wwPDB EM Validation Summary Report ⓘ

Aug 12, 2024 – 05:24 pm BST

PDB ID	:	8Q54
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)

The following versions of software and data (see references ⓘ) were used in the production of this report:

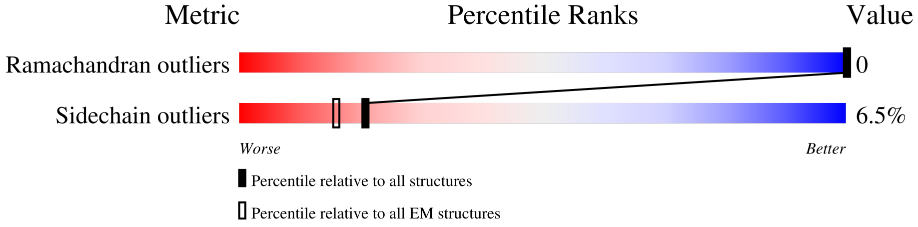
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance ⓘ

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

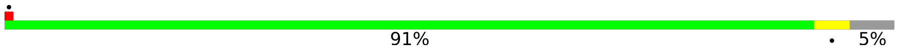
The reported resolution of this entry is 2.39 Å.

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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	
2	R	100	
2	b	100	
3	C	267	
3	S	267	
3	c	267	

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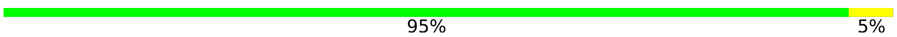
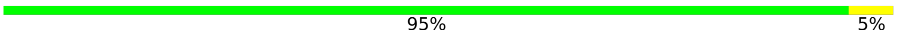
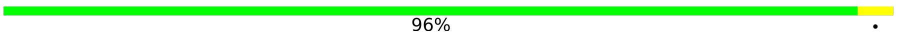
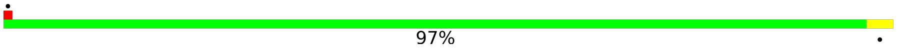
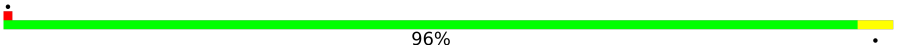
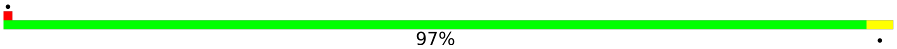
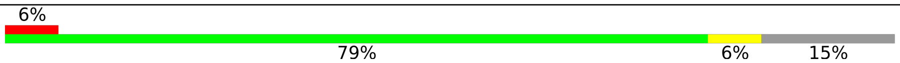
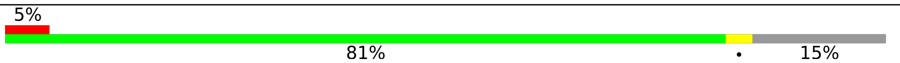
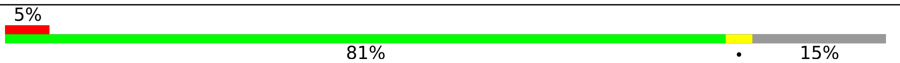
Mol	Chain	Length	Quality of chain
4	D	233	
4	T	233	
4	d	233	
5	E	295	
5	U	295	
5	e	295	
6	F	68	
6	V	68	
6	f	68	
7	G	86	
7	W	86	
7	g	86	

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	E	303[B]	-	X	-	-
11	COM	U	303[A]	-	X	-	-
11	COM	U	303[C]	-	X	-	-
11	COM	e	303[A]	-	X	-	-
11	COM	e	303[B]	-	X	-	-
9	JCV	E	304	X	-	-	-
9	JCV	E	306	X	-	-	-
9	JCV	S	301	X	-	-	-
9	JCV	U	305	X	-	-	-
9	JCV	W	101	X	-	-	-
9	JCV	c	301	X	-	-	-

2 Entry composition

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
			Total	C	H	N	O	S		
1	A	61	962	297	499	78	83	5	0	0
1	a	61	962	297	499	78	83	5	0	0
1	Q	61	962	297	499	78	83	5	0	0

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

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

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

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

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

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

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

- 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 4390 1420 2203 363 388 16	0	0
5	e	294	Total C H N O S 4390 1420 2203 363 388 16	0	0
5	U	294	Total C H N O S 4390 1420 2203 363 388 16	0	0

- 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 1069 329 564 90 84 2	0	0
6	f	67	Total C H N O S 1069 329 564 90 84 2	0	0
6	V	67	Total C H N O S 1069 329 564 90 84 2	0	0

- 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 1164 368 598 92 106	0	0
7	g	73	Total C H N O 1164 368 598 92 106	0	0
7	W	73	Total C H N O 1164 368 598 92 106	0	0

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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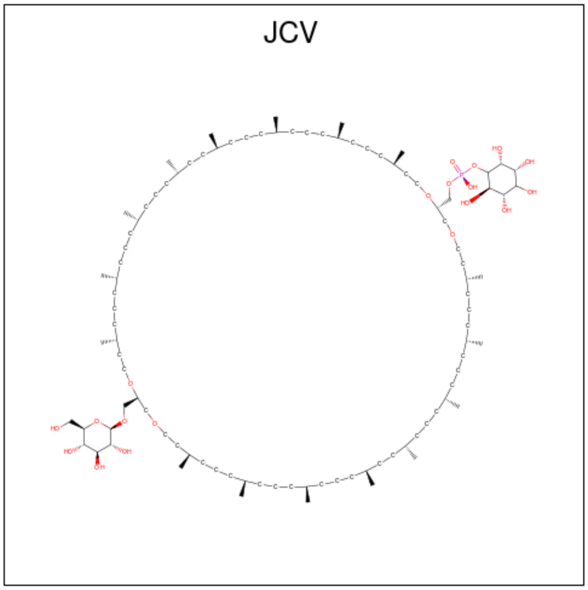
Mol	Chain	Residues	Atoms	AltConf
8	R	1	Total Mg 1 1	0

- 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 (three-letter code: JCV) (formula: $C_{98}H_{193}O_{19}P$).



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

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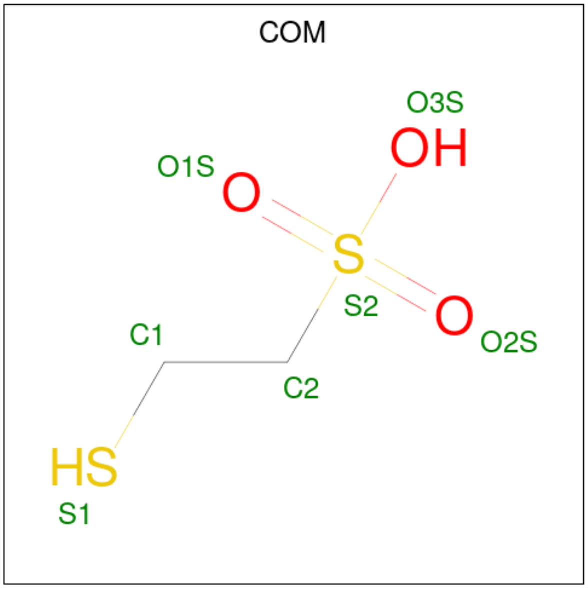
Mol	Chain	Residues	Atoms				AltConf
9	S	1	Total 118	C 98	O 19	P 1	0
9	U	1	Total 114	C 94	O 19	P 1	0
9	U	1	Total 118	C 98	O 19	P 1	0
9	W	1	Total 118	C 98	O 19	P 1	0

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 11 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: $C_2H_6O_3S_2$).



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

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

- Molecule 12 is water.

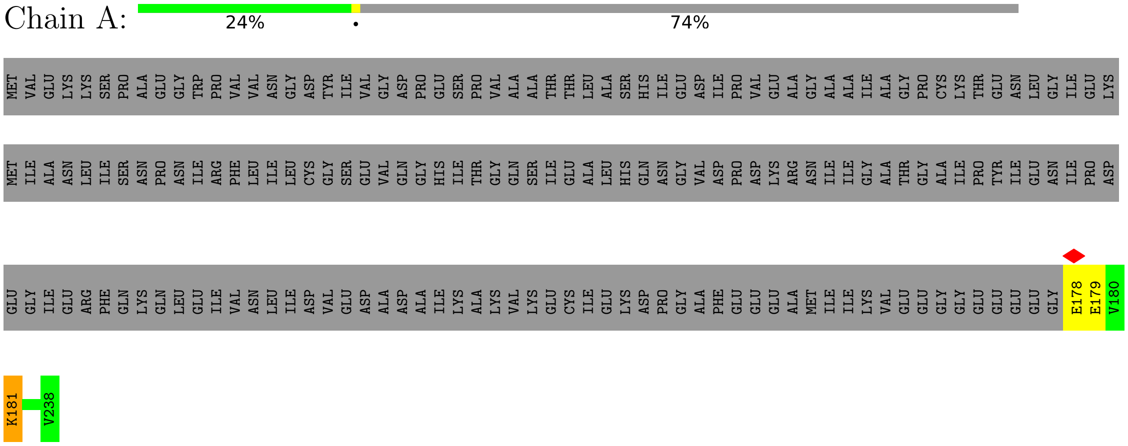
Mol	Chain	Residues	Atoms	AltConf
12	A	2	Total O 2 2	0
12	B	2	Total O 2 2	0
12	C	2	Total O 2 2	0
12	D	2	Total O 2 2	0
12	E	18	Total O 18 18	0
12	F	3	Total O 3 3	0
12	a	1	Total O 1 1	0
12	b	2	Total O 2 2	0
12	c	1	Total O 1 1	0
12	d	4	Total O 4 4	0
12	e	20	Total O 20 20	0
12	f	1	Total O 1 1	0
12	Q	1	Total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

3 Residue-property plots

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

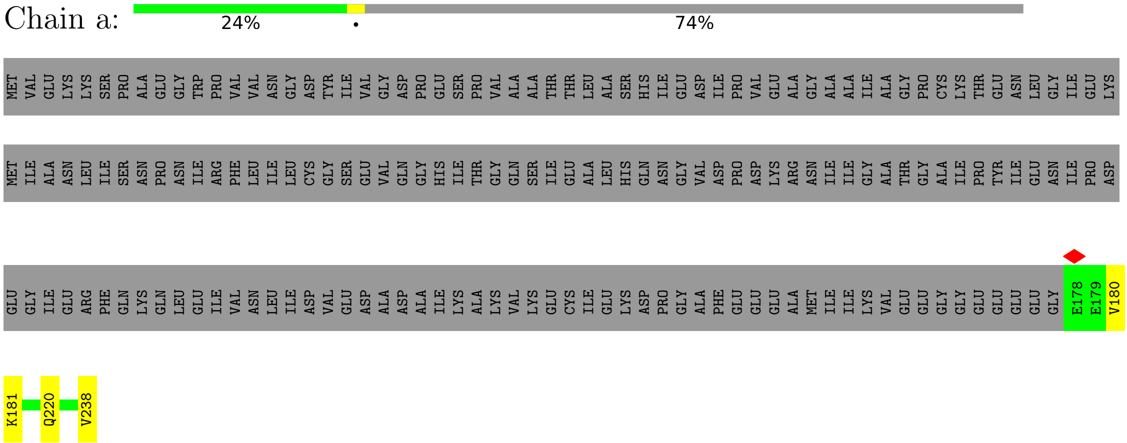
- Molecule 1: Tetrahydromethanopterin S-methyltransferase subunit A 1

Chain A:



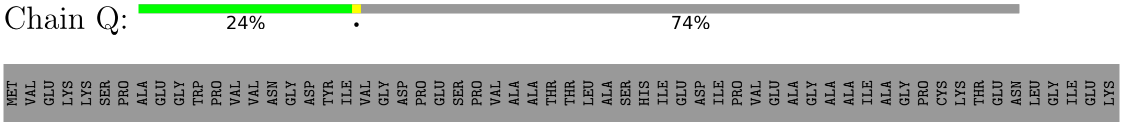
- Molecule 1: Tetrahydromethanopterin S-methyltransferase subunit A 1

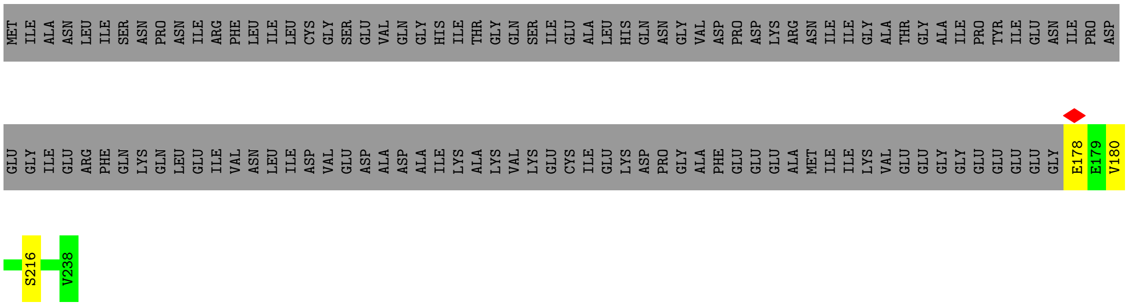
Chain a:



- Molecule 1: Tetrahydromethanopterin S-methyltransferase subunit A 1

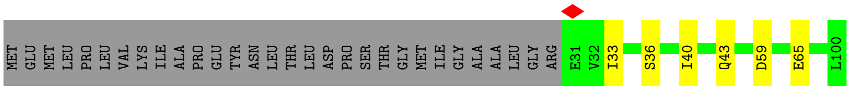
Chain Q:





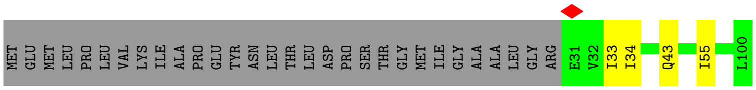
- Molecule 2: Tetrahydromethanopterin S-methyltransferase subunit B

Chain B:



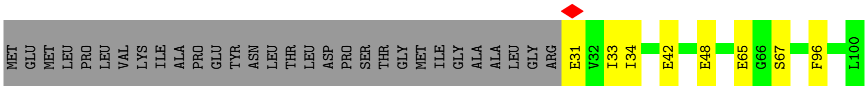
- Molecule 2: Tetrahydromethanopterin S-methyltransferase subunit B

Chain b:



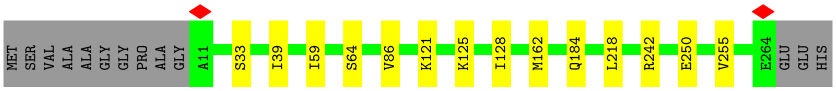
- Molecule 2: Tetrahydromethanopterin S-methyltransferase subunit B

Chain R:



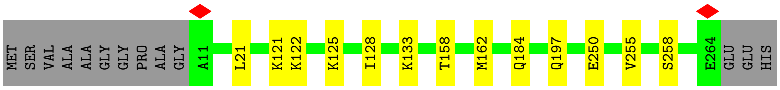
- Molecule 3: Tetrahydromethanopterin S-methyltransferase subunit C

Chain C:



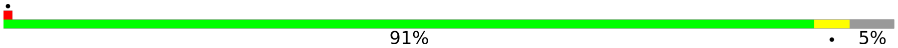
- Molecule 3: Tetrahydromethanopterin S-methyltransferase subunit C

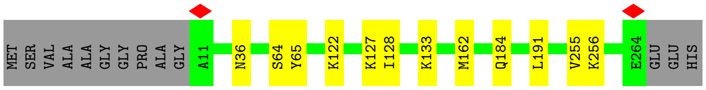
Chain c:



- Molecule 3: Tetrahydromethanopterin S-methyltransferase subunit C

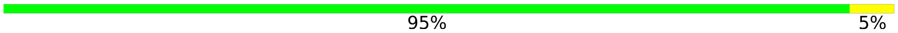
Chain S:

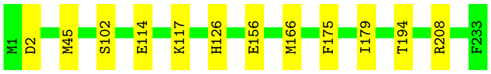




- Molecule 4: Tetrahydromethanopterin S-methyltransferase subunit D

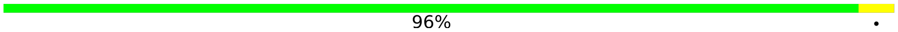
Chain D:





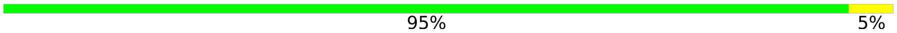
- Molecule 4: Tetrahydromethanopterin S-methyltransferase subunit D

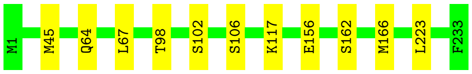
Chain d:



- Molecule 4: Tetrahydromethanopterin S-methyltransferase subunit D

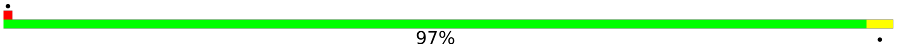
Chain T:

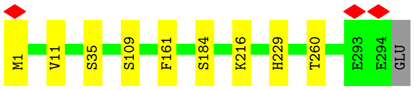




- Molecule 5: Tetrahydromethanopterin S-methyltransferase subunit E

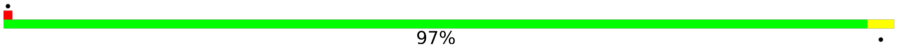
Chain E:

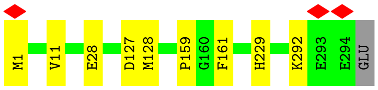




- Molecule 5: Tetrahydromethanopterin S-methyltransferase subunit E

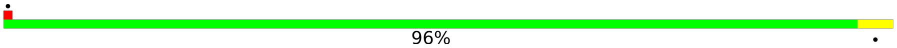
Chain e:

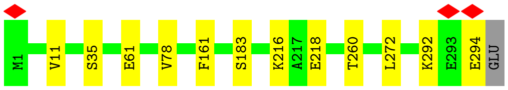




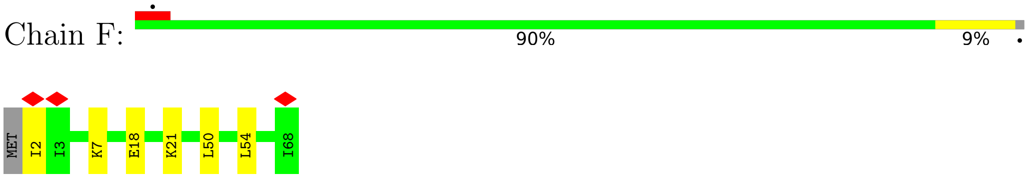
- Molecule 5: Tetrahydromethanopterin S-methyltransferase subunit E

Chain U:

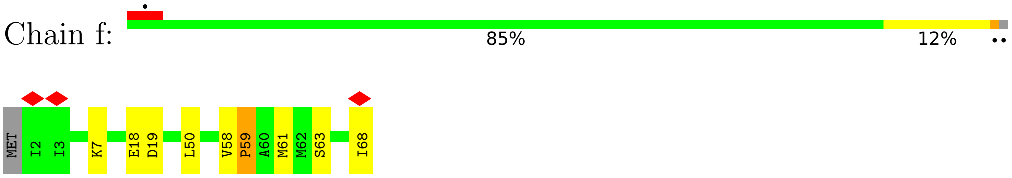




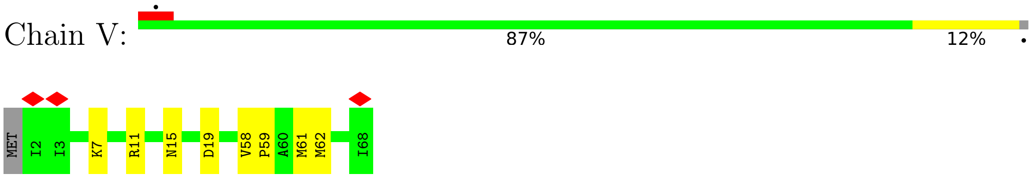
- Molecule 6: Tetrahydromethanopterin S-methyltransferase subunit F



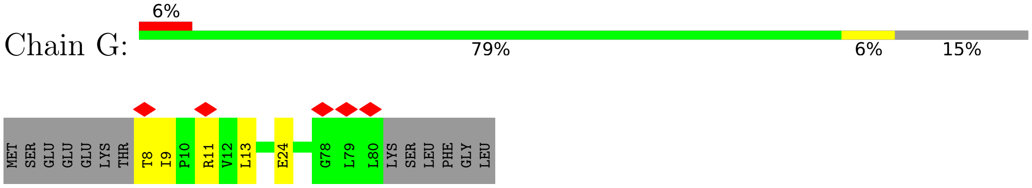
- Molecule 6: Tetrahydromethanopterin S-methyltransferase subunit F



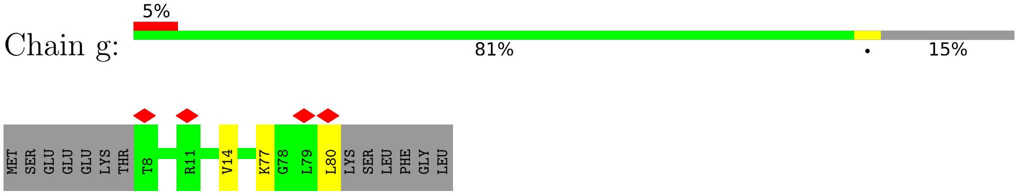
- Molecule 6: Tetrahydromethanopterin S-methyltransferase subunit F



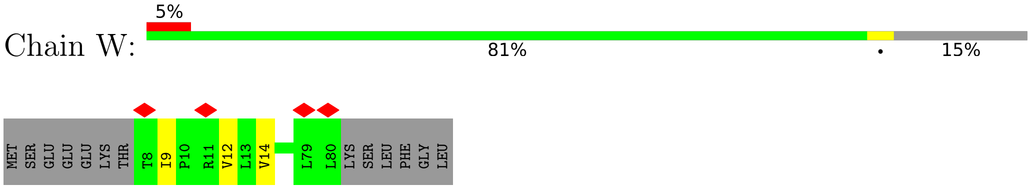
- Molecule 7: Tetrahydromethanopterin S-methyltransferase subunit G



- 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 $(e^-/\text{Å}^2)$	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: COM, MG, NA, JCV

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.72	1/467 (0.2%)	0.65	0/626
1	Q	0.64	0/467	0.67	0/626
1	a	0.70	1/467 (0.2%)	0.68	0/626
2	B	0.69	0/538	0.73	0/733
2	R	0.66	0/538	0.72	0/733
2	b	0.74	0/538	0.79	0/733
3	C	0.65	0/1878	0.78	0/2566
3	S	0.57	0/1878	0.70	0/2566
3	c	0.55	0/1894	0.65	0/2587
4	D	0.66	0/1624	0.75	0/2207
4	T	0.51	0/1624	0.60	0/2207
4	d	0.50	0/1624	0.57	0/2207
5	E	0.53	0/2242	0.64	1/3055 (0.0%)
5	U	0.60	2/2242 (0.1%)	0.66	1/3055 (0.0%)
5	e	0.60	1/2242 (0.0%)	0.69	1/3055 (0.0%)
6	F	0.77	0/509	0.80	0/684
6	V	0.94	2/509 (0.4%)	0.87	1/684 (0.1%)
6	f	0.99	2/509 (0.4%)	0.89	2/684 (0.3%)
7	G	0.45	0/571	0.63	0/770
7	W	0.47	0/571	0.56	0/770
7	g	0.58	0/571	0.70	0/770
All	All	0.61	9/23503 (0.0%)	0.69	6/31944 (0.0%)

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 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	59	PRO	N-CA	13.31	1.69	1.47
6	f	59	PRO	N-CA	13.07	1.69	1.47
1	A	181	LYS	C-N	10.87	1.54	1.34
1	a	181	LYS	C-N	10.49	1.54	1.34
5	U	61	GLU	C-N	9.77	1.52	1.34

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	59	PRO	CA-N-CD	-7.96	100.36	111.50
6	V	59	PRO	CA-N-CD	-6.63	102.22	111.50
5	e	161	PHE	CB-CA-C	6.01	122.43	110.40
5	U	161	PHE	CB-CA-C	5.98	122.35	110.40
5	E	161	PHE	CB-CA-C	5.32	121.04	110.40

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 ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	47 (94%)	3 (6%)	19	31
1	Q	50/193 (26%)	47 (94%)	3 (6%)	19	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	50/193 (26%)	47 (94%)	3 (6%)	19	31
2	B	58/82 (71%)	52 (90%)	6 (10%)	7	10
2	R	58/82 (71%)	50 (86%)	8 (14%)	3	4
2	b	58/82 (71%)	54 (93%)	4 (7%)	15	25
3	C	191/196 (97%)	176 (92%)	15 (8%)	12	19
3	S	191/196 (97%)	178 (93%)	13 (7%)	16	25
3	c	192/196 (98%)	178 (93%)	14 (7%)	14	22
4	D	155/155 (100%)	143 (92%)	12 (8%)	13	20
4	T	155/155 (100%)	144 (93%)	11 (7%)	14	23
4	d	155/155 (100%)	145 (94%)	10 (6%)	17	27
5	E	228/229 (100%)	220 (96%)	8 (4%)	36	55
5	U	228/229 (100%)	218 (96%)	10 (4%)	28	45
5	e	228/229 (100%)	222 (97%)	6 (3%)	46	66
6	F	54/55 (98%)	48 (89%)	6 (11%)	6	8
6	V	54/55 (98%)	48 (89%)	6 (11%)	6	8
6	f	54/55 (98%)	46 (85%)	8 (15%)	3	3
7	G	61/73 (84%)	56 (92%)	5 (8%)	11	17
7	W	61/73 (84%)	58 (95%)	3 (5%)	25	40
7	g	61/73 (84%)	58 (95%)	3 (5%)	25	40
All	All	2392/2949 (81%)	2235 (93%)	157 (7%)	21	26

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	S	64	SER
5	U	218	GLU
3	S	128	ILE
4	T	98	THR
6	V	15	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
4	T	64	GLN

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Mol	Chain	Res	Type
1	Q	196	ASN
6	f	24	ASN
5	e	40	GLN
7	g	47	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 monosaccharides 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	$\#\|Z\| >$
11	COM	e	303[B]	-	6,6,6	1.78	3 (50%)	7,8,8	2.80	4 (57%
11	COM	E	303[A]	-	6,6,6	1.82	2 (33%)	7,8,8	2.78	4 (57%
9	JCV	g	101	-	120,120,120	1.11	10 (8%)	148,154,154	0.71	0
9	JCV	e	305	-	120,120,120	1.15	11 (9%)	148,154,154	1.19	16 (10%
9	JCV	U	304	-	116,116,120	1.10	9 (7%)	141,146,154	0.73	0
11	COM	U	303[C]	-	6,6,6	1.84	3 (50%)	7,8,8	2.80	3 (42%
11	COM	E	303[B]	-	6,6,6	1.77	2 (33%)	7,8,8	2.79	4 (57%
9	JCV	E	305	-	120,120,120	1.32	12 (10%)	148,154,154	1.47	24 (16%

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| >$
9	JCV	W	101	-	120,120,120	1.13	11 (9%)	148,154,154	0.87	2 (1%)
9	JCV	E	306	-	120,120,120	1.13	10 (8%)	148,154,154	0.68	0
11	COM	U	303[A]	-	6,6,6	1.78	3 (50%)	7,8,8	2.75	4 (57%
9	JCV	C	301	-	120,120,120	1.13	12 (10%)	148,154,154	0.66	0
9	JCV	E	304	-	120,120,120	1.25	14 (11%)	148,154,154	1.62	23 (15%
9	JCV	e	304	-	120,120,120	1.32	12 (10%)	148,154,154	1.48	26 (17%
9	JCV	S	301	-	120,120,120	1.10	8 (6%)	148,154,154	1.29	20 (13%
11	COM	e	303[A]	-	6,6,6	1.31	1 (16%)	7,8,8	3.78	4 (57%
9	JCV	U	305	-	120,120,120	1.13	11 (9%)	148,154,154	0.67	0
9	JCV	c	301	-	120,120,120	1.13	10 (8%)	148,154,154	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[B]	-	-	1/4/4/4	-
11	COM	E	303[A]	-	-	4/4/4/4	-
9	JCV	g	101	-	-	51/126/170/170	0/2/2/2
9	JCV	e	305	-	-	62/126/170/170	0/2/2/2
9	JCV	U	304	-	-	34/118/162/170	0/2/2/2
11	COM	U	303[C]	-	-	3/4/4/4	-
11	COM	E	303[B]	-	-	2/4/4/4	-
9	JCV	E	305	-	-	29/126/170/170	0/2/2/2
9	JCV	W	101	-	2/2/30/30	61/126/170/170	0/2/2/2
9	JCV	E	306	-	1/1/30/30	55/126/170/170	0/2/2/2
11	COM	U	303[A]	-	-	4/4/4/4	-
9	JCV	C	301	-	-	71/126/170/170	0/2/2/2
9	JCV	E	304	-	1/1/30/30	54/126/170/170	0/2/2/2
9	JCV	e	304	-	-	44/126/170/170	0/2/2/2
9	JCV	S	301	-	2/2/30/30	51/126/170/170	0/2/2/2
11	COM	e	303[A]	-	-	3/4/4/4	-
9	JCV	U	305	-	1/1/30/30	72/126/170/170	0/2/2/2
9	JCV	c	301	-	2/2/30/30	71/126/170/170	0/2/2/2

The worst 5 of 144 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	305	JCV	OY1-CG7	-6.30	1.32	1.43
9	e	304	JCV	OY1-CG7	-5.88	1.33	1.43
9	e	305	JCV	OY1-CG7	-5.14	1.34	1.43
9	C	301	JCV	OY1-CG7	-4.27	1.35	1.43
9	g	101	JCV	OY1-CG7	-4.24	1.36	1.43

The worst 5 of 134 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	E	304	JCV	OX4-CX2-CX3	-8.22	91.35	110.35
11	e	303[A]	COM	O3S-S2-C2	6.47	116.24	105.77
9	E	304	JCV	CX6-CX1-CX2	6.09	119.63	110.85
11	e	303[A]	COM	O3S-S2-O1S	-5.50	97.83	111.27
9	e	304	JCV	CX4-CX3-CX2	-5.36	101.46	110.82

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 672 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	301	JCV	C52-C51-OG2-CG2
9	C	301	JCV	C30M-C30-C31-C32
9	C	301	JCV	C55-C56-C57-C57M
9	C	301	JCV	C80M-C80-C81-C82
9	C	301	JCV	CG1-O1-P-O2

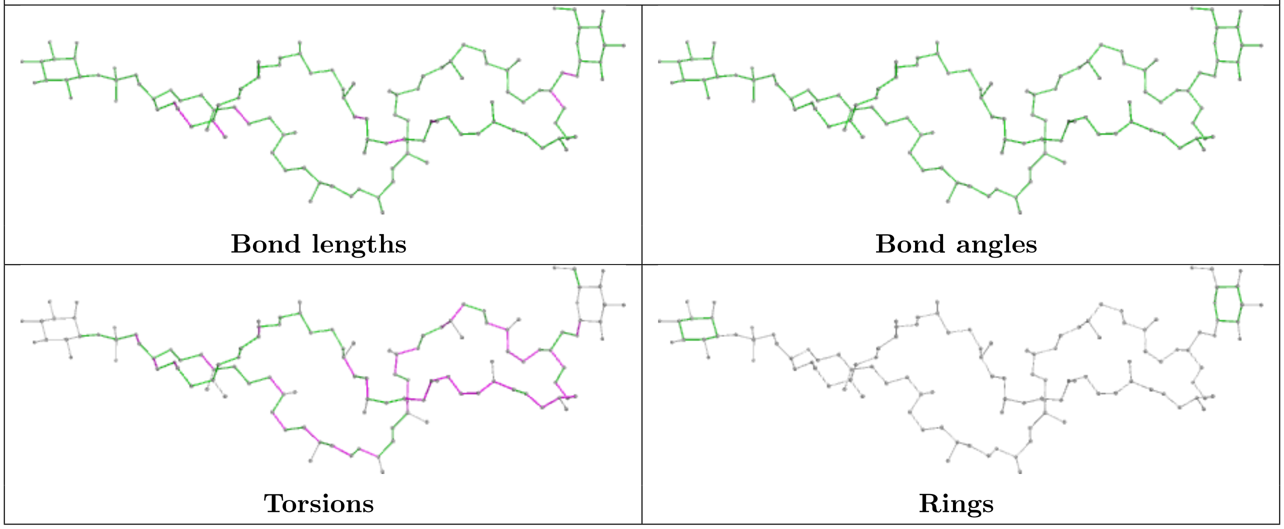
There are no ring outliers.

No monomer is involved in short contacts.

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 then 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.

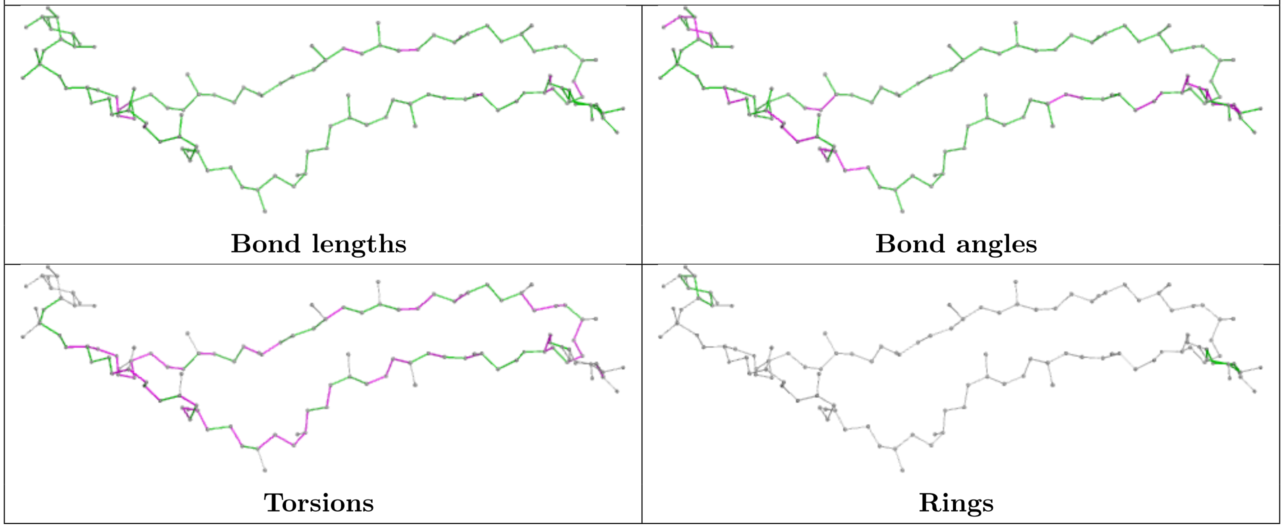
Ligand JCV g 101



Bond lengths **Bond angles**

Torsions **Rings**

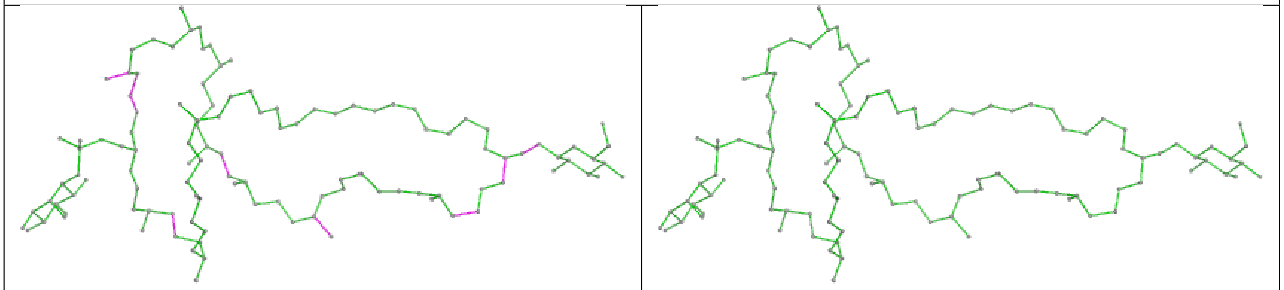
Ligand JCV e 305



Bond lengths **Bond angles**

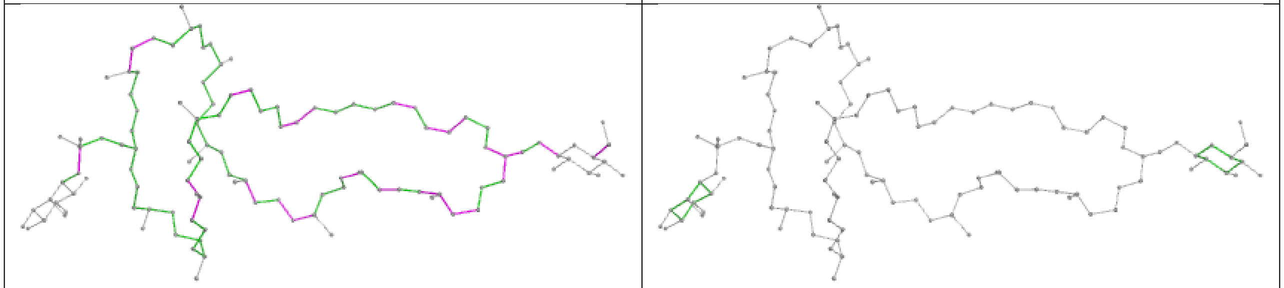
Torsions **Rings**

Ligand JCV U 304



Bond lengths

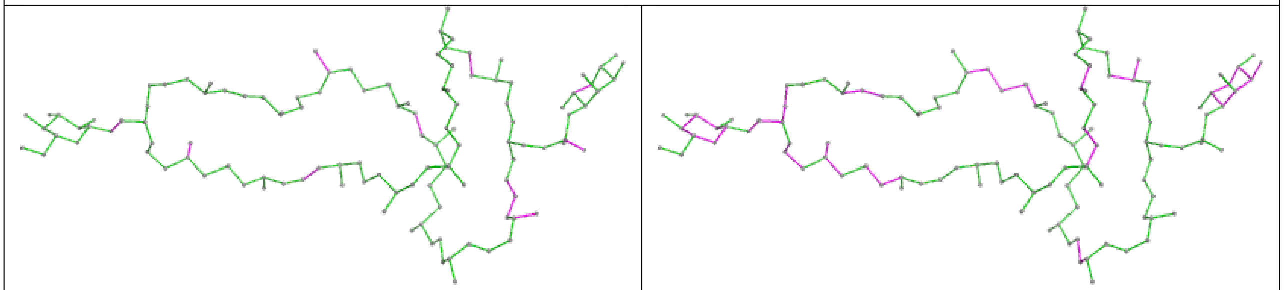
Bond angles



Torsions

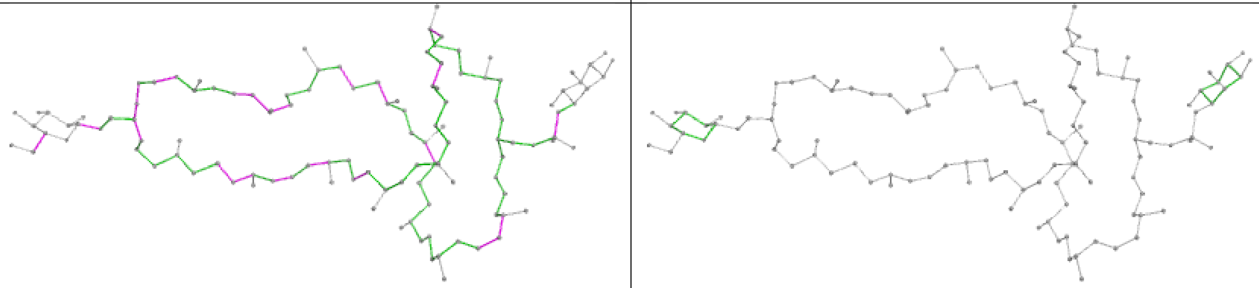
Rings

Ligand JCV E 305



Bond lengths

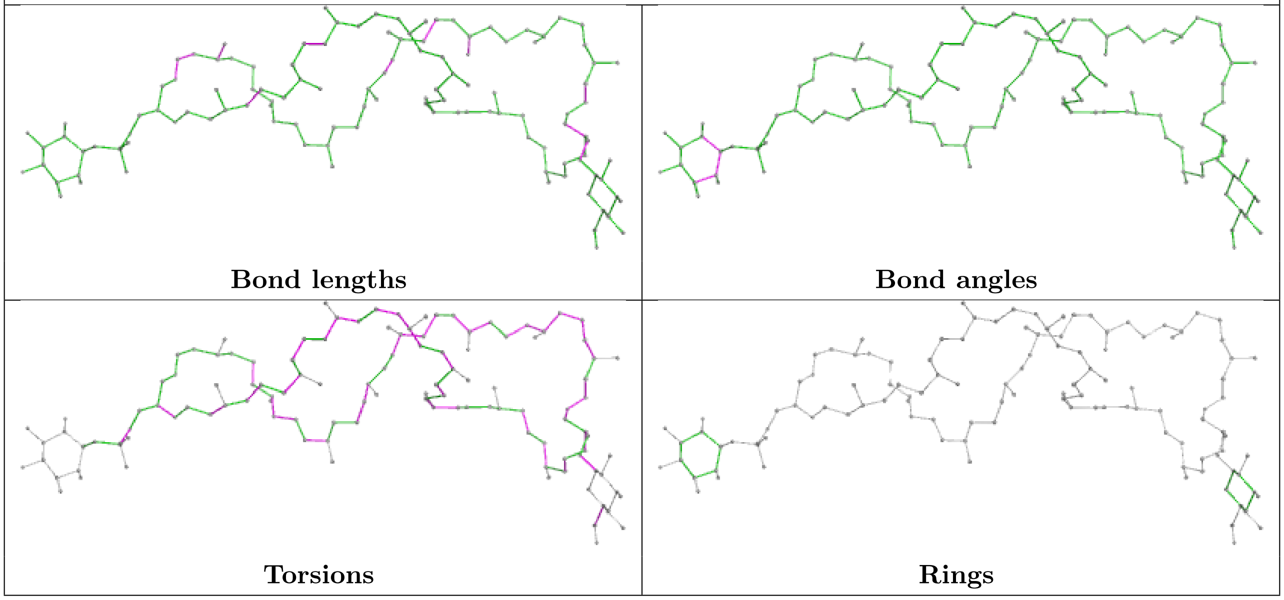
Bond angles



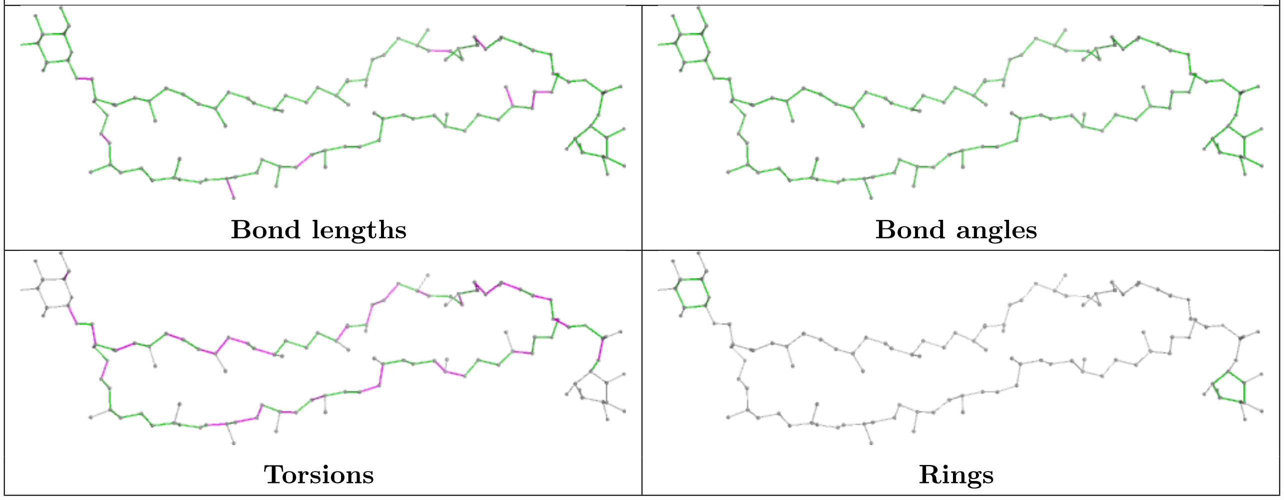
Torsions

Rings

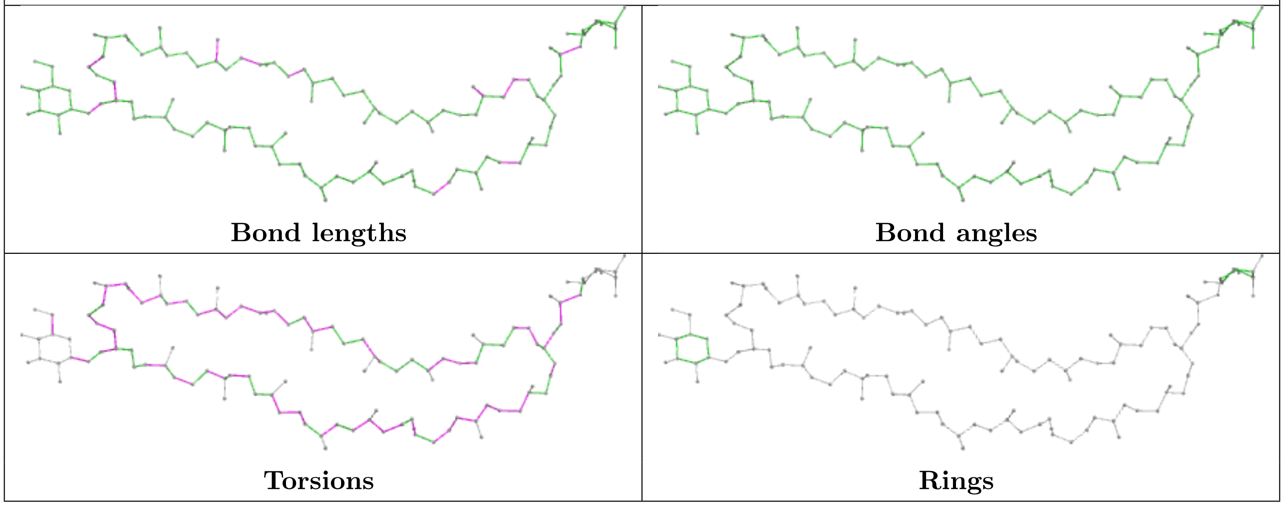
Ligand JCV W 101



Ligand JCV E 306



Ligand JCV C 301



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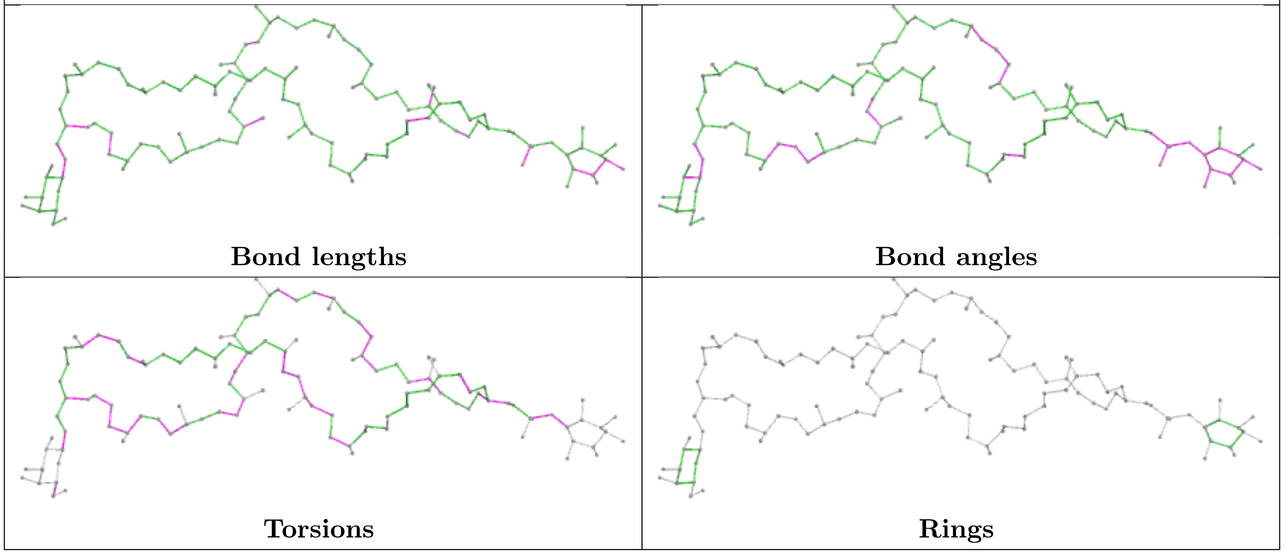

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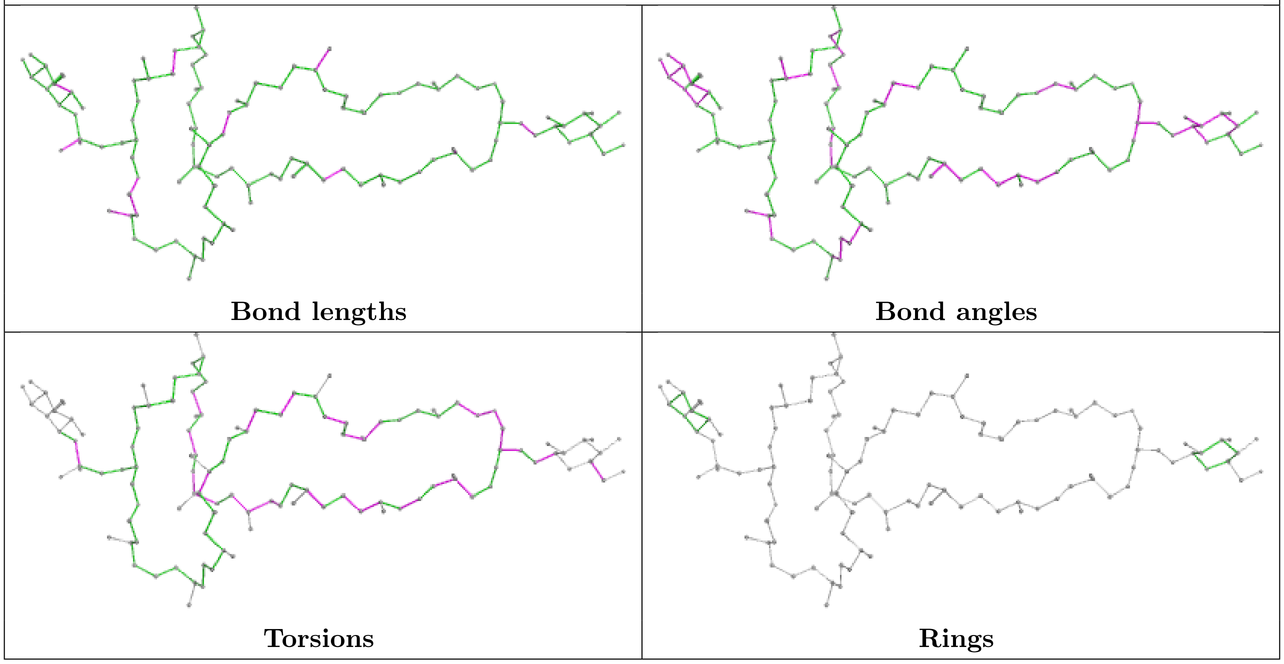
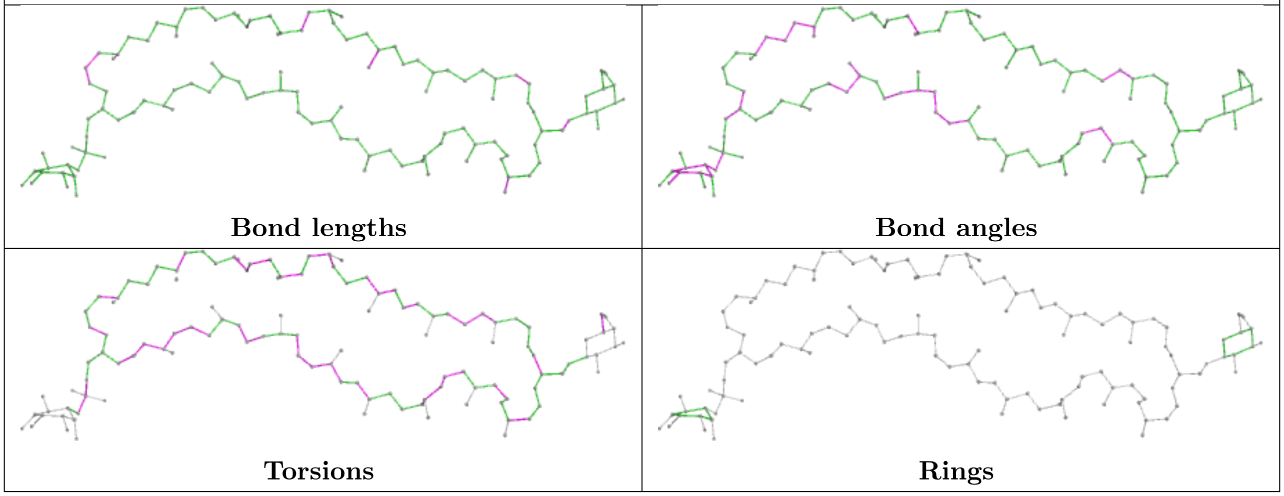


Ligand JCV S 301



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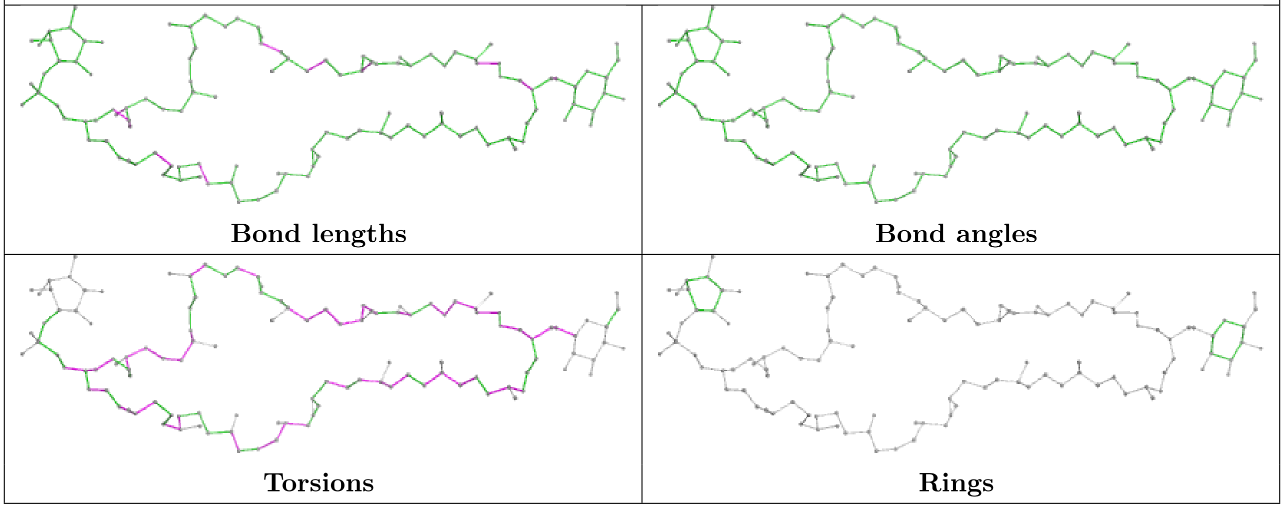
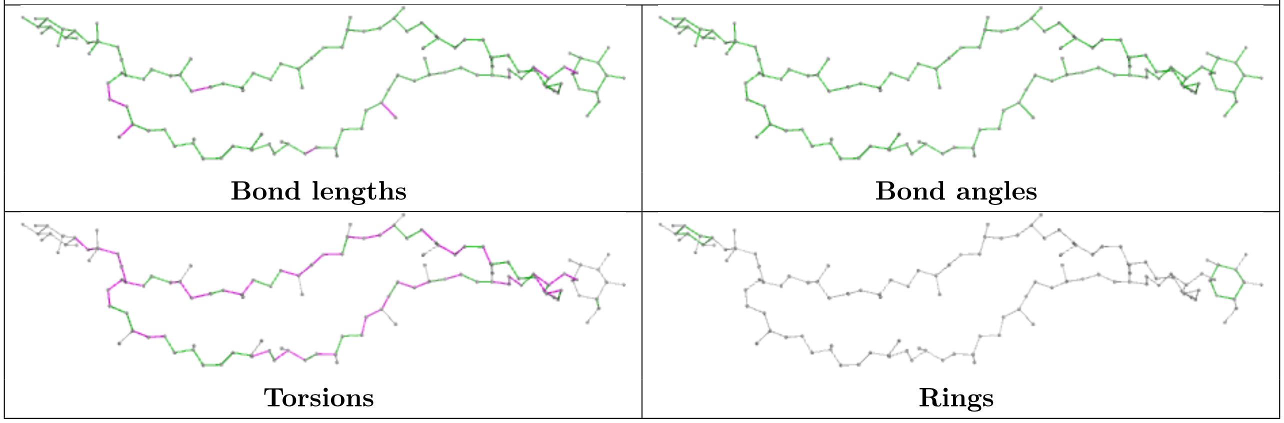


Ligand JCV c 301



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

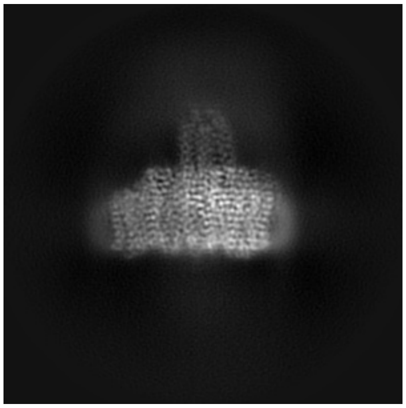
6 Map visualisation ⓘ

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.

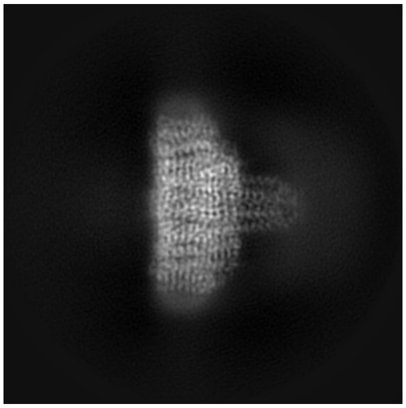
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ

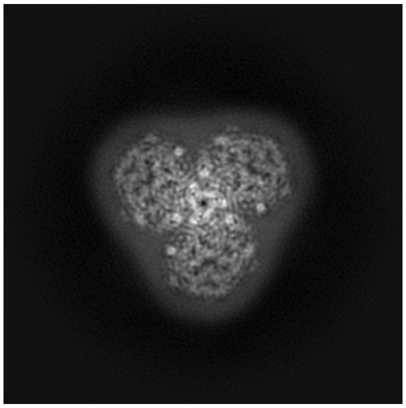
6.1.1 Primary map



X

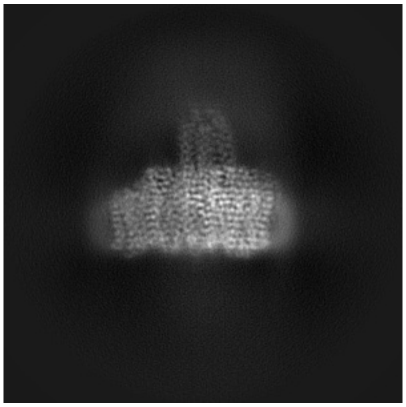


Y

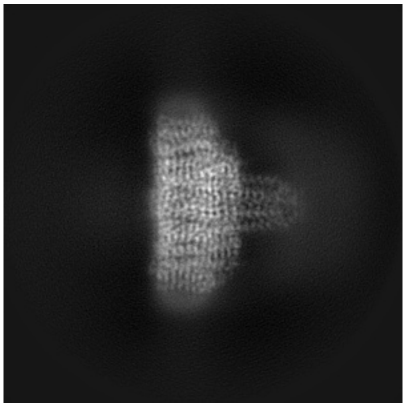


Z

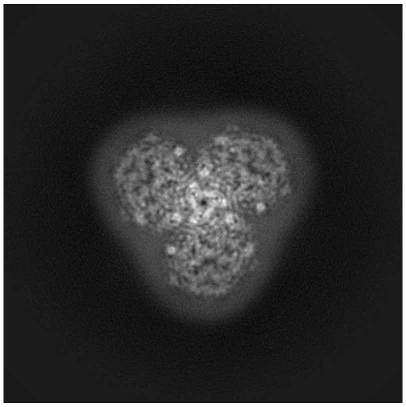
6.1.2 Raw map



X



Y

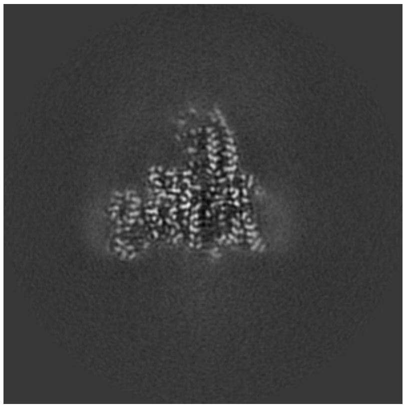


Z

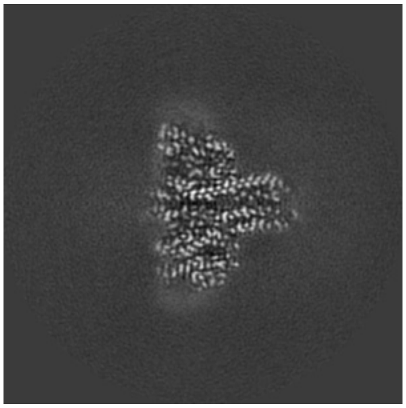
The images above show the map projected in three orthogonal directions.

6.2 Central slices

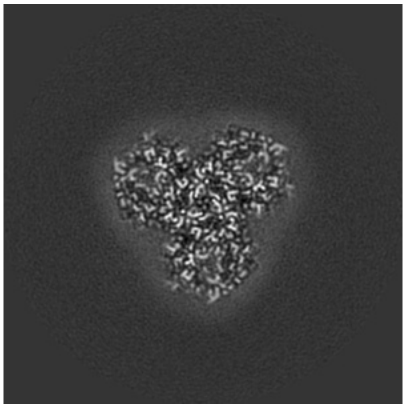
6.2.1 Primary map



X Index: 160

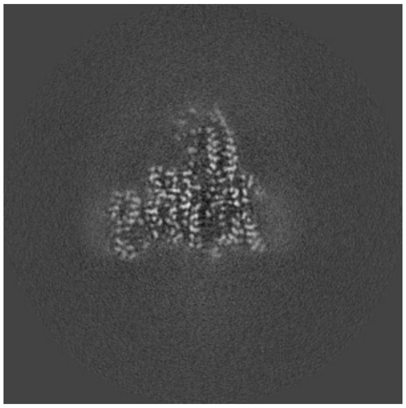


Y Index: 160

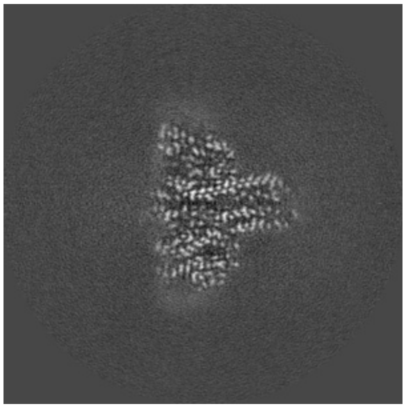


Z Index: 160

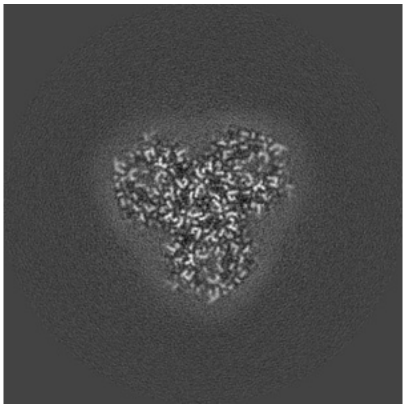
6.2.2 Raw map



X Index: 160



Y Index: 160

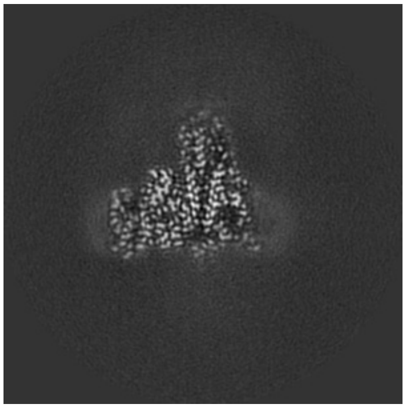


Z Index: 160

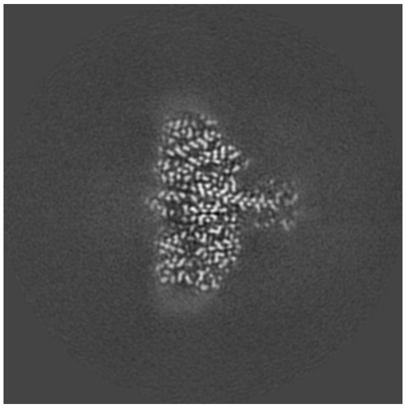
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

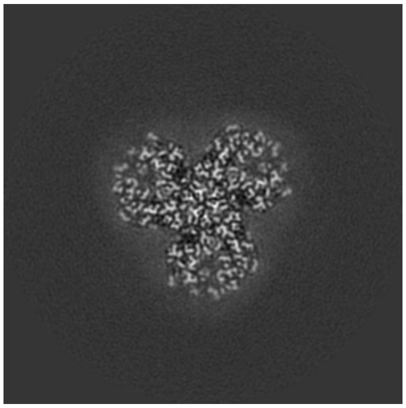
6.3.1 Primary map



X Index: 155

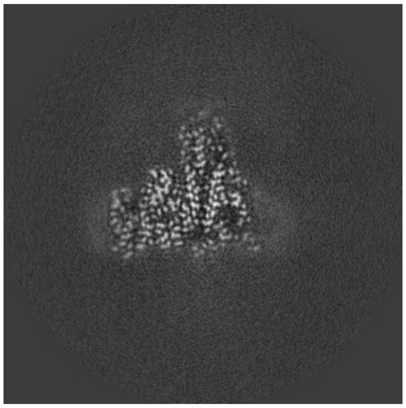


Y Index: 167

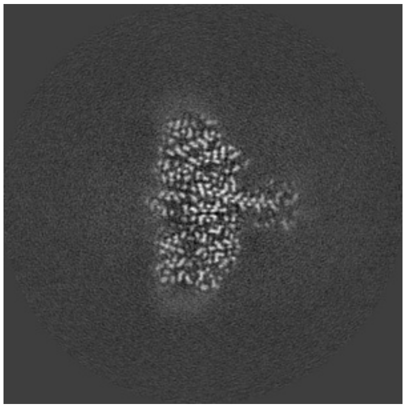


Z Index: 165

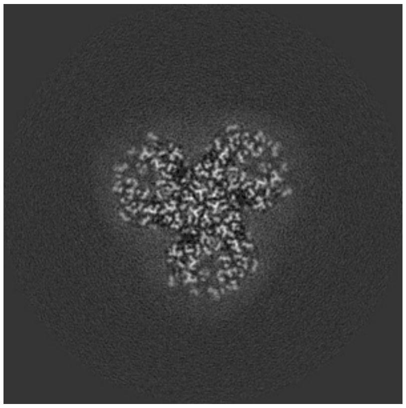
6.3.2 Raw map



X Index: 155



Y Index: 167

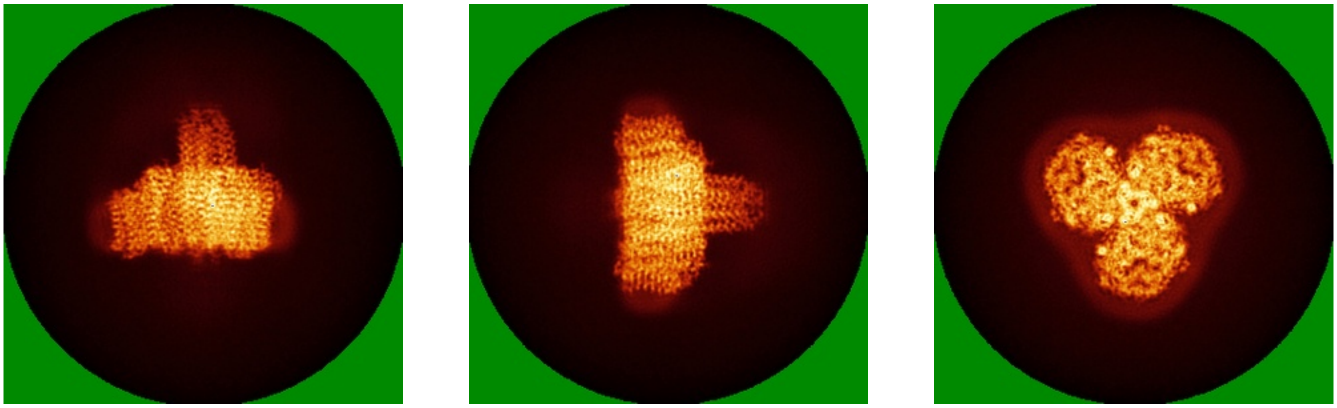


Z Index: 165

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

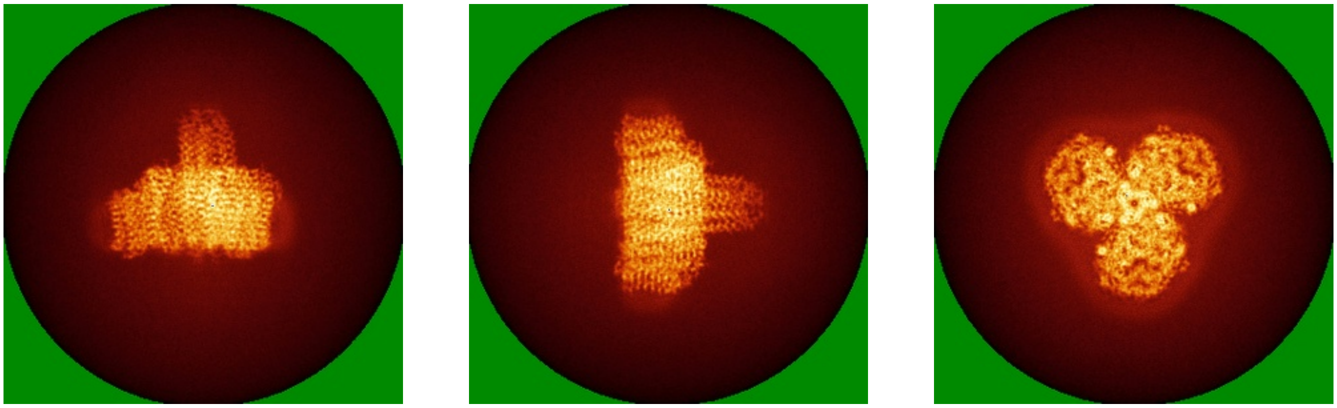
6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



X Y Z

6.4.2 Raw map

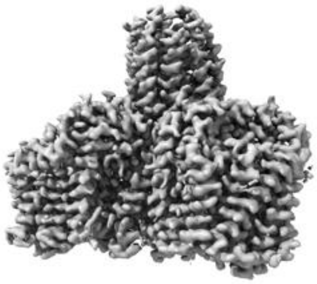


X Y Z

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.

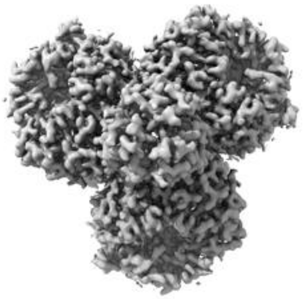
6.5 Orthogonal surface views (i)

6.5.1 Primary map



X

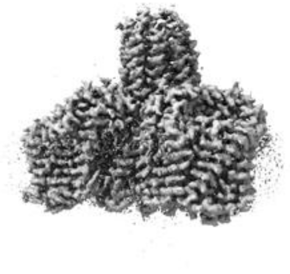
Y



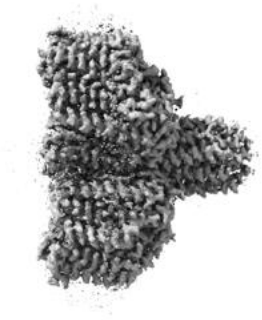
Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

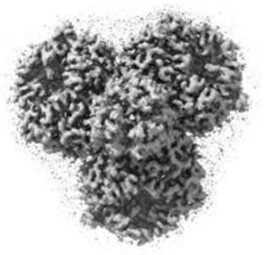
6.5.2 Raw map



X



Y



Z

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.

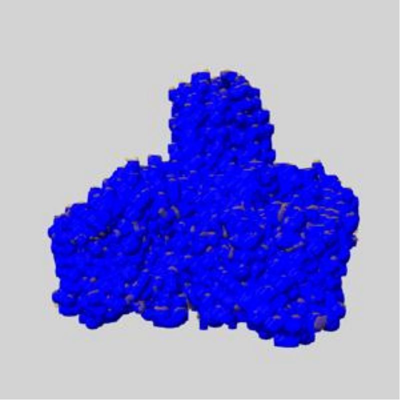
6.6 Mask visualisation

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

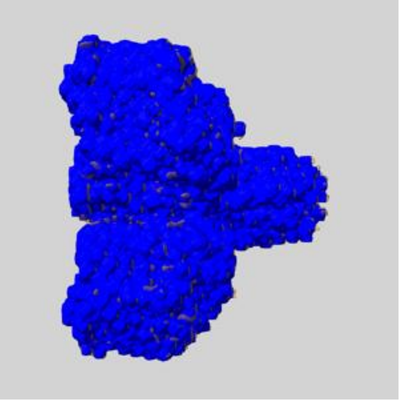
A mask typically either:

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

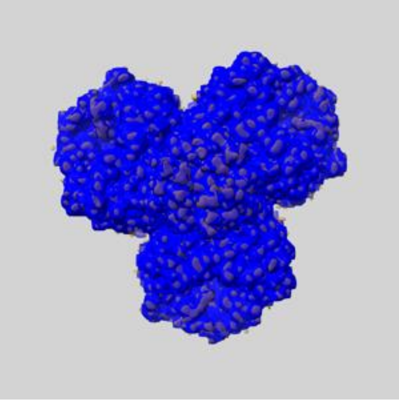
6.6.1 emd_18162_msk_1.map



X



Y

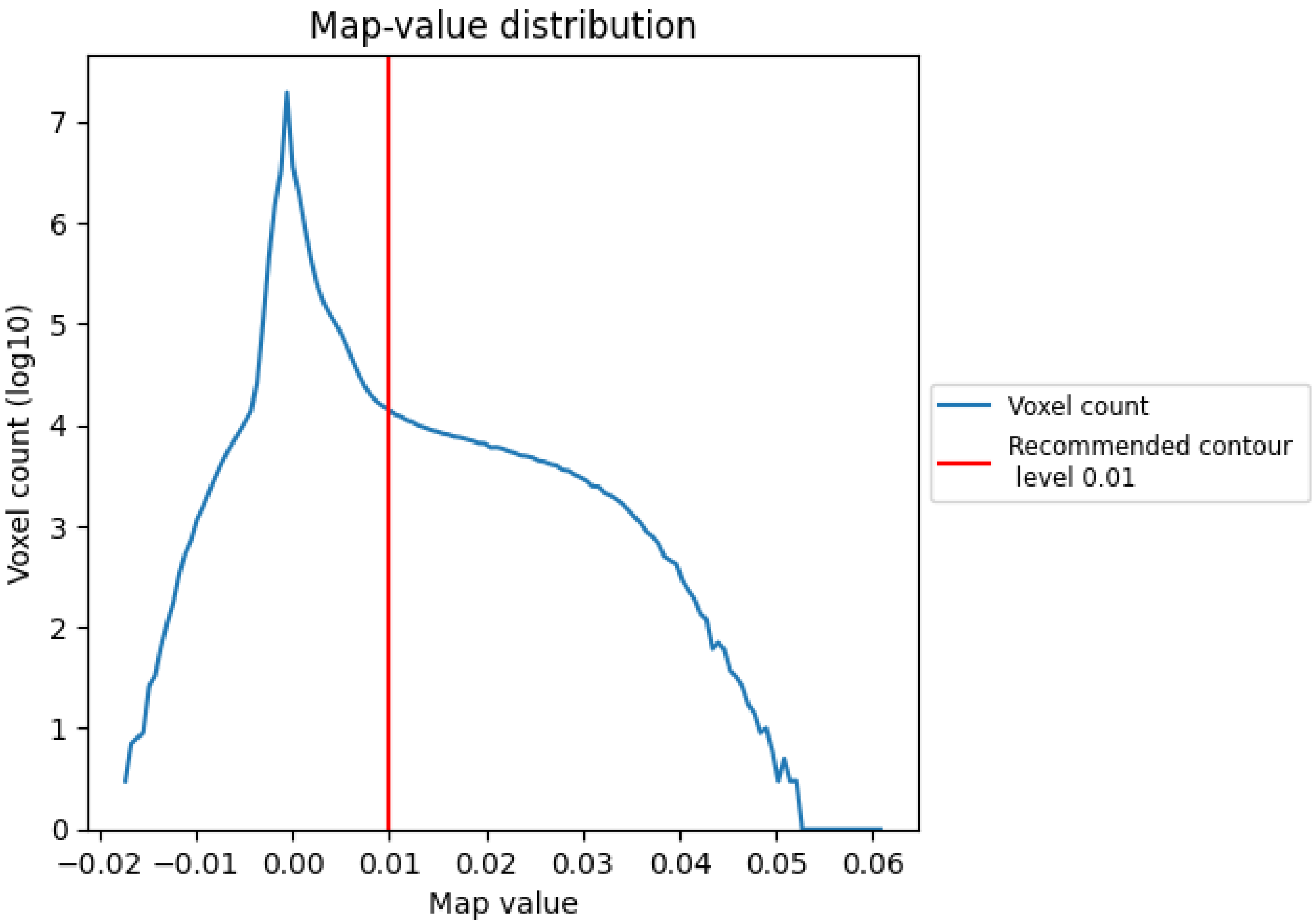


Z

7 Map analysis (i)

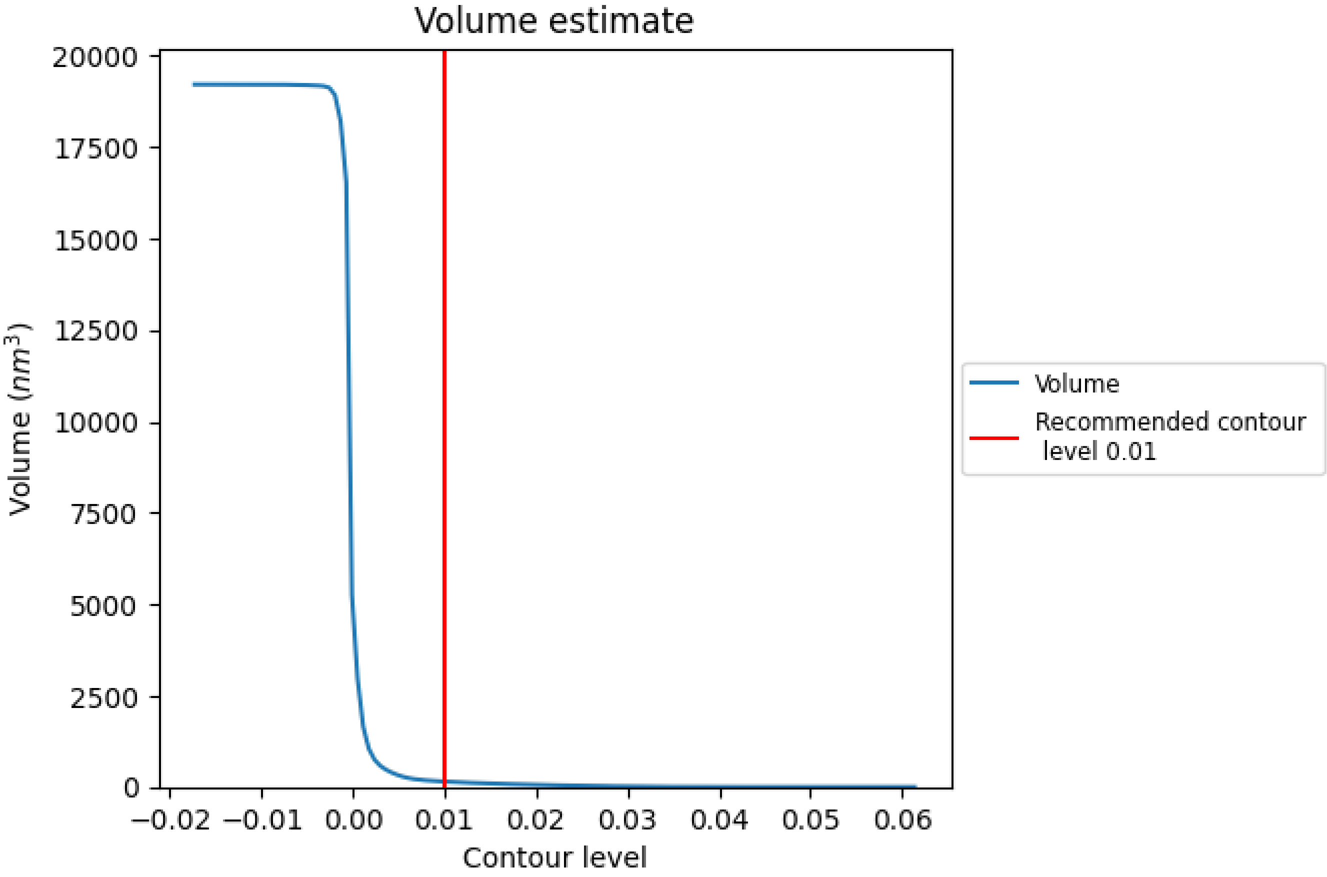
This section contains the results of statistical analysis of the map.

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.

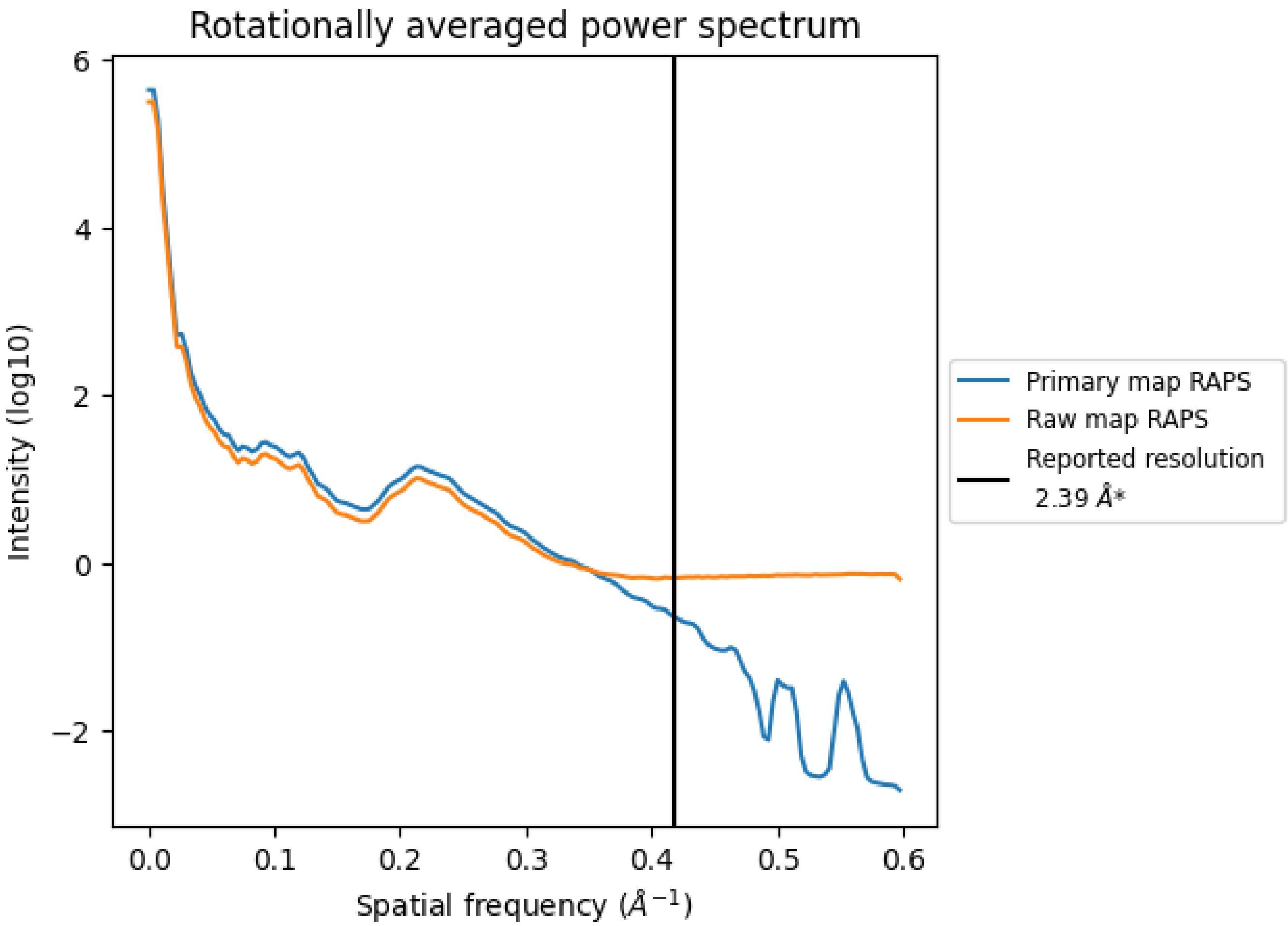
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 148 nm^3; 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 ⓘ

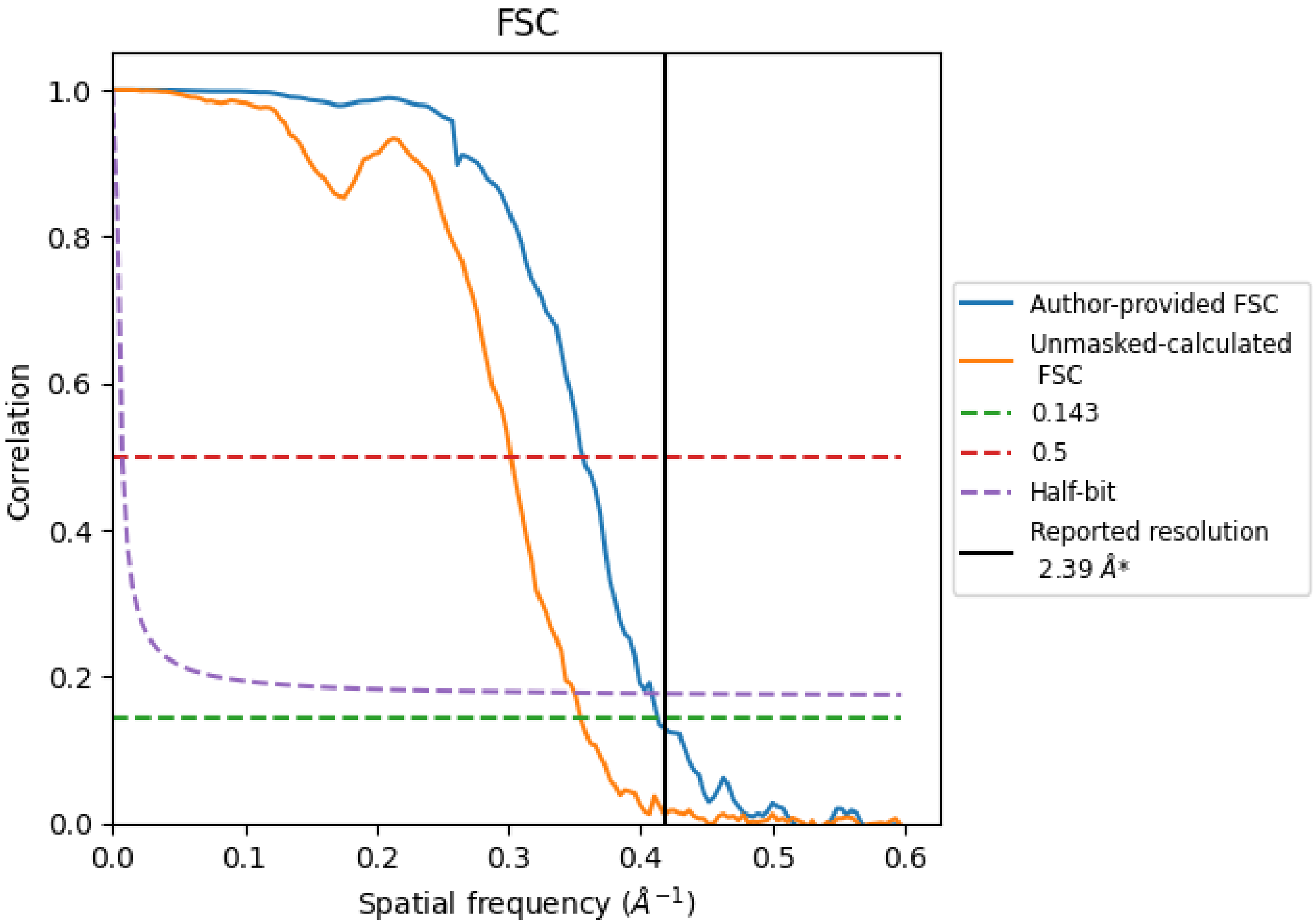


*Reported resolution corresponds to spatial frequency of 0.418 Å^{-1}

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.418 $Å^{-1}$

8.2 Resolution estimates

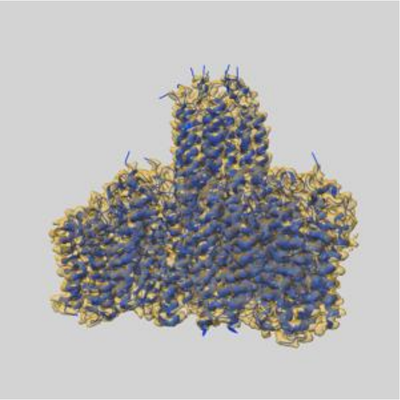
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.39	-	-
Author-provided FSC curve	2.42	2.81	2.45
Unmasked-calculated*	2.82	3.31	2.86

*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 %

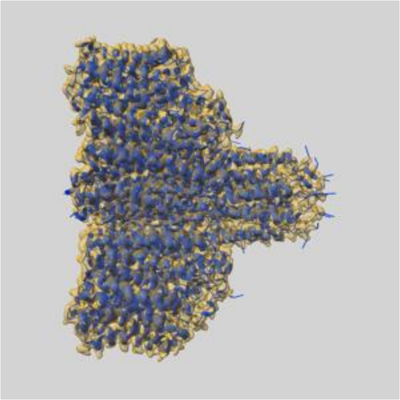
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18162 and PDB model 8Q54. Per-residue inclusion information can be found in section 3 on page 9.

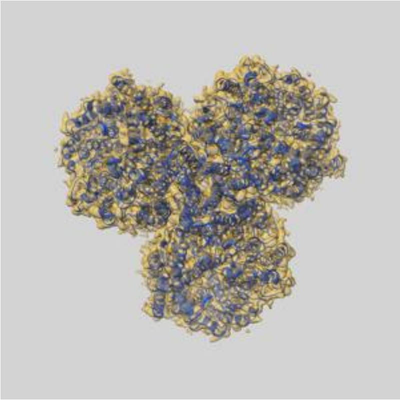
9.1 Map-model overlay



X



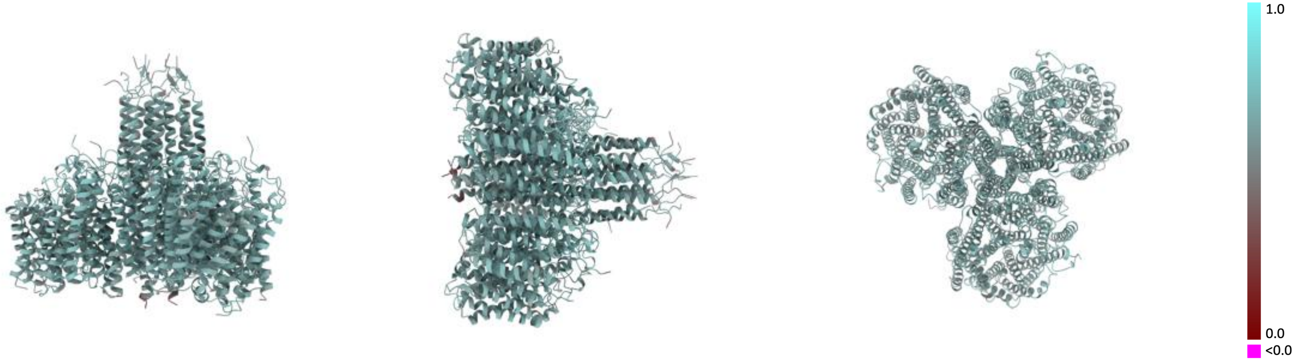
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

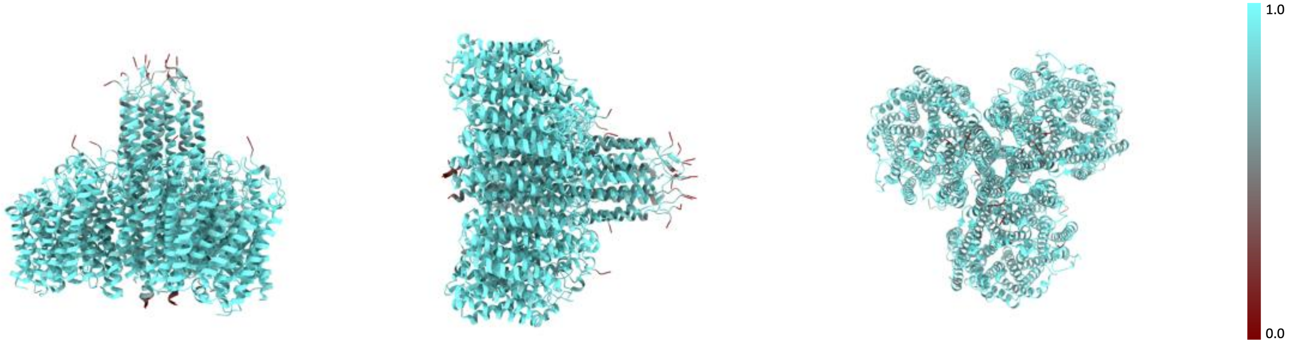
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

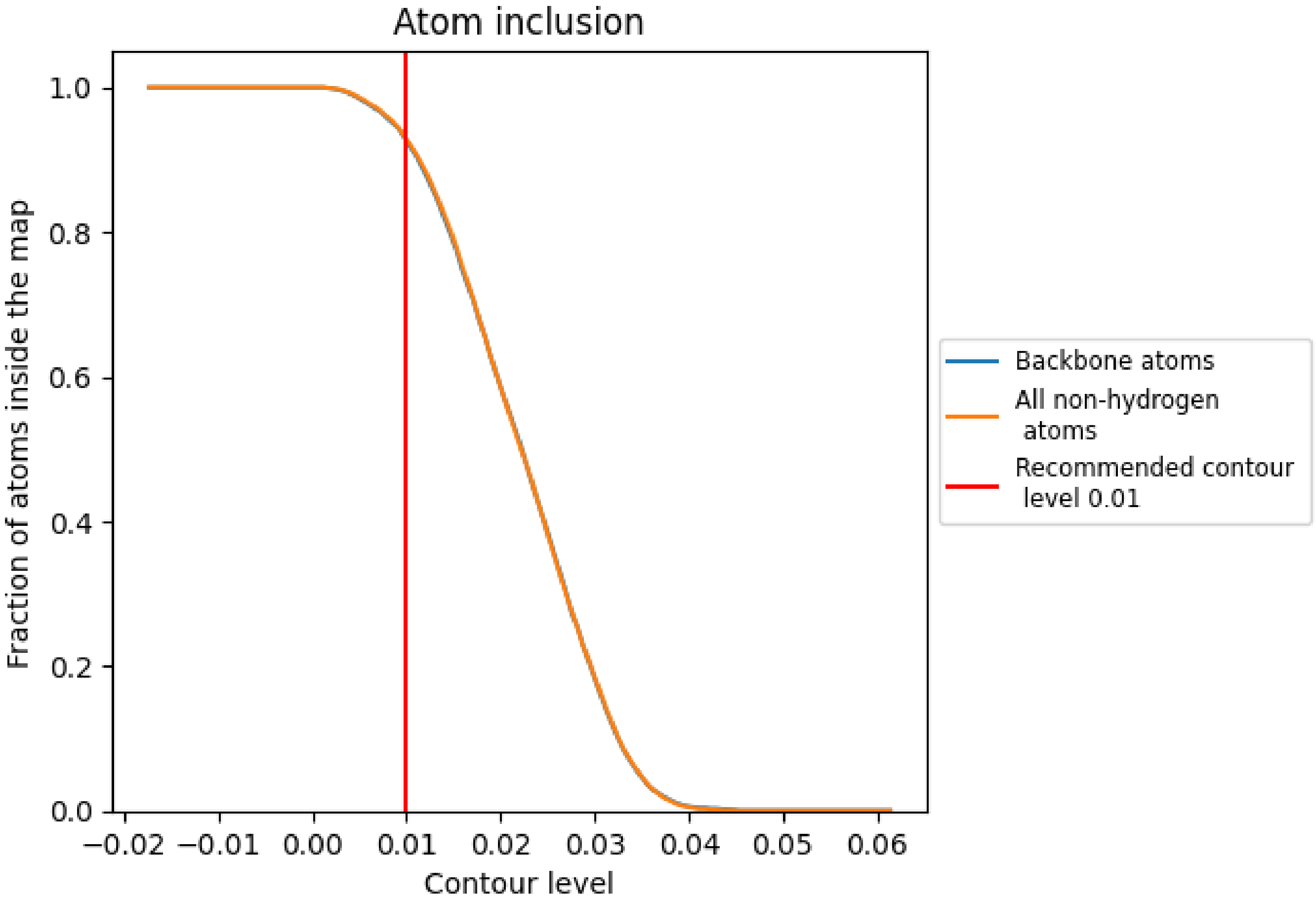
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

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 ⓘ



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