%)
2	R	0.92	2/538 (0.4%)	0.99	0/733
2	b	1.04	4/538 (0.7%)	1.13	2/733 (0.3%)
3	C	0.95	6/1878 (0.3%)	1.15	12/2566 (0.5%)
3	S	0.81	4/1878 (0.2%)	1.01	6/2566 (0.2%)
3	c	0.77	3/1894 (0.2%)	0.88	1/2587 (0.0%)
4	D	0.95	5/1624 (0.3%)	1.08	10/2207 (0.5%)
4	T	0.67	1/1624 (0.1%)	0.77	2/2207 (0.1%)
4	d	0.62	0/1624	0.70	3/2207 (0.1%)
5	E	0.66	7/2242 (0.3%)	0.78	6/3055 (0.2%)
5	U	0.79	8/2242 (0.4%)	0.84	8/3055 (0.3%)
5	e	0.77	6/2242 (0.3%)	0.87	10/3055 (0.3%)
6	F	1.20	5/509 (1.0%)	1.27	4/684 (0.6%)
6	V	1.32	7/509 (1.4%)	1.55	10/684 (1.5%)
6	f	1.38	7/509 (1.4%)	1.64	10/684 (1.5%)
7	G	0.59	1/571 (0.2%)	0.75	1/770 (0.1%)
7	W	0.60	1/571 (0.2%)	0.63	0/770
7	g	0.85	2/571 (0.4%)	1.18	6/770 (0.8%)
All	All	0.85	84/23503 (0.4%)	0.97	97/31944 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	e	0	1

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	LYS	C-N	17.32	1.54	1.33
6	V	59	PRO	N-CA	16.62	1.69	1.47
6	f	59	PRO	N-CA	16.36	1.69	1.47
1	a	181	LYS	C-N	16.31	1.54	1.33
5	U	61	GLU	C-N	13.67	1.52	1.33

The worst 5 of 97 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	58	VAL	CA-C-N	16.77	136.69	119.24
6	f	58	VAL	C-N-CA	16.77	136.69	119.24
6	V	58	VAL	CA-C-N	14.29	135.61	119.32
6	V	58	VAL	C-N-CA	14.29	135.61	119.32
3	S	67	LEU	N-CA-C	-10.47	99.95	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	e	128	MET	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	463	499	499	10	0
1	Q	463	499	499	8	0
1	a	463	499	499	8	0
2	B	531	545	545	13	0
2	R	531	545	545	9	0
2	b	531	545	545	8	0
3	C	1831	1955	1947	26	0
3	S	1831	1955	1947	33	0
3	c	1842	1964	1955	19	0
4	D	1596	1668	1668	33	0
4	T	1596	1668	1668	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	d	1596	1668	1668	12	0
5	E	2187	2203	2203	22	0
5	U	2187	2203	2203	22	0
5	e	2187	2203	2203	21	0
6	F	505	564	564	10	0
6	V	505	564	564	16	0
6	f	505	564	564	13	0
7	G	566	598	598	19	0
7	W	566	598	598	19	0
7	g	566	598	598	15	0
8	B	1	0	0	0	0
8	R	1	0	0	0	0
8	b	1	0	0	0	0
9	C	118	0	0	1	0
9	E	354	0	0	8	0
9	S	118	0	0	10	0
9	U	232	0	0	1	0
9	W	118	0	0	2	0
9	c	118	0	0	1	0
9	e	236	0	0	8	0
9	g	118	0	0	0	0
10	E	2	0	0	0	0
10	U	2	0	0	0	0
10	e	2	0	0	0	0
11	E	14	10	12	1	0
11	U	14	10	12	4	0
11	e	14	10	12	2	0
12	A	2	0	0	0	0
12	B	2	0	0	0	0
12	C	2	0	0	0	0
12	D	2	0	0	0	0
12	E	18	0	0	0	0
12	F	3	0	0	0	0
12	Q	1	0	0	0	0
12	R	2	0	0	0	0
12	S	1	0	0	0	0
12	T	3	0	0	0	0
12	U	21	0	0	0	0
12	V	2	0	0	0	0
12	a	1	0	0	0	0
12	b	2	0	0	0	0
12	c	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	d	4	0	0	0	0
12	e	20	0	0	0	0
12	f	1	0	0	0	0
All	All	24599	24135	24116	310	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 6.

The worst 5 of 310 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)
6:V:59:PRO:N	6:V:59:PRO:CA	1.69	1.45
6:f:59:PRO:N	6:f:59:PRO:CA	1.69	1.31
2:B:31:GLU:O	7:g:10:PRO:HB3	1.35	1.24
1:a:238:VAL:HG23	1:a:238:VAL:OXT	1.50	1.04
1:a:238:VAL:OXT	1:a:238:VAL:CG2	2.06	1.02

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	59/238 (25%)	55 (93%)	4 (7%)	0	100	100
1	Q	59/238 (25%)	57 (97%)	2 (3%)	0	100	100
1	a	59/238 (25%)	56 (95%)	3 (5%)	0	100	100
2	B	68/100 (68%)	67 (98%)	1 (2%)	0	100	100
2	R	68/100 (68%)	68 (100%)	0	0	100	100
2	b	68/100 (68%)	68 (100%)	0	0	100	100
3	C	254/267 (95%)	247 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	S	254/267 (95%)	246 (97%)	8 (3%)	0	100	100
3	c	256/267 (96%)	250 (98%)	6 (2%)	0	100	100
4	D	231/233 (99%)	226 (98%)	5 (2%)	0	100	100
4	T	231/233 (99%)	227 (98%)	4 (2%)	0	100	100
4	d	231/233 (99%)	228 (99%)	3 (1%)	0	100	100
5	E	292/295 (99%)	283 (97%)	9 (3%)	0	100	100
5	U	292/295 (99%)	286 (98%)	6 (2%)	0	100	100
5	e	292/295 (99%)	287 (98%)	5 (2%)	0	100	100
6	F	65/68 (96%)	64 (98%)	1 (2%)	0	100	100
6	V	65/68 (96%)	65 (100%)	0	0	100	100
6	f	65/68 (96%)	63 (97%)	2 (3%)	0	100	100
7	G	71/86 (83%)	71 (100%)	0	0	100	100
7	W	71/86 (83%)	71 (100%)	0	0	100	100
7	g	71/86 (83%)	69 (97%)	2 (3%)	0	100	100
All	All	3122/3861 (81%)	3054 (98%)	68 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	50/193 (26%)	46 (92%)	4 (8%)	11	19
1	Q	50/193 (26%)	47 (94%)	3 (6%)	17	31
1	a	50/193 (26%)	47 (94%)	3 (6%)	17	31
2	B	58/82 (71%)	53 (91%)	5 (9%)	10	16
2	R	58/82 (71%)	48 (83%)	10 (17%)	2	2
2	b	58/82 (71%)	51 (88%)	7 (12%)	5	7
3	C	191/196 (97%)	179 (94%)	12 (6%)	16	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	S	191/196 (97%)	178 (93%)	13 (7%)	14	25
3	c	192/196 (98%)	179 (93%)	13 (7%)	14	25
4	D	155/155 (100%)	143 (92%)	12 (8%)	12	20
4	T	155/155 (100%)	145 (94%)	10 (6%)	15	27
4	d	155/155 (100%)	146 (94%)	9 (6%)	18	32
5	E	228/229 (100%)	220 (96%)	8 (4%)	32	53
5	U	228/229 (100%)	219 (96%)	9 (4%)	28	48
5	e	228/229 (100%)	220 (96%)	8 (4%)	32	53
6	F	54/55 (98%)	47 (87%)	7 (13%)	4	5
6	V	54/55 (98%)	45 (83%)	9 (17%)	2	3
6	f	54/55 (98%)	44 (82%)	10 (18%)	1	2
7	G	61/73 (84%)	56 (92%)	5 (8%)	10	18
7	W	61/73 (84%)	58 (95%)	3 (5%)	22	39
7	g	61/73 (84%)	55 (90%)	6 (10%)	7	12
All	All	2392/2949 (81%)	2226 (93%)	166 (7%)	16	24

5 of 166 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	R	34	ILE
4	T	223	LEU
2	R	65	GLU
3	S	161	THR
5	U	229	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
5	e	229	HIS
6	f	24	ASN
7	W	23	ASN
3	S	179	ASN
4	T	64	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 9 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	COM	e	303[A]	-	6,6,6	1.32	1 (16%)	8,8,8	3.24	5 (62%)
9	JCV	S	301	-	120,120,120	1.13	8 (6%)	147,154,154	1.28	17 (11%)
9	JCV	g	101	-	120,120,120	1.14	11 (9%)	147,154,154	0.71	0
11	COM	U	303[C]	-	6,6,6	1.87	3 (50%)	8,8,8	2.35	3 (37%)
9	JCV	e	305	-	120,120,120	1.18	11 (9%)	147,154,154	1.18	16 (10%)
11	COM	e	303[B]	-	6,6,6	1.81	3 (50%)	8,8,8	2.34	4 (50%)
9	JCV	W	101	-	120,120,120	1.15	12 (10%)	147,154,154	0.87	2 (1%)
9	JCV	c	301	-	120,120,120	1.16	13 (10%)	147,154,154	0.67	0
9	JCV	U	304	-	116,116,120	1.13	10 (8%)	140,146,154	0.73	0
9	JCV	E	306	-	120,120,120	1.16	12 (10%)	147,154,154	0.68	0
11	COM	E	303[A]	-	6,6,6	1.85	3 (50%)	8,8,8	2.33	4 (50%)
9	JCV	E	305	-	120,120,120	1.35	12 (10%)	147,154,154	1.47	23 (15%)
11	COM	E	303[B]	-	6,6,6	1.80	3 (50%)	8,8,8	2.36	3 (37%)
9	JCV	U	305	-	120,120,120	1.16	12 (10%)	147,154,154	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >
9	JCV	e	304	-	120,120,120	1.35	12 (10%)	147,154,154	1.49	28 (19%)
11	COM	U	303[A]	-	6,6,6	1.81	3 (50%)	8,8,8	2.31	4 (50%)
9	JCV	E	304	-	120,120,120	1.27	14 (11%)	147,154,154	1.61	21 (14%)
9	JCV	C	301	-	120,120,120	1.16	12 (10%)	147,154,154	0.66	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
11	COM	e	303[A]	-	-	3/4/4/4	-
9	JCV	S	301	-	2/2/30/30	49/126/170/170	0/2/2/2
9	JCV	g	101	-	-	52/126/170/170	0/2/2/2
11	COM	U	303[C]	-	-	3/4/4/4	-
9	JCV	e	305	-	-	59/126/170/170	0/2/2/2
11	COM	e	303[B]	-	-	0/4/4/4	-
9	JCV	W	101	-	2/2/30/30	58/126/170/170	0/2/2/2
9	JCV	c	301	-	2/2/30/30	69/126/170/170	0/2/2/2
9	JCV	U	304	-	-	30/118/162/170	0/2/2/2
9	JCV	E	306	-	1/1/30/30	48/126/170/170	0/2/2/2
11	COM	E	303[A]	-	-	4/4/4/4	-
9	JCV	E	305	-	-	24/126/170/170	0/2/2/2
11	COM	E	303[B]	-	-	1/4/4/4	-
9	JCV	U	305	-	1/1/30/30	69/126/170/170	0/2/2/2
9	JCV	e	304	-	-	37/126/170/170	0/2/2/2
11	COM	U	303[A]	-	-	3/4/4/4	-
9	JCV	E	304	-	1/1/30/30	53/126/170/170	0/2/2/2
9	JCV	C	301	-	-	69/126/170/170	0/2/2/2

The worst 5 of 155 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	305	JCV	OY1-CG7	-6.62	1.32	1.43
9	e	304	JCV	OY1-CG7	-6.18	1.33	1.43
9	e	305	JCV	OY1-CG7	-5.41	1.34	1.43
9	C	301	JCV	OY1-CG7	-4.49	1.35	1.43
9	g	101	JCV	OY1-CG7	-4.46	1.36	1.43

The worst 5 of 130 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	304	JCV	OX4-CX2-CX3	-8.07	91.35	110.38
9	E	304	JCV	CX6-CX1-CX2	6.32	119.63	110.86
9	E	304	JCV	O4-CX1-CX2	5.76	120.92	108.73
11	e	303[A]	COM	O3S-S2-O1S	-5.42	97.83	111.40
9	e	304	JCV	CX4-CX3-CX2	-5.34	101.46	110.83

5 of 9 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	E	304	JCV	CY4
9	E	306	JCV	CG6
9	c	301	JCV	C80
9	c	301	JCV	C68
9	S	301	JCV	C61

5 of 631 torsion outliers are listed below:

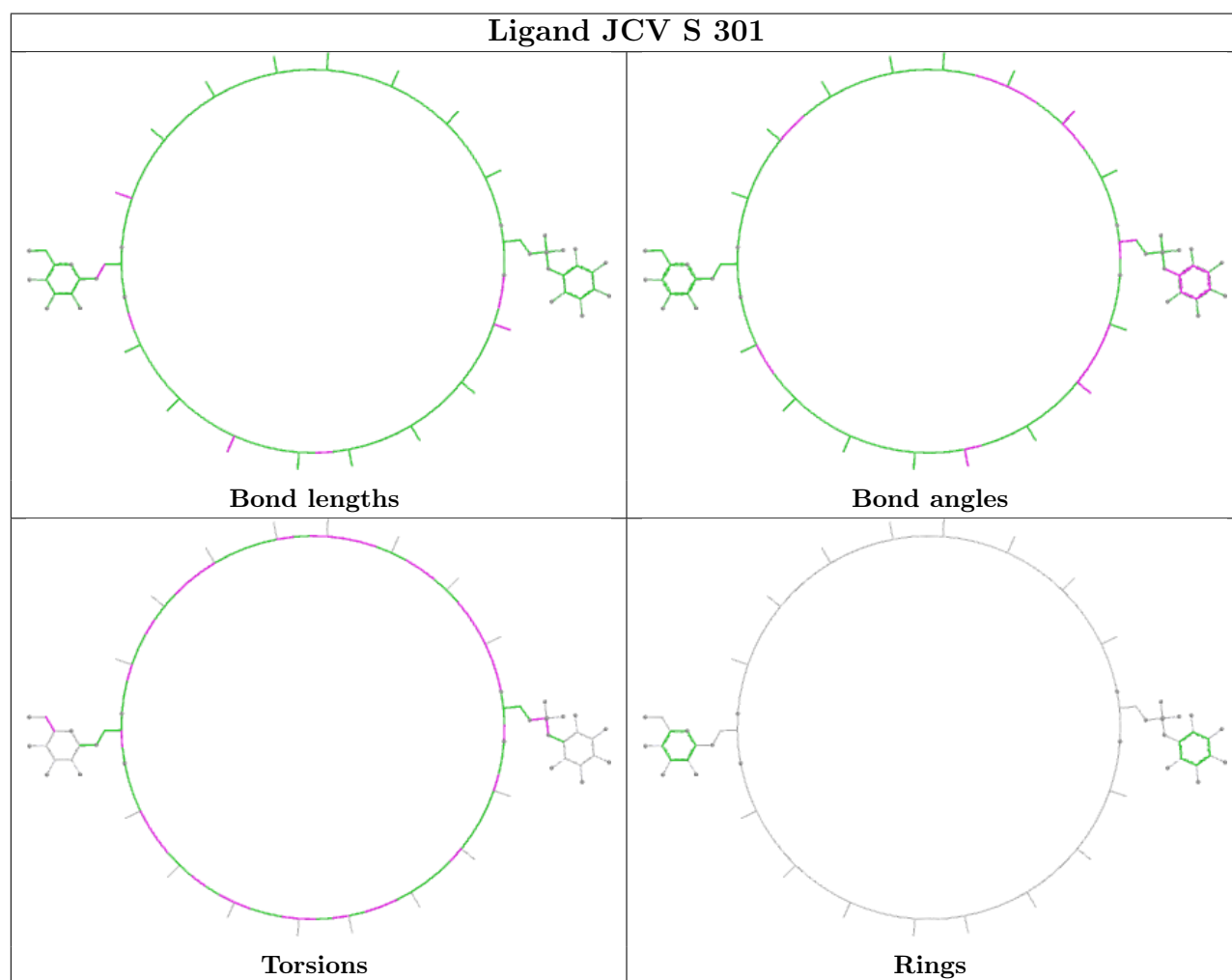
Mol	Chain	Res	Type	Atoms
9	C	301	JCV	C52-C51-OG2-CG2
9	C	301	JCV	C29-C30-C31-C32
9	C	301	JCV	C30M-C30-C31-C32
9	C	301	JCV	C55-C56-C57-C57M
9	C	301	JCV	C80M-C80-C81-C82

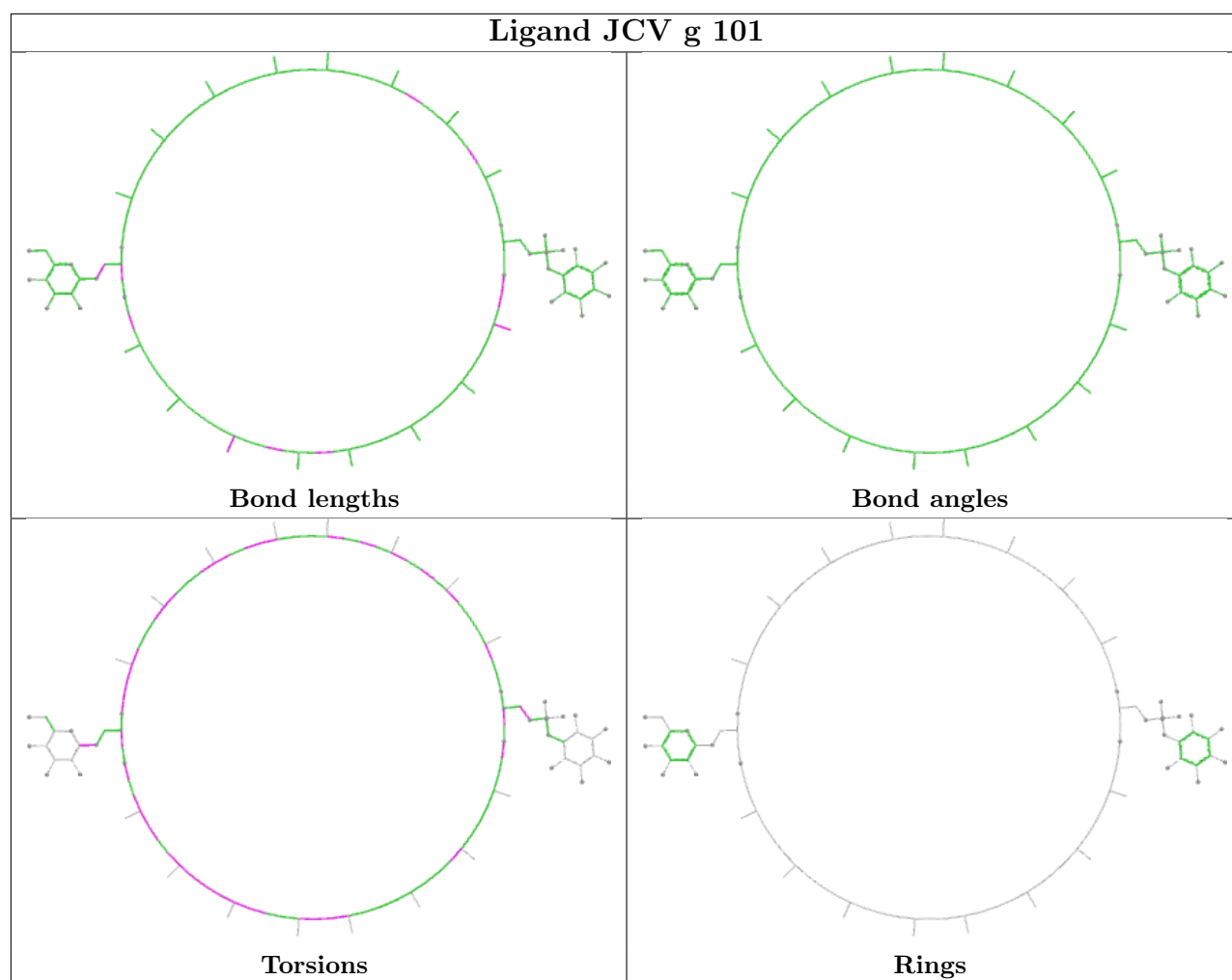
There are no ring outliers.

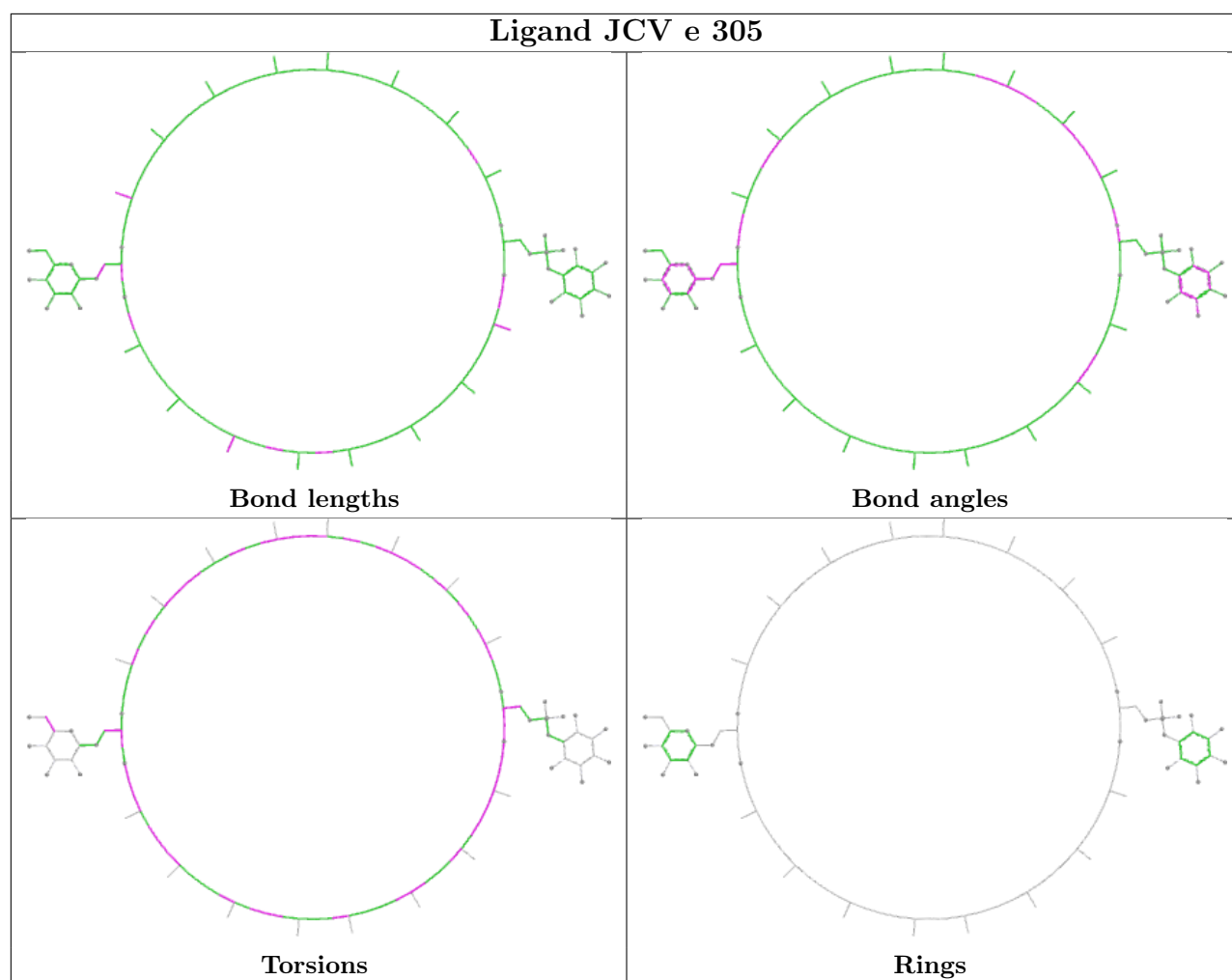
13 monomers are involved in 36 short contacts:

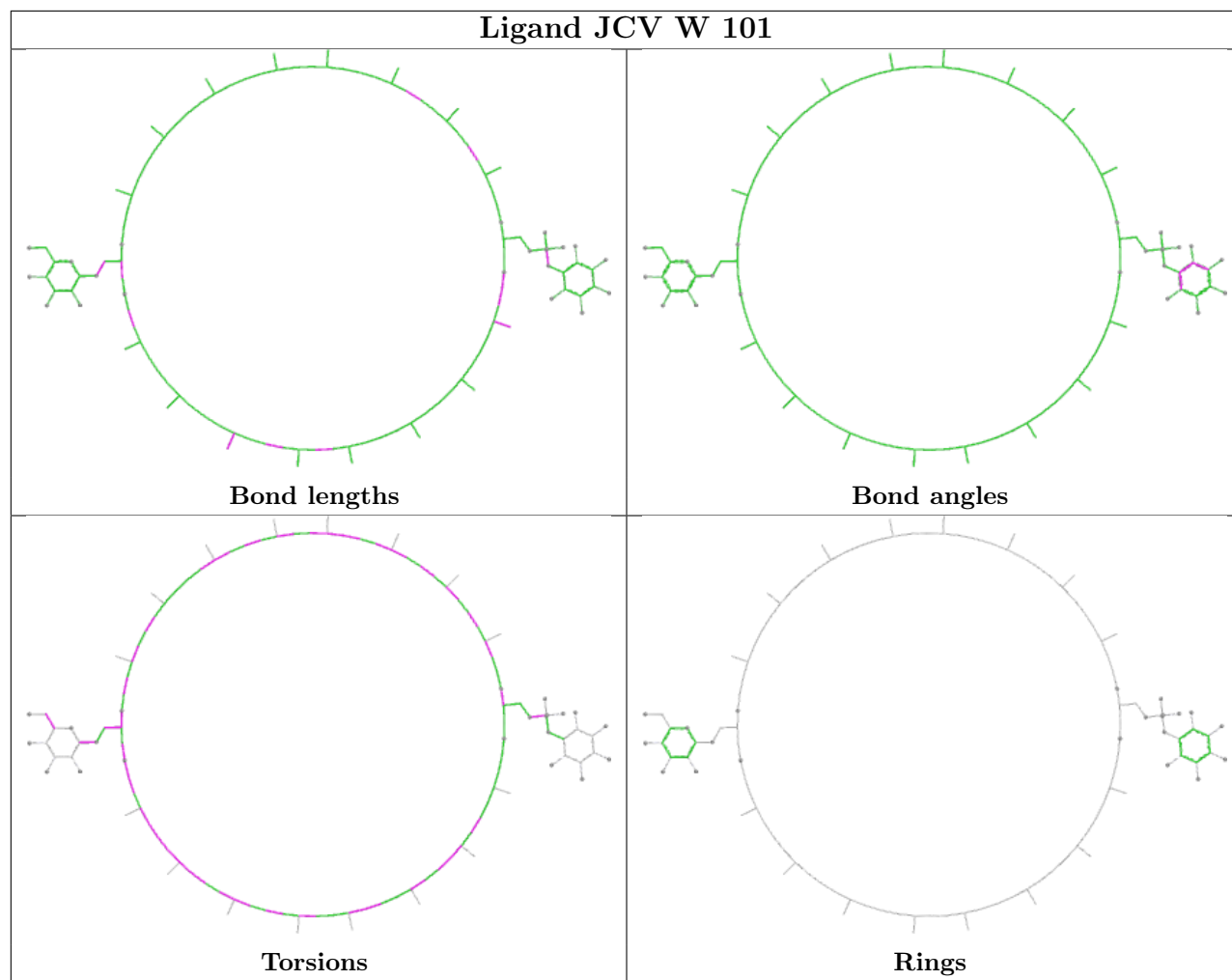
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	e	303[A]	COM	1	0
9	S	301	JCV	10	0
11	U	303[C]	COM	1	0
9	e	305	JCV	8	0
11	e	303[B]	COM	1	0
9	W	101	JCV	2	0
9	c	301	JCV	1	0
9	U	304	JCV	1	0
9	E	306	JCV	1	0
11	E	303[B]	COM	1	0
11	U	303[A]	COM	3	0
9	E	304	JCV	7	0
9	C	301	JCV	1	0

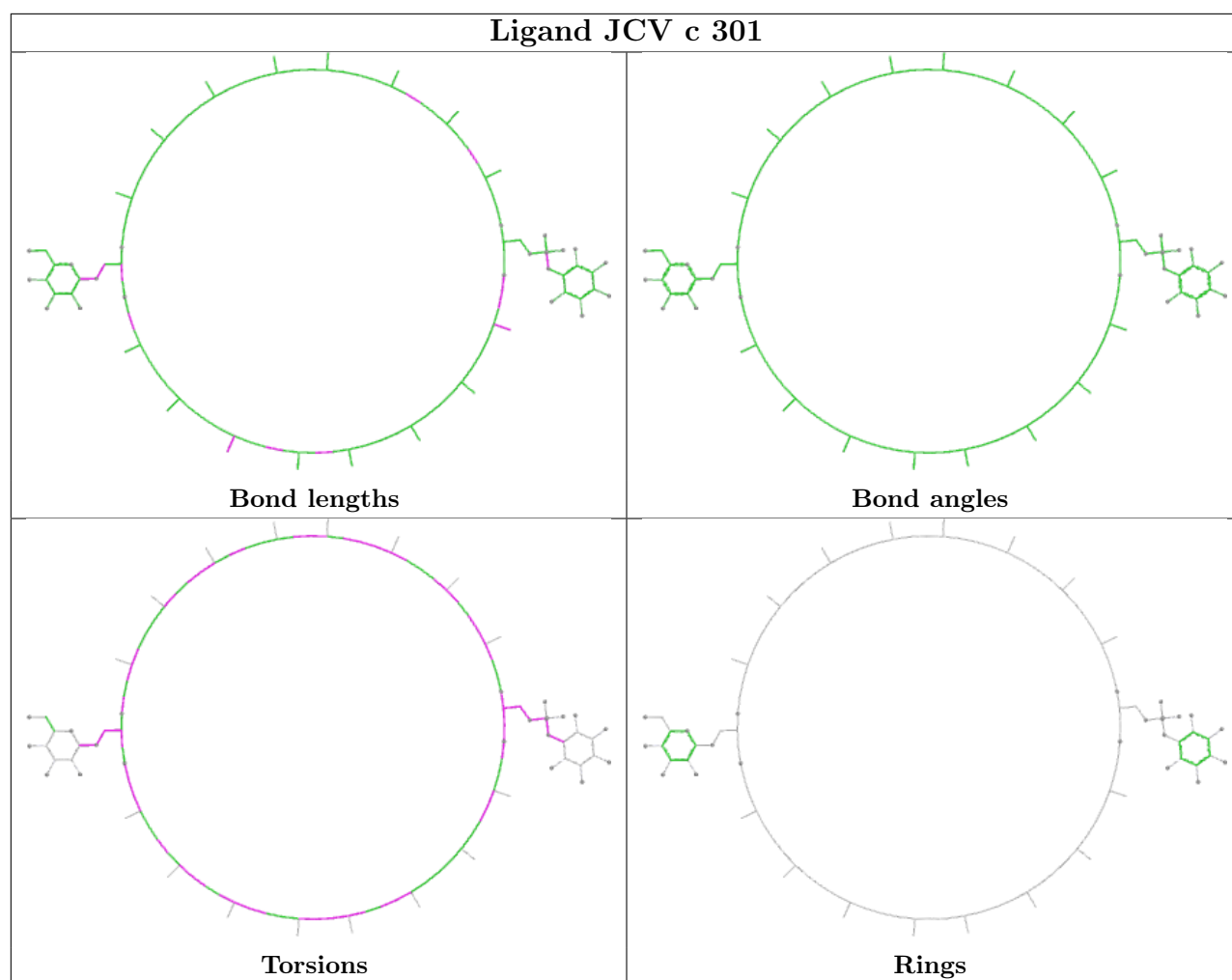
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

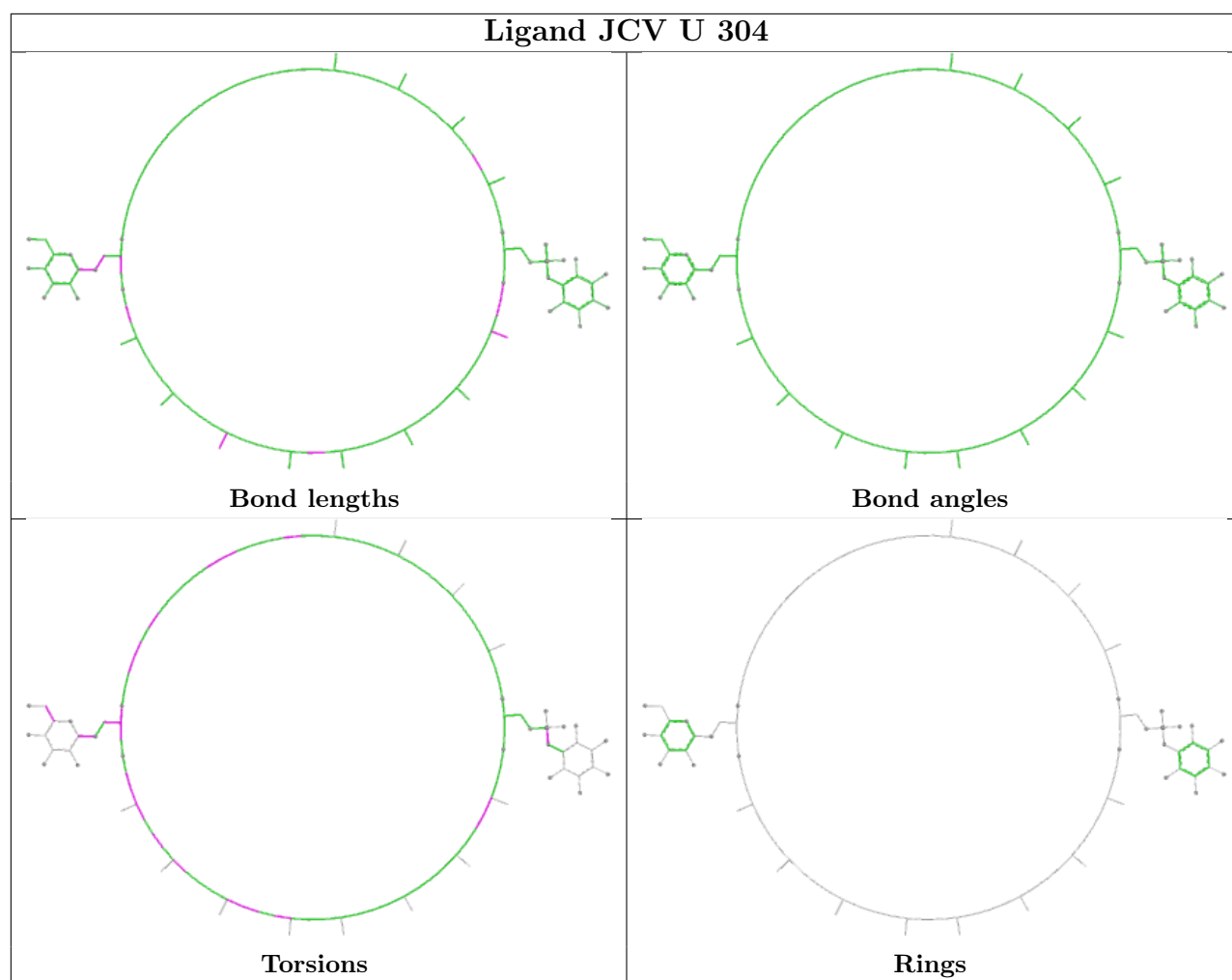


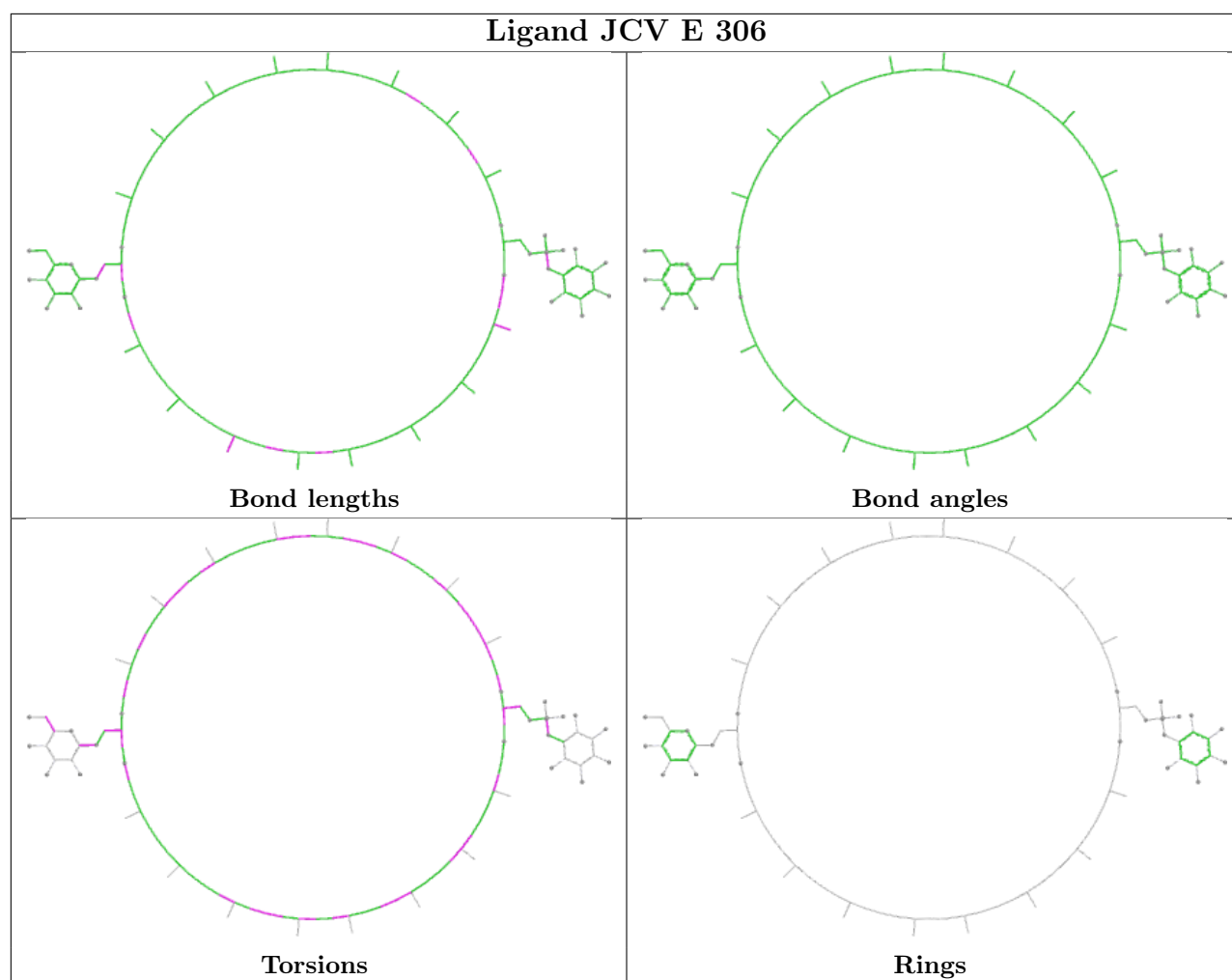


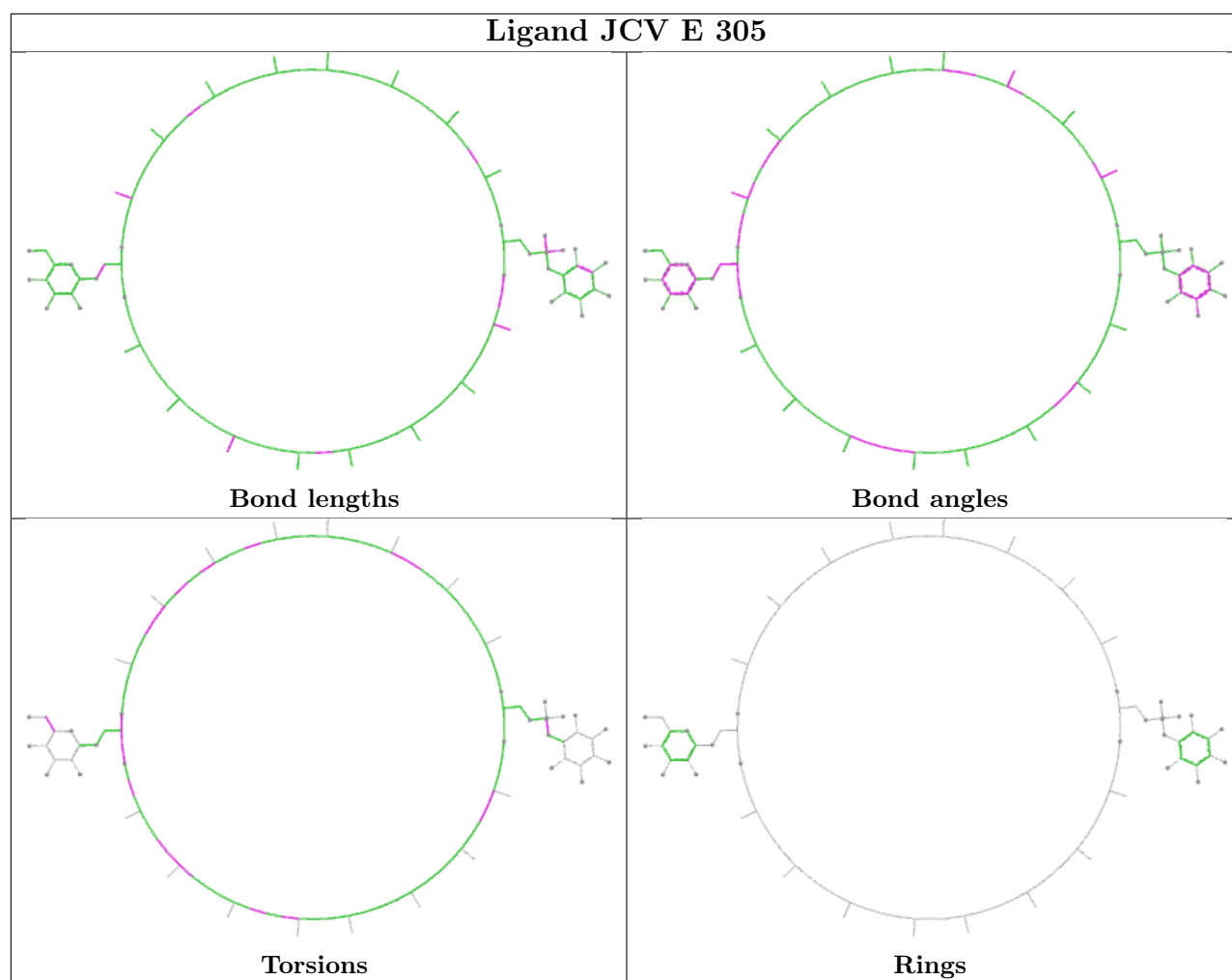


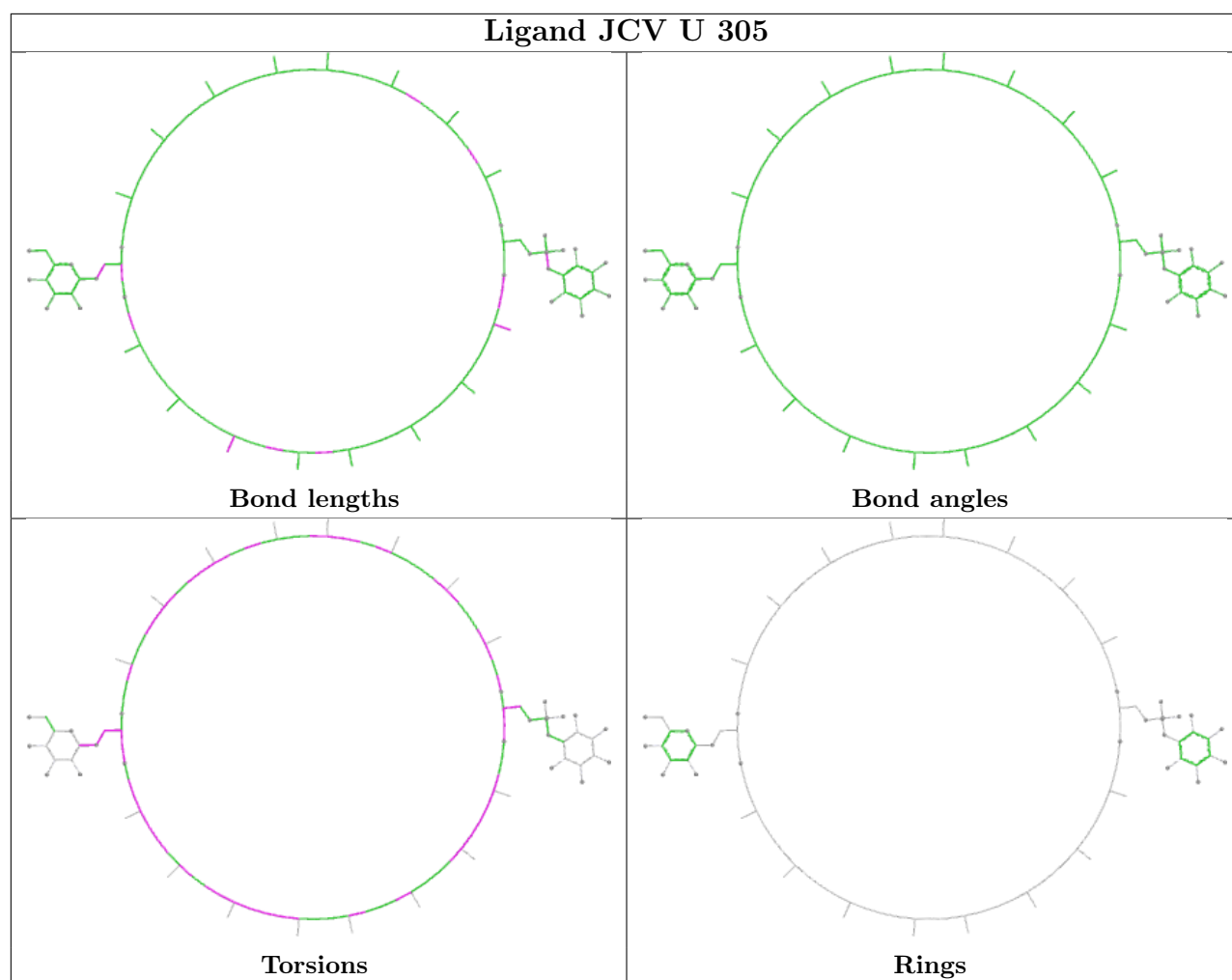


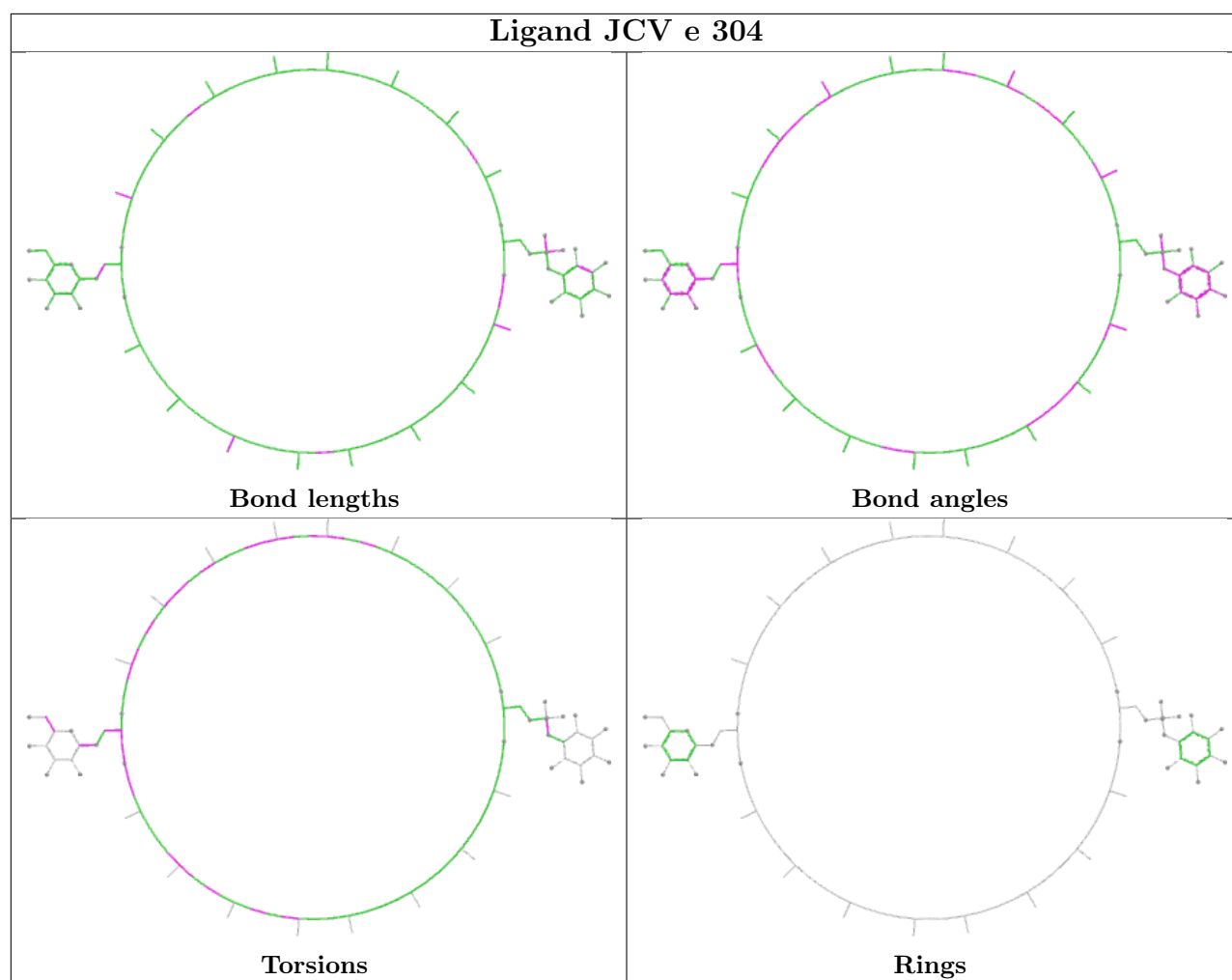


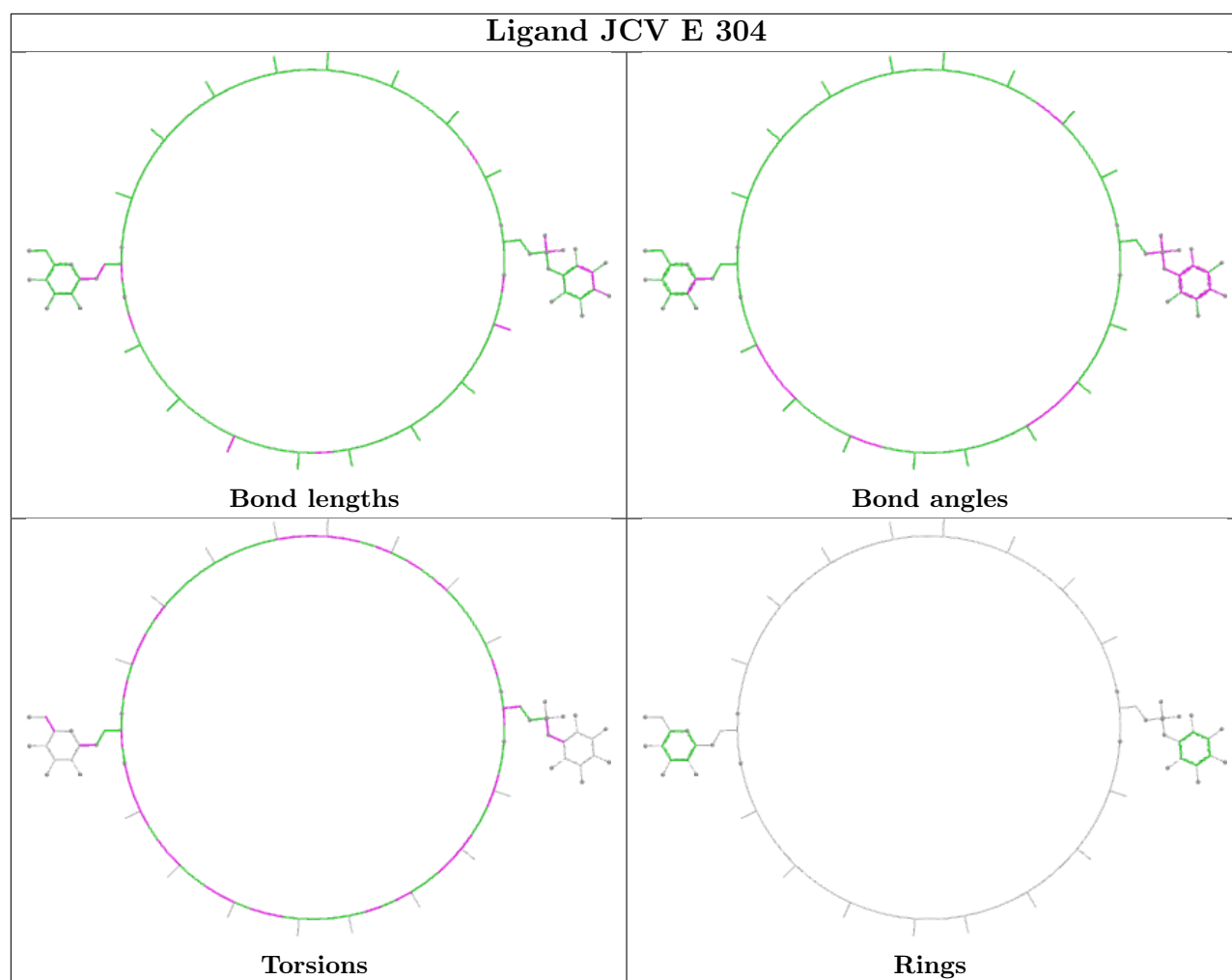


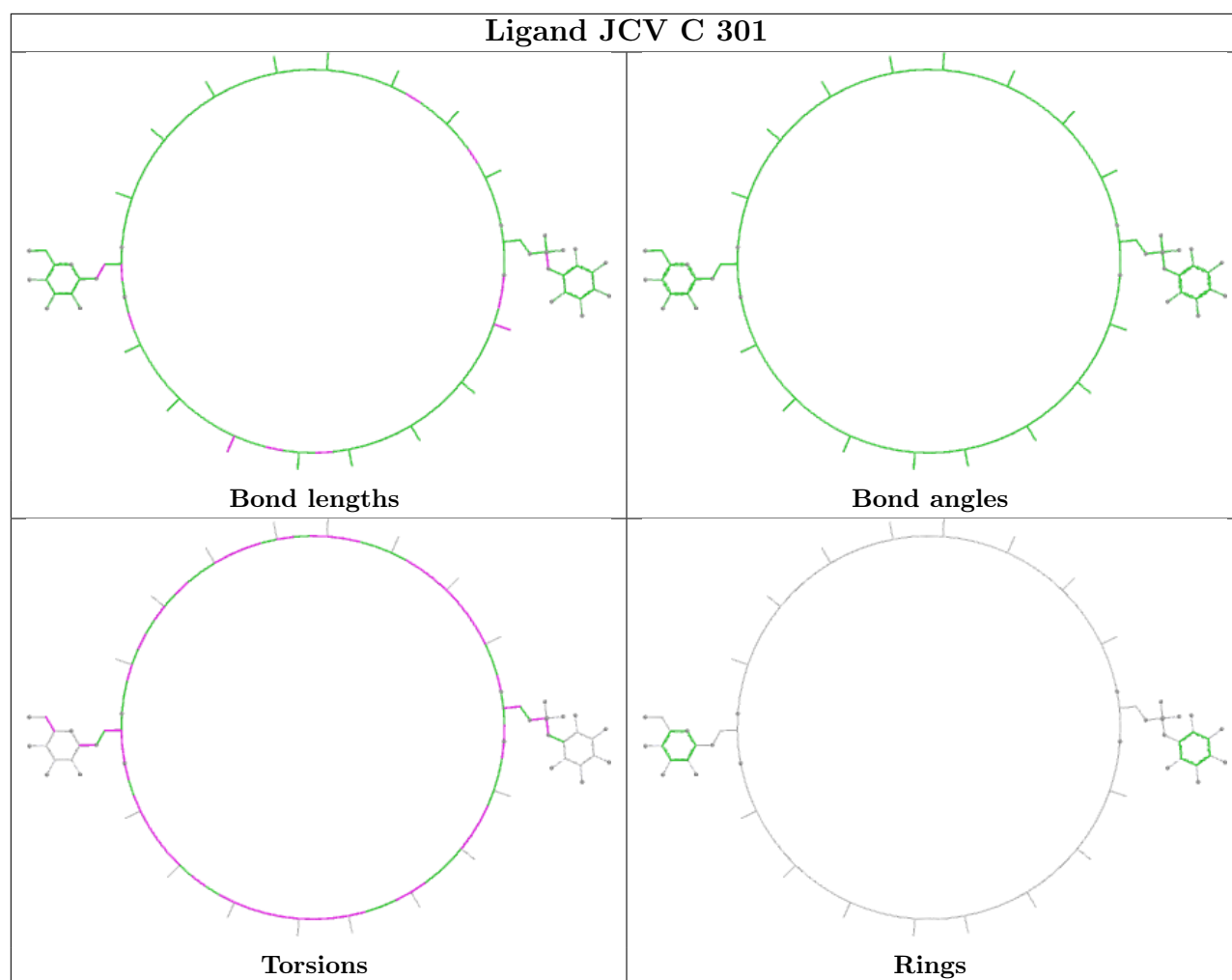












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

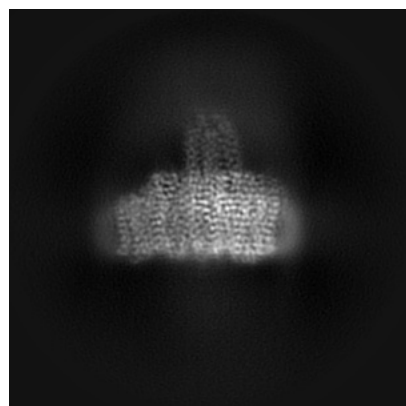
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18162. These allow visual inspection of the internal detail of the map and identification of artifacts.

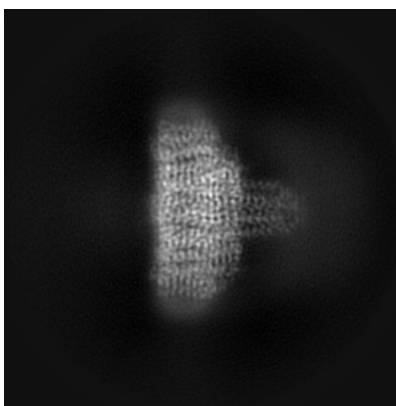
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

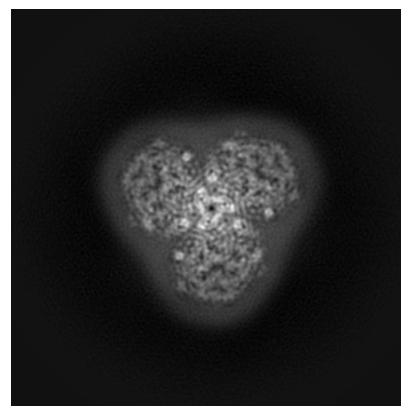
6.1.1 Primary map



X

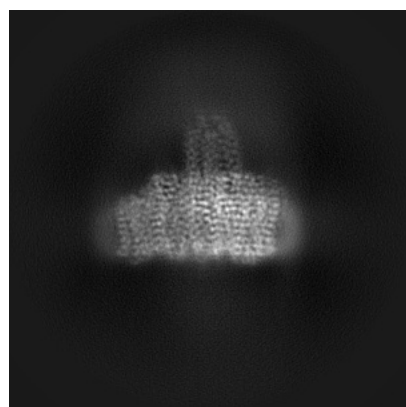


Y

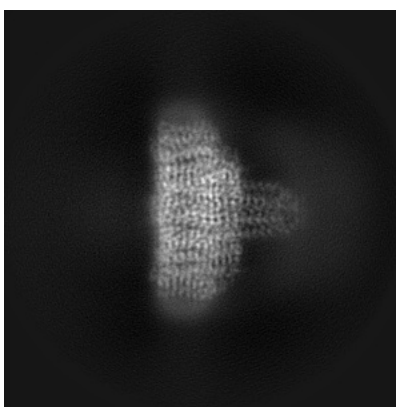


Z

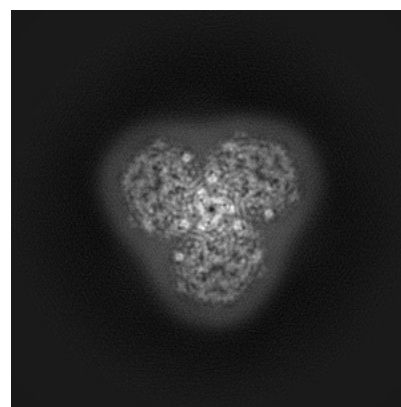
6.1.2 Raw map



X



Y

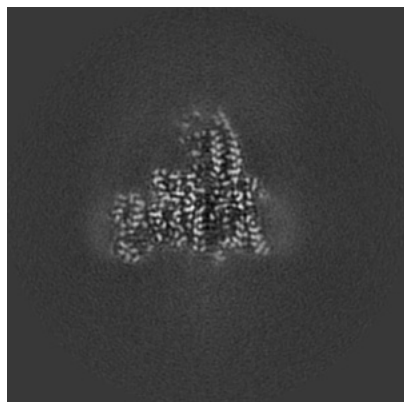


Z

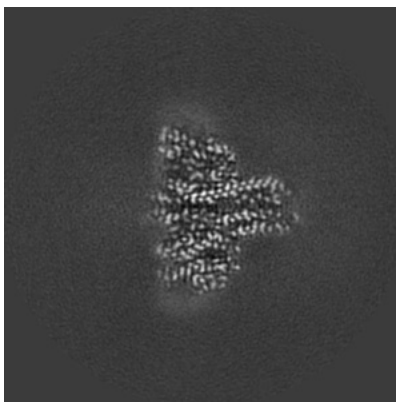
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

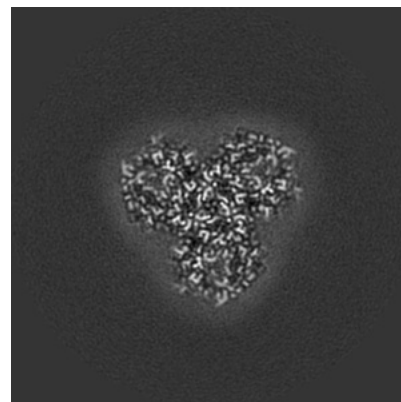
6.2.1 Primary map



X Index: 160

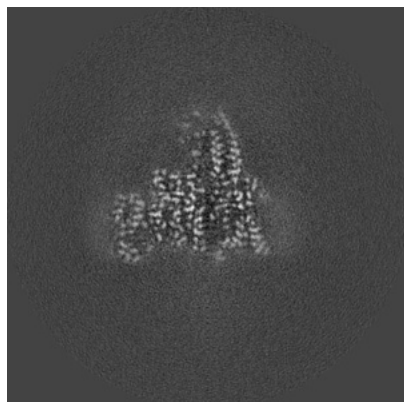


Y Index: 160

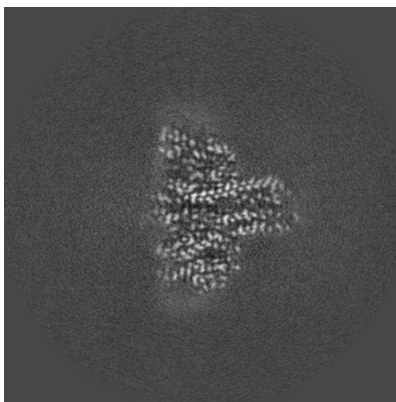


Z Index: 160

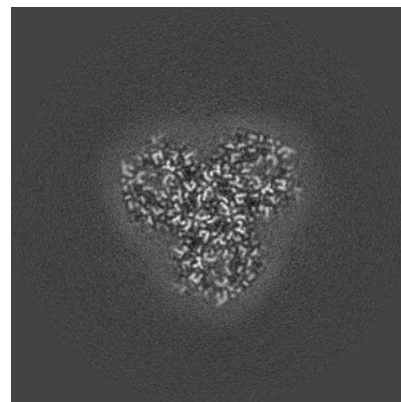
6.2.2 Raw map



X Index: 160



Y Index: 160

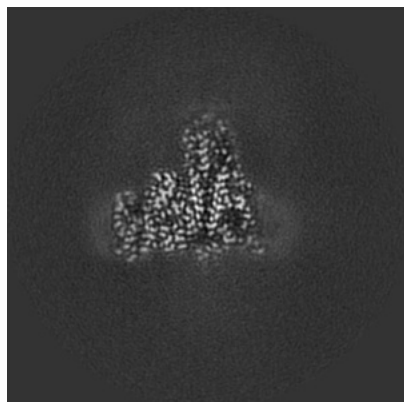


Z Index: 160

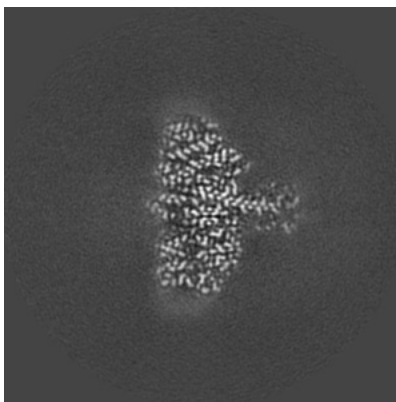
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

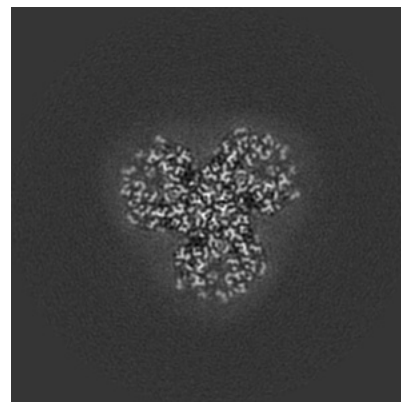
6.3.1 Primary map



X Index: 155

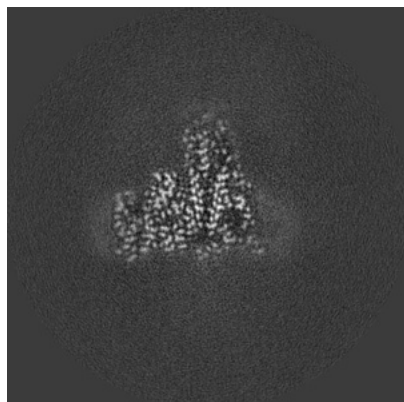


Y Index: 167

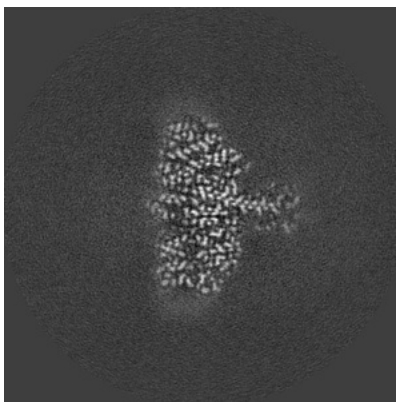


Z Index: 165

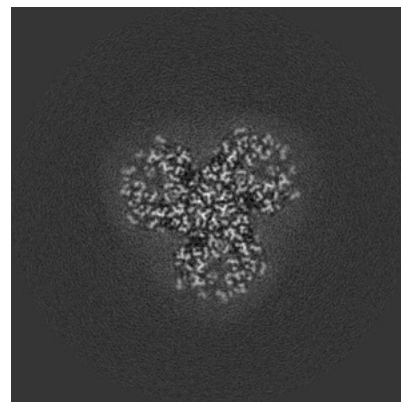
6.3.2 Raw map



X Index: 155



Y Index: 167

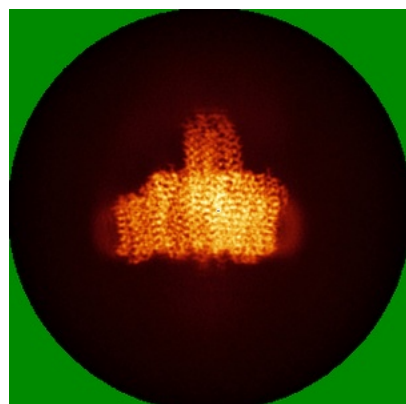


Z Index: 165

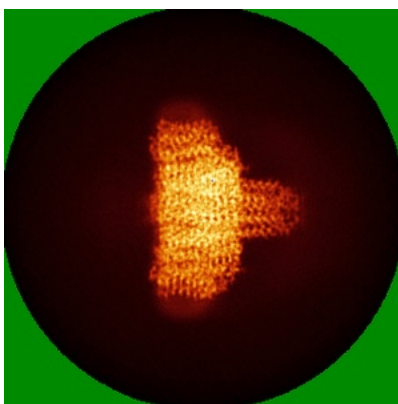
The images above show the largest variance slices of the map in three orthogonal directions.

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

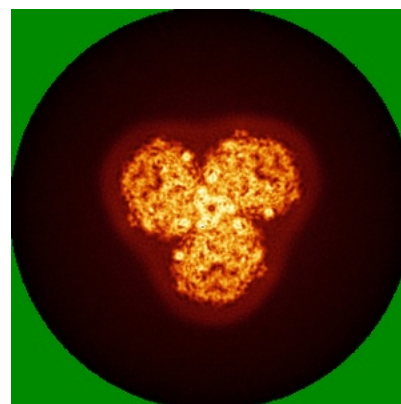
6.4.1 Primary map



X

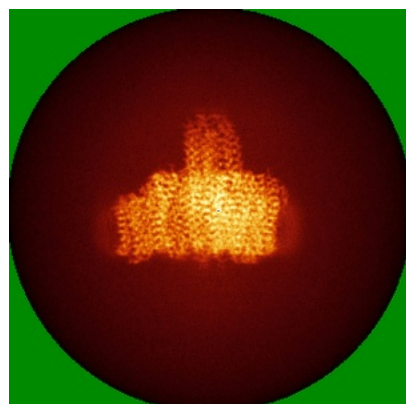


Y

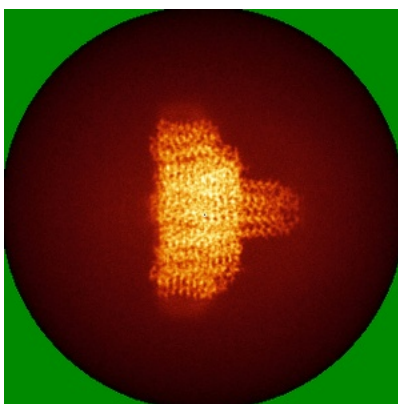


Z

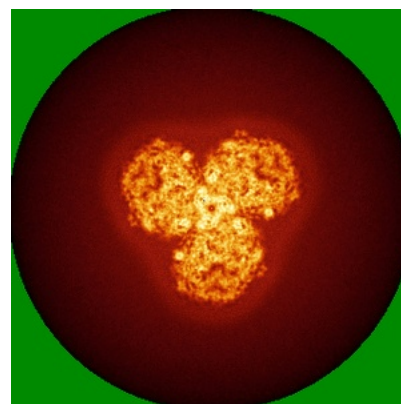
6.4.2 Raw map



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](#)

This section was not generated.

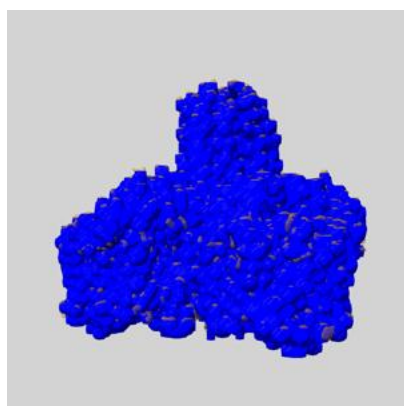
6.6 Mask visualisation [i](#)

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

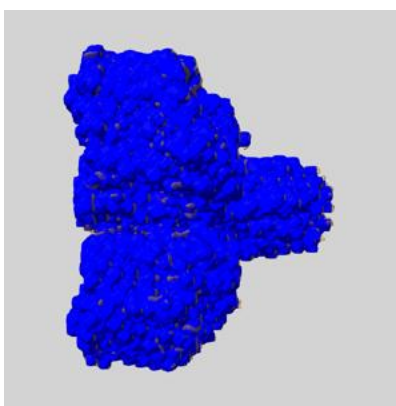
A mask typically either:

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

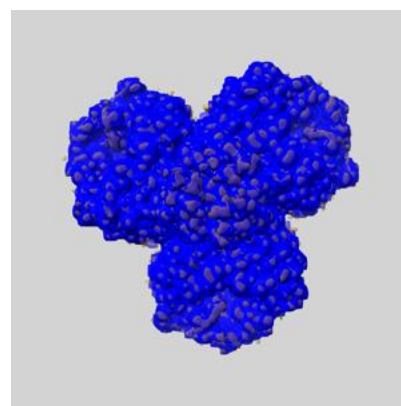
6.6.1 emd_18162_msk_1.map [i](#)



X



Y

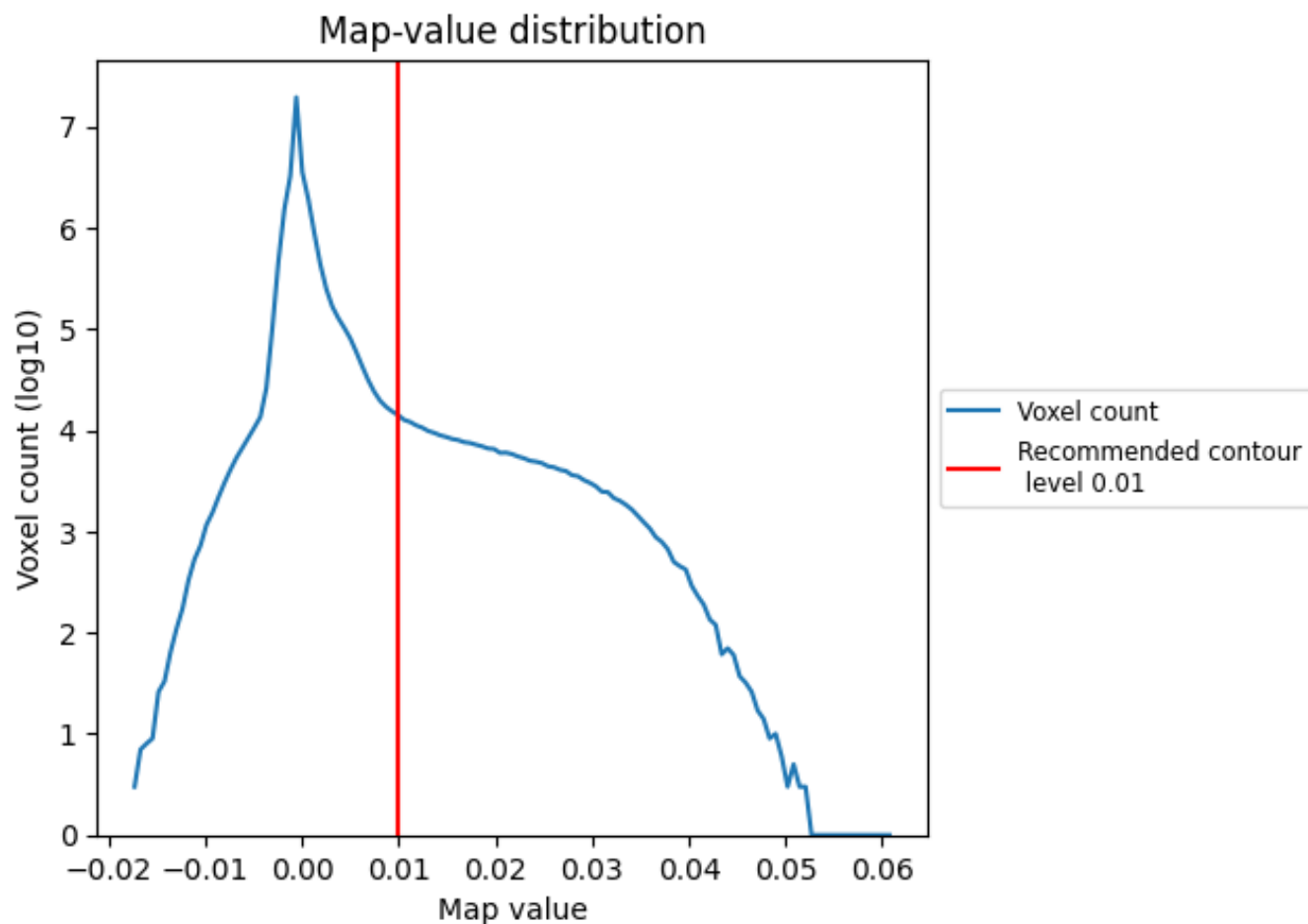


Z

7 Map analysis [i](#)

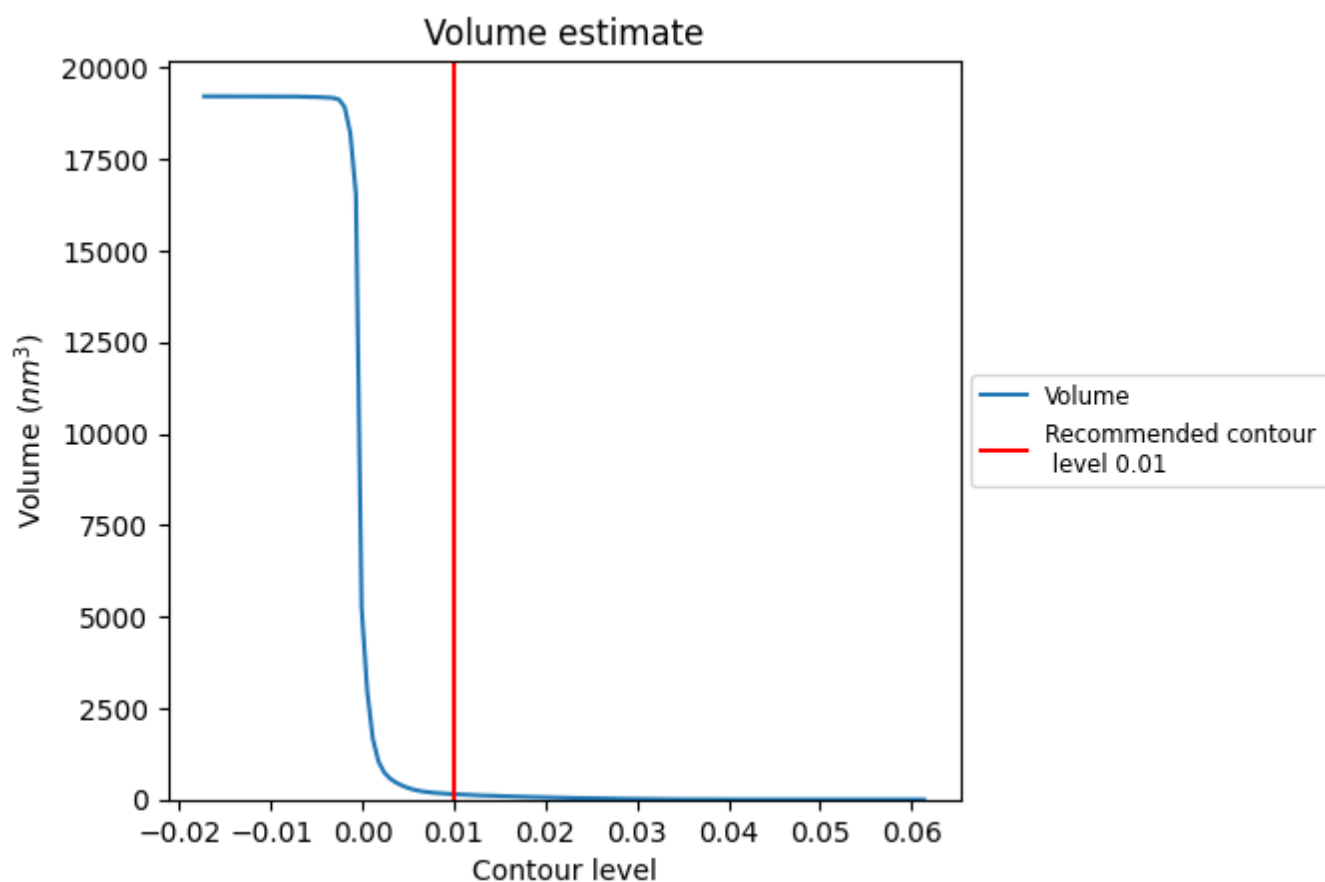
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

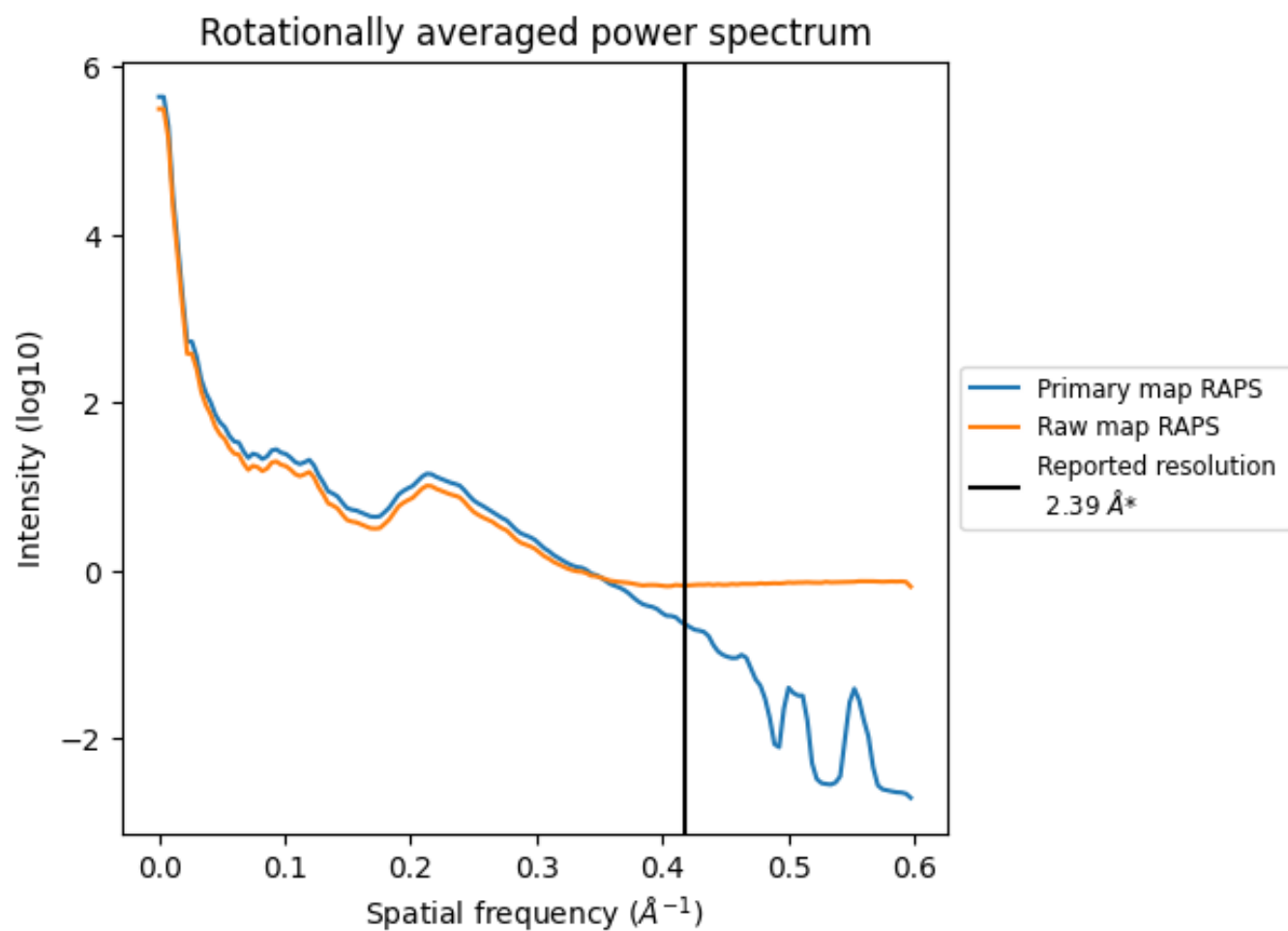
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 148 nm³; this corresponds to an approximate mass of 133 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 ⓘ

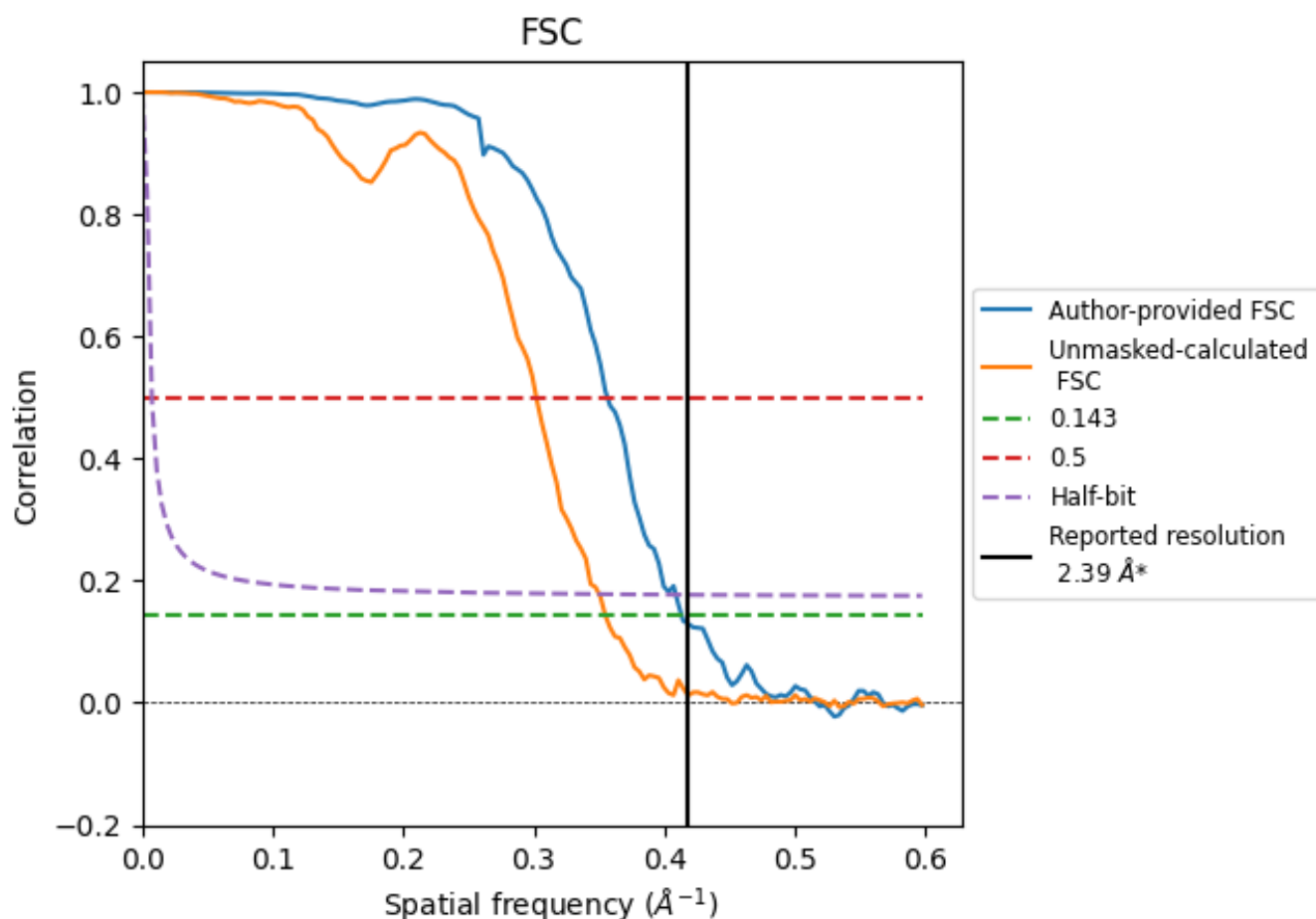


*Reported resolution corresponds to spatial frequency of 0.418 Å⁻¹

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 0.418 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.39	-	-
Author-provided FSC curve	2.42	2.81	2.45
Unmasked-calculated*	2.82	3.31	2.86

*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 2.82 differs from the reported value 2.39 by more than 10 %

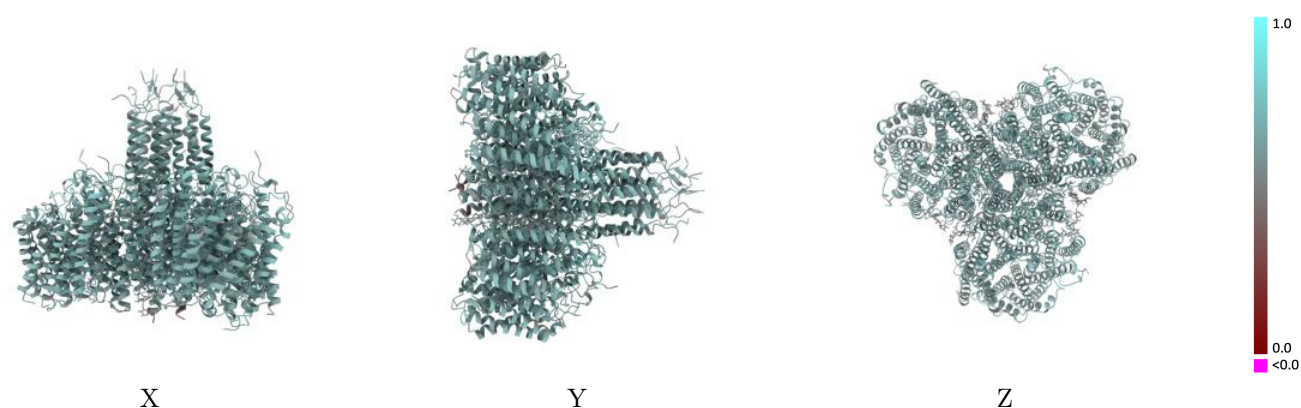
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-18162 and PDB model 8Q54. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)

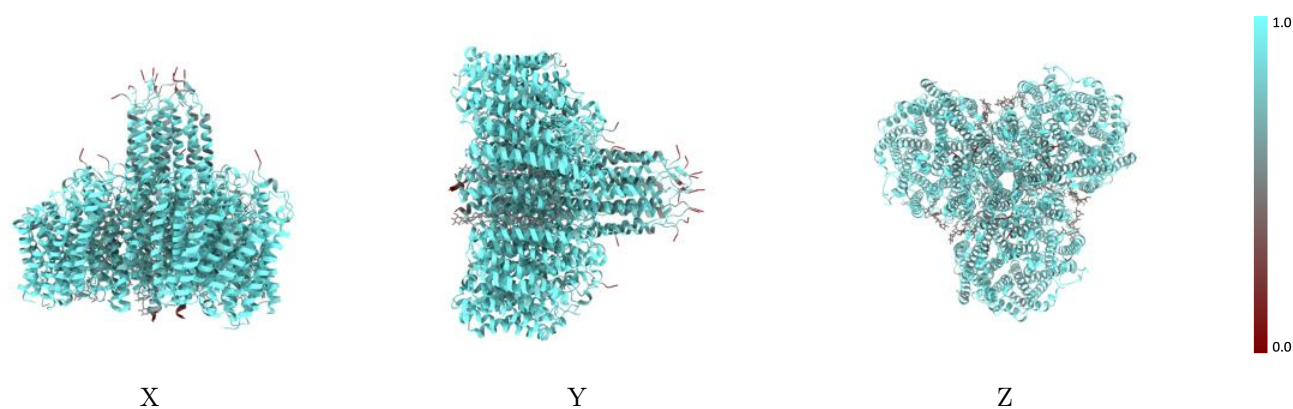
This section was not generated.

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



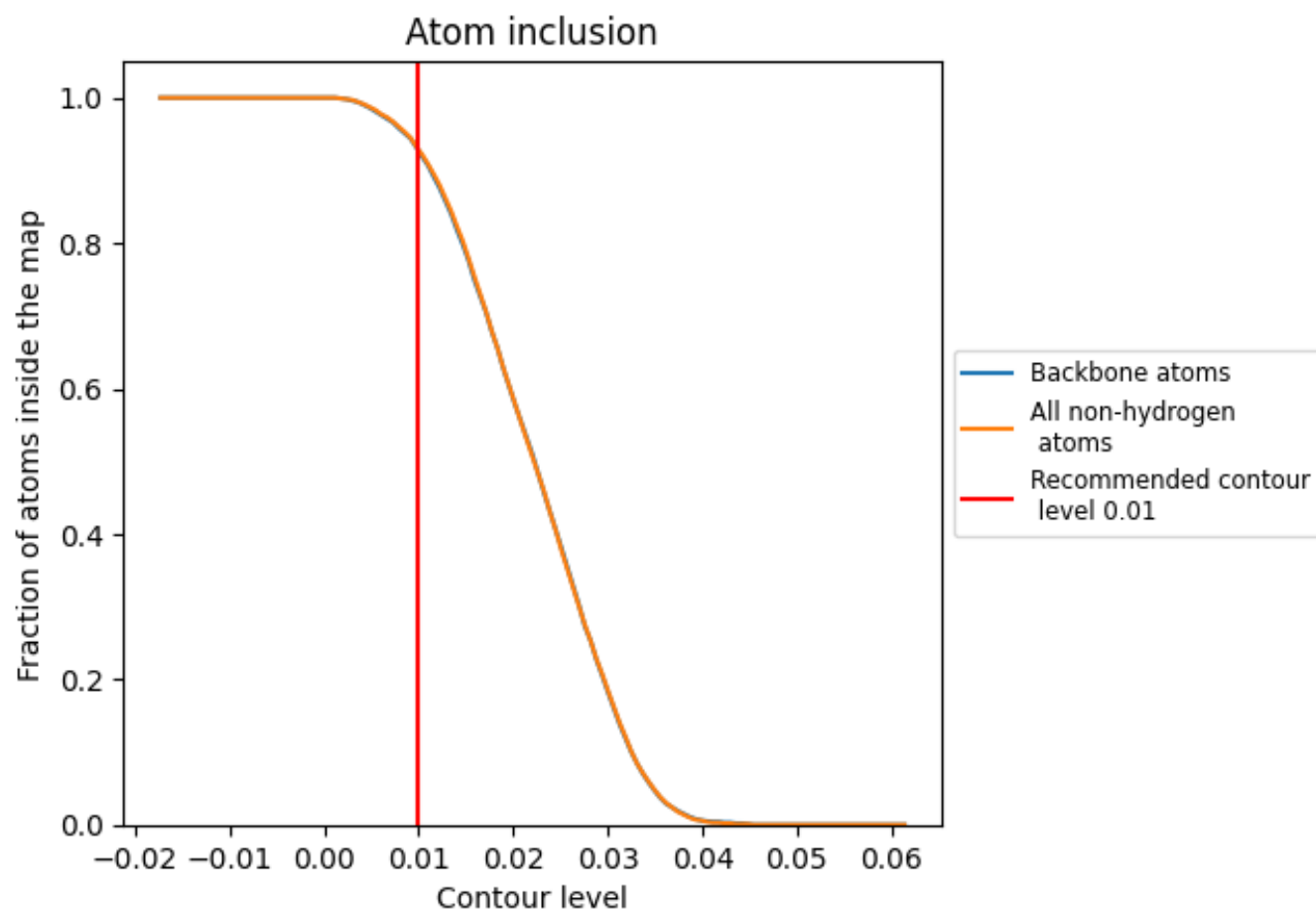
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9280	 0.6320
A	 0.9250	 0.6360
B	 0.9090	 0.6340
C	 0.9110	 0.6160
D	 0.9600	 0.6290
E	 0.9270	 0.6430
F	 0.8970	 0.6350
G	 0.8500	 0.6140
Q	 0.9190	 0.6440
R	 0.9130	 0.6370
S	 0.9210	 0.6130
T	 0.9630	 0.6370
U	 0.9380	 0.6490
V	 0.8990	 0.6270
W	 0.8170	 0.6080
a	 0.9230	 0.6420
b	 0.9180	 0.6350
c	 0.9130	 0.6180
d	 0.9670	 0.6370
e	 0.9410	 0.6490
f	 0.8950	 0.6300
g	 0.8140	 0.6100

