Full wwPDB EM Validation Report ⓘ

Jul 3, 2024 – 07:19 pm BST

PDB ID	:	8Q3V
EMDB ID	:	EMD-18135
Title	:	Cryo-EM structure of the methanogenic Na+ translocating N5-methyl-H4MPT:CoM methyltransferase complex
Authors	:	Aziz, I.; Vonck, J.; Ermler, U.
Deposited on	:	2023-08-04
Resolution	:	2.08 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

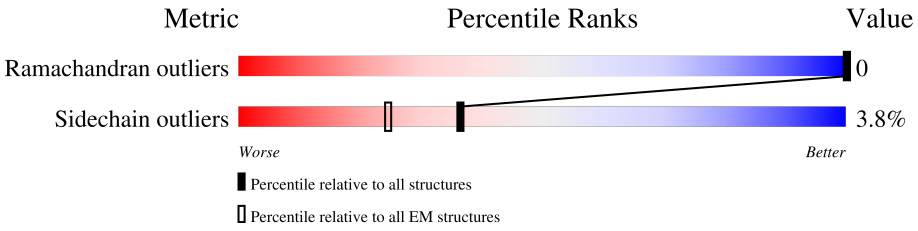
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.08 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	24% · 74%
1	Q	238	25% · 74%
1	a	238	25% · 74%
2	B	100	70% 30%
2	R	100	70% 30%
2	b	100	70% 30%
3	C	267	93% · 5%
3	S	267	93% · 5%
3	c	267	93% · 5%

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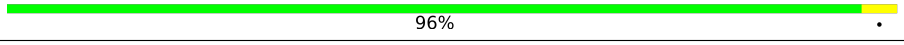
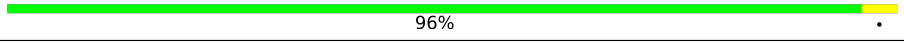
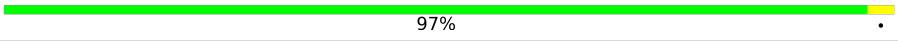
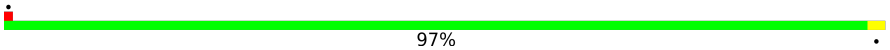
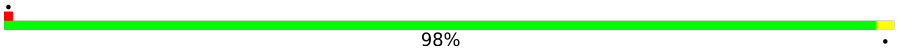
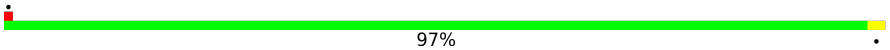
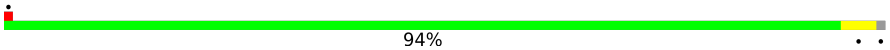
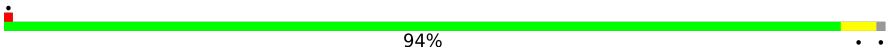
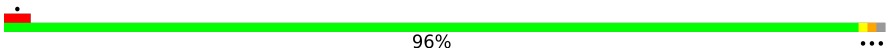
Mol	Chain	Length	Quality of chain
4	D	233	
4	T	233	
4	d	233	
5	E	295	
5	U	295	
5	e	295	
6	F	68	
6	V	68	
6	f	68	
7	G	86	
7	W	86	
7	g	86	

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
9	JCV	C	301	X	-	-	-
9	JCV	F	102	X	-	-	-
9	JCV	G	101	X	-	-	-
9	JCV	V	101	X	-	-	-
9	JCV	W	101	X	-	-	-
9	JCV	c	301	X	-	-	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 24720 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tetrahydromethanopterin S-methyltransferase subunit A 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	61	Total	C	N	O	S	0	0
			463	297	78	83	5		
1	a	61	Total	C	N	O	S	0	0
			463	297	78	83	5		
1	Q	61	Total	C	N	O	S	0	0
			463	297	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	N	O	S	0	0
			531	346	78	106	1		
2	b	70	Total	C	N	O	S	0	0
			531	346	78	106	1		
2	R	70	Total	C	N	O	S	0	0
			531	346	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	N	O	S	1	0
			1831	1207	296	317	11		
3	c	253	Total	C	N	O	S	2	0
			1837	1210	299	317	11		
3	S	254	Total	C	N	O	S	1	0
			1831	1207	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	N	O	S	0	0
			1596	1038	257	288	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	233	Total	C	N	O	S	0	0
			1596	1038	257	288	13		
4	T	233	Total	C	N	O	S	0	0
			1596	1038	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	N	O	S	0	0
			2187	1420	363	388	16		
5	e	294	Total	C	N	O	S	0	0
			2187	1420	363	388	16		
5	U	294	Total	C	N	O	S	0	0
			2187	1420	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	N	O	S	0	0
			505	329	90	84	2		
6	f	67	Total	C	N	O	S	0	0
			505	329	90	84	2		
6	V	67	Total	C	N	O	S	0	0
			505	329	90	84	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	74	Total	C	N	O	0	0
			575	374	94	107		
7	g	76	Total	C	N	O	0	0
			589	383	96	110		
7	W	75	Total	C	N	O	0	0
			581	377	95	109		

- Molecule 8 is MAGNESIUM ION (three-letter code: 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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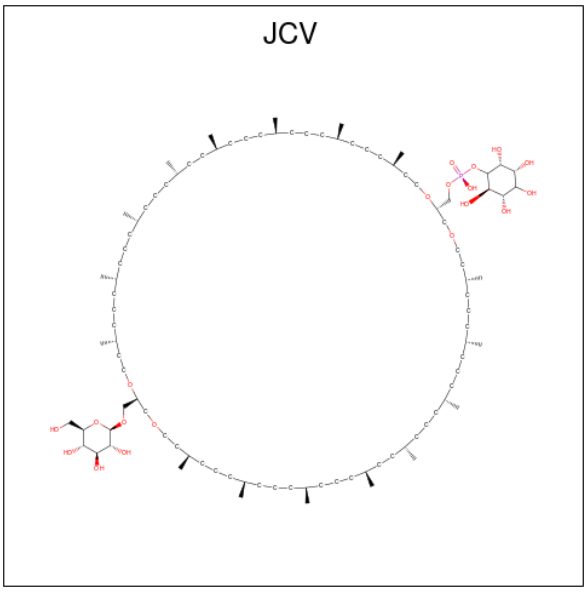
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
8	R	1	1	1	0

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



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
9	C	1	118	98	19	1	0
9	F	1	118	98	19	1	0
9	F	1	118	98	19	1	0
9	G	1	118	98	19	1	0
9	G	1	114	94	19	1	0
9	c	1	118	98	19	1	0
9	e	1	118	98	19	1	0
9	f	1	118	98	19	1	0

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Mol	Chain	Residues	Atoms				AltConf
9	g	1	Total	C	O	P	0
			118	98	19	1	
9	S	1	Total	C	O	P	0
			118	98	19	1	
9	V	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 (three-letter code: 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 water.

Mol	Chain	Residues	Atoms		AltConf
11	A	5	Total	O	0
			5	5	
11	B	5	Total	O	0
			5	5	
11	C	11	Total	O	0
			11	11	
11	D	8	Total	O	0
			8	8	
11	E	34	Total	O	1
			35	35	
11	F	7	Total	O	0
			7	7	
11	G	3	Total	O	0
			3	3	
11	a	5	Total	O	0
			5	5	
11	b	5	Total	O	0
			5	5	
11	c	8	Total	O	0
			8	8	

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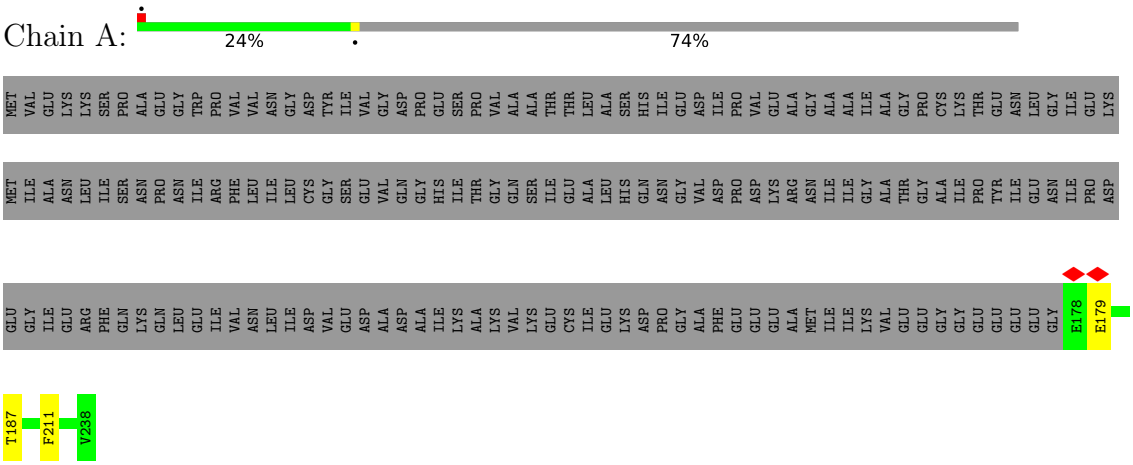
Mol	Chain	Residues	Atoms	AltConf
11	d	8	Total O 8 8	0
11	e	29	Total O 29 29	0
11	f	6	Total O 6 6	0
11	g	4	Total O 4 4	0
11	Q	5	Total O 5 5	0
11	R	5	Total O 5 5	0
11	S	11	Total O 11 11	0
11	T	8	Total O 8 8	0
11	U	31	Total O 31 31	0
11	V	6	Total O 6 6	0
11	W	4	Total O 4 4	0

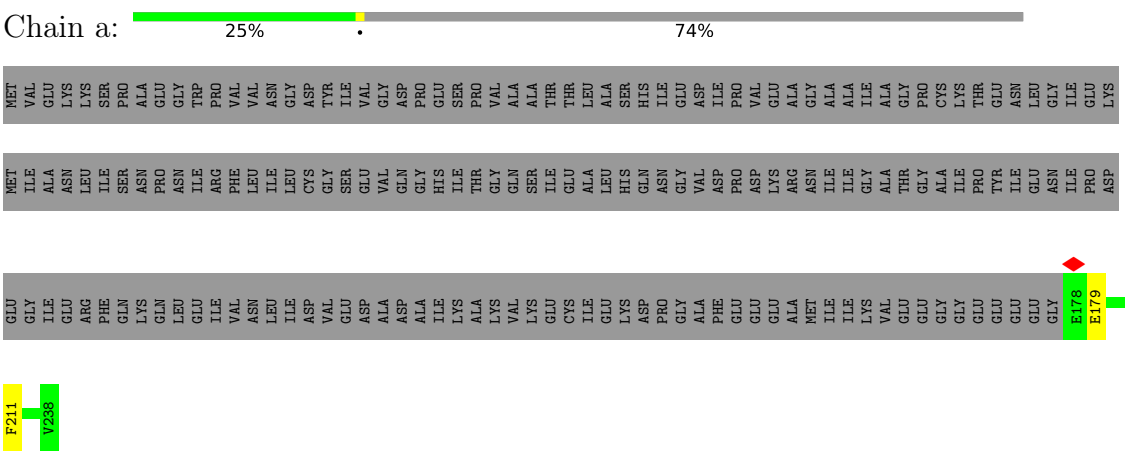
3 Residue-property plots (i)

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

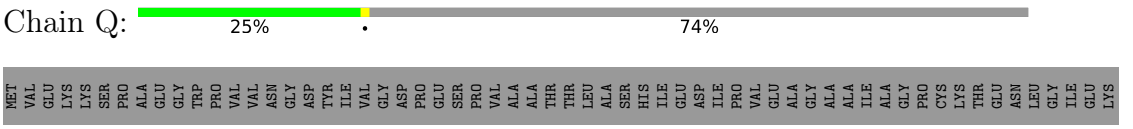
• Molecule 1: Tetrahydromethanopterin S-methyltransferase subunit A 1

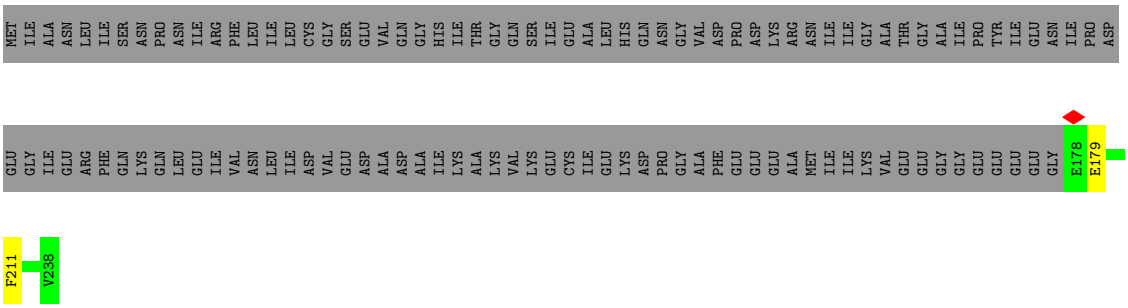


• Molecule 1: Tetrahydromethanopterin S-methyltransferase subunit A 1



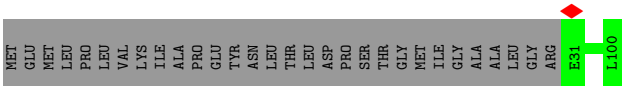
• Molecule 1: Tetrahydromethanopterin S-methyltransferase subunit A 1





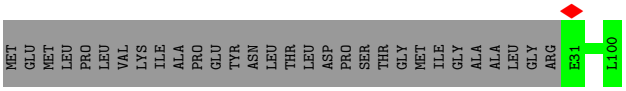
• Molecule 2: Tetrahydromethanopterin S-methyltransferase subunit B

Chain B:



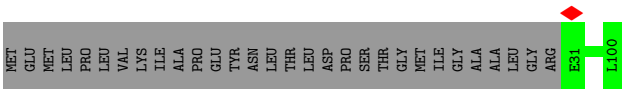
• Molecule 2: Tetrahydromethanopterin S-methyltransferase subunit B

Chain b:



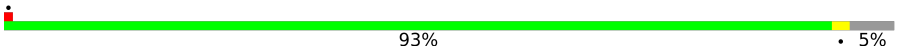
• Molecule 2: Tetrahydromethanopterin S-methyltransferase subunit B

Chain R:



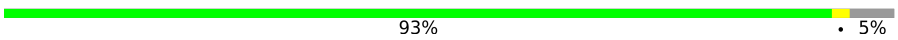
• Molecule 3: Tetrahydromethanopterin S-methyltransferase subunit C

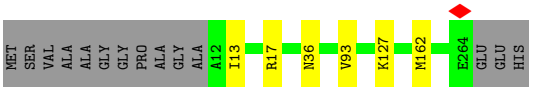
Chain C:



• Molecule 3: Tetrahydromethanopterin S-methyltransferase subunit C

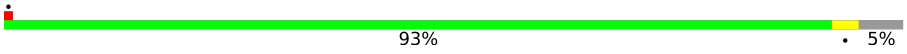
Chain c:





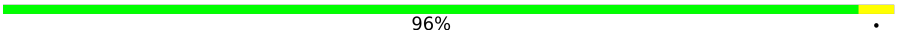
• Molecule 3: Tetrahydromethanopterin S-methyltransferase subunit C

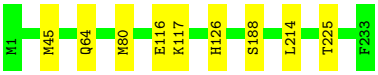
Chain S:



• Molecule 4: Tetrahydromethanopterin S-methyltransferase subunit D

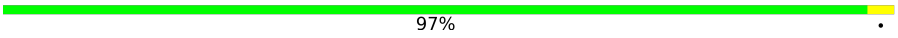
Chain D:





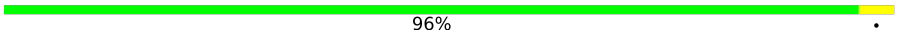
• Molecule 4: Tetrahydromethanopterin S-methyltransferase subunit D

Chain d:



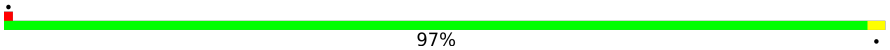
• Molecule 4: Tetrahydromethanopterin S-methyltransferase subunit D

Chain T:



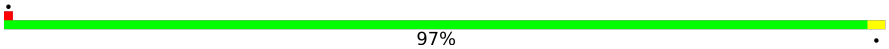
• Molecule 5: Tetrahydromethanopterin S-methyltransferase subunit E

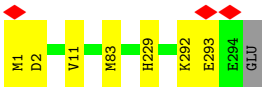
Chain E:



• Molecule 5: Tetrahydromethanopterin S-methyltransferase subunit E

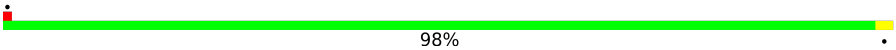
Chain e:

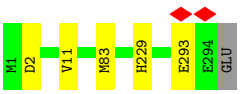




• Molecule 5: Tetrahydromethanopterin S-methyltransferase subunit E

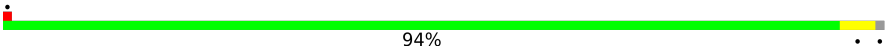
Chain U:

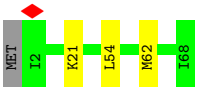




• Molecule 6: Tetrahydromethanopterin S-methyltransferase subunit F

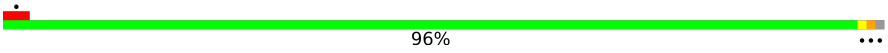
Chain F:

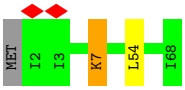




• Molecule 6: Tetrahydromethanopterin S-methyltransferase subunit F

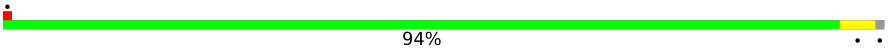
Chain f:

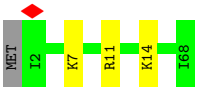




• Molecule 6: Tetrahydromethanopterin S-methyltransferase subunit F

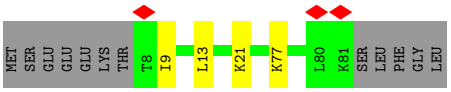
Chain V:





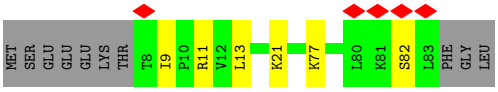
• Molecule 7: Tetrahydromethanopterin S-methyltransferase subunit G

Chain G:



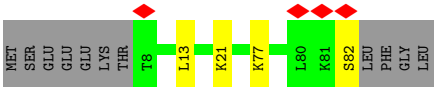
• Molecule 7: Tetrahydromethanopterin S-methyltransferase subunit G

Chain g:



• Molecule 7: Tetrahydromethanopterin S-methyltransferase subunit G

Chain W:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138464	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 ($e^-/Å^2$)	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	0.095	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	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: NA, MG, 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	0.53	0/467	0.67	0/626
1	Q	0.57	0/467	0.64	0/626
1	a	0.60	0/467	0.62	0/626
2	B	0.32	0/538	0.48	0/733
2	R	0.33	0/538	0.49	0/733
2	b	0.46	0/538	0.55	0/733
3	C	0.40	0/1867	0.57	0/2550
3	S	0.37	0/1867	0.56	0/2550
3	c	0.36	0/1873	0.55	0/2557
4	D	0.32	0/1624	0.55	0/2207
4	T	0.39	0/1624	0.58	1/2207 (0.0%)
4	d	0.36	0/1624	0.56	0/2207
5	E	0.42	0/2242	0.57	0/3055
5	U	0.42	0/2242	0.59	0/3055
5	e	0.42	0/2242	0.59	0/3055
6	F	0.47	0/509	0.71	0/684
6	V	0.43	0/509	0.70	0/684
6	f	0.61	1/509 (0.2%)	0.79	1/684 (0.1%)
7	G	0.40	0/580	0.63	0/781
7	W	0.40	0/586	0.60	0/789
7	g	0.39	0/594	0.62	0/800
All	All	0.41	1/23507 (0.0%)	0.59	2/31942 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	7	LYS	C-N	8.28	1.50	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	T	117	LYS	CA-CB-CG	7.56	130.04	113.40
6	f	54	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	59/238 (25%)	59 (100%)	0	0	100	100
1	Q	59/238 (25%)	59 (100%)	0	0	100	100
1	a	59/238 (25%)	59 (100%)	0	0	100	100
2	B	68/100 (68%)	68 (100%)	0	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	253/267 (95%)	250 (99%)	3 (1%)	0	100	100
3	S	253/267 (95%)	250 (99%)	3 (1%)	0	100	100
3	c	253/267 (95%)	250 (99%)	3 (1%)	0	100	100
4	D	231/233 (99%)	228 (99%)	3 (1%)	0	100	100
4	T	231/233 (99%)	228 (99%)	3 (1%)	0	100	100
4	d	231/233 (99%)	228 (99%)	3 (1%)	0	100	100
5	E	292/295 (99%)	282 (97%)	10 (3%)	0	100	100
5	U	292/295 (99%)	282 (97%)	10 (3%)	0	100	100
5	e	292/295 (99%)	283 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	65/68 (96%)	65 (100%)	0	0	100	100
6	V	65/68 (96%)	65 (100%)	0	0	100	100
6	f	65/68 (96%)	65 (100%)	0	0	100	100
7	G	72/86 (84%)	72 (100%)	0	0	100	100
7	W	73/86 (85%)	73 (100%)	0	0	100	100
7	g	74/86 (86%)	74 (100%)	0	0	100	100
All	All	3123/3861 (81%)	3076 (98%)	47 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	50/193 (26%)	47 (94%)	3 (6%)	19	15
1	Q	50/193 (26%)	48 (96%)	2 (4%)	31	31
1	a	50/193 (26%)	48 (96%)	2 (4%)	31	31
2	B	58/82 (71%)	58 (100%)	0	100	100
2	R	58/82 (71%)	58 (100%)	0	100	100
2	b	58/82 (71%)	58 (100%)	0	100	100
3	C	190/196 (97%)	184 (97%)	6 (3%)	39	40
3	S	190/196 (97%)	182 (96%)	8 (4%)	30	29
3	c	191/196 (97%)	185 (97%)	6 (3%)	40	41
4	D	155/155 (100%)	146 (94%)	9 (6%)	20	16
4	T	155/155 (100%)	147 (95%)	8 (5%)	23	20
4	d	155/155 (100%)	147 (95%)	8 (5%)	23	20
5	E	228/229 (100%)	221 (97%)	7 (3%)	40	41
5	U	228/229 (100%)	223 (98%)	5 (2%)	52	55
5	e	228/229 (100%)	221 (97%)	7 (3%)	40	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	F	54/55 (98%)	51 (94%)	3 (6%)	21 18
6	V	54/55 (98%)	51 (94%)	3 (6%)	21 18
6	f	54/55 (98%)	53 (98%)	1 (2%)	57 61
7	G	62/73 (85%)	58 (94%)	4 (6%)	17 13
7	W	63/73 (86%)	59 (94%)	4 (6%)	18 14
7	g	64/73 (88%)	58 (91%)	6 (9%)	8 5
All	All	2395/2949 (81%)	2303 (96%)	92 (4%)	36 33

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	GLU
1	A	187	THR
1	A	211	PHE
3	C	17	ARG
3	C	36	ASN
3	C	93	VAL
3	C	127	LYS
3	C	162	MET
3	C	263	LYS
4	D	45	MET
4	D	64	GLN
4	D	80	MET
4	D	116	GLU
4	D	117	LYS
4	D	126	HIS
4	D	188	SER
4	D	214	LEU
4	D	225	THR
5	E	11	VAL
5	E	83	MET
5	E	184	SER
5	E	229	HIS
5	E	292	LYS
5	E	293	GLU
5	E	294	GLU
6	F	21	LYS
6	F	54	LEU
6	F	62	MET
7	G	9	ILE

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Mol	Chain	Res	Type
7	G	13	LEU
7	G	21	LYS
7	G	77	LYS
1	a	179	GLU
1	a	211	PHE
3	c	13	ILE
3	c	17	ARG
3	c	36	ASN
3	c	93	VAL
3	c	127	LYS
3	c	162	MET
4	d	1	MET
4	d	45	MET
4	d	64	GLN
4	d	80	MET
4	d	117	LYS
4	d	126	HIS
4	d	188	SER
4	d	214	LEU
5	e	1	MET
5	e	2	ASP
5	e	11	VAL
5	e	83	MET
5	e	229	HIS
5	e	292	LYS
5	e	293	GLU
6	f	7	LYS
7	g	9	ILE
7	g	11	ARG
7	g	13	LEU
7	g	21	LYS
7	g	77	LYS
7	g	82	SER
1	Q	179	GLU
1	Q	211	PHE
3	S	13	ILE
3	S	17	ARG
3	S	36	ASN
3	S	93	VAL
3	S	127	LYS
3	S	162	MET
3	S	184[A]	GLN

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Mol	Chain	Res	Type
3	S	184[B]	GLN
4	T	45	MET
4	T	64	GLN
4	T	80	MET
4	T	116	GLU
4	T	126	HIS
4	T	166	MET
4	T	188	SER
4	T	214	LEU
5	U	2	ASP
5	U	11	VAL
5	U	83	MET
5	U	229	HIS
5	U	293	GLU
6	V	7	LYS
6	V	11	ARG
6	V	14	LYS
7	W	13	LEU
7	W	21	LYS
7	W	77	LYS
7	W	82	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	208	ASN
5	E	117	GLN
7	G	47	GLN
1	a	208	ASN
5	e	117	GLN
6	f	6	ASN
7	g	47	GLN
1	Q	208	ASN
2	R	43	GLN
5	U	117	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
9	JCV	c	301	-	120,120,120	1.16	12 (10%)	148,154,154	1.11	10 (6%)
9	JCV	W	101	-	120,120,120	1.14	11 (9%)	148,154,154	0.97	5 (3%)
9	JCV	e	303	-	120,120,120	1.17	11 (9%)	148,154,154	0.71	2 (1%)
9	JCV	V	101	-	120,120,120	1.15	12 (10%)	148,154,154	0.83	1 (0%)
9	JCV	C	301	-	120,120,120	1.11	10 (8%)	148,154,154	1.04	10 (6%)
9	JCV	F	101	-	120,120,120	1.12	9 (7%)	148,154,154	0.70	0
9	JCV	G	101	-	120,120,120	1.15	11 (9%)	148,154,154	0.89	5 (3%)
9	JCV	S	301	-	120,120,120	1.15	11 (9%)	148,154,154	0.65	0
9	JCV	F	102	-	120,120,120	1.12	11 (9%)	148,154,154	1.01	9 (6%)
9	JCV	G	102	-	116,116,120	1.10	9 (7%)	141,146,154	0.65	0
9	JCV	g	101	-	120,120,120	1.13	11 (9%)	148,154,154	0.66	0
9	JCV	f	100	-	120,120,120	1.12	9 (7%)	148,154,154	0.67	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
9	JCV	c	301	-	2/2/30/30	71/126/170/170	0/2/2/2
9	JCV	W	101	-	2/2/30/30	39/126/170/170	0/2/2/2
9	JCV	V	101	-	1/1/30/30	62/126/170/170	0/2/2/2
9	JCV	e	303	-	-	55/126/170/170	0/2/2/2
9	JCV	C	301	-	1/1/30/30	63/126/170/170	0/2/2/2
9	JCV	F	101	-	-	18/126/170/170	0/2/2/2
9	JCV	G	101	-	1/1/30/30	55/126/170/170	0/2/2/2
9	JCV	S	301	-	-	48/126/170/170	0/2/2/2
9	JCV	F	102	-	1/1/30/30	63/126/170/170	0/2/2/2
9	JCV	G	102	-	-	30/118/162/170	0/2/2/2
9	JCV	g	101	-	-	36/126/170/170	0/2/2/2
9	JCV	f	100	-	-	28/126/170/170	0/2/2/2

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	f	100	JCV	OY1-CG7	-4.29	1.35	1.43
9	e	303	JCV	OY1-CG7	-4.26	1.35	1.43
9	F	101	JCV	OY1-CG7	-4.22	1.36	1.43
9	V	101	JCV	OY1-CG7	-4.20	1.36	1.43
9	c	301	JCV	OY1-CG7	-4.18	1.36	1.43
9	g	101	JCV	OY1-CG7	-4.18	1.36	1.43
9	G	102	JCV	OY1-CG7	-4.17	1.36	1.43
9	C	301	JCV	OY1-CG7	-4.16	1.36	1.43
9	W	101	JCV	OY1-CG7	-4.12	1.36	1.43
9	S	301	JCV	OY1-CG7	-4.06	1.36	1.43
9	F	102	JCV	OY1-CG7	-4.05	1.36	1.43
9	G	101	JCV	OY1-CG7	-3.73	1.36	1.43
9	e	303	JCV	C22M-C22	3.59	1.64	1.52
9	V	101	JCV	C22M-C22	3.37	1.63	1.52
9	C	301	JCV	C22M-C22	3.33	1.63	1.52
9	G	101	JCV	C22M-C22	3.32	1.63	1.52
9	W	101	JCV	C22M-C22	3.32	1.63	1.52
9	g	101	JCV	C22M-C22	3.31	1.63	1.52
9	S	301	JCV	C22M-C22	3.30	1.63	1.52
9	f	100	JCV	C22M-C22	3.27	1.63	1.52
9	F	101	JCV	C22M-C22	3.24	1.63	1.52
9	G	102	JCV	C22M-C22	3.24	1.63	1.52
9	c	301	JCV	C31-C32	3.18	1.61	1.50
9	e	303	JCV	C31-C32	3.18	1.61	1.50
9	G	101	JCV	C31-C32	3.09	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	101	JCV	C31-C32	3.02	1.61	1.50
9	g	101	JCV	C31-C32	3.02	1.61	1.50
9	S	301	JCV	C31-C32	3.00	1.61	1.50
9	W	101	JCV	C31-C32	2.96	1.61	1.50
9	F	101	JCV	C31-C32	2.93	1.61	1.50
9	G	101	JCV	OY1-CY1	2.91	1.45	1.40
9	f	100	JCV	C31-C32	2.91	1.60	1.50
9	S	301	JCV	C2-C1	2.90	1.60	1.50
9	G	102	JCV	C31-C32	2.89	1.60	1.50
9	C	301	JCV	C31-C32	2.88	1.60	1.50
9	F	102	JCV	OG3-C1	-2.88	1.29	1.42
9	F	101	JCV	C2-C1	2.86	1.60	1.50
9	G	102	JCV	C2-C1	2.85	1.60	1.50
9	f	100	JCV	C2-C1	2.84	1.60	1.50
9	V	101	JCV	OG3-C1	-2.82	1.29	1.42
9	e	303	JCV	C2-C1	2.80	1.60	1.50
9	C	301	JCV	OG3-C1	-2.80	1.29	1.42
9	g	101	JCV	C2-C1	2.76	1.60	1.50
9	e	303	JCV	C55-C54	2.76	1.64	1.52
9	G	101	JCV	C2-C1	2.75	1.60	1.50
9	F	102	JCV	C22M-C22	2.75	1.61	1.52
9	C	301	JCV	C3M-C3	-2.74	1.44	1.52
9	c	301	JCV	C3M-C3	-2.73	1.44	1.52
9	W	101	JCV	CG8-CG6	2.71	1.59	1.50
9	S	301	JCV	C55-C54	2.71	1.63	1.52
9	c	301	JCV	C2-C1	2.70	1.60	1.50
9	F	101	JCV	C55-C54	2.68	1.63	1.52
9	W	101	JCV	C55-C54	2.68	1.63	1.52
9	F	102	JCV	C31-C32	2.68	1.60	1.50
9	g	101	JCV	C55-C54	2.67	1.63	1.52
9	G	102	JCV	C55-C54	2.67	1.63	1.52
9	W	101	JCV	C2-C1	2.67	1.60	1.50
9	f	100	JCV	C55-C54	2.65	1.63	1.52
9	G	101	JCV	C55-C54	2.65	1.63	1.52
9	c	301	JCV	C22M-C22	2.65	1.61	1.52
9	G	101	JCV	OG3-C1	-2.59	1.30	1.42
9	W	101	JCV	OG3-C1	-2.57	1.30	1.42
9	G	102	JCV	OG3-C1	-2.53	1.31	1.42
9	F	102	JCV	CG8-CG6	2.53	1.58	1.50
9	f	100	JCV	OG3-C1	-2.52	1.31	1.42
9	F	101	JCV	OG3-C1	-2.50	1.31	1.42
9	c	301	JCV	OG3-C1	-2.50	1.31	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	e	303	JCV	OG3-C1	-2.49	1.31	1.42
9	g	101	JCV	OG3-C1	-2.48	1.31	1.42
9	F	102	JCV	C2-C1	2.48	1.59	1.50
9	c	301	JCV	CG8-CG6	2.46	1.58	1.50
9	V	101	JCV	C3M-C3	-2.45	1.45	1.52
9	F	102	JCV	C55-C54	2.43	1.62	1.52
9	F	101	JCV	CG8-CG6	2.41	1.58	1.50
9	V	101	JCV	CG8-CG6	2.41	1.58	1.50
9	F	102	JCV	C3M-C3	-2.38	1.45	1.52
9	C	301	JCV	C80M-C80	-2.38	1.45	1.52
9	C	301	JCV	C2-C1	2.36	1.59	1.50
9	S	301	JCV	OG3-C1	-2.36	1.31	1.42
9	g	101	JCV	CG8-CG6	2.36	1.57	1.50
9	C	301	JCV	CG8-CG6	2.32	1.57	1.50
9	S	301	JCV	CG8-CG6	2.30	1.57	1.50
9	V	101	JCV	C2-C1	2.27	1.58	1.50
9	S	301	JCV	P-O4	2.27	1.66	1.60
9	f	100	JCV	C17-C16	-2.25	1.46	1.53
9	e	303	JCV	CG8-CG6	2.23	1.57	1.50
9	c	301	JCV	C55-C54	2.23	1.61	1.52
9	f	100	JCV	CG8-CG6	2.21	1.57	1.50
9	G	102	JCV	C17-C16	-2.20	1.46	1.53
9	F	101	JCV	C17-C16	-2.20	1.46	1.53
9	S	301	JCV	C17-C16	-2.19	1.46	1.53
9	F	102	JCV	C80M-C80	-2.17	1.45	1.52
9	C	301	JCV	C55-C54	2.16	1.61	1.52
9	F	102	JCV	C59-C60	2.14	1.61	1.52
9	V	101	JCV	C55-C54	2.14	1.61	1.52
9	G	102	JCV	CG8-CG6	2.13	1.57	1.50
9	G	101	JCV	CG8-CG6	2.12	1.57	1.50
9	V	101	JCV	C80M-C80	-2.12	1.46	1.52
9	e	303	JCV	C3M-C3	-2.12	1.46	1.52
9	c	301	JCV	C17-C16	-2.12	1.46	1.53
9	V	101	JCV	C17-C16	-2.11	1.46	1.53
9	G	101	JCV	C17-C16	-2.10	1.47	1.53
9	G	102	JCV	C3M-C3	-2.10	1.46	1.52
9	C	301	JCV	C20-C19	2.09	1.61	1.52
9	c	301	JCV	C59-C60	2.09	1.61	1.52
9	c	301	JCV	CG3-CG2	2.08	1.57	1.50
9	e	303	JCV	C17-C16	-2.07	1.47	1.53
9	c	301	JCV	C20-C19	2.07	1.61	1.52
9	g	101	JCV	C3M-C3	-2.07	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	101	JCV	C3M-C3	-2.06	1.46	1.52
9	W	101	JCV	C59-C60	2.05	1.61	1.52
9	S	301	JCV	C59-C60	2.05	1.60	1.52
9	W	101	JCV	C17-C16	-2.05	1.47	1.53
9	F	102	JCV	C17-C16	-2.04	1.47	1.53
9	e	303	JCV	C20-C19	2.04	1.60	1.52
9	g	101	JCV	C17-C16	-2.03	1.47	1.53
9	V	101	JCV	C20-C19	2.03	1.60	1.52
9	W	101	JCV	C20-C19	2.03	1.60	1.52
9	F	101	JCV	C3M-C3	-2.03	1.46	1.52
9	e	303	JCV	C59-C60	2.02	1.60	1.52
9	V	101	JCV	C59-C60	2.02	1.60	1.52
9	G	101	JCV	C59-C60	2.02	1.60	1.52
9	g	101	JCV	C59-C60	2.02	1.60	1.52
9	f	100	JCV	C3M-C3	-2.02	1.46	1.52
9	G	101	JCV	C3M-C3	-2.02	1.46	1.52
9	g	101	JCV	C20-C19	2.02	1.60	1.52
9	S	301	JCV	CG3-CG2	2.01	1.56	1.50

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	W	101	JCV	CX6-CX1-CX2	4.52	117.37	110.85
9	c	301	JCV	CX5-CX6-CX1	4.38	119.67	109.68
9	c	301	JCV	CX6-CX1-CX2	3.98	116.59	110.85
9	G	101	JCV	CX6-CX1-CX2	3.76	116.28	110.85
9	F	102	JCV	OX4-CX2-CX1	3.75	119.89	109.94
9	G	101	JCV	OY1-CY1-CY2	3.43	113.66	108.30
9	W	101	JCV	CX3-CX2-CX1	3.42	117.48	109.68
9	V	101	JCV	CG3-CG2-CG1	-3.28	104.03	111.79
9	c	301	JCV	C5-C4-C3	-3.15	105.74	115.92
9	F	102	JCV	CX3-CX2-CX1	3.11	116.78	109.68
9	W	101	JCV	CX5-CX6-CX1	3.00	116.53	109.68
9	G	101	JCV	CG7-OY1-CY1	2.99	119.57	113.74
9	C	301	JCV	C70-C71-C72	-2.85	106.70	115.92
9	G	101	JCV	CX3-CX2-CX1	2.79	116.06	109.68
9	c	301	JCV	C28-C29-C30	-2.78	106.93	115.92
9	c	301	JCV	OG3-CG3-CG2	2.75	115.90	109.44
9	F	102	JCV	C20-C19-C18	-2.58	107.57	115.92
9	C	301	JCV	C70-C69-C68	-2.56	107.65	115.92
9	C	301	JCV	OX2-CX4-CX5	2.52	116.17	110.35
9	C	301	JCV	O4-CX1-CX2	-2.51	102.83	108.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	301	JCV	C5-C4-C3	-2.47	107.93	115.92
9	C	301	JCV	C28-C29-C30	-2.46	107.97	115.92
9	F	102	JCV	O3-P-O2	-2.46	100.10	112.24
9	F	102	JCV	C24-C25-C26	-2.44	108.02	115.92
9	c	301	JCV	O4-CX1-CX2	-2.38	103.13	108.66
9	e	303	JCV	CX3-CX2-CX1	2.37	115.10	109.68
9	C	301	JCV	OG3-CG3-CG2	2.33	114.91	109.44
9	G	101	JCV	CX4-CX3-CX2	2.32	114.88	110.82
9	e	303	JCV	CX6-CX5-CX4	2.25	114.75	110.82
9	W	101	JCV	C82-OG4-CG6	2.24	120.55	115.40
9	C	301	JCV	CX3-CX2-CX1	2.22	114.76	109.68
9	W	101	JCV	CG3-CG2-CG1	-2.22	106.53	111.79
9	C	301	JCV	C74-C73-C72	-2.19	108.85	115.92
9	c	301	JCV	CX6-CX5-CX4	2.17	114.60	110.82
9	C	301	JCV	C28-C27-C26	-2.13	109.02	115.92
9	c	301	JCV	C9-C8-C7	-2.13	109.02	115.92
9	F	102	JCV	OG3-CG3-CG2	-2.08	104.53	109.44
9	c	301	JCV	OX3-CX3-CX4	-2.08	105.54	110.35
9	F	102	JCV	CX6-CX1-CX2	2.06	113.82	110.85
9	F	102	JCV	OX4-CX2-CX3	2.05	115.08	110.35
9	c	301	JCV	C18M-C18-C17	-2.05	103.88	111.29
9	F	102	JCV	C5-C4-C3	-2.01	109.42	115.92

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	C	301	JCV	CX6
9	F	102	JCV	CG6
9	G	101	JCV	CX6
9	c	301	JCV	C68
9	c	301	JCV	C80
9	V	101	JCV	C22
9	W	101	JCV	CG2
9	W	101	JCV	C26

All (568) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	301	JCV	C52-C51-OG2-CG2
9	C	301	JCV	CG2-CG3-OG3-C1
9	C	301	JCV	C15-C16-C17-C18
9	C	301	JCV	C24-C25-C26-C26M

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Mol	Chain	Res	Type	Atoms
9	C	301	JCV	C30M-C30-C31-C32
9	C	301	JCV	C65-C66-C67-C68
9	C	301	JCV	CX2-CX1-O4-P
9	C	301	JCV	CX6-CX1-O4-P
9	C	301	JCV	CX1-O4-P-O3
9	F	101	JCV	CX1-O4-P-O3
9	F	102	JCV	C13-C14-C15-C15M
9	F	102	JCV	C1-C2-C3-C3M
9	F	102	JCV	C30M-C30-C31-C32
9	F	102	JCV	C51-C52-C53-C53M
9	F	102	JCV	C65-C66-C67-C68
9	F	102	JCV	C81-C82-OG4-CG6
9	F	102	JCV	CY2-CY1-OY1-CG7
9	F	102	JCV	OY5-CY1-OY1-CG7
9	F	102	JCV	CX1-O4-P-O2
9	F	102	JCV	CX1-O4-P-O3
9	G	101	JCV	OG2-CG2-CG3-OG3
9	G	101	JCV	C15-C16-C17-C18
9	G	101	JCV	C80M-C80-C81-C82
9	G	101	JCV	CY2-CY1-OY1-CG7
9	G	102	JCV	CY2-CY1-OY1-CG7
9	G	102	JCV	OY5-CY1-OY1-CG7
9	G	102	JCV	CX1-O4-P-O3
9	c	301	JCV	C30M-C30-C31-C32
9	c	301	JCV	OY5-CY1-OY1-CG7
9	e	303	JCV	C20-C21-C22-C22M
9	e	303	JCV	C30M-C30-C31-C32
9	e	303	JCV	C81-C82-OG4-CG6
9	f	100	JCV	C80M-C80-C81-C82
9	f	100	JCV	CX1-O4-P-O3
9	S	301	JCV	CX1-O4-P-O1
9	V	101	JCV	C51-C52-C53-C53M
9	V	101	JCV	C65-C66-C67-C68
9	V	101	JCV	C80M-C80-C81-C82
9	W	101	JCV	C81-C82-OG4-CG6
9	W	101	JCV	CG8-CG6-OG4-C82
9	W	101	JCV	CG6-CG8-OG6-C32
9	f	100	JCV	OY5-CY5-CY6-OY6
9	e	303	JCV	C31-C32-OG6-CG8
9	C	301	JCV	C30-C31-C32-OG6
9	e	303	JCV	C30-C31-C32-OG6
9	c	301	JCV	CY4-CY5-CY6-OY6

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Mol	Chain	Res	Type	Atoms
9	C	301	JCV	C4-C5-C6-C7
9	G	101	JCV	C73-C74-C75-C76
9	f	100	JCV	CY4-CY5-CY6-OY6
9	C	301	JCV	C61-C62-C63-C64
9	F	102	JCV	C11-C12-C13-C14
9	G	101	JCV	C3-C4-C5-C6
9	c	301	JCV	C54-C55-C56-C57
9	S	301	JCV	C11-C12-C13-C14
9	S	301	JCV	C19-C20-C21-C22
9	V	101	JCV	C53-C54-C55-C56
9	f	100	JCV	OG4-CG6-CG7-OY1
9	C	301	JCV	C11M-C11-C12-C13
9	C	301	JCV	C13-C14-C15-C15M
9	C	301	JCV	C22M-C22-C23-C24
9	C	301	JCV	C26M-C26-C27-C28
9	C	301	JCV	C55-C56-C57-C57M
9	C	301	JCV	C72M-C72-C73-C74
9	C	301	JCV	C76M-C76-C77-C78
9	F	101	JCV	C72M-C72-C73-C74
9	F	102	JCV	C11M-C11-C12-C13
9	F	102	JCV	C20-C21-C22-C22M
9	F	102	JCV	C5-C6-C7-C7M
9	F	102	JCV	C68M-C68-C69-C70
9	F	102	JCV	C70-C71-C72-C72M
9	G	101	JCV	C76M-C76-C77-C78
9	c	301	JCV	C24-C25-C26-C26M
9	c	301	JCV	C59-C60-C61-C61M
9	c	301	JCV	C63-C64-C65-C65M
9	c	301	JCV	C66-C67-C68-C68M
9	e	303	JCV	C26M-C26-C27-C28
9	e	303	JCV	C65M-C65-C66-C67
9	g	101	JCV	C63-C64-C65-C65M
9	S	301	JCV	C53M-C53-C54-C55
9	S	301	JCV	C5-C6-C7-C7M
9	V	101	JCV	C20-C21-C22-C22M
9	V	101	JCV	C61M-C61-C62-C63
9	V	101	JCV	C66-C67-C68-C68M
9	V	101	JCV	C68M-C68-C69-C70
9	V	101	JCV	C76M-C76-C77-C78
9	C	301	JCV	C54-C55-C56-C57
9	F	101	JCV	OY5-CY5-CY6-OY6
9	g	101	JCV	C68-C69-C70-C71

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Mol	Chain	Res	Type	Atoms
9	V	101	JCV	C3-C4-C5-C6
9	V	101	JCV	C57-C58-C59-C60
9	G	101	JCV	C4-C5-C6-C7
9	c	301	JCV	C57-C58-C59-C60
9	e	303	JCV	C76-C77-C78-C79
9	G	101	JCV	C79-C80-C81-C82
9	G	101	JCV	C27-C28-C29-C30
9	G	101	JCV	C68-C69-C70-C71
9	G	101	JCV	C76-C77-C78-C79
9	e	303	JCV	C72-C73-C74-C75
9	S	301	JCV	C53-C54-C55-C56
9	V	101	JCV	C69-C70-C71-C72
9	W	101	JCV	C68-C69-C70-C71
9	W	101	JCV	C76-C77-C78-C79
9	F	102	JCV	C53-C54-C55-C56
9	G	101	JCV	C11-C12-C13-C14
9	c	301	JCV	C23-C24-C25-C26
9	c	301	JCV	C69-C70-C71-C72
9	W	101	JCV	OY5-CY5-CY6-OY6
9	C	301	JCV	C69-C70-C71-C72
9	G	101	JCV	C23-C24-C25-C26
9	c	301	JCV	C53-C54-C55-C56
9	S	301	JCV	C62-C63-C64-C65
9	C	301	JCV	C23-C24-C25-C26
9	c	301	JCV	C62-C63-C64-C65
9	W	101	JCV	C18-C19-C20-C21
9	C	301	JCV	C60-C61-C62-C63
9	F	102	JCV	C60-C61-C62-C63
9	G	101	JCV	C13-C14-C15-C16
9	G	101	JCV	C20-C21-C22-C23
9	c	301	JCV	C9-C10-C11-C12
9	S	301	JCV	C71-C72-C73-C74
9	V	101	JCV	C9-C10-C11-C12
9	S	301	JCV	C26-C27-C28-C29
9	W	101	JCV	OY5-CY1-OY1-CG7
9	V	101	JCV	C4-C5-C6-C7
9	e	303	JCV	C62-C63-C64-C65
9	S	301	JCV	C76-C77-C78-C79
9	V	101	JCV	C54-C55-C56-C57
9	V	101	JCV	C58-C59-C60-C61
9	C	301	JCV	C53-C54-C55-C56
9	G	101	JCV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
9	V	101	JCV	C7-C8-C9-C10
9	c	301	JCV	OY5-CY5-CY6-OY6
9	F	102	JCV	C61-C62-C63-C64
9	c	301	JCV	C7-C8-C9-C10
9	g	101	JCV	C23-C24-C25-C26
9	W	101	JCV	C27-C28-C29-C30
9	C	301	JCV	CG1-O1-P-O4
9	c	301	JCV	CG1-O1-P-O4
9	e	303	JCV	C54-C55-C56-C57
9	F	102	JCV	C22-C23-C24-C25
9	V	101	JCV	C76-C77-C78-C79
9	F	102	JCV	OG3-C1-C2-C3
9	G	101	JCV	CX1-O4-P-O1
9	c	301	JCV	CX1-O4-P-O1
9	C	301	JCV	C26-C27-C28-C29
9	c	301	JCV	C11-C12-C13-C14
9	f	100	JCV	CY2-CY1-OY1-CG7
9	W	101	JCV	CY2-CY1-OY1-CG7
9	g	101	JCV	C18-C19-C20-C21
9	c	301	JCV	C9-C10-C11-C11M
9	e	303	JCV	C72M-C72-C73-C74
9	g	101	JCV	C20-C21-C22-C22M
9	V	101	JCV	C68-C69-C70-C71
9	F	102	JCV	C52-C51-OG2-CG2
9	S	301	JCV	C52-C51-OG2-CG2
9	S	301	JCV	CG2-CG3-OG3-C1
9	f	100	JCV	OY5-CY1-OY1-CG7
9	W	101	JCV	C62-C63-C64-C65
9	G	101	JCV	C62-C63-C64-C65
9	C	301	JCV	C68-C69-C70-C71
9	F	102	JCV	C54-C55-C56-C57
9	e	303	JCV	CY4-CY5-CY6-OY6
9	F	102	JCV	C80-C81-C82-OG4
9	c	301	JCV	C30-C31-C32-OG6
9	g	101	JCV	C80-C81-C82-OG4
9	W	101	JCV	OG2-C51-C52-C53
9	F	101	JCV	C59-C60-C61-C62
9	F	102	JCV	C5-C6-C7-C8
9	G	101	JCV	C28-C29-C30-C31
9	G	101	JCV	C70-C71-C72-C73
9	G	101	JCV	C75-C76-C77-C78
9	G	102	JCV	C63-C64-C65-C66

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Mol	Chain	Res	Type	Atoms
9	e	303	JCV	C9-C10-C11-C12
9	e	303	JCV	C64-C65-C66-C67
9	e	303	JCV	C71-C72-C73-C74
9	f	100	JCV	C59-C60-C61-C62
9	g	101	JCV	C20-C21-C22-C23
9	S	301	JCV	C28-C29-C30-C31
9	S	301	JCV	C52-C53-C54-C55
9	V	101	JCV	C10-C11-C12-C13
9	V	101	JCV	C20-C21-C22-C23
9	C	301	JCV	C11-C10-C9-C8
9	c	301	JCV	C72-C73-C74-C75
9	G	102	JCV	C71-C72-C73-C74
9	e	303	JCV	C73-C74-C75-C76
9	f	100	JCV	C62-C63-C64-C65
9	F	102	JCV	C11-C10-C9-C8
9	C	301	JCV	C31-C32-OG6-CG8
9	G	102	JCV	OG4-CG6-CG8-OG6
9	G	102	JCV	C76-C77-C78-C79
9	c	301	JCV	C73-C74-C75-C76
9	G	102	JCV	CY4-CY5-CY6-OY6
9	F	102	JCV	C28-C29-C30-C30M
9	F	102	JCV	C61M-C61-C62-C63
9	G	101	JCV	C20-C21-C22-C22M
9	G	101	JCV	C70-C71-C72-C72M
9	c	301	JCV	C13-C14-C15-C15M
9	e	303	JCV	C9-C10-C11-C11M
9	e	303	JCV	C57M-C57-C58-C59
9	e	303	JCV	C7M-C7-C8-C9
9	e	303	JCV	C78-C79-C80-C80M
9	g	101	JCV	C65M-C65-C66-C67
9	S	301	JCV	C28-C29-C30-C30M
9	V	101	JCV	C11M-C11-C12-C13
9	V	101	JCV	C22M-C22-C23-C24
9	V	101	JCV	C7M-C7-C8-C9
9	W	101	JCV	C20-C21-C22-C22M
9	W	101	JCV	C26M-C26-C27-C28
9	W	101	JCV	C28-C29-C30-C30M
9	W	101	JCV	C78-C79-C80-C80M
9	G	102	JCV	OY5-CY5-CY6-OY6
9	F	102	JCV	CG2-CG3-OG3-C1
9	e	303	JCV	CG6-CG8-OG6-C32
9	G	101	JCV	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
9	e	303	JCV	C58-C59-C60-C61
9	S	301	JCV	C27-C28-C29-C30
9	V	101	JCV	O1-CG1-CG2-CG3
9	c	301	JCV	C61-C62-C63-C64
9	g	101	JCV	C27-C28-C29-C30
9	c	301	JCV	C29-C30-C31-C32
9	V	101	JCV	C51-C52-C53-C54
9	S	301	JCV	C72-C73-C74-C75
9	F	102	JCV	CG1-CG2-CG3-OG3
9	c	301	JCV	CG8-CG6-CG7-OY1
9	e	303	JCV	CG8-CG6-CG7-OY1
9	f	100	JCV	CG8-CG6-CG7-OY1
9	S	301	JCV	CG8-CG6-CG7-OY1
9	V	101	JCV	CG7-CG6-CG8-OG6
9	g	101	JCV	CY4-CY5-CY6-OY6
9	C	301	JCV	CX1-O4-P-O1
9	F	101	JCV	CX1-O4-P-O1
9	F	102	JCV	CX1-O4-P-O1
9	f	100	JCV	CX1-O4-P-O1
9	S	301	JCV	C57-C58-C59-C60
9	C	301	JCV	CG6-CG8-OG6-C32
9	G	101	JCV	C18-C19-C20-C21
9	W	101	JCV	C19-C20-C21-C22
9	F	102	JCV	OY5-CY5-CY6-OY6
9	f	100	JCV	C19-C20-C21-C22
9	F	101	JCV	C19-C20-C21-C22
9	S	301	JCV	C68-C69-C70-C71
9	V	101	JCV	C62-C63-C64-C65
9	c	301	JCV	CY2-CY1-OY1-CG7
9	g	101	JCV	CY2-CY1-OY1-CG7
9	V	101	JCV	CY2-CY1-OY1-CG7
9	e	303	JCV	OG2-CG2-CG3-OG3
9	W	101	JCV	OG2-CG2-CG3-OG3
9	c	301	JCV	C15-C16-C17-C18
9	V	101	JCV	C26-C27-C28-C29
9	C	301	JCV	C10-C11-C12-C13
9	C	301	JCV	C52-C53-C54-C55
9	C	301	JCV	C55-C56-C57-C58
9	F	102	JCV	C10-C11-C12-C13
9	F	102	JCV	C28-C29-C30-C31
9	F	102	JCV	C67-C68-C69-C70
9	G	101	JCV	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
9	G	101	JCV	C78-C79-C80-C81
9	c	301	JCV	C13-C14-C15-C16
9	c	301	JCV	C25-C26-C27-C28
9	c	301	JCV	C28-C29-C30-C31
9	c	301	JCV	C59-C60-C61-C62
9	c	301	JCV	C64-C65-C66-C67
9	e	303	JCV	C20-C21-C22-C23
9	e	303	JCV	C52-C53-C54-C55
9	e	303	JCV	C56-C57-C58-C59
9	e	303	JCV	C6-C7-C8-C9
9	g	101	JCV	C63-C64-C65-C66
9	g	101	JCV	C64-C65-C66-C67
9	S	301	JCV	C6-C7-C8-C9
9	S	301	JCV	C74-C75-C76-C77
9	V	101	JCV	C21-C22-C23-C24
9	V	101	JCV	C6-C7-C8-C9
9	W	101	JCV	C20-C21-C22-C23
9	W	101	JCV	C25-C26-C27-C28
9	W	101	JCV	C28-C29-C30-C31
9	W	101	JCV	C78-C79-C80-C81
9	C	301	JCV	C53M-C53-C54-C55
9	F	102	JCV	C76M-C76-C77-C78
9	G	101	JCV	C15M-C15-C16-C17
9	G	101	JCV	C59-C60-C61-C61M
9	c	301	JCV	C28-C29-C30-C30M
9	c	301	JCV	C65M-C65-C66-C67
9	g	101	JCV	C28-C29-C30-C30M
9	S	301	JCV	C57M-C57-C58-C59
9	S	301	JCV	C7M-C7-C8-C9
9	S	301	JCV	C74-C75-C76-C76M
9	V	101	JCV	C26M-C26-C27-C28
9	V	101	JCV	C53M-C53-C54-C55
9	V	101	JCV	C70-C71-C72-C72M
9	W	101	JCV	C55-C56-C57-C57M
9	g	101	JCV	C81-C82-OG4-CG6
9	g	101	JCV	OY5-CY1-OY1-CG7
9	G	101	JCV	C12-C13-C14-C15
9	e	303	JCV	OY5-CY5-CY6-OY6
9	G	102	JCV	C19-C20-C21-C22
9	G	102	JCV	CX1-O4-P-O1
9	F	102	JCV	C1-C2-C3-C4
9	F	102	JCV	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
9	f	100	JCV	C79-C80-C81-C82
9	V	101	JCV	C79-C80-C81-C82
9	F	101	JCV	CG8-CG6-OG4-C82
9	G	101	JCV	CG1-CG2-CG3-OG3
9	G	101	JCV	CG7-CG6-CG8-OG6
9	G	102	JCV	CG8-CG6-CG7-OY1
9	G	102	JCV	CG7-CG6-CG8-OG6
9	c	301	JCV	CG3-CG2-OG2-C51
9	e	303	JCV	CG1-CG2-CG3-OG3
9	V	101	JCV	CG8-CG6-OG4-C82
9	W	101	JCV	CG1-CG2-CG3-OG3
9	C	301	JCV	CX1-O4-P-O2
9	F	101	JCV	CX1-O4-P-O2
9	G	102	JCV	CX1-O4-P-O2
9	c	301	JCV	CX1-O4-P-O3
9	f	100	JCV	CX1-O4-P-O2
9	c	301	JCV	C26-C27-C28-C29
9	f	100	JCV	C76-C77-C78-C79
9	c	301	JCV	CG2-CG3-OG3-C1
9	c	301	JCV	O1-CG1-CG2-OG2
9	C	301	JCV	OG2-CG2-CG3-OG3
9	G	101	JCV	OG4-CG6-CG8-OG6
9	G	102	JCV	OG2-CG2-CG3-OG3
9	g	101	JCV	OG2-CG2-CG3-OG3
9	S	301	JCV	OG4-CG6-CG7-OY1
9	V	101	JCV	OY5-CY1-OY1-CG7
9	C	301	JCV	C62-C63-C64-C65
9	e	303	JCV	C68-C69-C70-C71
9	C	301	JCV	C61M-C61-C62-C63
9	F	102	JCV	C59-C60-C61-C61M
9	G	101	JCV	C63-C64-C65-C65M
9	c	301	JCV	C26M-C26-C27-C28
9	c	301	JCV	C55-C56-C57-C57M
9	e	303	JCV	C3M-C3-C4-C5
9	g	101	JCV	C66-C67-C68-C68M
9	g	101	JCV	C76M-C76-C77-C78
9	S	301	JCV	C26M-C26-C27-C28
9	C	301	JCV	CG2-CG1-O1-P
9	G	101	JCV	CG2-CG1-O1-P
9	S	301	JCV	CG2-CG1-O1-P
9	G	101	JCV	C57-C58-C59-C60
9	G	101	JCV	OG2-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
9	e	303	JCV	C26-C27-C28-C29
9	G	101	JCV	O1-CG1-CG2-CG3
9	e	303	JCV	O1-CG1-CG2-CG3
9	C	301	JCV	C75-C76-C77-C78
9	F	101	JCV	C71-C72-C73-C74
9	F	102	JCV	C13-C14-C15-C16
9	F	102	JCV	C75-C76-C77-C78
9	G	101	JCV	C59-C60-C61-C62
9	G	101	JCV	C63-C64-C65-C66
9	G	101	JCV	C71-C72-C73-C74
9	G	102	JCV	C59-C60-C61-C62
9	c	301	JCV	C63-C64-C65-C66
9	e	303	JCV	C16-C17-C18-C19
9	f	100	JCV	C71-C72-C73-C74
9	g	101	JCV	C28-C29-C30-C31
9	g	101	JCV	C66-C67-C68-C69
9	g	101	JCV	C75-C76-C77-C78
9	S	301	JCV	C14-C15-C16-C17
9	S	301	JCV	C56-C57-C58-C59
9	V	101	JCV	C17-C18-C19-C20
9	V	101	JCV	C25-C26-C27-C28
9	V	101	JCV	C52-C53-C54-C55
9	V	101	JCV	C70-C71-C72-C73
9	W	101	JCV	C55-C56-C57-C58
9	W	101	JCV	C60-C61-C62-C63
9	W	101	JCV	C63-C64-C65-C66
9	W	101	JCV	C75-C76-C77-C78
9	e	303	JCV	CX1-O4-P-O1
9	C	301	JCV	C29-C30-C31-C32
9	F	102	JCV	C51-C52-C53-C54
9	C	301	JCV	CG7-CG6-CG8-OG6
9	G	102	JCV	CG1-CG2-CG3-OG3
9	e	303	JCV	CG2-CG3-OG3-C1
9	c	301	JCV	C58-C59-C60-C61
9	F	102	JCV	C2-C1-OG3-CG3
9	G	101	JCV	C31-C32-OG6-CG8
9	c	301	JCV	C2-C1-OG3-CG3
9	c	301	JCV	OG4-CG6-CG7-OY1
9	g	101	JCV	OG4-CG6-CG8-OG6
9	c	301	JCV	CX6-CX1-O4-P
9	G	101	JCV	C72M-C72-C73-C74
9	G	102	JCV	C63-C64-C65-C65M

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Mol	Chain	Res	Type	Atoms
9	c	301	JCV	C18M-C18-C19-C20
9	c	301	JCV	C78-C79-C80-C80M
9	f	100	JCV	C59-C60-C61-C61M
9	V	101	JCV	C18M-C18-C19-C20
9	W	101	JCV	C76M-C76-C77-C78
9	C	301	JCV	C80-C81-C82-OG4
9	F	101	JCV	C30-C31-C32-OG6
9	F	101	JCV	C80-C81-C82-OG4
9	G	101	JCV	OG3-C1-C2-C3
9	c	301	JCV	OG2-C51-C52-C53
9	e	303	JCV	OG2-C51-C52-C53
9	f	100	JCV	C30-C31-C32-OG6
9	S	301	JCV	OG3-C1-C2-C3
9	S	301	JCV	C30-C31-C32-OG6
9	V	101	JCV	OG2-C51-C52-C53
9	F	102	JCV	C27-C28-C29-C30
9	F	101	JCV	C81-C82-OG4-CG6
9	f	100	JCV	C81-C82-OG4-CG6
9	G	102	JCV	CG2-CG3-OG3-C1
9	W	101	JCV	CX1-O4-P-O1
9	c	301	JCV	CG1-O1-P-O2
9	c	301	JCV	CG1-O1-P-O3
9	W	101	JCV	CG1-O1-P-O3
9	S	301	JCV	OY5-CY1-OY1-CG7
9	c	301	JCV	O1-CG1-CG2-CG3
9	S	301	JCV	O1-CG1-CG2-CG3
9	F	101	JCV	C68-C69-C70-C71
9	G	101	JCV	C69-C70-C71-C72
9	W	101	JCV	C26-C27-C28-C29
9	C	301	JCV	C78-C79-C80-C81
9	F	102	JCV	C6-C7-C8-C9
9	F	102	JCV	C70-C71-C72-C73
9	G	102	JCV	C64-C65-C66-C67
9	c	301	JCV	C17-C18-C19-C20
9	c	301	JCV	C56-C57-C58-C59
9	c	301	JCV	C74-C75-C76-C77
9	e	303	JCV	C25-C26-C27-C28
9	e	303	JCV	C2-C3-C4-C5
9	f	100	JCV	C67-C68-C69-C70
9	g	101	JCV	C55-C56-C57-C58
9	S	301	JCV	O1-CG1-CG2-OG2
9	S	301	JCV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
9	S	301	JCV	C78-C79-C80-C81
9	V	101	JCV	C60-C61-C62-C63
9	V	101	JCV	C74-C75-C76-C77
9	g	101	JCV	C22-C23-C24-C25
9	F	101	JCV	CG6-CG8-OG6-C32
9	e	303	JCV	C29-C30-C31-C32
9	F	102	JCV	C57-C58-C59-C60
9	C	301	JCV	CY4-CY5-CY6-OY6
9	C	301	JCV	CG1-CG2-CG3-OG3
9	C	301	JCV	C1-C2-C3-C3M
9	e	303	JCV	C1-C2-C3-C3M
9	e	303	JCV	C51-C52-C53-C53M
9	g	101	JCV	CG7-CG6-CG8-OG6
9	C	301	JCV	OG4-CG6-CG8-OG6
9	F	102	JCV	OG2-CG2-CG3-OG3
9	G	102	JCV	OG4-CG6-CG7-OY1
9	e	303	JCV	OG4-CG6-CG7-OY1
9	S	301	JCV	OG4-CG6-CG8-OG6
9	c	301	JCV	C18-C19-C20-C21
9	G	101	JCV	CG6-CG7-OY1-CY1
9	C	301	JCV	C78-C79-C80-C80M
9	F	101	JCV	C59-C60-C61-C61M
9	F	102	JCV	C16-C17-C18-C18M
9	F	102	JCV	C74-C75-C76-C76M
9	G	101	JCV	C13-C14-C15-C15M
9	G	101	JCV	C78-C79-C80-C80M
9	G	102	JCV	C59-C60-C61-C61M
9	f	100	JCV	C72M-C72-C73-C74
9	V	101	JCV	C24-C25-C26-C26M
9	V	101	JCV	C74-C75-C76-C76M
9	W	101	JCV	C61M-C61-C62-C63
9	S	301	JCV	C18-C19-C20-C21
9	g	101	JCV	C76-C77-C78-C79
9	F	102	JCV	C31-C32-OG6-CG8
9	F	102	JCV	O1-CG1-CG2-OG2
9	G	101	JCV	O1-CG1-CG2-OG2
9	V	101	JCV	O1-CG1-CG2-OG2
9	C	301	JCV	C3-C4-C5-C6
9	g	101	JCV	OY5-CY5-CY6-OY6
9	V	101	JCV	CG2-CG3-OG3-C1
9	W	101	JCV	C30-C31-C32-OG6
9	V	101	JCV	OG4-CG6-CG8-OG6

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Mol	Chain	Res	Type	Atoms
9	e	303	JCV	CG1-O1-P-O4
9	G	102	JCV	C1-C2-C3-C4
9	c	301	JCV	C78-C79-C80-C81
9	F	102	JCV	C7M-C7-C8-C9
9	G	102	JCV	C65M-C65-C66-C67
9	c	301	JCV	C57M-C57-C58-C59
9	e	303	JCV	C16-C17-C18-C18M
9	S	301	JCV	C15M-C15-C16-C17
9	S	301	JCV	C72M-C72-C73-C74
9	S	301	JCV	C78-C79-C80-C80M
9	V	101	JCV	C9-C10-C11-C11M
9	V	101	JCV	C55-C56-C57-C57M
9	V	101	JCV	C78-C79-C80-C80M
9	W	101	JCV	C63-C64-C65-C65M
9	g	101	JCV	C52-C51-OG2-CG2
9	c	301	JCV	CG6-CG8-OG6-C32
9	V	101	JCV	C30-C31-C32-OG6
9	W	101	JCV	C80-C81-C82-OG4
9	C	301	JCV	C22-C23-C24-C25
9	c	301	JCV	C22-C23-C24-C25
9	F	102	JCV	C19-C20-C21-C22
9	S	301	JCV	C51-C52-C53-C54
9	C	301	JCV	C57M-C57-C58-C59
9	c	301	JCV	C53M-C53-C54-C55
9	c	301	JCV	C74-C75-C76-C76M
9	g	101	JCV	CG1-CG2-CG3-OG3
9	G	102	JCV	C80-C81-C82-OG4
9	C	301	JCV	C71-C72-C73-C74
9	F	102	JCV	C21-C22-C23-C24
9	c	301	JCV	C66-C67-C68-C69
9	g	101	JCV	C60-C61-C62-C63
9	V	101	JCV	C66-C67-C68-C69
9	V	101	JCV	C67-C68-C69-C70
9	V	101	JCV	C75-C76-C77-C78
9	V	101	JCV	C78-C79-C80-C81
9	F	102	JCV	CG6-CG8-OG6-C32
9	F	102	JCV	C12-C13-C14-C15
9	e	303	JCV	O1-CG1-CG2-OG2
9	F	102	JCV	C15-C16-C17-C18
9	F	102	JCV	C24-C25-C26-C26M
9	f	100	JCV	C66-C67-C68-C68M
9	g	101	JCV	C53-C54-C55-C56

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Mol	Chain	Res	Type	Atoms
9	c	301	JCV	C52-C51-OG2-CG2
9	f	100	JCV	CG6-CG8-OG6-C32
9	g	101	JCV	C61-C62-C63-C64
9	S	301	JCV	C69-C70-C71-C72
9	G	102	JCV	C79-C80-C81-C82
9	W	101	JCV	C12-C13-C14-C15
9	f	100	JCV	C9-C10-C11-C12
9	S	301	JCV	C5-C6-C7-C8
9	e	303	JCV	CG2-CG1-O1-P
9	C	301	JCV	C2-C1-OG3-CG3
9	C	301	JCV	C58-C59-C60-C61
9	e	303	JCV	C4-C5-C6-C7
9	e	303	JCV	C77-C78-C79-C80
9	C	301	JCV	C5-C6-C7-C7M
9	G	101	JCV	C28-C29-C30-C30M
9	G	101	JCV	C65M-C65-C66-C67
9	G	101	JCV	C68M-C68-C69-C70
9	c	301	JCV	C76M-C76-C77-C78
9	f	100	JCV	C68M-C68-C69-C70
9	g	101	JCV	C61M-C61-C62-C63
9	V	101	JCV	C72M-C72-C73-C74
9	S	301	JCV	CG7-CG6-CG8-OG6
9	W	101	JCV	C61-C62-C63-C64
9	C	301	JCV	C21-C22-C23-C24
9	F	102	JCV	C16-C17-C18-C19
9	F	102	JCV	C20-C21-C22-C23
9	G	101	JCV	C64-C65-C66-C67
9	G	102	JCV	C9-C10-C11-C12
9	S	301	JCV	C24-C25-C26-C27
9	V	101	JCV	C24-C25-C26-C27
9	f	100	JCV	C3-C4-C5-C6
9	c	301	JCV	C22M-C22-C23-C24
9	e	303	JCV	C70-C71-C72-C72M
9	S	301	JCV	C24-C25-C26-C26M
9	F	102	JCV	C30-C31-C32-OG6
9	G	102	JCV	C30-C31-C32-OG6
9	G	101	JCV	C2-C1-OG3-CG3
9	f	100	JCV	C68-C69-C70-C71
9	C	301	JCV	C73-C74-C75-C76
9	g	101	JCV	C12-C13-C14-C15
9	C	301	JCV	CG1-O1-P-O3
9	V	101	JCV	CG1-O1-P-O2

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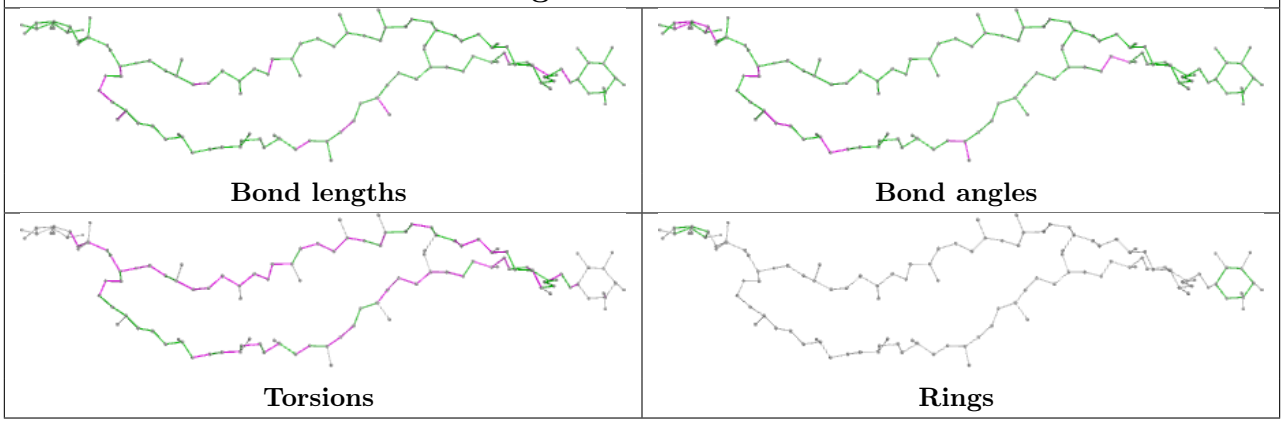
Mol	Chain	Res	Type	Atoms
9	W	101	JCV	CG1-O1-P-O2
9	F	101	JCV	CY4-CY5-CY6-OY6
9	C	301	JCV	C63-C64-C65-C65M
9	F	102	JCV	C63-C64-C65-C65M
9	G	102	JCV	C9-C10-C11-C11M
9	f	100	JCV	C9-C10-C11-C11M
9	G	102	JCV	C3-C4-C5-C6
9	C	301	JCV	C24-C25-C26-C27
9	C	301	JCV	C2-C3-C4-C5
9	F	101	JCV	C9-C10-C11-C12
9	c	301	JCV	C21-C22-C23-C24
9	c	301	JCV	C24-C25-C26-C27
9	c	301	JCV	C75-C76-C77-C78
9	e	303	JCV	C55-C56-C57-C58
9	e	303	JCV	C70-C71-C72-C73
9	g	101	JCV	C29-C30-C31-C32
9	F	101	JCV	C3-C4-C5-C6
9	e	303	JCV	C22-C23-C24-C25

There are no ring outliers.

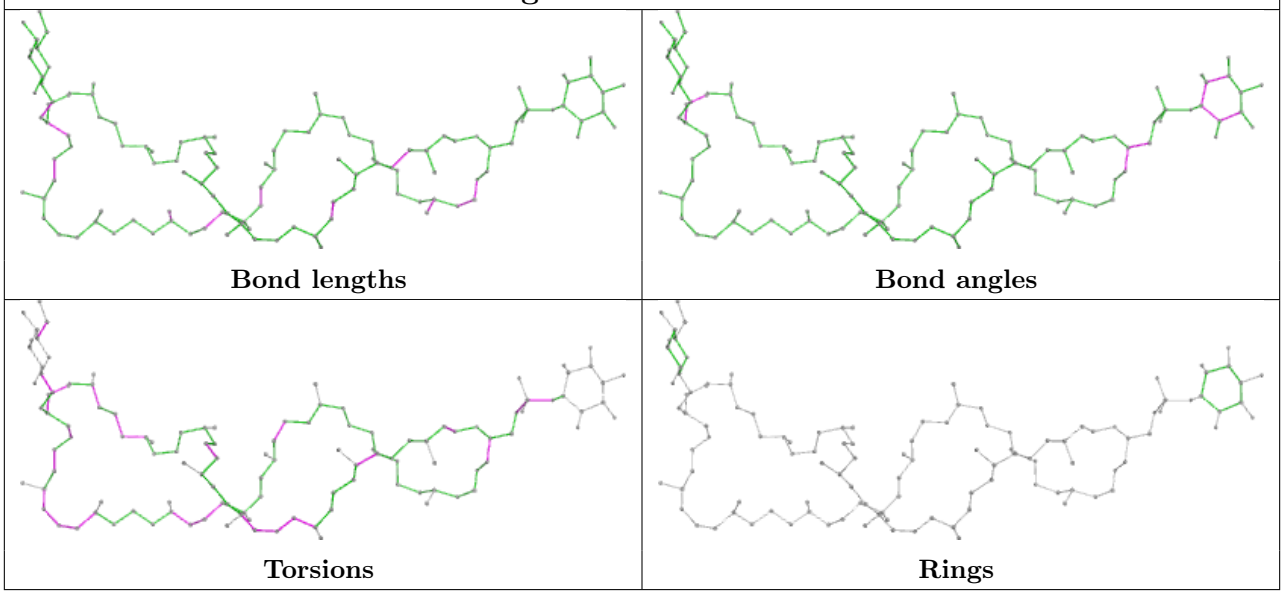
No monomer is involved in short contacts.

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.

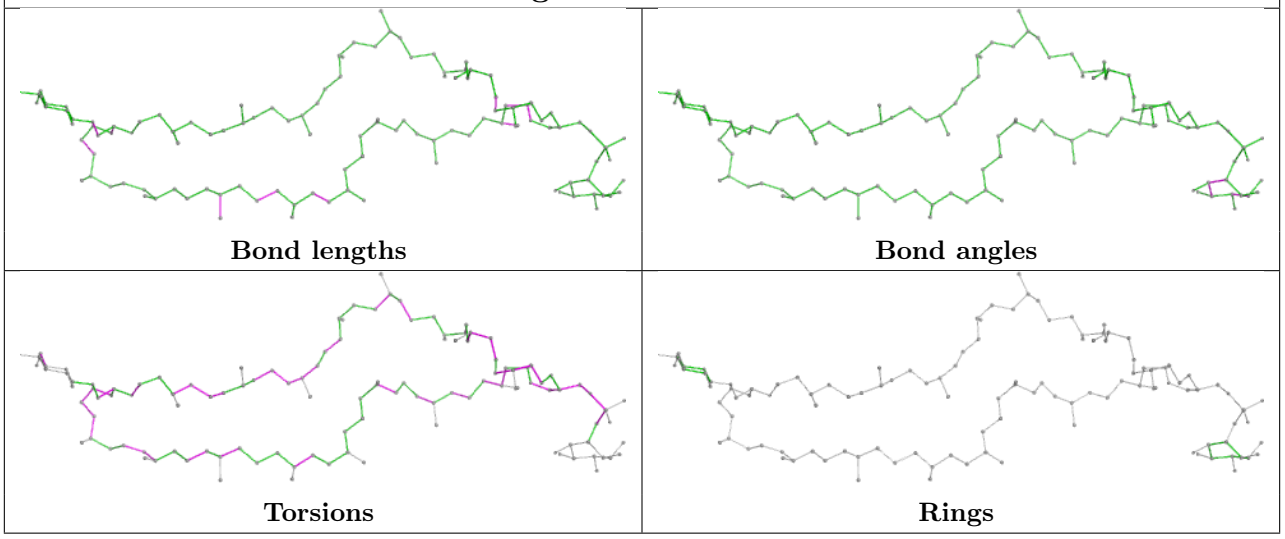
Ligand JCV c 301



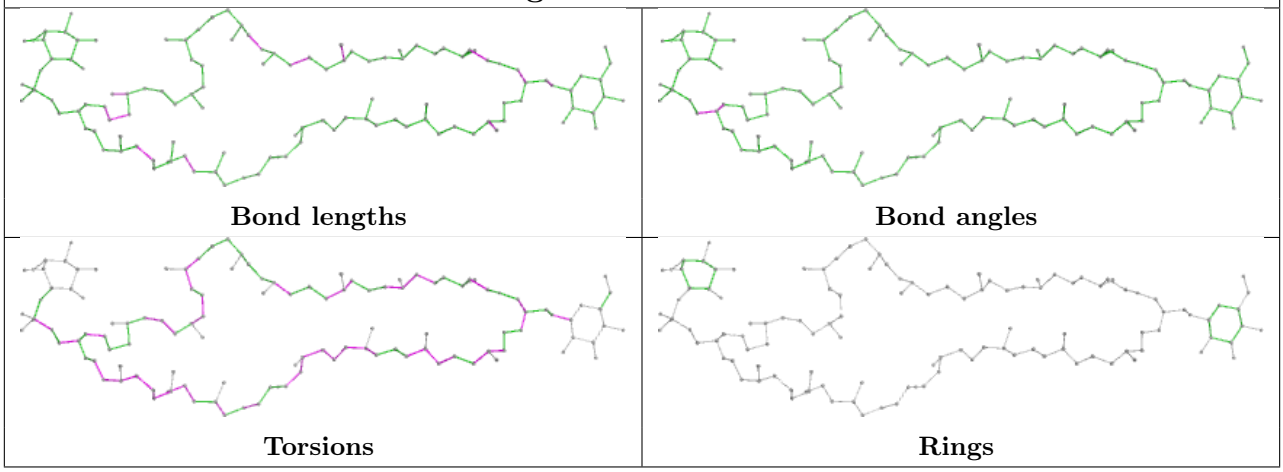
Ligand JCV W 101



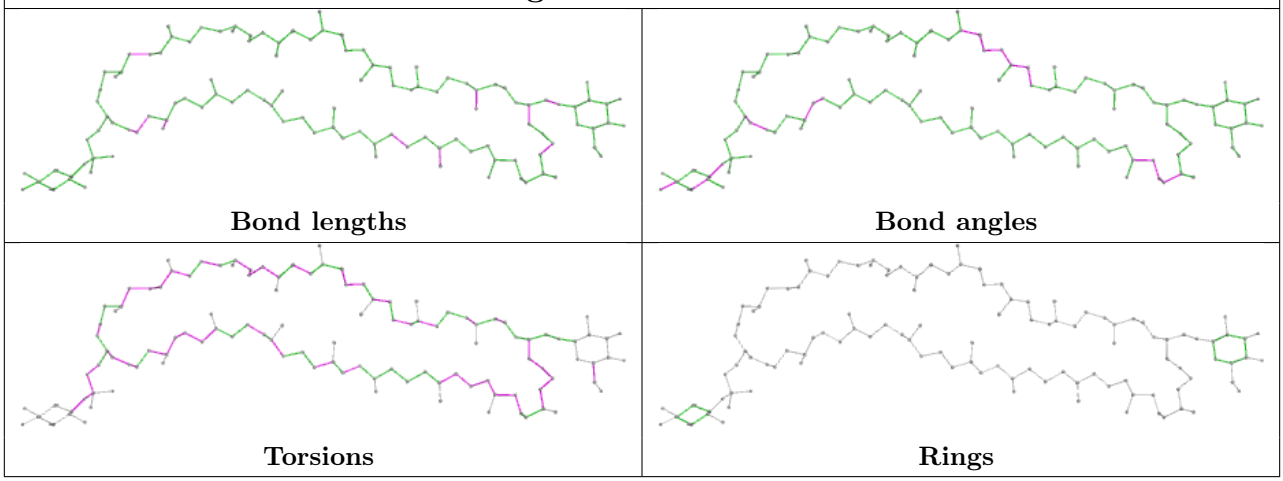
Ligand JCV e 303



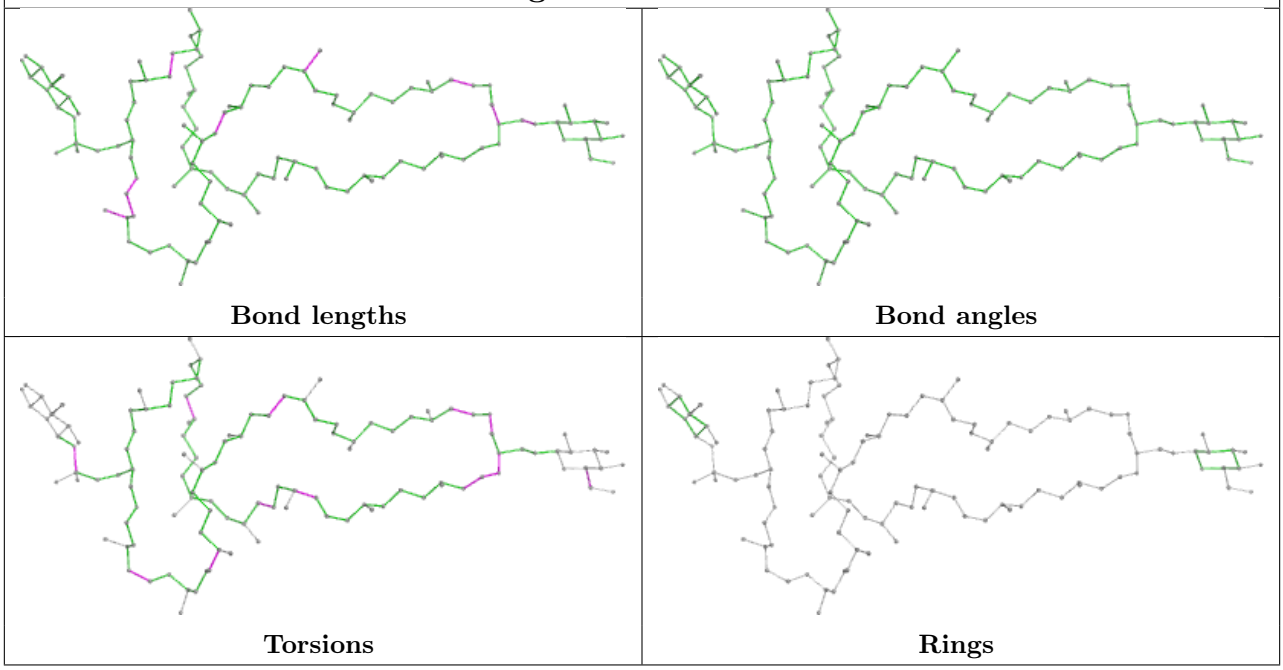
Ligand JCV V 101



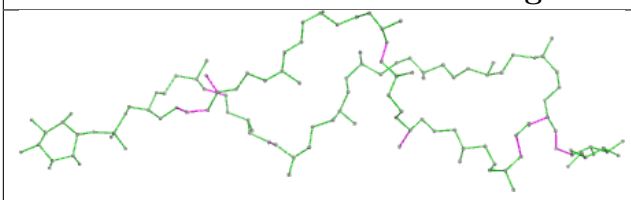
Ligand JCV C 301



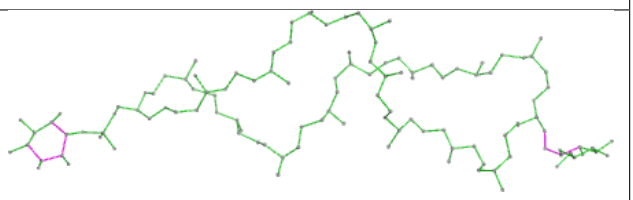
Ligand JCV F 101



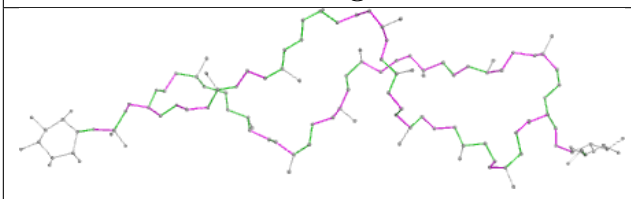
Ligand JCV G 101



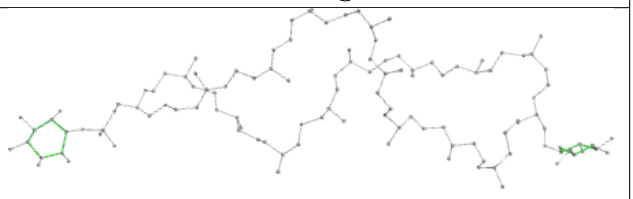
Bond lengths



Bond angles

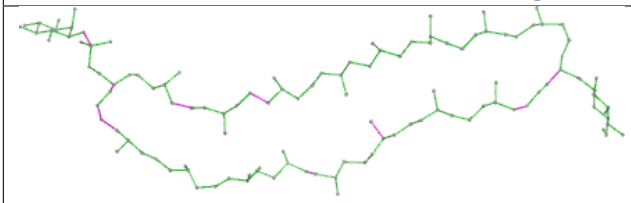


Torsions

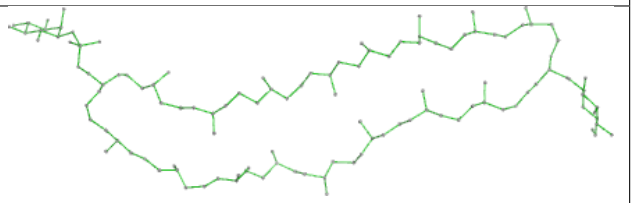


Rings

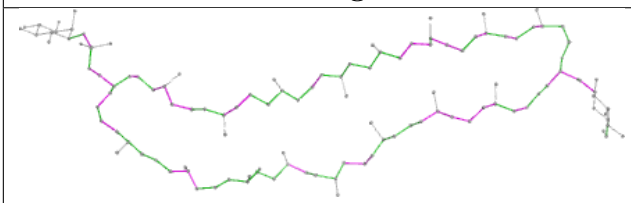
Ligand JCV S 301



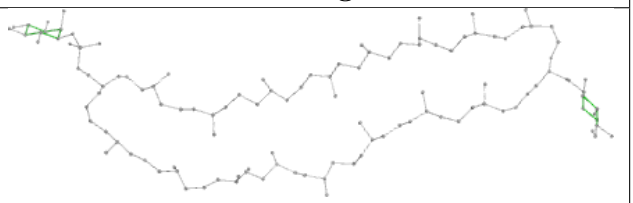
Bond lengths



Bond angles

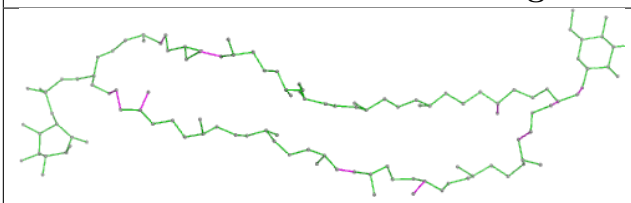


Torsions

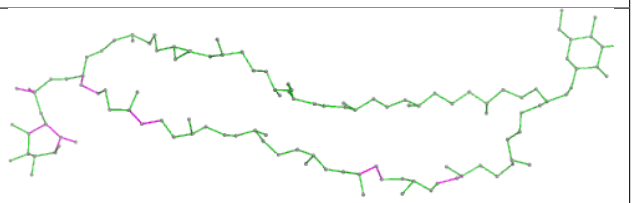


Rings

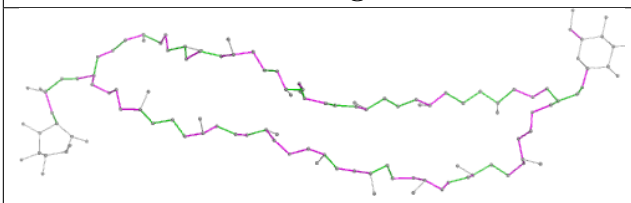
Ligand JCV F 102



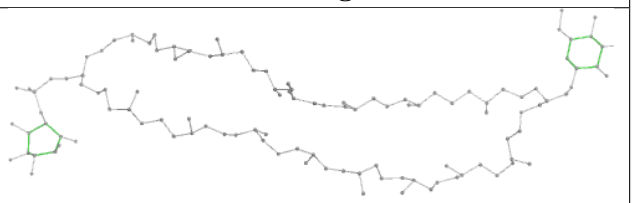
Bond lengths



Bond angles

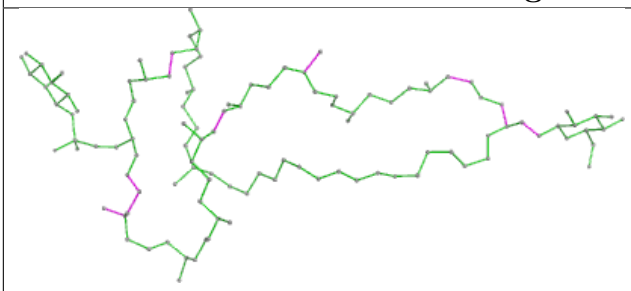


Torsions

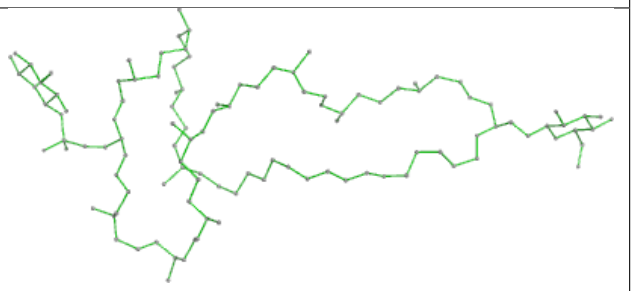


Rings

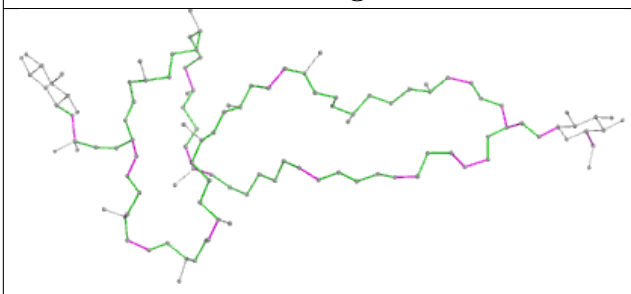
Ligand JCV G 102



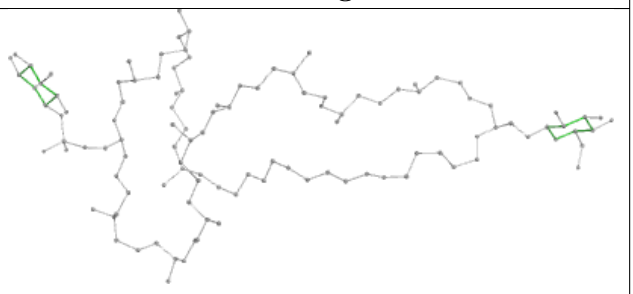
Bond lengths



Bond angles

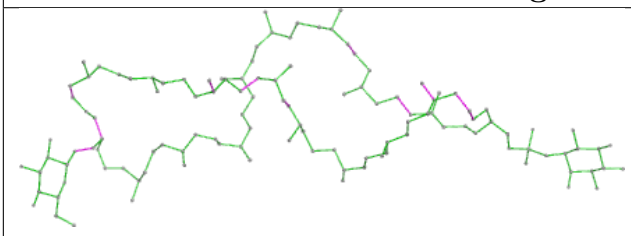


Torsions

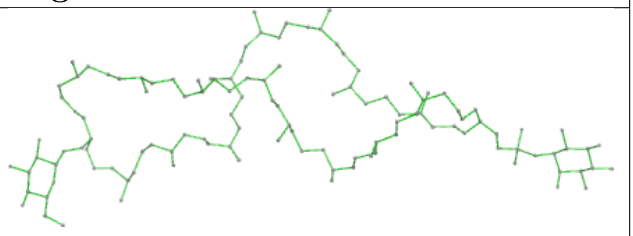


Rings

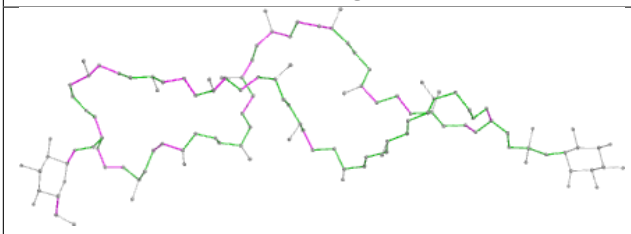
Ligand JCV g 101



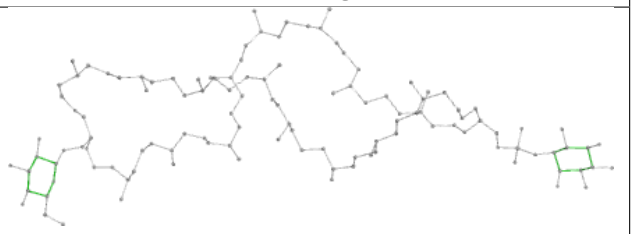
Bond lengths



Bond angles

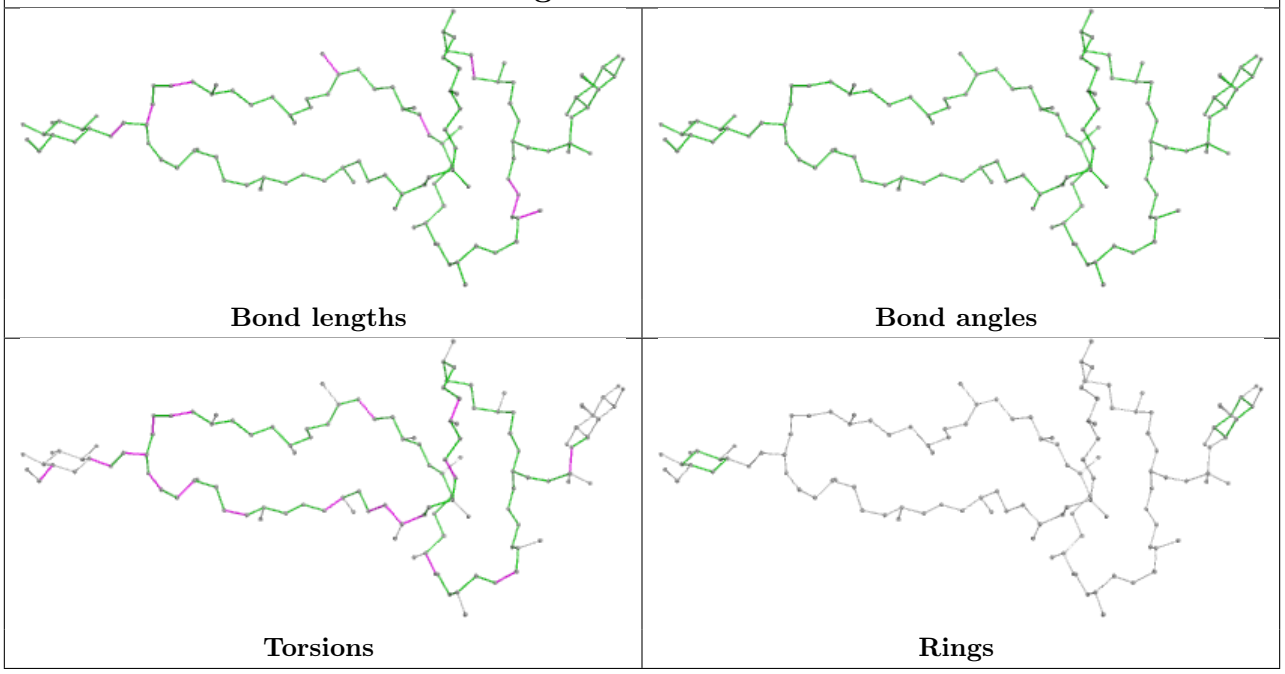


Torsions



Rings

Ligand JCV f 100



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.

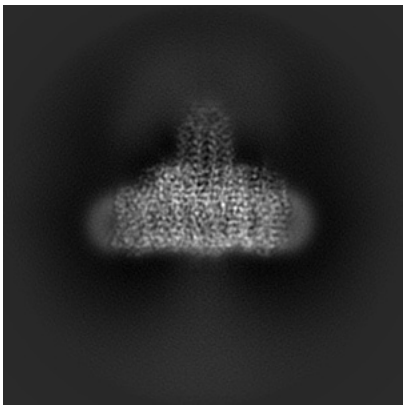
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18135. These allow visual inspection of the internal detail of the map and identification of artifacts.

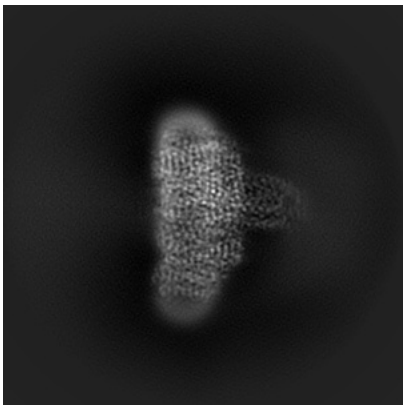
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

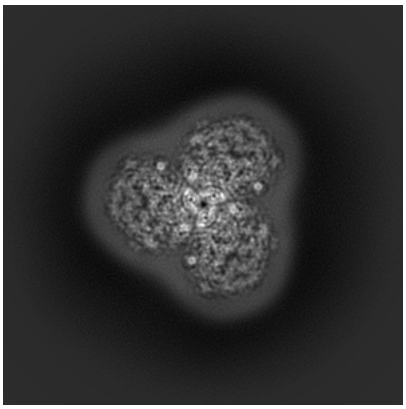
6.1.1 Primary map



X

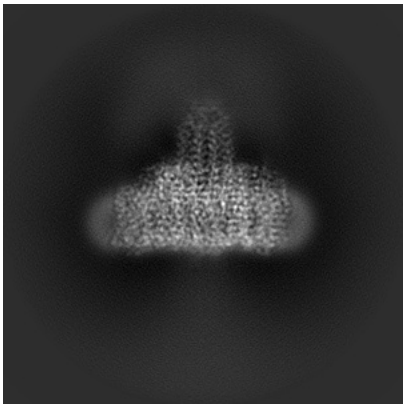


Y

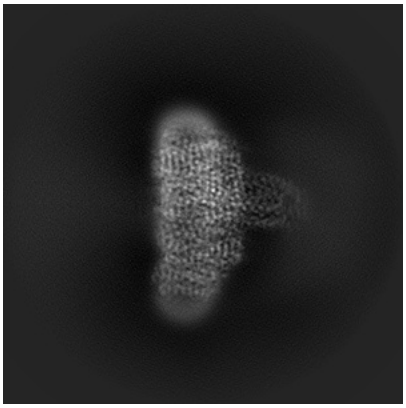


Z

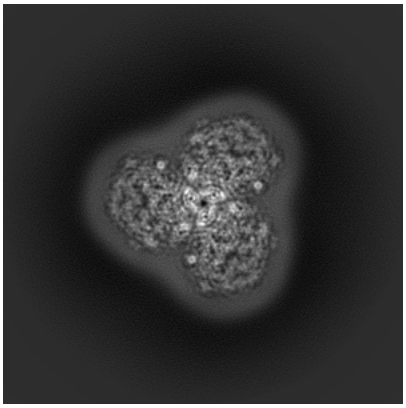
6.1.2 Raw map



X



Y

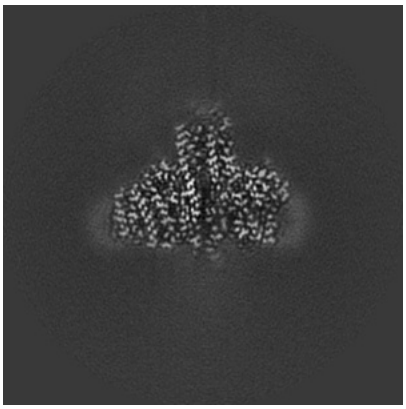


Z

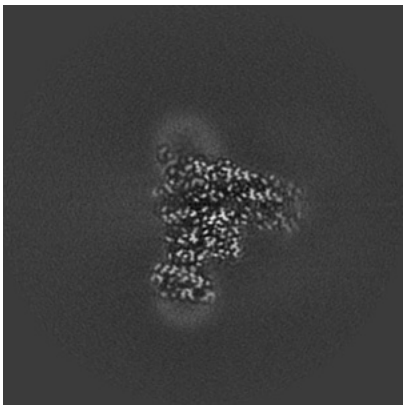
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

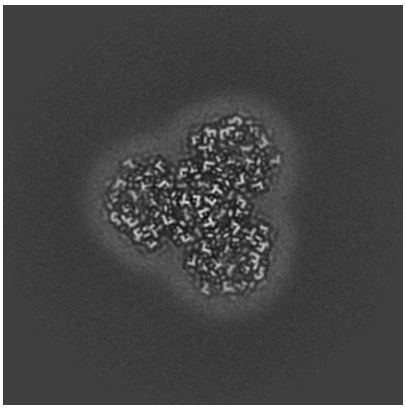
6.2.1 Primary map



X Index: 160

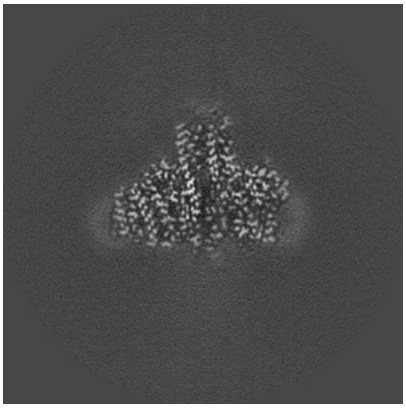


Y Index: 160

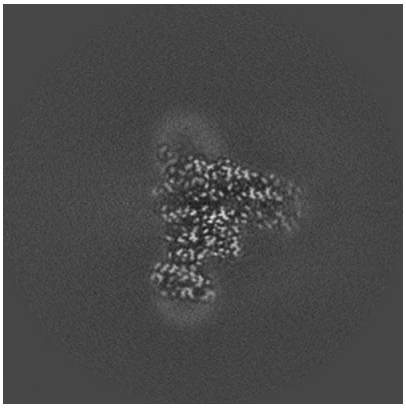


Z Index: 160

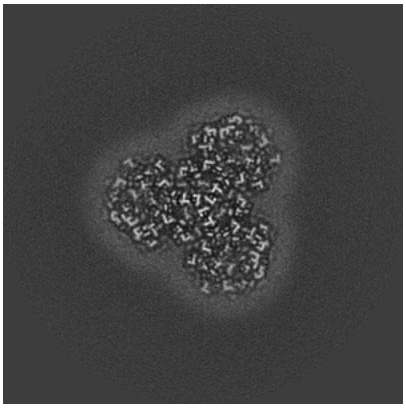
6.2.2 Raw map



X Index: 160



Y Index: 160

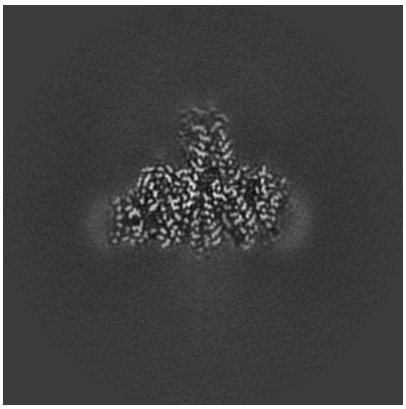


Z Index: 160

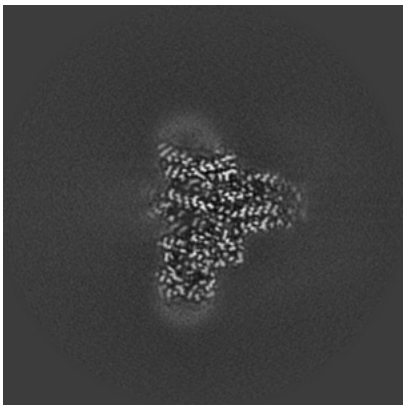
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

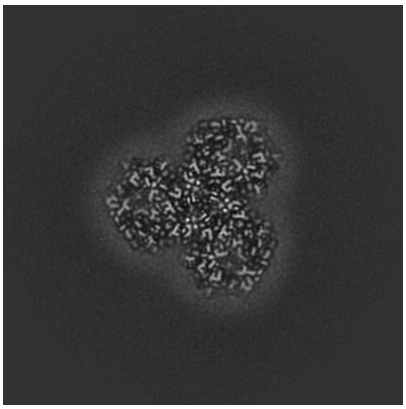
6.3.1 Primary map



X Index: 165

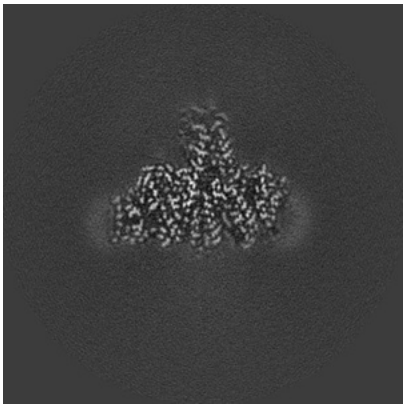


Y Index: 154

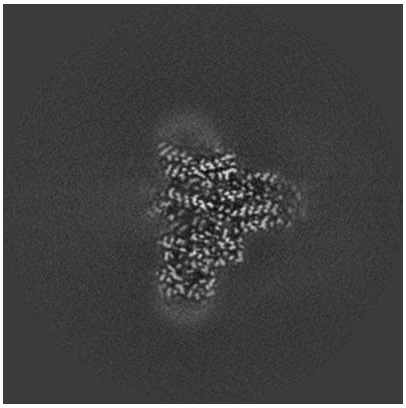


Z Index: 163

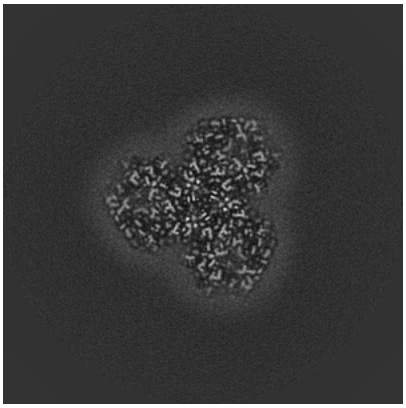
6.3.2 Raw map



X Index: 165



Y Index: 154

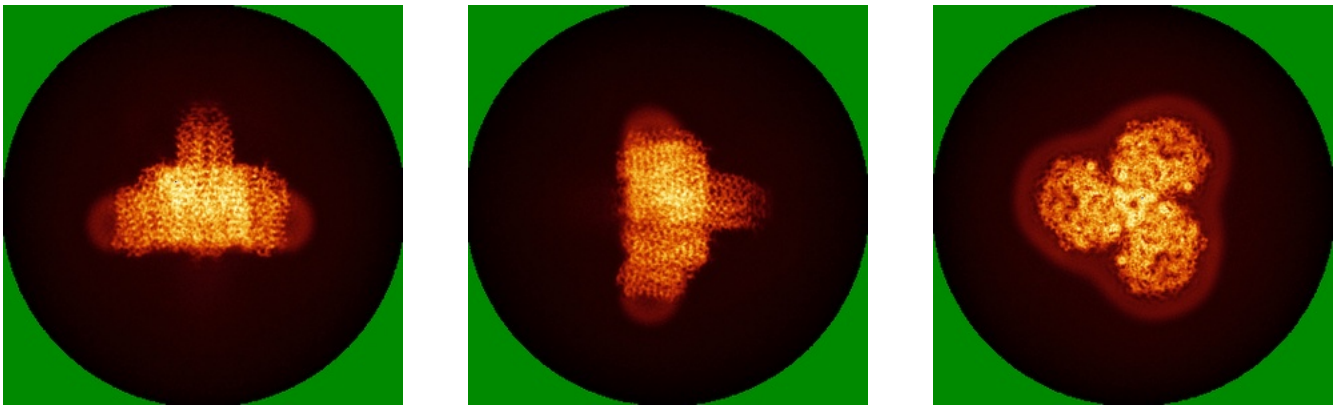


Z Index: 163

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

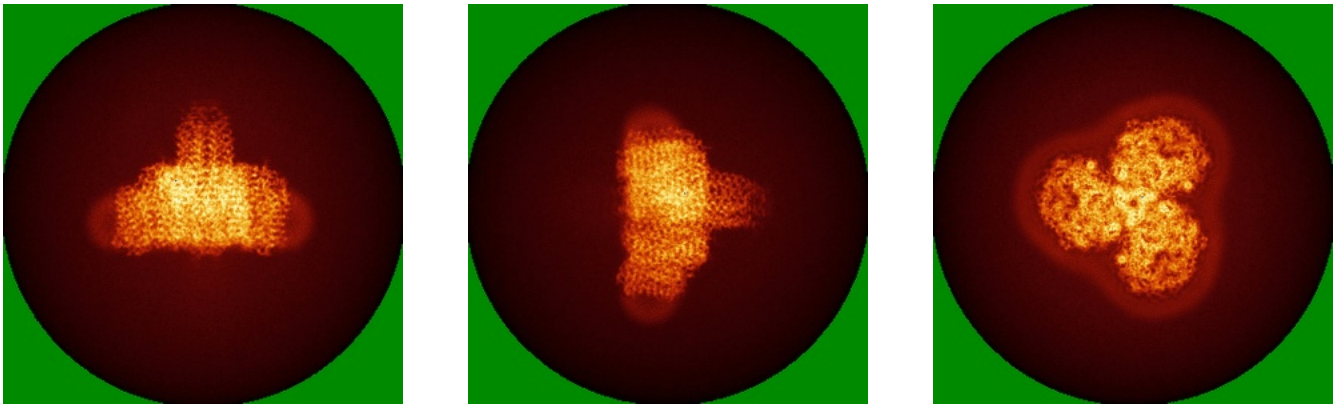
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

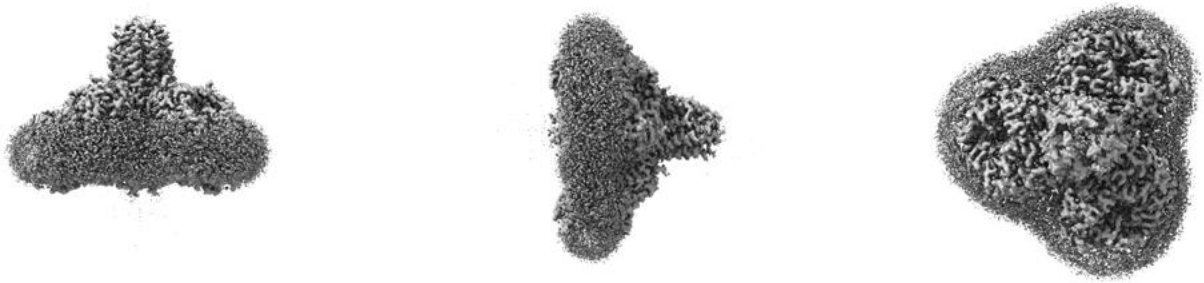
6.5 Orthogonal surface views (i)

6.5.1 Primary map

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.

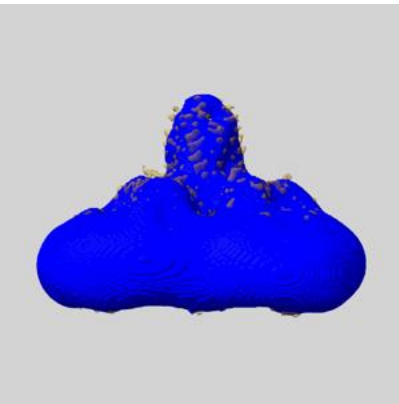
6.6 Mask visualisation (i)

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

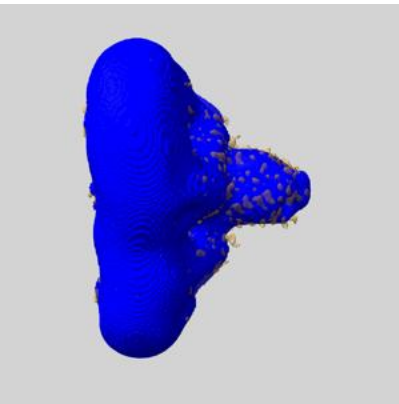
A mask typically either:

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

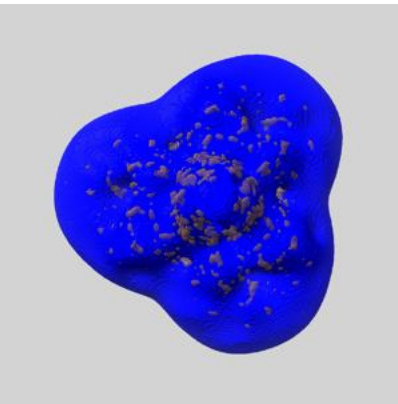
6.6.1 emd_18135_msk_1.map (i)



X



Y

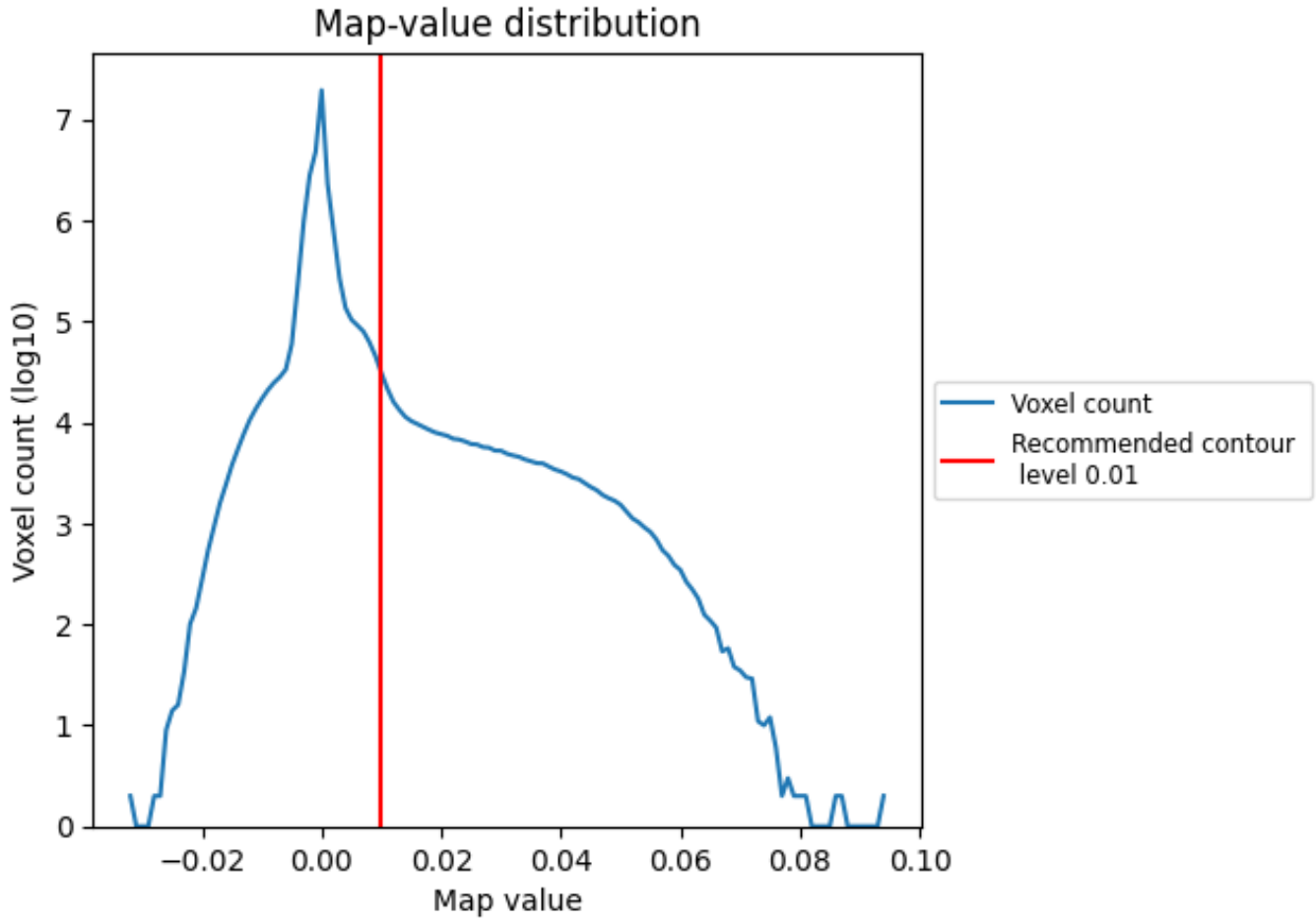


Z

7 Map analysis

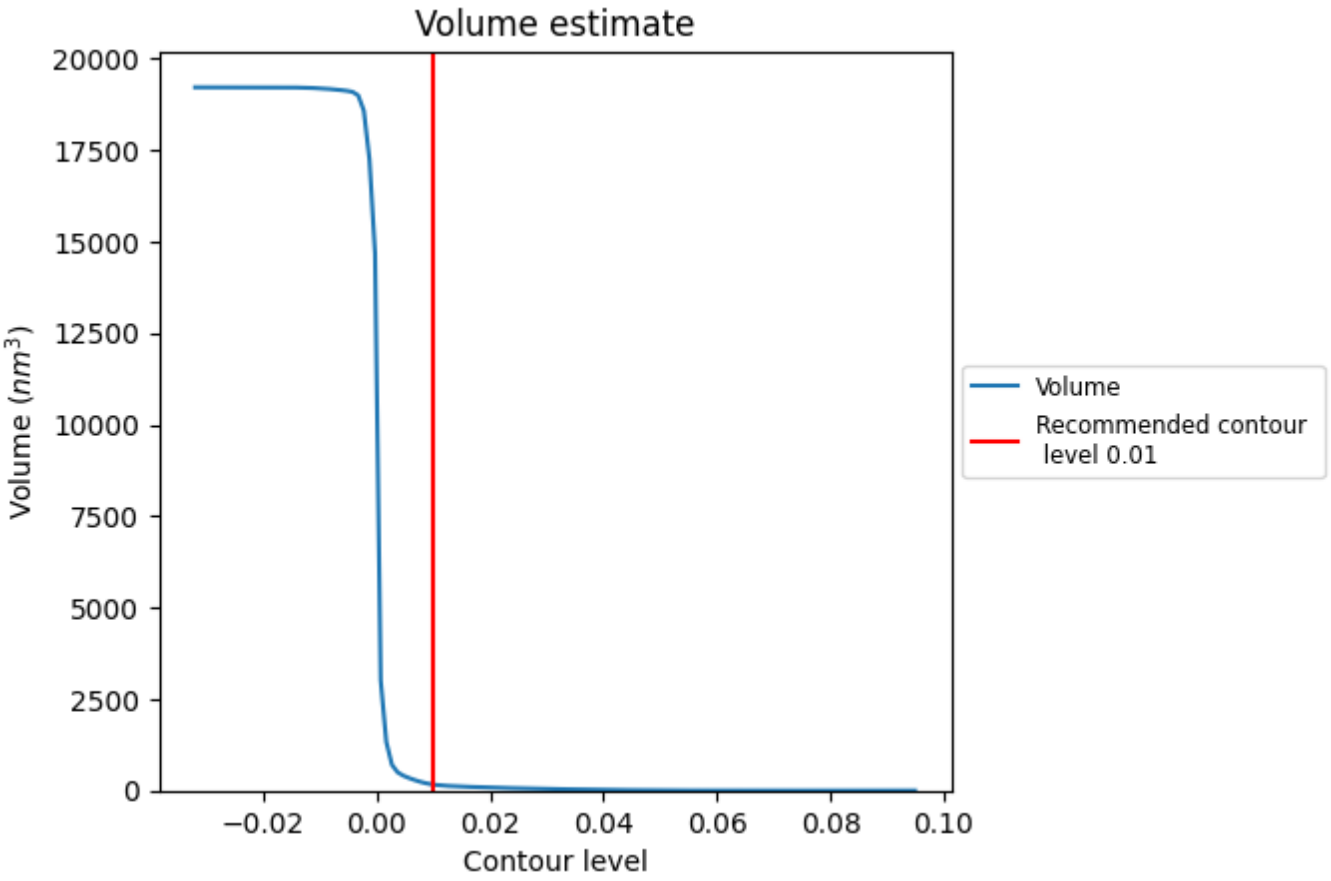
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

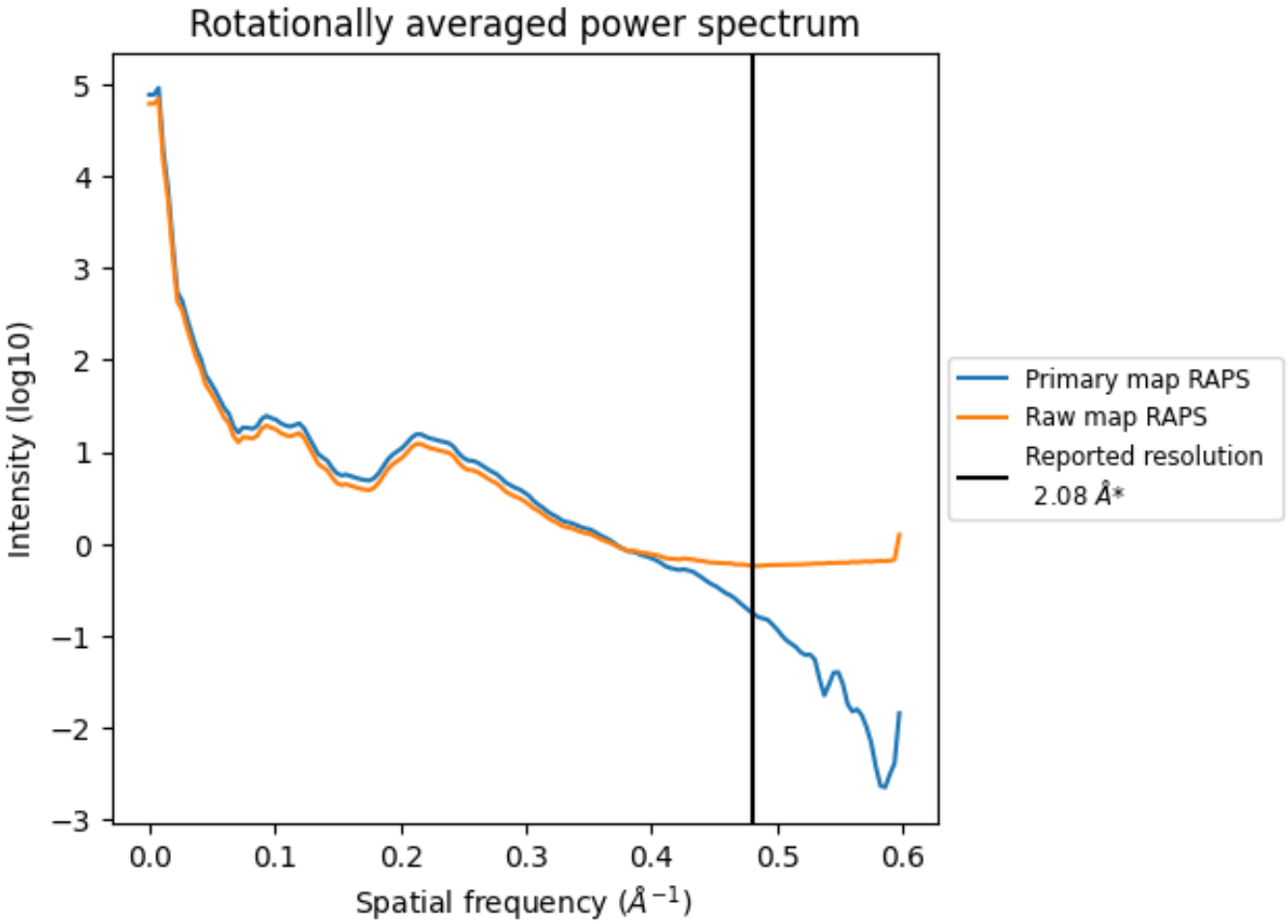
7.2 Volume estimate



The volume at the recommended contour level is 165 nm^3; this corresponds to an approximate mass of 149 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 (i)

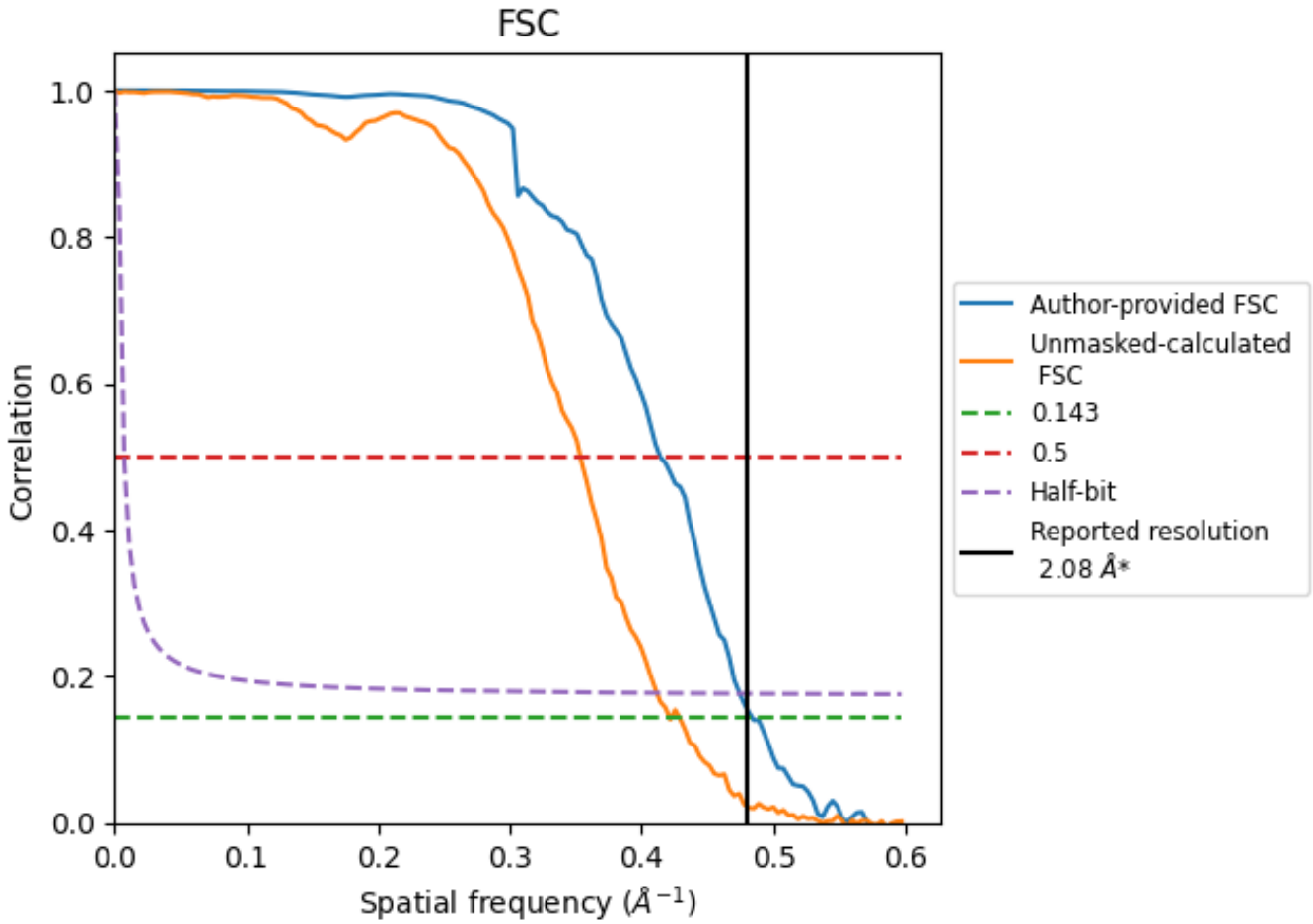


*Reported resolution corresponds to spatial frequency of 0.481 Å^{-1}

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 0.481 Å^{-1}

8.2 Resolution estimates (i)

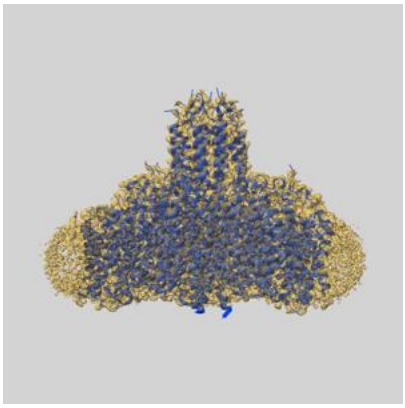
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.08	-	-
Author-provided FSC curve	2.07	2.41	2.11
Unmasked-calculated*	2.37	2.83	2.43

*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 2.37 differs from the reported value 2.08 by more than 10 %

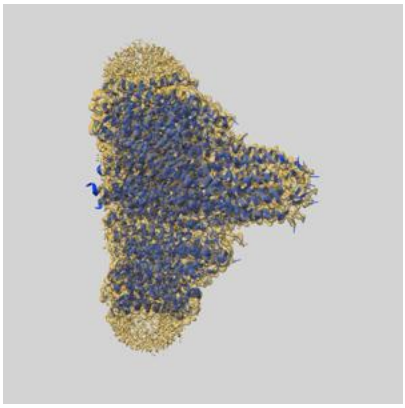
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18135 and PDB model 8Q3V. Per-residue inclusion information can be found in section 3 on page 9.

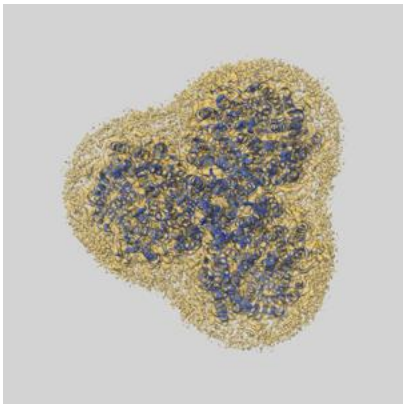
9.1 Map-model overlay



X



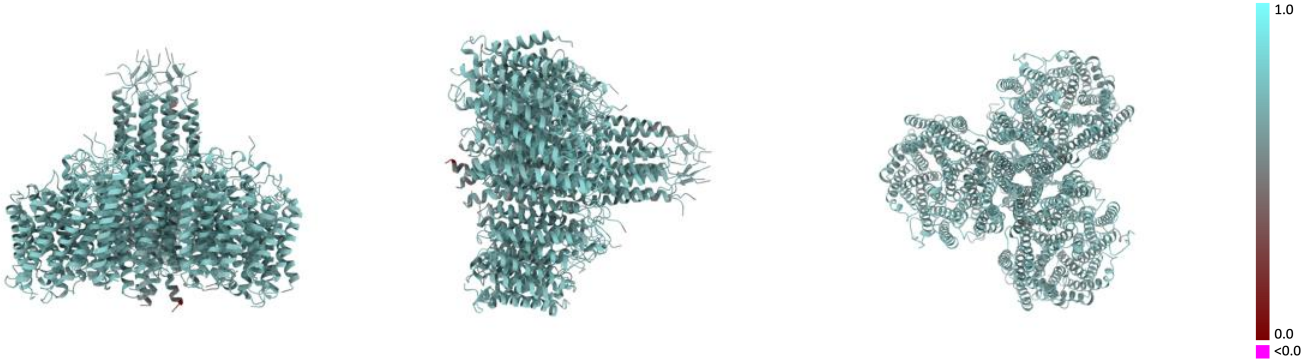
Y



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.

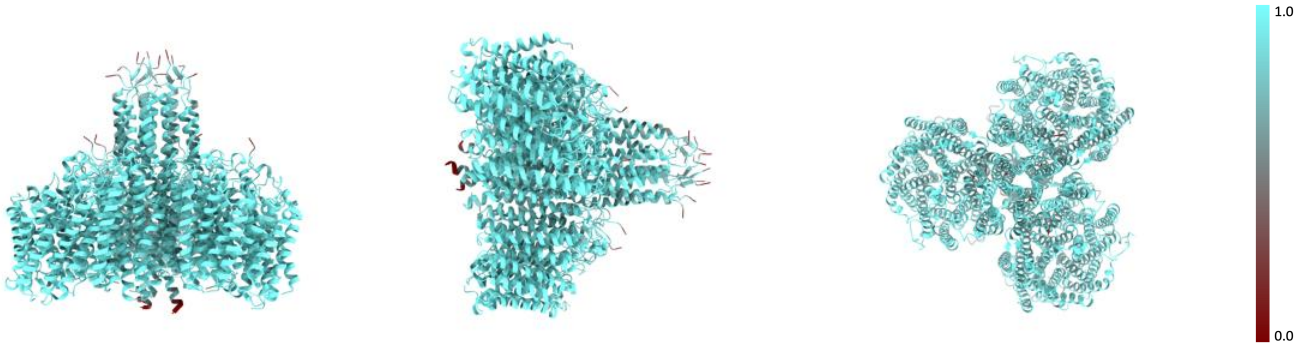
9.2 Q-score mapped to coordinate model (i)



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.

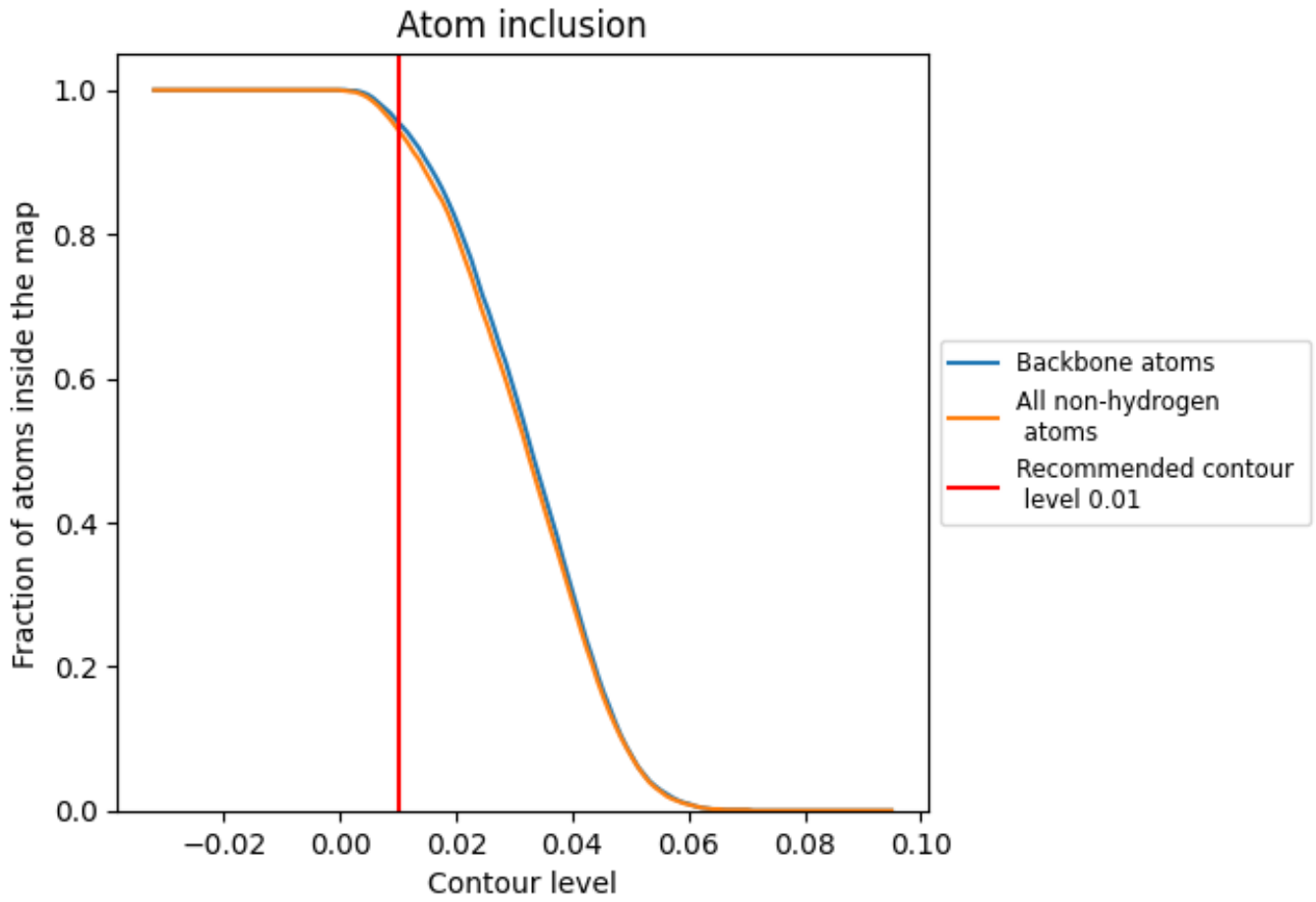
9.3 Atom inclusion mapped to coordinate model (i)



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 (i)



At the recommended contour level, 96% of all backbone atoms, 94% 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	0.9450	0.6860
A	0.9470	0.7010
B	0.9350	0.6950
C	0.9540	0.6770
D	0.9820	0.6930
E	0.9800	0.7120
F	0.8770	0.6490
G	0.8490	0.6520
Q	0.9470	0.7020
R	0.9320	0.6910
S	0.9450	0.6710
T	0.9800	0.6910
U	0.9820	0.7130
V	0.8600	0.6470
W	0.8350	0.6460
a	0.9520	0.7010
b	0.9350	0.6940
c	0.9490	0.6760
d	0.9840	0.6940
e	0.9520	0.6990
f	0.9300	0.6740
g	0.8080	0.6420