wwPDB EM Validation Summary Report (i)

Apr 10, 2025 – 02:14 pm BST

PDB ID	:	9H1L / pdb_00009h1l
EMDB ID	:	EMD-51767
Title	:	Methyl-coenzyme M reductase activation complex binding to the A2 component after incubation with ATP
Authors	:	Ramirez-Amador, F.; Paul, S.; Kumar, A.; Schuller, J.M.
Deposited on	:	2024-10-09
Resolution	:	2.14 Å(reported)
Based on initial model	:	.

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

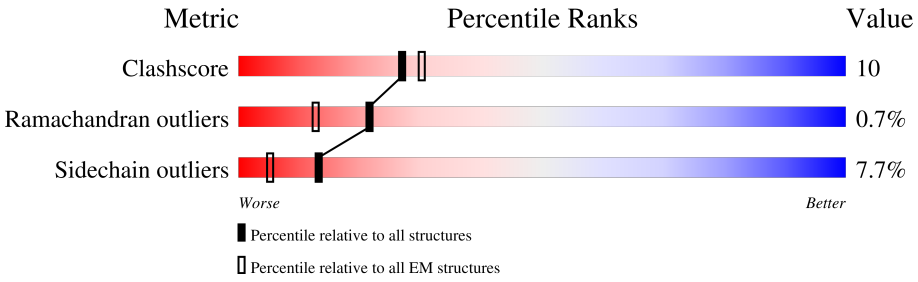
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.14 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



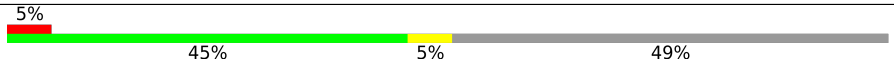
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	J	501	29% 58% 30% 9%
2	A	260	81% 18%
2	B	260	81% 18%
3	D	443	84% 15%
3	E	443	84% 15%
4	C	553	80% 18%
4	F	553	80% 13% 6%
5	G	183	47% 15% 38%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	H	304	
7	I	234	
8	K	531	
9	L	93	

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
13	SHT	F	602	X	-	X	-
4	GL3	C	448	-	-	X	-
4	SMC	C	455	-	-	X	-

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 32524 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 UPF0288 protein MmarC6_0796.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	499	Total	C	N	O	S	0	0
			3962	2517	647	790	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	500	SER	LYS	variant	UNP A9A8E0

- Molecule 2 is a protein called Methyl-coenzyme M reductase subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	259	Total	C	N	O	S	0	0
			2071	1293	369	397	12		
2	B	259	Total	C	N	O	S	0	0
			2071	1293	369	397	12		

- Molecule 3 is a protein called Methyl-coenzyme M reductase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	442	Total	C	N	O	S	0	0
			3263	2066	546	630	21		
3	D	442	Total	C	N	O	S	0	0
			3263	2066	546	630	21		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	173	GLY	SER	conflict	UNP A0A2L1CBB3
D	173	GLY	SER	conflict	UNP A0A2L1CBB3

- Molecule 4 is a protein called Methyl-coenzyme M reductase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	550	Total	C	N	O	S	0	0
			4284	2707	731	826	20		
4	F	520	Total	C	N	O	S	0	0
			4039	2556	684	779	20		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	51	SER	ALA	variant	UNP A0A2L1CBB0
F	51	SER	ALA	variant	UNP A0A2L1CBB0

- Molecule 5 is a protein called Methanogenesis marker protein 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	114	Total	C	N	O	S	0	0
			931	600	152	172	7		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	109	VAL	ILE	variant	UNP G0H411
G	129	ILE	VAL	variant	UNP G0H411
G	167	GLU	GLN	variant	UNP G0H411
G	168	GLU	ASP	variant	UNP G0H411
G	171	ASN	ASP	variant	UNP G0H411

- Molecule 6 is a protein called Methanogenesis marker protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	296	Total	C	N	O	S	0	0
			2393	1530	411	440	12		

- Molecule 7 is a protein called Methyl-coenzyme M reductase operon protein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	194	Total	C	N	O	S	0	0
			1469	929	261	271	8		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-35	MET	-	initiating methionine	UNP G0H3B1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	-34	SER	-	expression tag	UNP G0H3B1
I	-33	ALA	-	expression tag	UNP G0H3B1
I	-32	TRP	-	expression tag	UNP G0H3B1
I	-31	SER	-	expression tag	UNP G0H3B1
I	-30	HIS	-	expression tag	UNP G0H3B1
I	-29	PRO	-	expression tag	UNP G0H3B1
I	-28	GLN	-	expression tag	UNP G0H3B1
I	-27	PHE	-	expression tag	UNP G0H3B1
I	-26	GLU	-	expression tag	UNP G0H3B1
I	-25	LYS	-	expression tag	UNP G0H3B1
I	-24	GLY	-	expression tag	UNP G0H3B1
I	-23	GLY	-	expression tag	UNP G0H3B1
I	-22	GLY	-	expression tag	UNP G0H3B1
I	-21	SER	-	expression tag	UNP G0H3B1
I	-20	GLY	-	expression tag	UNP G0H3B1
I	-19	GLY	-	expression tag	UNP G0H3B1
I	-18	GLY	-	expression tag	UNP G0H3B1
I	-17	SER	-	expression tag	UNP G0H3B1
I	-16	GLY	-	expression tag	UNP G0H3B1
I	-15	GLY	-	expression tag	UNP G0H3B1
I	-14	SER	-	expression tag	UNP G0H3B1
I	-13	ALA	-	expression tag	UNP G0H3B1
I	-12	TRP	-	expression tag	UNP G0H3B1
I	-11	SER	-	expression tag	UNP G0H3B1
I	-10	HIS	-	expression tag	UNP G0H3B1
I	-9	PRO	-	expression tag	UNP G0H3B1
I	-8	GLN	-	expression tag	UNP G0H3B1
I	-7	PHE	-	expression tag	UNP G0H3B1
I	-6	GLU	-	expression tag	UNP G0H3B1
I	-5	LYS	-	expression tag	UNP G0H3B1
I	-4	SER	-	expression tag	UNP G0H3B1
I	-3	ALA	-	expression tag	UNP G0H3B1
I	-2	GLY	-	expression tag	UNP G0H3B1
I	-1	SER	-	expression tag	UNP G0H3B1
I	0	GLY	-	expression tag	UNP G0H3B1

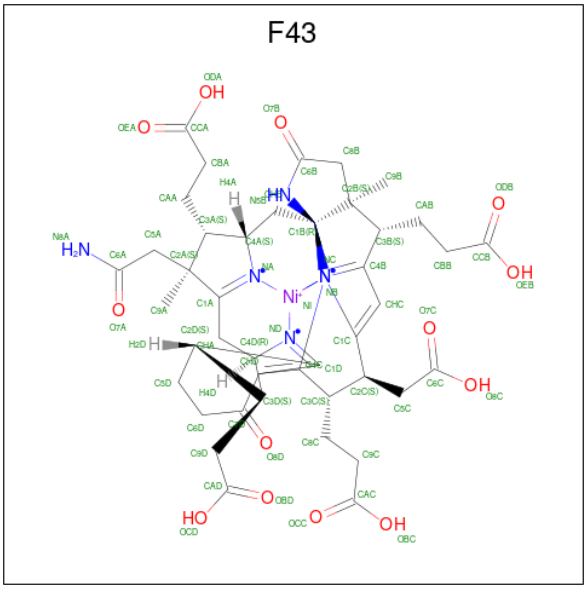
- Molecule 8 is a protein called Glycine betaine/carnitine/choline transport ATP-binding protein OpuCA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	521	Total	C	N	O	S	0	0
			4089	2598	693	774	24		

- Molecule 9 is a protein called DUF2098 domain-containing protein.

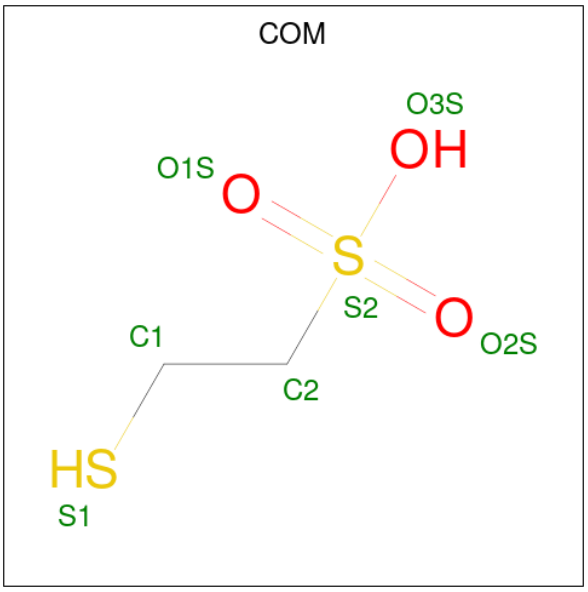
Mol	Chain	Residues	Atoms				AltConf	Trace
9	L	47	Total	C	N	O	0	0
			390	251	61	78		

- Molecule 10 is FACTOR 430 (CCD ID: F43) (formula: $C_{42}H_{51}N_6NiO_{13}$).



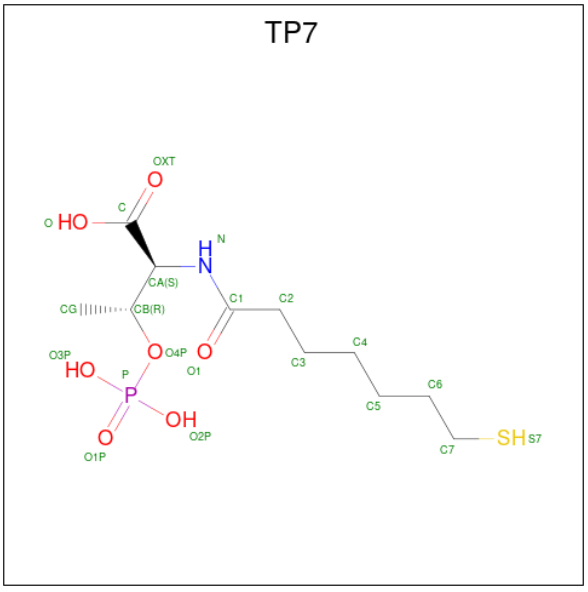
Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	Ni	O	0
			62	42	6	1	13	
10	E	1	Total	C	N	Ni	O	0
			62	42	6	1	13	

- Molecule 11 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: $C_2H_6O_3S_2$).



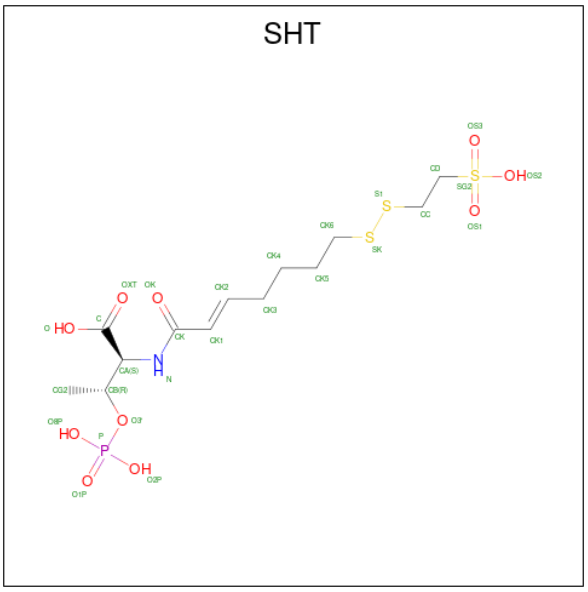
Mol	Chain	Residues	Atoms				AltConf
11	C	1	Total	C	O	S	0
			7	2	3	2	

- Molecule 12 is Coenzyme B (CCD ID: TP7) (formula: $C_{11}H_{22}NO_7PS$).



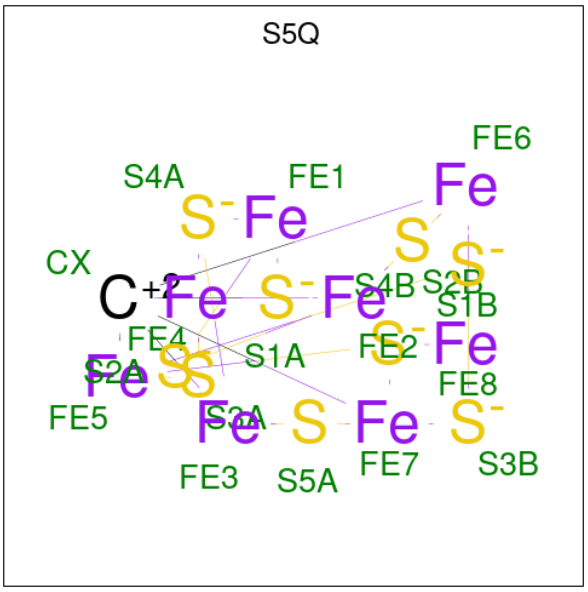
Mol	Chain	Residues	Atoms						AltConf
12	F	1	Total	C	N	O	P	S	0
			21	11	1	7	1	1	

- Molecule 13 is O-PHOSPHONO-N-{(2E)-7-[(2-SULFOETHYL)DITHIO]HEPT-2-ENOYL}-L-THREONINE (CCD ID: SHT) (formula: $C_{13}H_{24}NO_{10}PS_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
13	F	1	Total	C	N	O	P	S	0
			28	13	1	10	1	3	

- Molecule 14 is FeFe cofactor (CCD ID: S5Q) (formula: CFe_8S_9) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
14	H	1	Total	C	Fe	S	0
			18	1	8	9	
14	I	1	Total	C	Fe	S	0
			18	1	8	9	

Continued on next page...

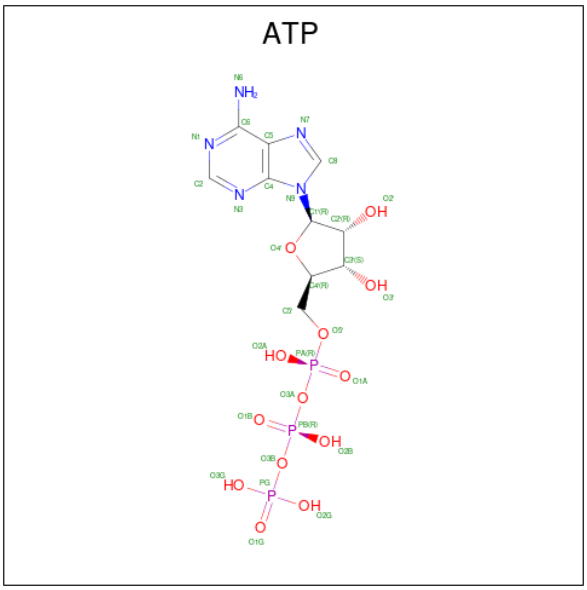
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
14	I	1	Total	C	Fe	S	0
			18	1	8	9	

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
15	K	1	Total	Zn	0
			1	1	

- Molecule 16 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
16	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
16	K	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

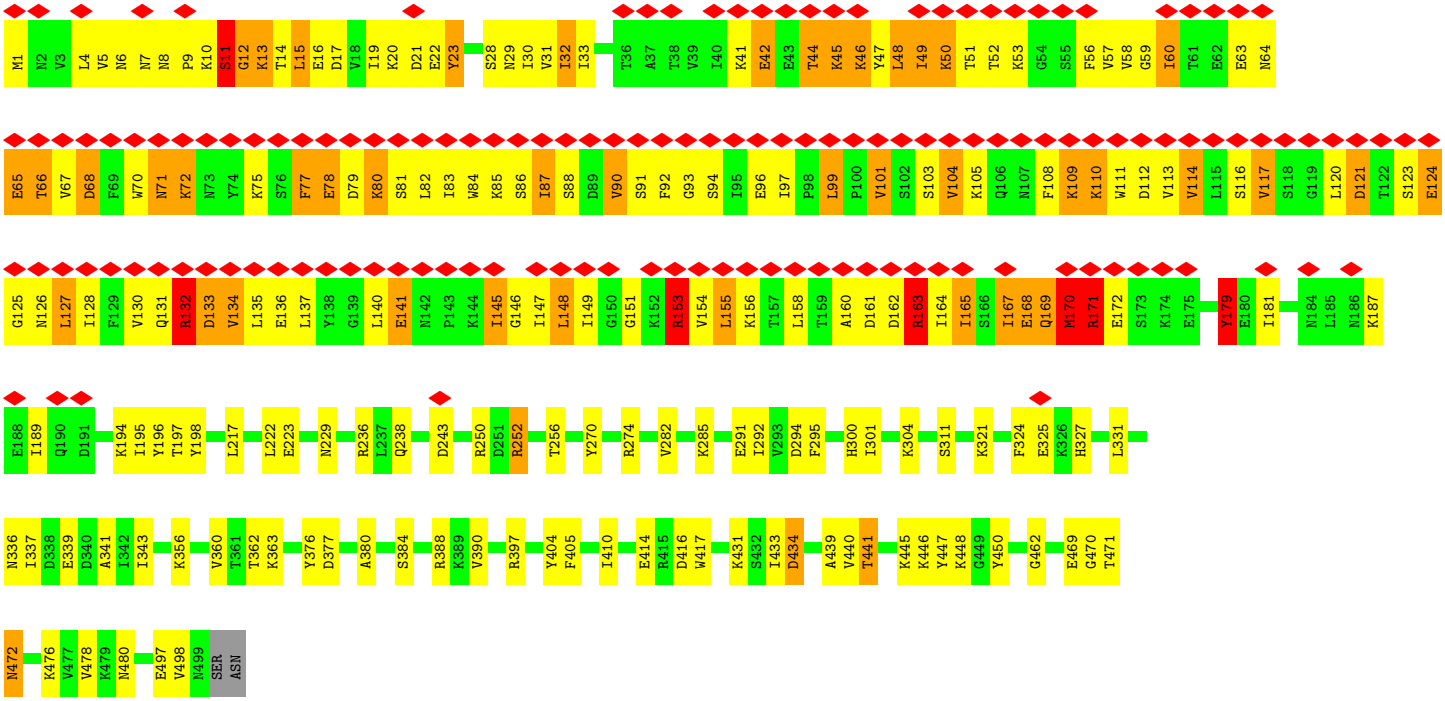
Mol	Chain	Residues	Atoms		AltConf
17	K	2	Total	Mg	0
			2	2	

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.

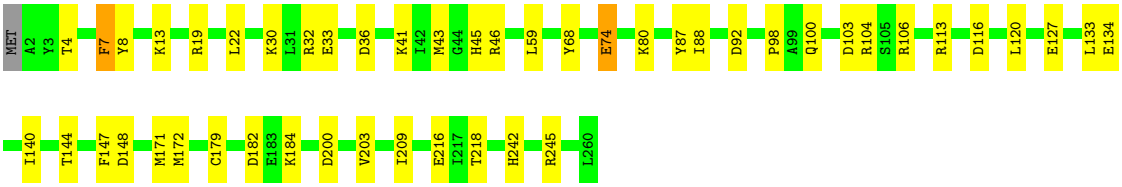
• Molecule 1: UPF0288 protein MmarC6_0796

Chain J:



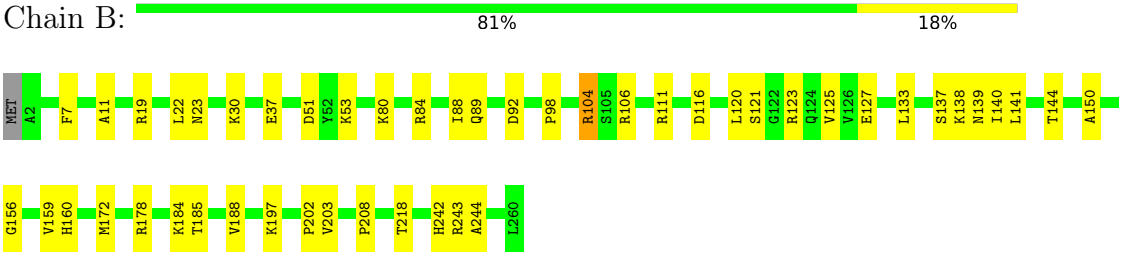
• Molecule 2: Methyl-coenzyme M reductase subunit gamma

Chain A:



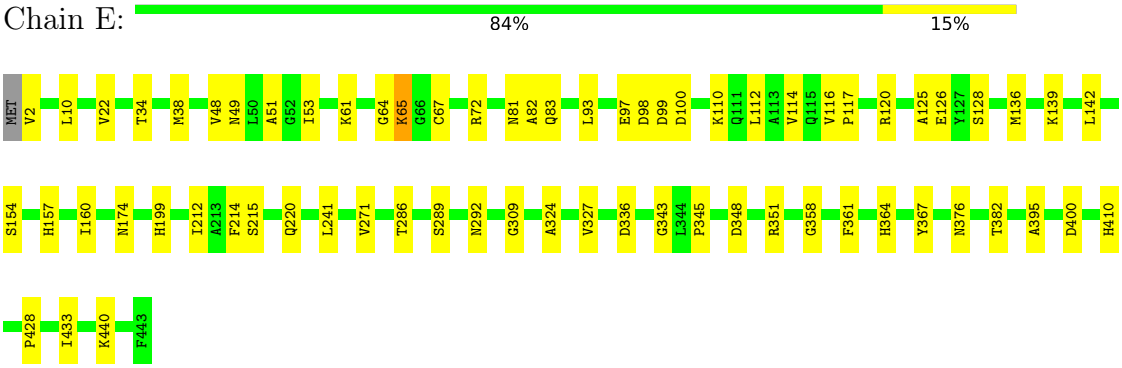
• Molecule 2: Methyl-coenzyme M reductase subunit gamma

Chain B:



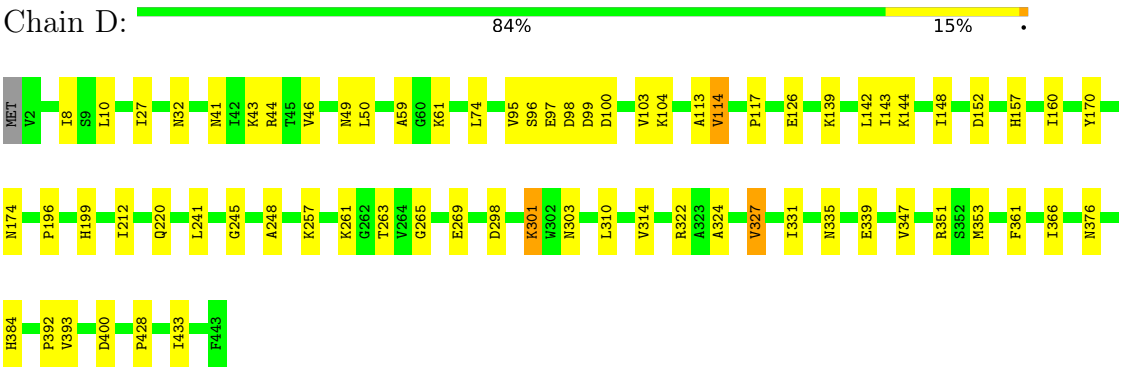
• Molecule 3: Methyl-coenzyme M reductase subunit beta

Chain E:



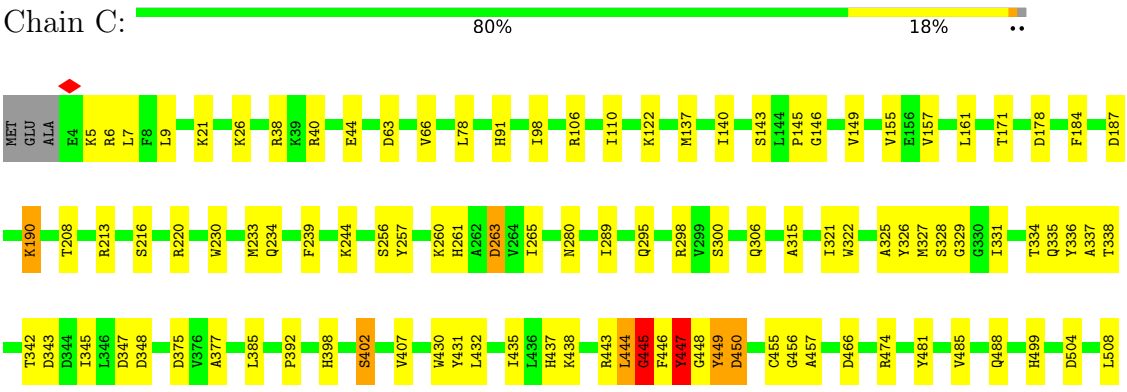
• Molecule 3: Methyl-coenzyme M reductase subunit beta

Chain D:



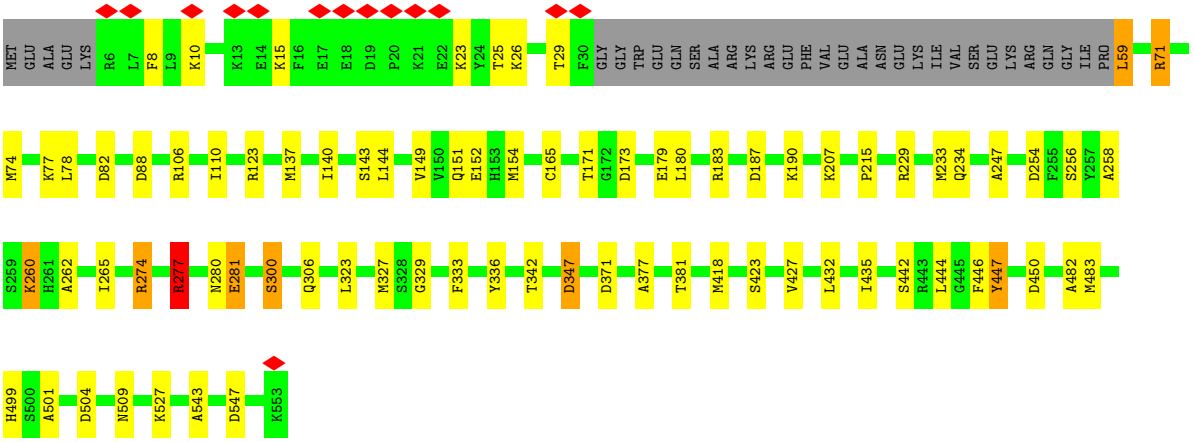
• Molecule 4: Methyl-coenzyme M reductase subunit alpha

Chain C:



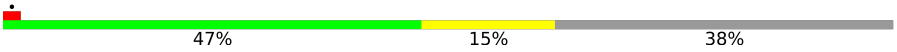
• Molecule 4: Methyl-coenzyme M reductase subunit alpha

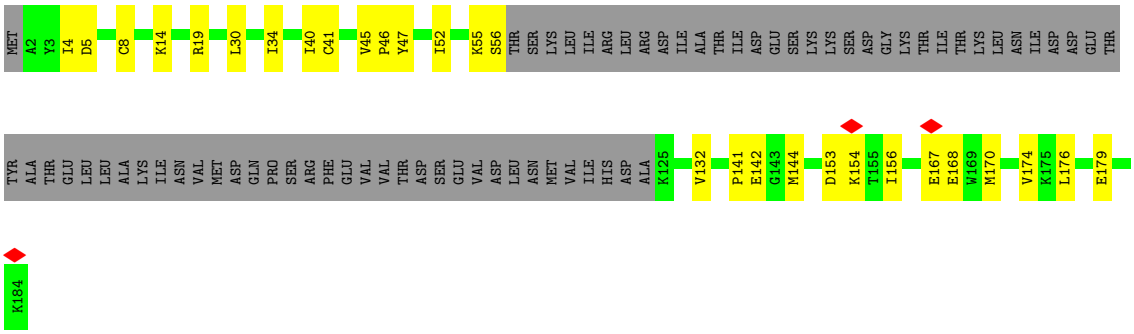
Chain F:



• Molecule 5: Methanogenesis marker protein 17

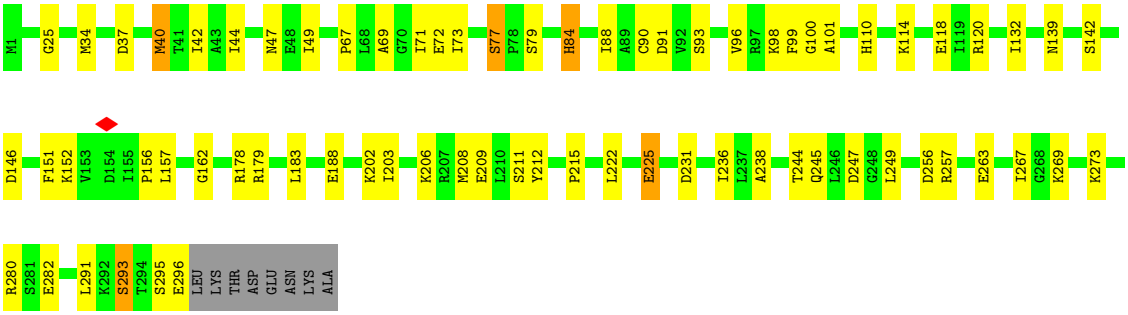
Chain G:





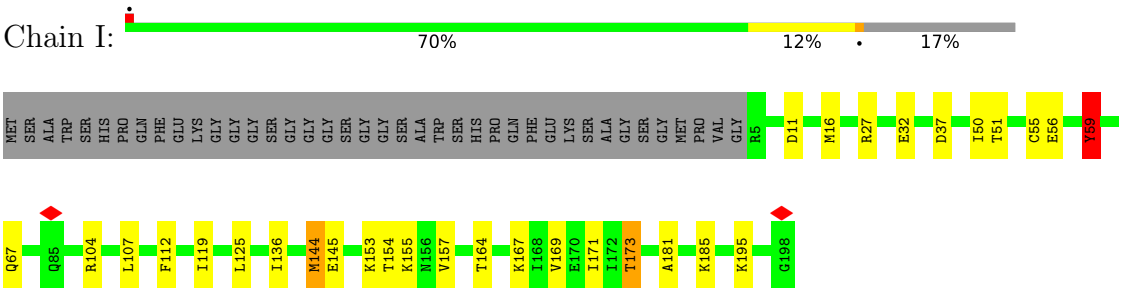
• Molecule 6: Methanogenesis marker protein 7

Chain H:



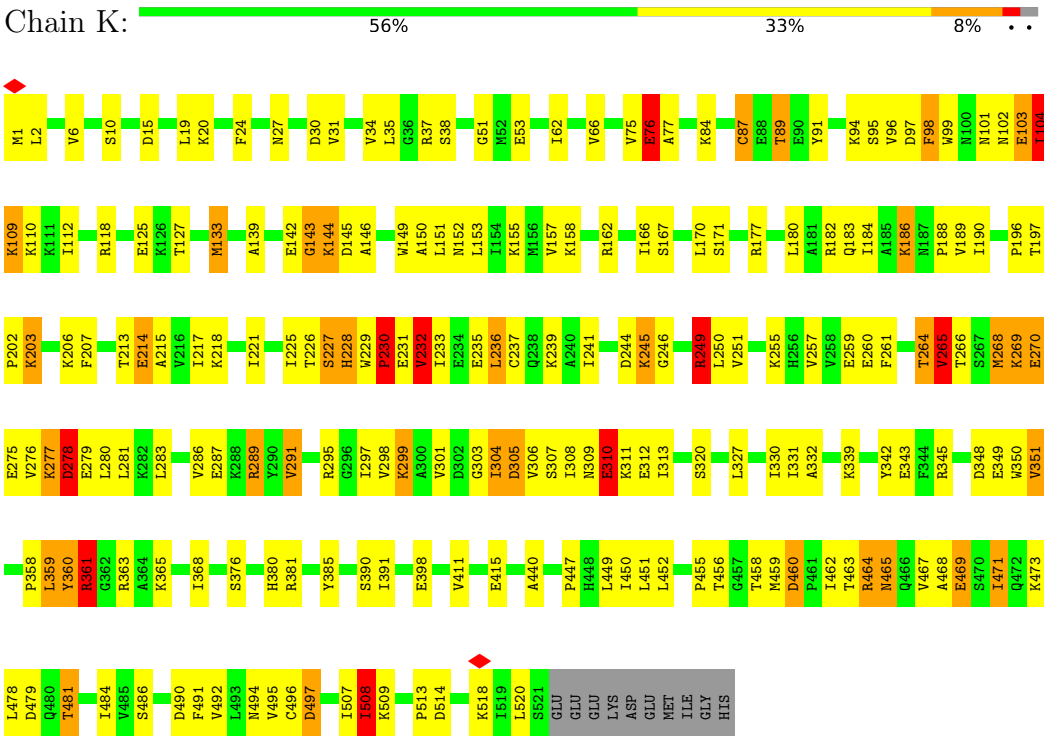
• Molecule 7: Methyl-coenzyme M reductase operon protein C

Chain I:



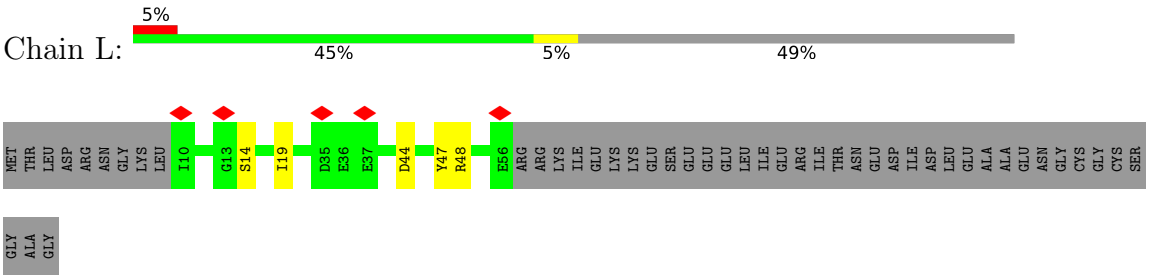
• Molecule 8: Glycine betaine/carnitine/choline transport ATP-binding protein OpuCA

Chain K:



• Molecule 9: DUF2098 domain-containing protein

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118247	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.175	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0197	Depositor
Map size (Å)	342.0, 342.0, 342.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.57, 0.57, 0.57	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AGM, S5Q, TP7, COM, ATP, ZN, MHS, SHT, GL3, MGN, F43, SMC

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	J	0.41	0/4026	0.74	6/5441 (0.1%)
2	A	0.28	0/2116	0.57	2/2861 (0.1%)
2	B	0.27	0/2116	0.54	0/2861
3	D	0.29	0/3319	0.50	1/4499 (0.0%)
3	E	0.29	0/3319	0.50	1/4499 (0.0%)
4	C	0.28	0/4328	0.64	3/5856 (0.1%)
4	F	0.28	0/4078	0.50	0/5522
5	G	0.28	0/943	0.54	0/1262
6	H	0.28	0/2435	0.52	0/3280
7	I	0.27	0/1490	0.58	2/2006 (0.1%)
8	K	0.52	1/4159 (0.0%)	0.94	28/5613 (0.5%)
9	L	0.28	0/398	0.58	0/542
All	All	0.34	1/32727 (0.0%)	0.64	43/44242 (0.1%)

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
1	J	0	6
2	A	0	1
4	F	0	2
6	H	0	1
8	K	0	7
All	All	0	17

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	230	PRO	N-CD	11.52	1.64	1.47

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	447	TYR	CB-CA-C	-26.05	58.31	110.40
1	J	32	ILE	O-C-N	21.22	156.65	122.70
1	J	32	ILE	CA-C-N	-18.02	77.56	117.20
8	K	354	THR	N-CA-CB	-14.10	83.50	110.30
4	C	447	TYR	N-CA-C	13.90	148.54	111.00

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	132	ARG	Sidechain
1	J	153	ARG	Sidechain
1	J	163	ARG	Sidechain
1	J	171	ARG	Sidechain
1	J	42	GLU	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	3962	0	3996	179	0
2	A	2071	0	2012	24	0
2	B	2071	0	2012	32	0
3	D	3263	0	3260	44	0
3	E	3263	0	3259	33	0
4	C	4284	0	4147	75	0
4	F	4039	0	3904	64	0
5	G	931	0	970	16	0
6	H	2393	0	2475	45	0
7	I	1469	0	1534	15	0
8	K	4089	0	4163	156	0
9	L	390	0	378	3	0
10	A	62	0	43	7	0
10	E	62	0	42	10	0
11	C	7	0	5	3	0
12	F	21	0	19	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	F	28	0	20	15	0
14	H	18	0	0	0	0
14	I	36	0	0	0	0
15	K	1	0	0	0	0
16	K	62	0	24	2	0
17	K	2	0	0	0	0
All	All	32524	0	32263	631	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 631 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:179:TYR:CE1	1:J:295:PHE:HB3	1.36	1.59
3:E:367:TYR:OH	10:E:601:F43:C5A	1.67	1.40
1:J:179:TYR:CD1	1:J:295:PHE:HB3	1.61	1.33
1:J:179:TYR:CE1	1:J:295:PHE:CB	2.16	1.26
1:J:42:GLU:HA	1:J:172:GLU:HB3	1.24	1.13

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	J	493/501 (98%)	435 (88%)	47 (10%)	11 (2%)	5 1
2	A	257/260 (99%)	253 (98%)	4 (2%)	0	100 100
2	B	257/260 (99%)	252 (98%)	5 (2%)	0	100 100
3	D	440/443 (99%)	422 (96%)	18 (4%)	0	100 100
3	E	440/443 (99%)	422 (96%)	17 (4%)	1 (0%)	44 43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	C	539/553 (98%)	515 (96%)	22 (4%)	2 (0%)	30 26
4	F	511/553 (92%)	490 (96%)	20 (4%)	1 (0%)	44 43
5	G	110/183 (60%)	107 (97%)	3 (3%)	0	100 100
6	H	294/304 (97%)	283 (96%)	11 (4%)	0	100 100
7	I	192/234 (82%)	183 (95%)	9 (5%)	0	100 100
8	K	519/531 (98%)	450 (87%)	57 (11%)	12 (2%)	5 1
9	L	45/93 (48%)	45 (100%)	0	0	100 100
All	All	4097/4358 (94%)	3857 (94%)	213 (5%)	27 (1%)	21 13

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	445	GLY
8	K	103	GLU
8	K	231	GLU
8	K	265	VAL
8	K	270	GLU

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	J	452/454 (100%)	377 (83%)	75 (17%)	2 0
2	A	223/224 (100%)	212 (95%)	11 (5%)	21 17
2	B	223/224 (100%)	219 (98%)	4 (2%)	54 57
3	D	341/342 (100%)	332 (97%)	9 (3%)	41 41
3	E	341/342 (100%)	327 (96%)	14 (4%)	26 23
4	C	437/439 (100%)	415 (95%)	22 (5%)	20 16
4	F	412/439 (94%)	389 (94%)	23 (6%)	17 13
5	G	104/168 (62%)	95 (91%)	9 (9%)	8 4
6	H	264/271 (97%)	248 (94%)	16 (6%)	15 11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	I	160/186 (86%)	149 (93%)	11 (7%)	13 8
8	K	449/458 (98%)	378 (84%)	71 (16%)	2 0
9	L	43/81 (53%)	41 (95%)	2 (5%)	22 18
All	All	3449/3628 (95%)	3182 (92%)	267 (8%)	13 5

5 of 267 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	K	269	LYS
8	K	291	VAL
8	K	471	ILE
3	E	114	VAL
3	E	98	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	459	ASN
8	K	102	ASN
8	K	210	ASN
8	K	228	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MHS	F	261	4	7,11,12	0.78	0	6,14,16	0.87	0
4	MGN	C	403	-	6,9,10	0.69	0	5,12,14	0.74	0
4	AGM	C	275	3,4	10,11,12	0.36	0	6,13,15	0.69	0
4	MHS	C	261	4	7,11,12	0.78	0	6,14,16	1.00	0
4	AGM	F	275	4	10,11,12	0.45	0	6,13,15	0.26	0
4	GL3	C	448	-	2,3,4	1.40	0	1,2,4	0.17	0
4	SMC	C	455	4	5,6,7	0.80	0	2,6,8	1.69	0
4	MGN	F	403	4	6,9,10	0.68	0	5,12,14	0.76	0
4	GL3	F	448	4	2,3,4	0.48	0	1,2,4	0.35	0
4	SMC	F	455	4	5,6,7	0.71	0	2,6,8	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MHS	F	261	4	-	2/5/6/8	0/1/1/1
4	MGN	C	403	-	-	1/7/9/12	-
4	AGM	C	275	3,4	-	1/10/11/13	-
4	MHS	C	261	4	-	2/5/6/8	0/1/1/1
4	AGM	F	275	4	-	6/10/11/13	-
4	GL3	C	448	-	-	1/1/1/2	-
4	SMC	C	455	4	-	2/3/5/7	-
4	MGN	F	403	4	-	0/7/9/12	-
4	GL3	F	448	4	-	1/1/1/2	-
4	SMC	F	455	4	-	2/3/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	261	MHS	O-C-CA-CB
4	C	448	GL3	S-C-CA-N
4	C	455	SMC	N-CA-CB-SG
4	C	455	SMC	CA-CB-SG-CS
4	F	261	MHS	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	261	MHS	1	0
4	C	448	GL3	12	0
4	C	455	SMC	4	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
12	TP7	F	601	-	19,20,20	0.68	0	24,26,26	0.58	0
16	ATP	K	603	17	26,33,33	0.88	0	31,52,52	0.81	1 (3%)
14	S5Q	I	202	7	18,30,30	2.61	11 (61%)	-		
13	SHT	F	602	-	26,27,27	2.04	7 (26%)	30,36,36	2.00	6 (20%)
10	F43	E	601	-	61,71,71	1.96	4 (6%)	64,118,118	1.03	5 (7%)
11	COM	C	601	10	6,6,6	1.81	3 (50%)	7,8,8	2.81	4 (57%)
14	S5Q	H	401	6	18,30,30	2.60	12 (66%)	-		
14	S5Q	I	201	7	18,30,30	2.59	11 (61%)	-		
10	F43	A	601	11,4	61,71,71	2.04	4 (6%)	64,118,118	1.11	4 (6%)
16	ATP	K	602	17	26,33,33	0.97	2 (7%)	31,52,52	0.75	1 (3%)

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
12	TP7	F	601	-	-	5/24/24/24	-
16	ATP	K	603	17	-	4/18/38/38	0/3/3/3
13	SHT	F	602	-	1/1/6/9	17/31/31/31	-
10	F43	E	601	-	-	9/28/185/185	-
11	COM	C	601	10	-	0/4/4/4	-
10	F43	A	601	11,4	-	14/28/185/185	-
16	ATP	K	602	17	-	3/18/38/38	0/3/3/3

The worst 5 of 54 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	601	F43	NI-NA	9.76	2.10	1.89
10	E	601	F43	NI-NA	9.38	2.09	1.89
10	A	601	F43	NI-NB	9.21	2.09	1.89
10	E	601	F43	NI-NB	9.08	2.09	1.89
10	A	601	F43	NI-ND	7.16	2.04	1.89

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	F	602	SHT	CK3-CK2-CK1	-6.48	111.95	125.85
13	F	602	SHT	OS1-SG2-CD	4.10	111.85	106.92
11	C	601	COM	O2S-S2-C2	3.90	111.61	106.92
11	C	601	COM	O1S-S2-C2	3.80	111.49	106.92
11	C	601	COM	O2S-S2-O1S	-3.77	100.91	113.95

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	F	602	SHT	CB

5 of 52 torsion outliers are listed below:

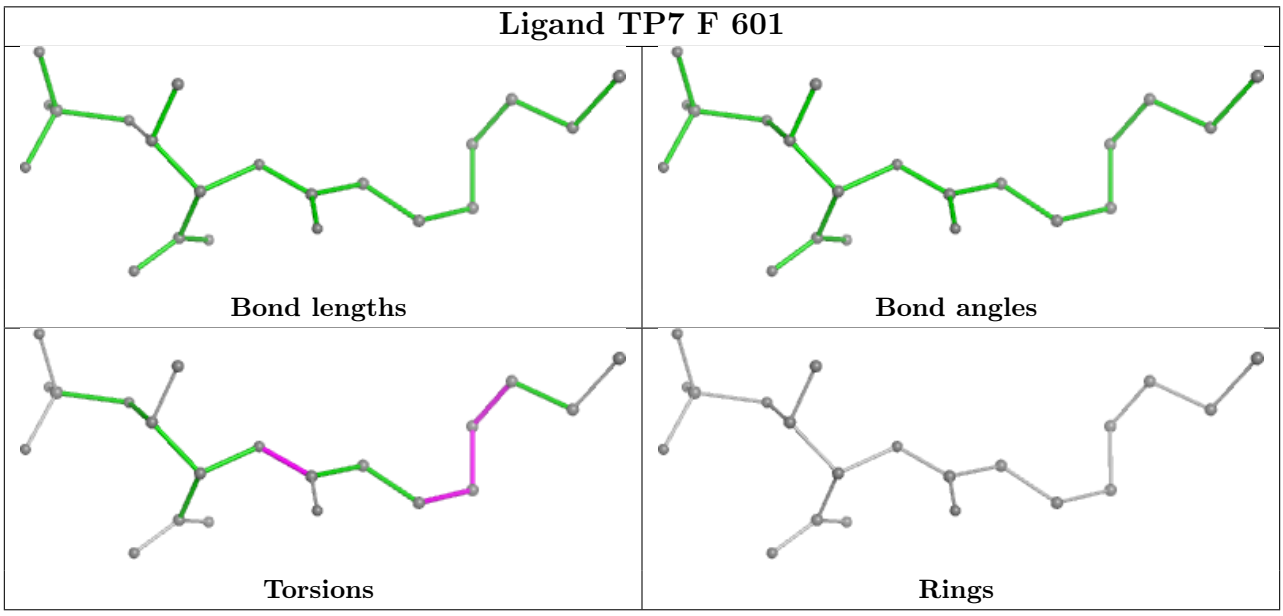
Mol	Chain	Res	Type	Atoms
10	A	601	F43	C2A-C3A-CAA-CBA
10	A	601	F43	C4A-C3A-CAA-CBA
10	E	601	F43	C1A-C2A-C5A-C6A
10	E	601	F43	C9A-C2A-C5A-C6A
10	E	601	F43	C2A-C3A-CAA-CBA

There are no ring outliers.

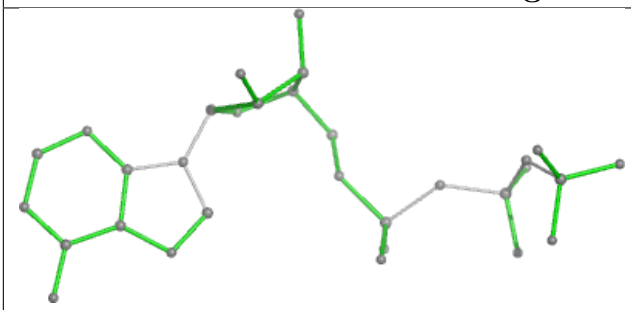
6 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	601	TP7	3	0
16	K	603	ATP	2	0
13	F	602	SHT	15	0
10	E	601	F43	10	0
11	C	601	COM	3	0
10	A	601	F43	7	0

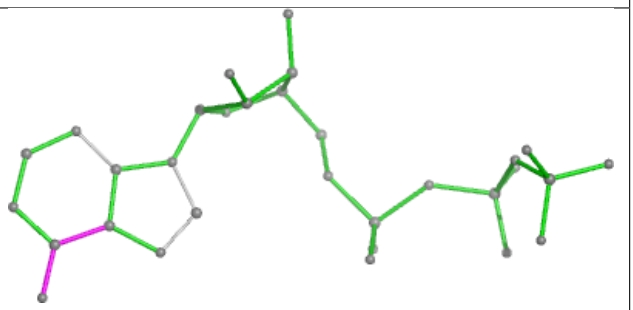
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



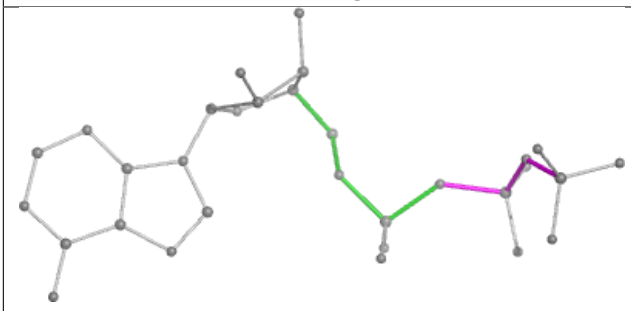
Ligand ATP K 603



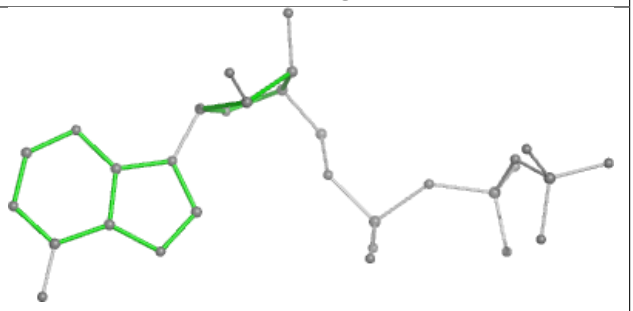
Bond lengths



Bond angles

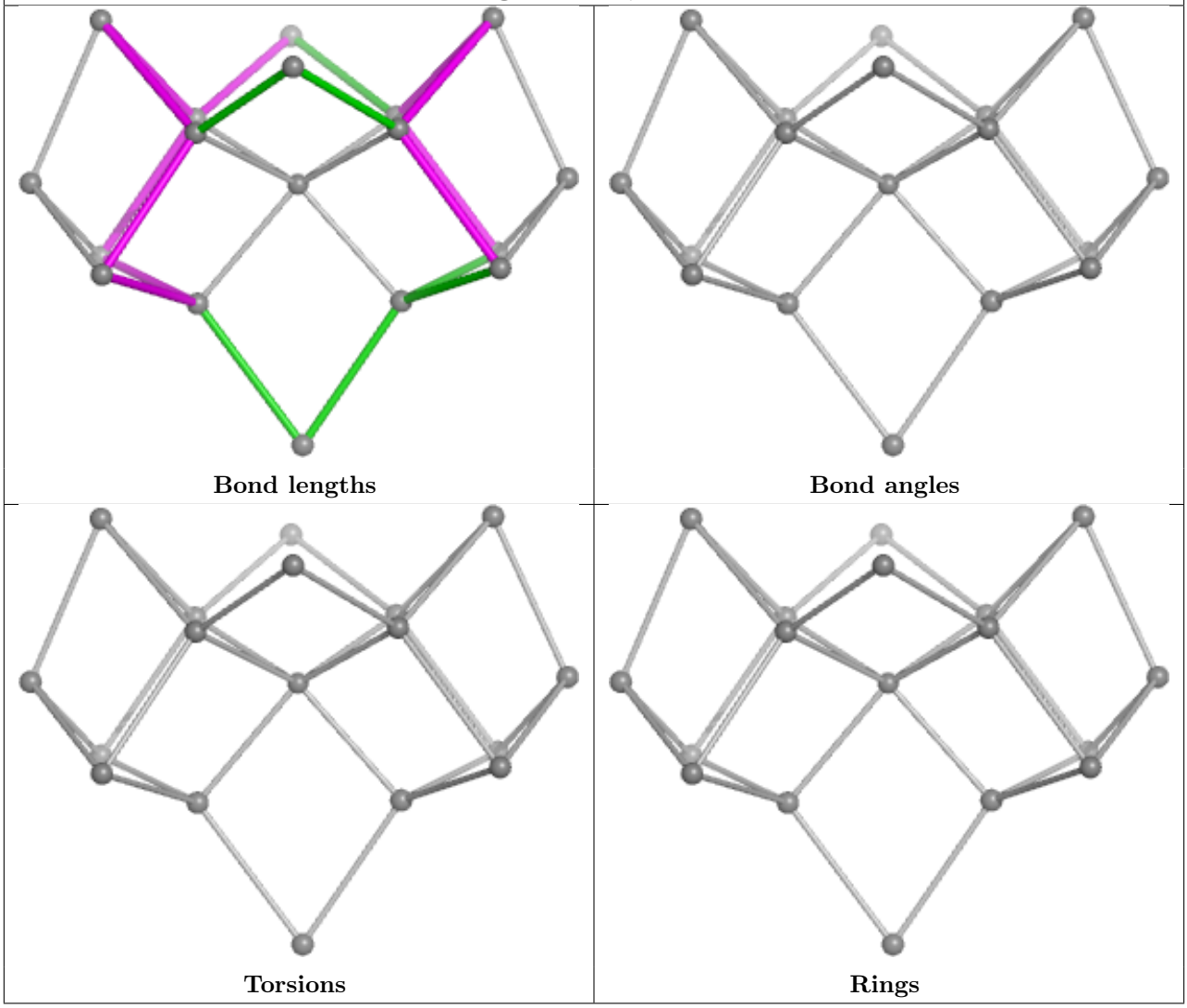


Torsions

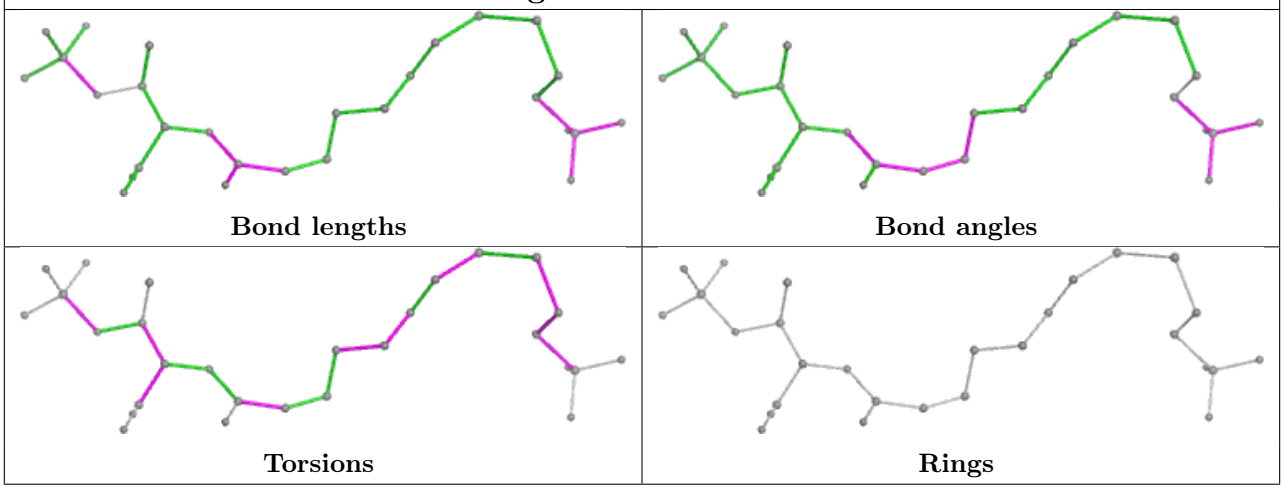


Rings

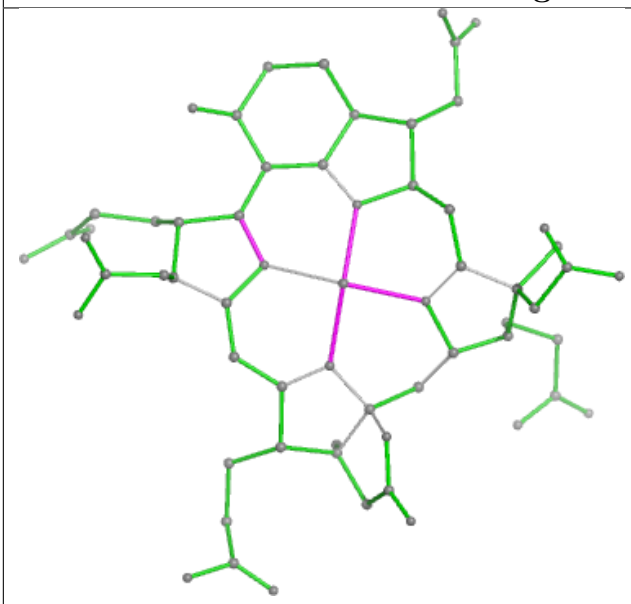
Ligand S5Q I 202



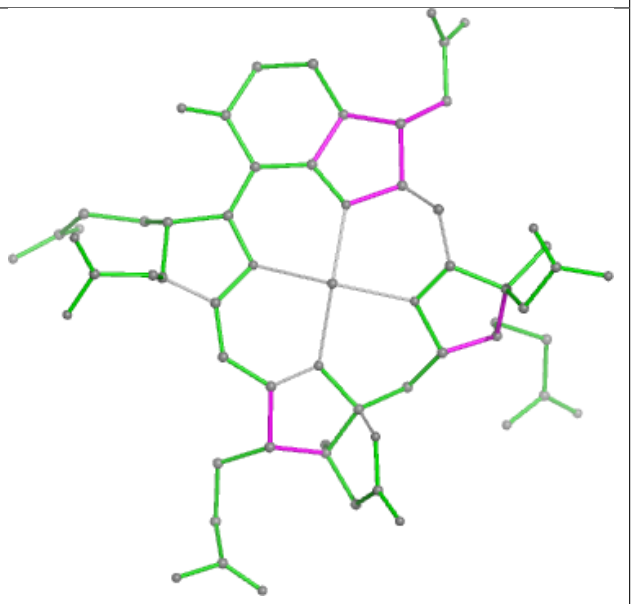
Ligand SHT F 602



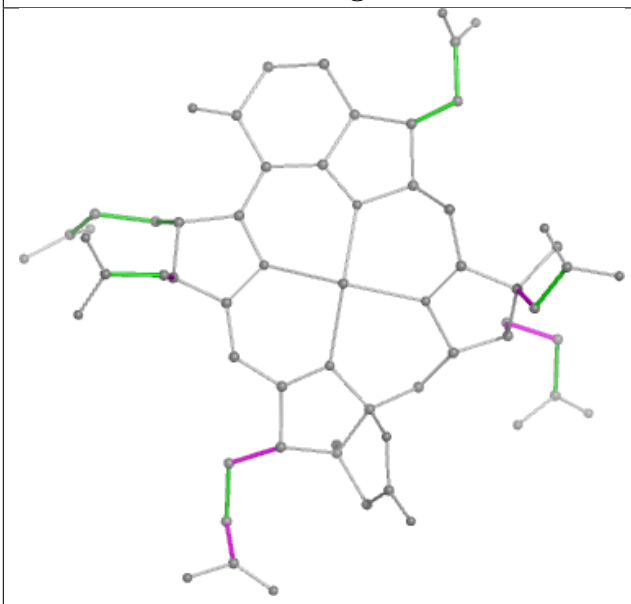
Ligand F43 E 601



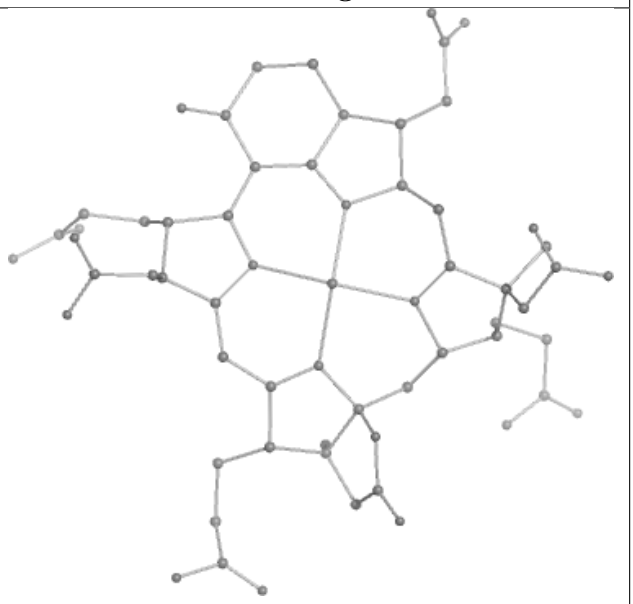
Bond lengths



Bond angles

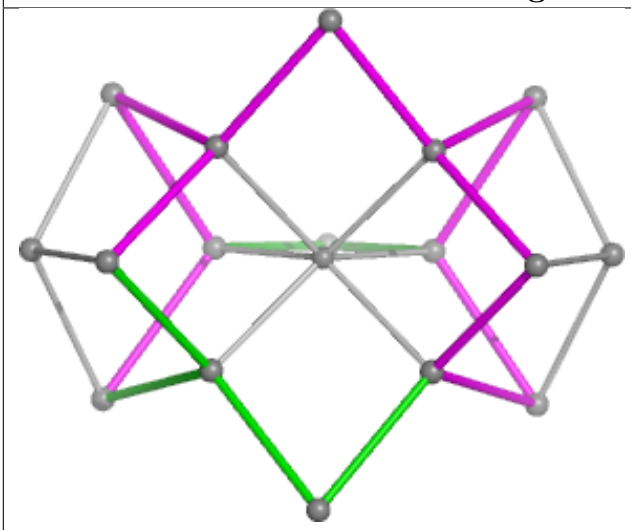


Torsions

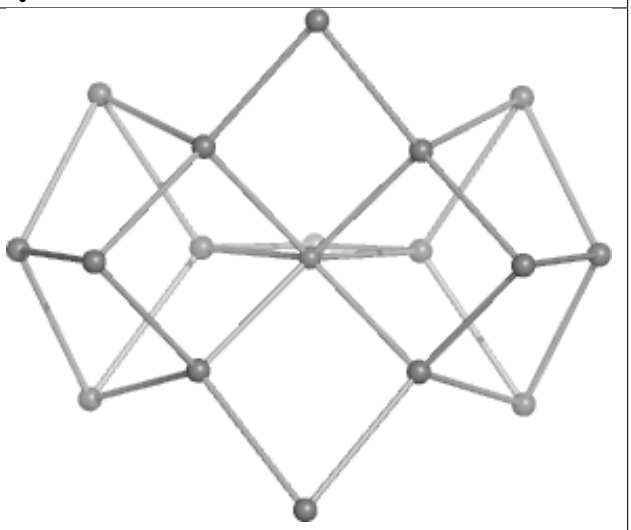


Rings

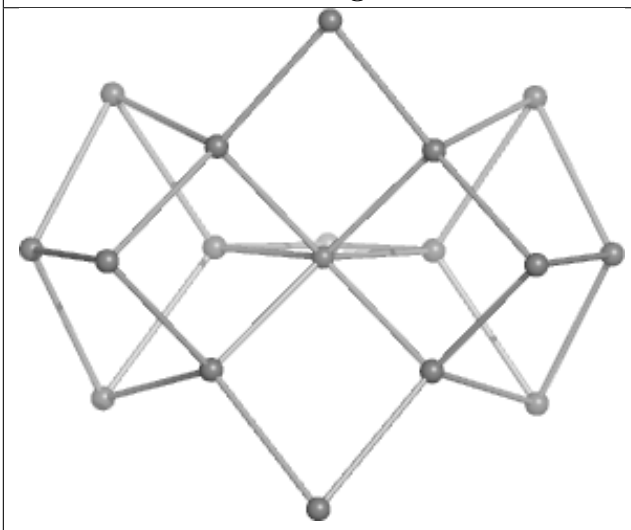
Ligand S5Q H 401



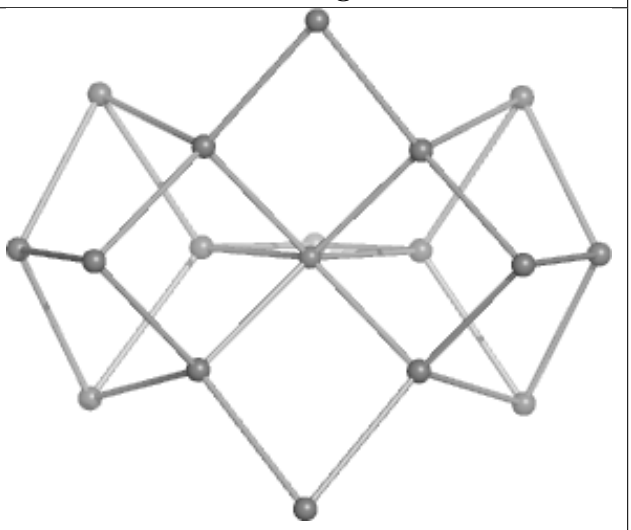
Bond lengths



Bond angles

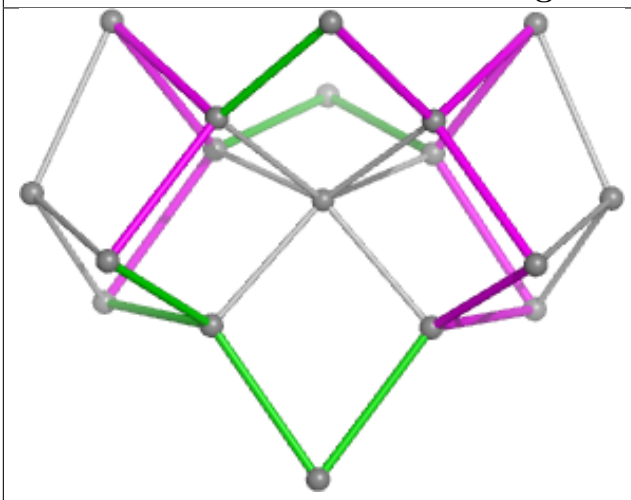


Torsions

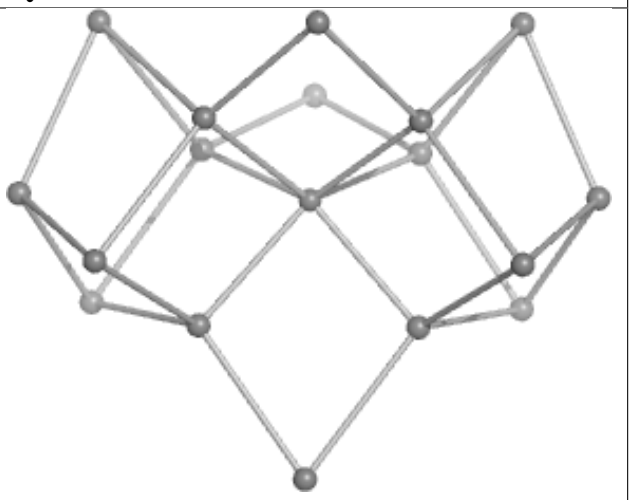


Rings

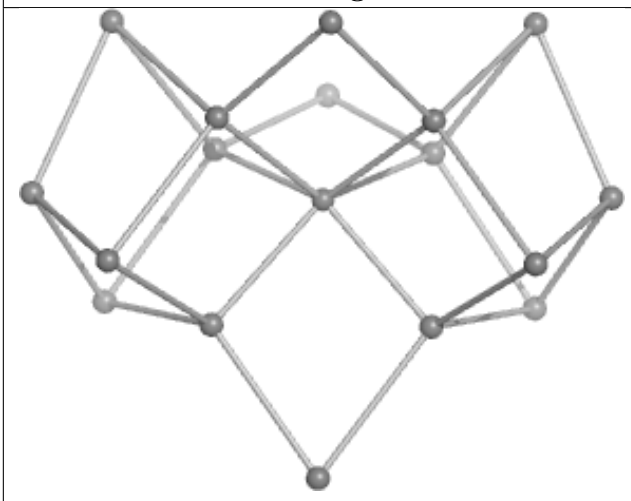
Ligand S5Q I 201



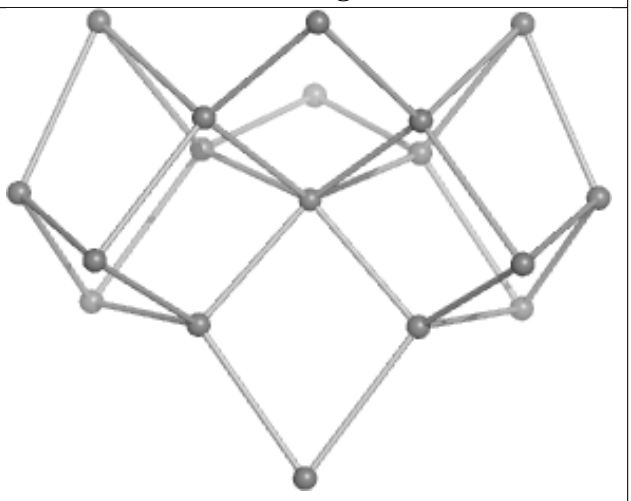
Bond lengths



Bond angles

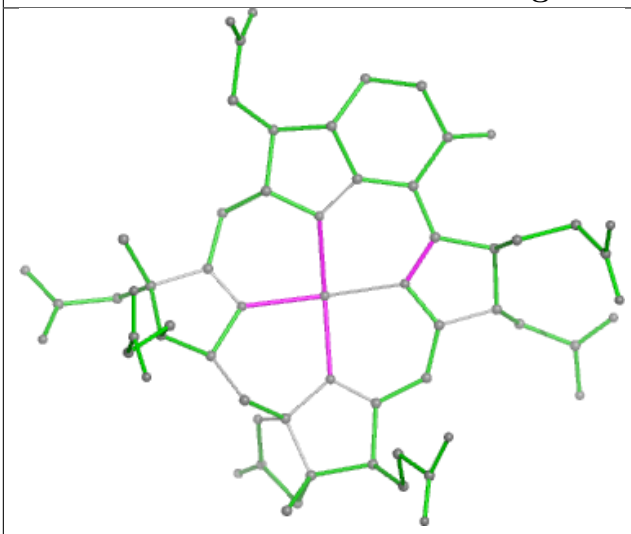


Torsions

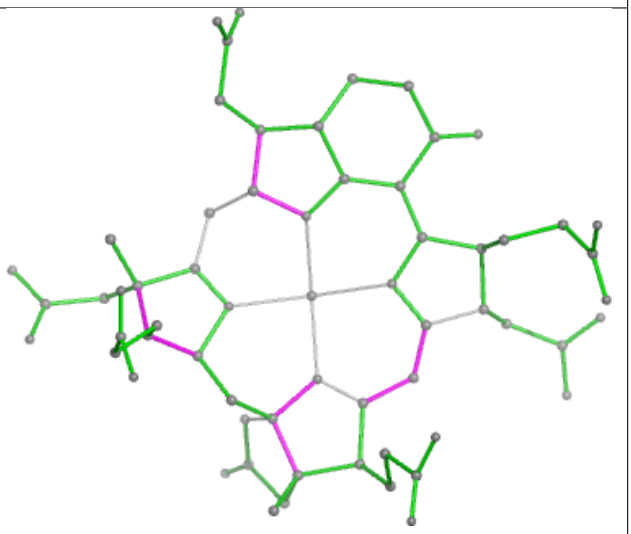


Rings

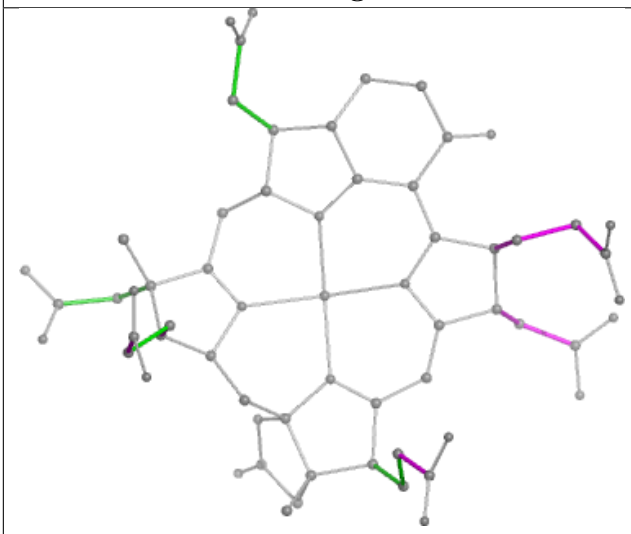
Ligand F43 A 601



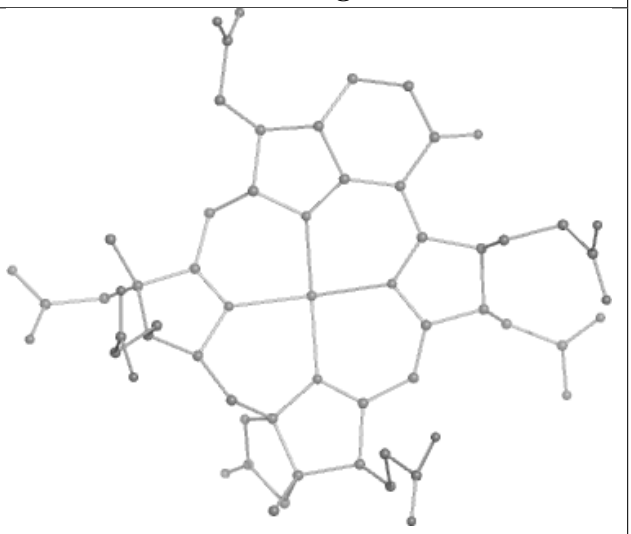
Bond lengths



Bond angles

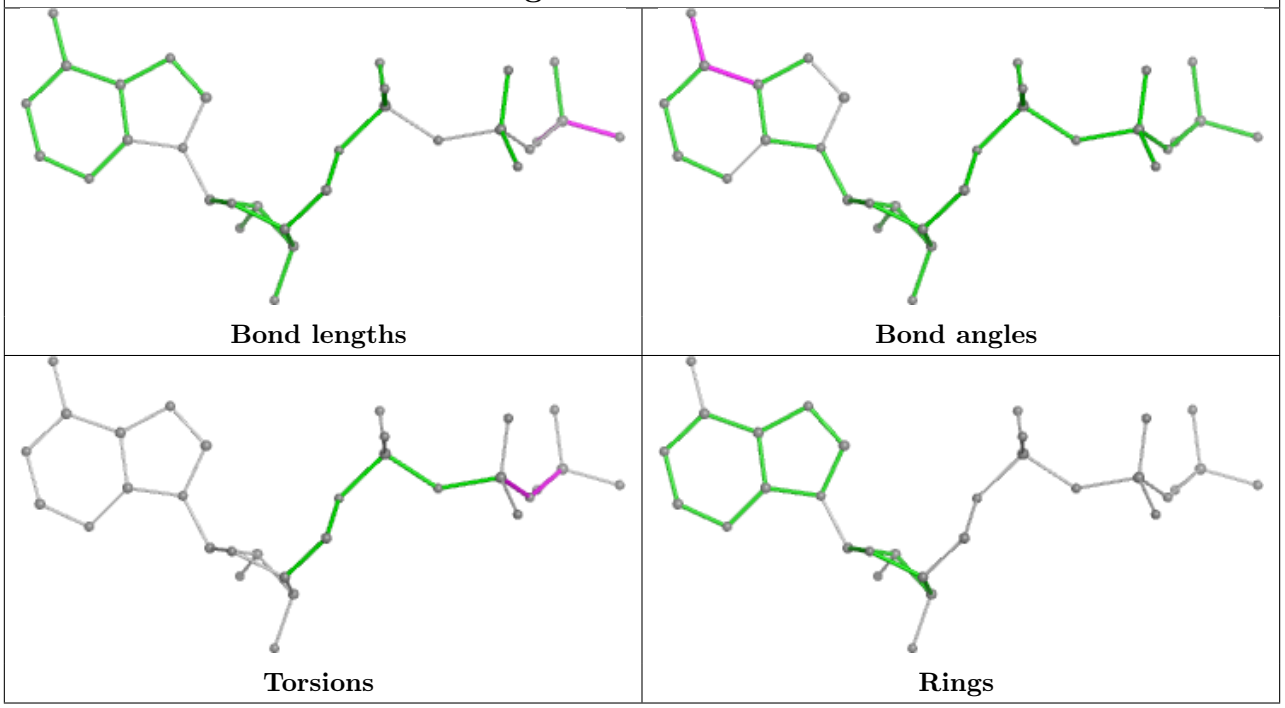


Torsions



Rings

Ligand ATP K 602



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	C	4
1	J	2

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	183:THR	C	184:ASN	N	3.52
1	C	402:SER	C	403:MGN	N	3.12
1	C	403:MGN	C	404:ARG	N	3.07
1	C	447:TYR	C	448:GL3	N	3.00
1	J	22:GLU	C	23:TYR	N	2.59

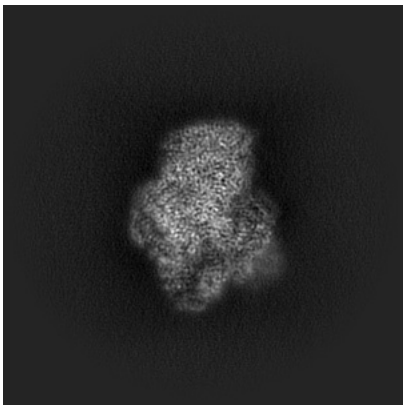
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51767. These allow visual inspection of the internal detail of the map and identification of artifacts.

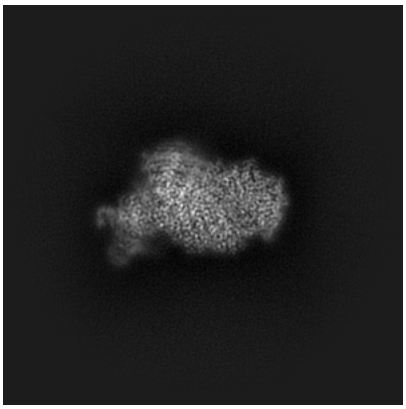
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

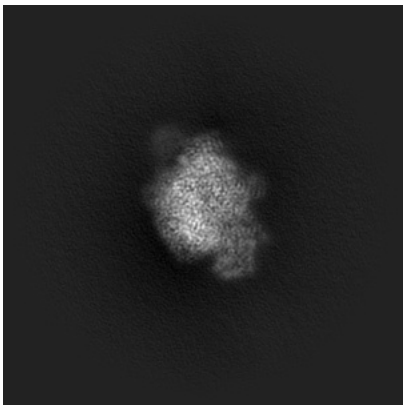
6.1.1 Primary map



X

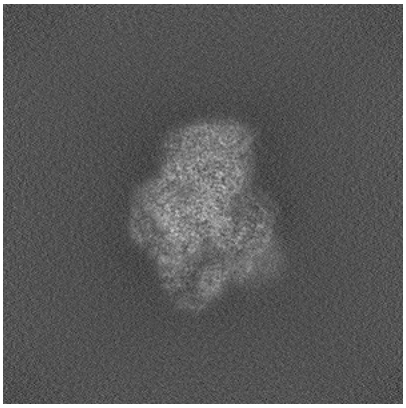


Y

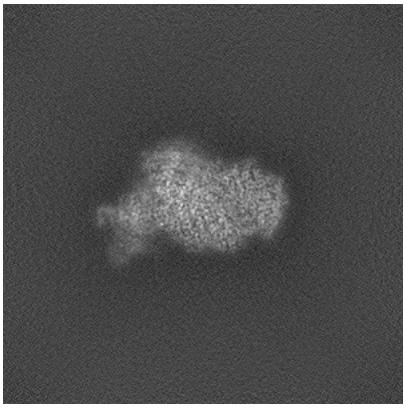


Z

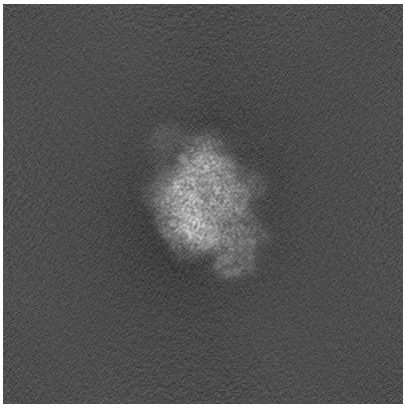
6.1.2 Raw map



X



Y

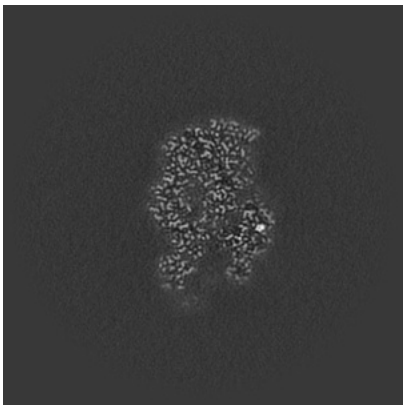


Z

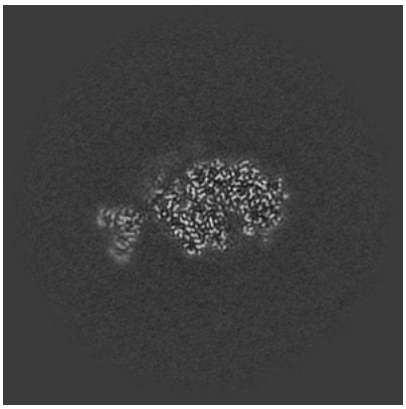
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

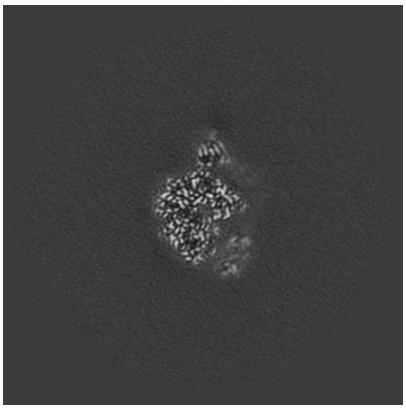
6.2.1 Primary map



X Index: 300

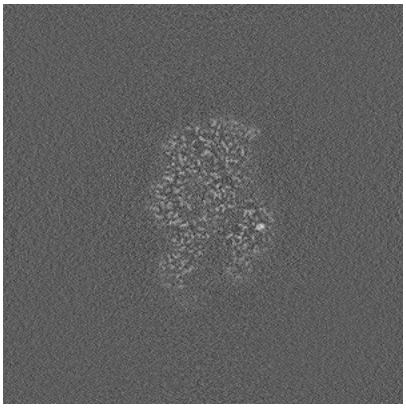


Y Index: 300

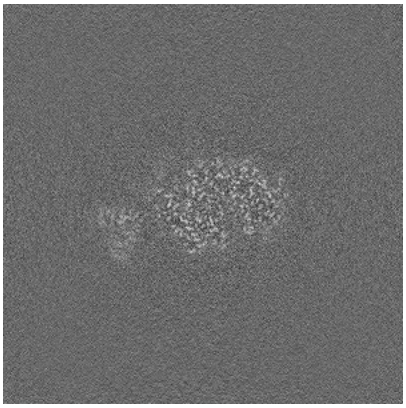


Z Index: 300

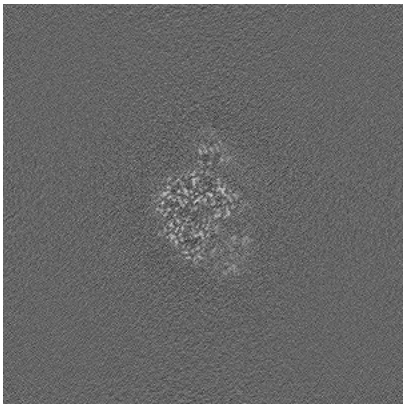
6.2.2 Raw map



X Index: 300



Y Index: 300

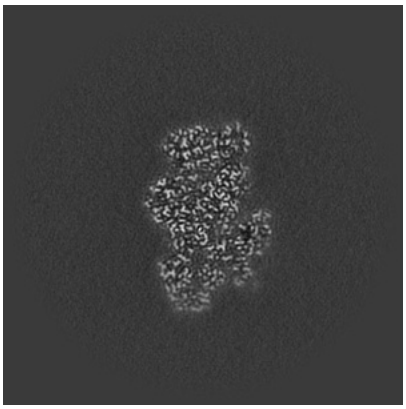


Z Index: 300

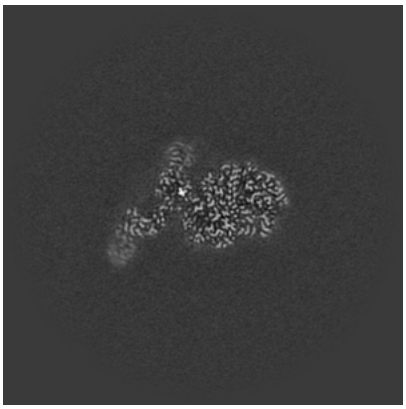
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

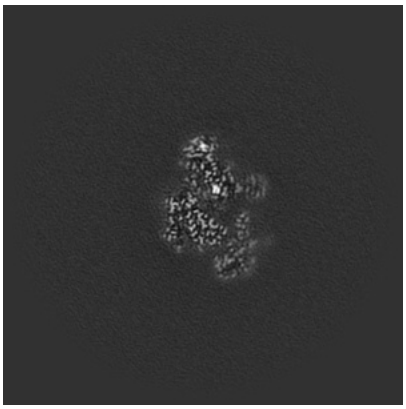
6.3.1 Primary map



X Index: 286

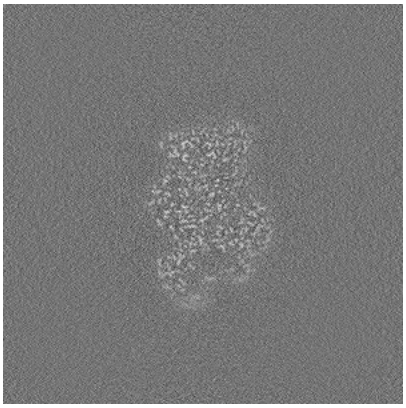


Y Index: 325

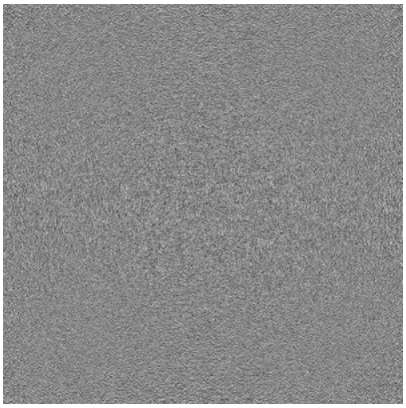


Z Index: 267

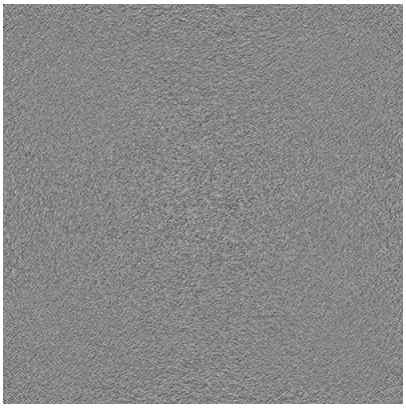
6.3.2 Raw map



X Index: 294



Y Index: 0

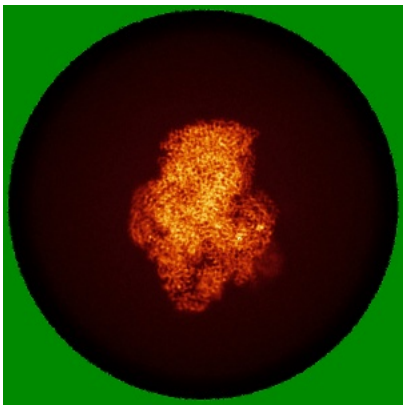


Z Index: 0

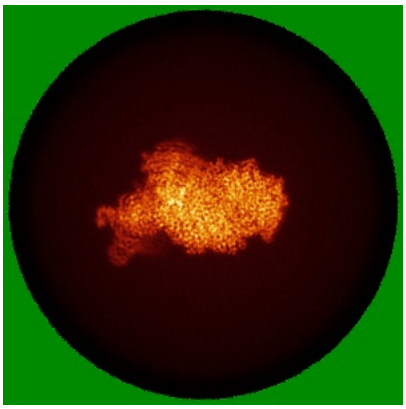
The images above show the largest variance slices of the map in three orthogonal directions.

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

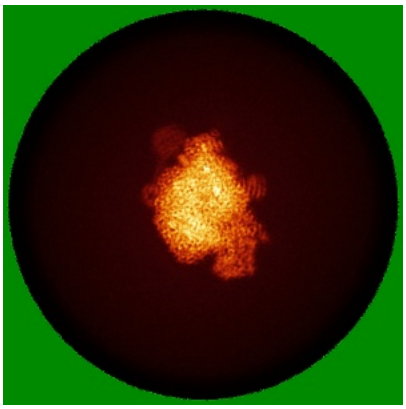
6.4.1 Primary map



X

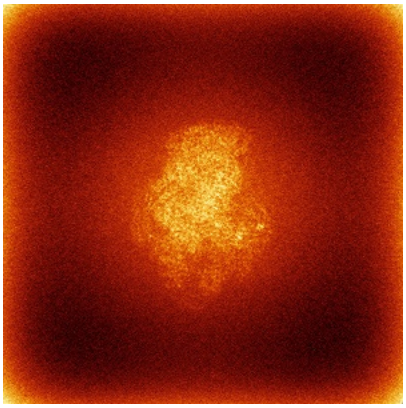


Y

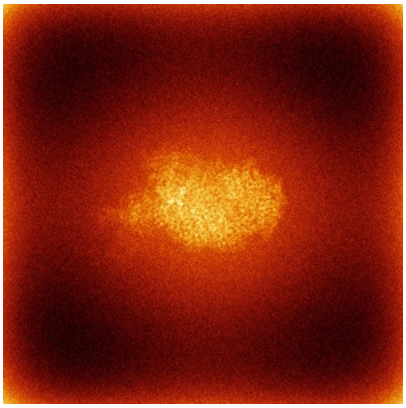


Z

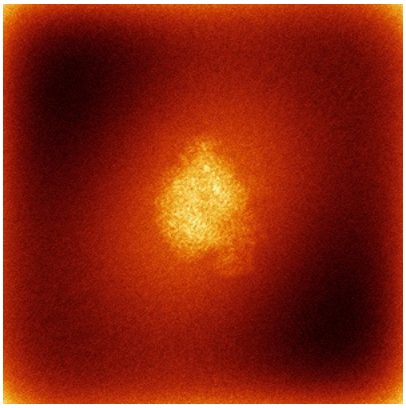
6.4.2 Raw map



X



Y

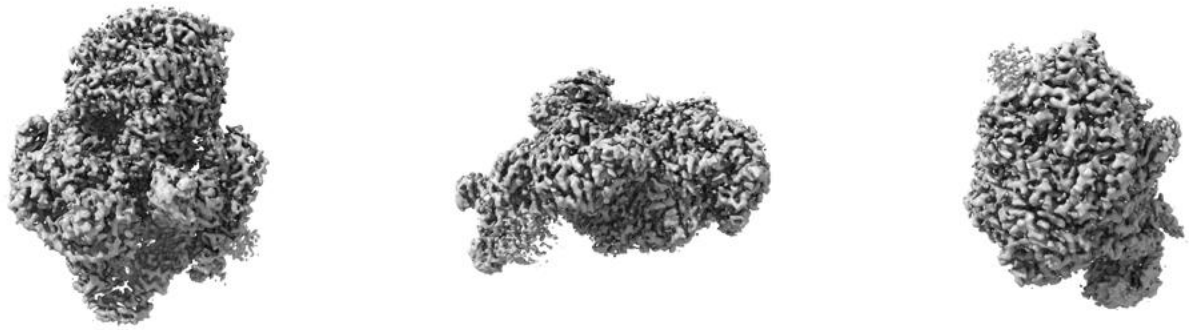


Z

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)

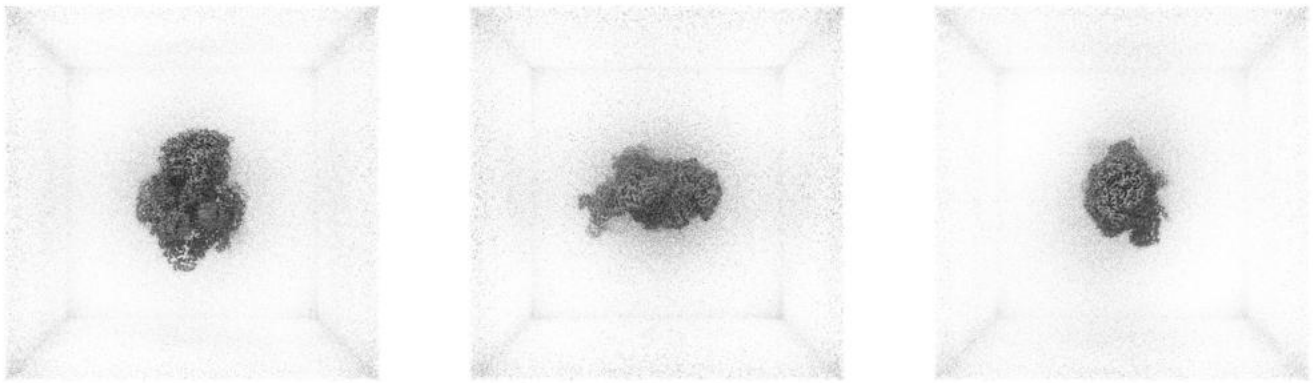
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0197. 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.

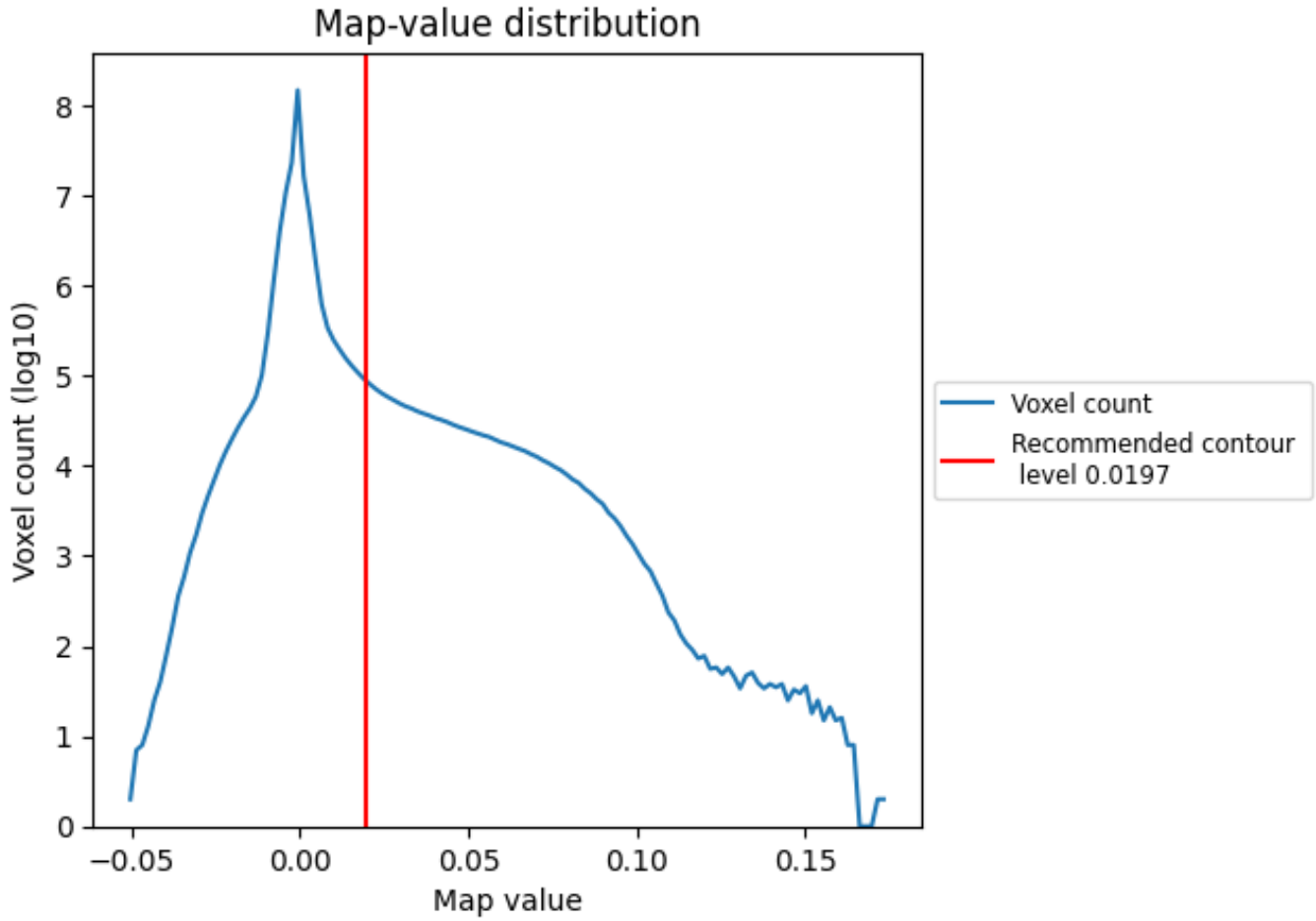
6.6 Mask visualisation (i)

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

7 Map analysis

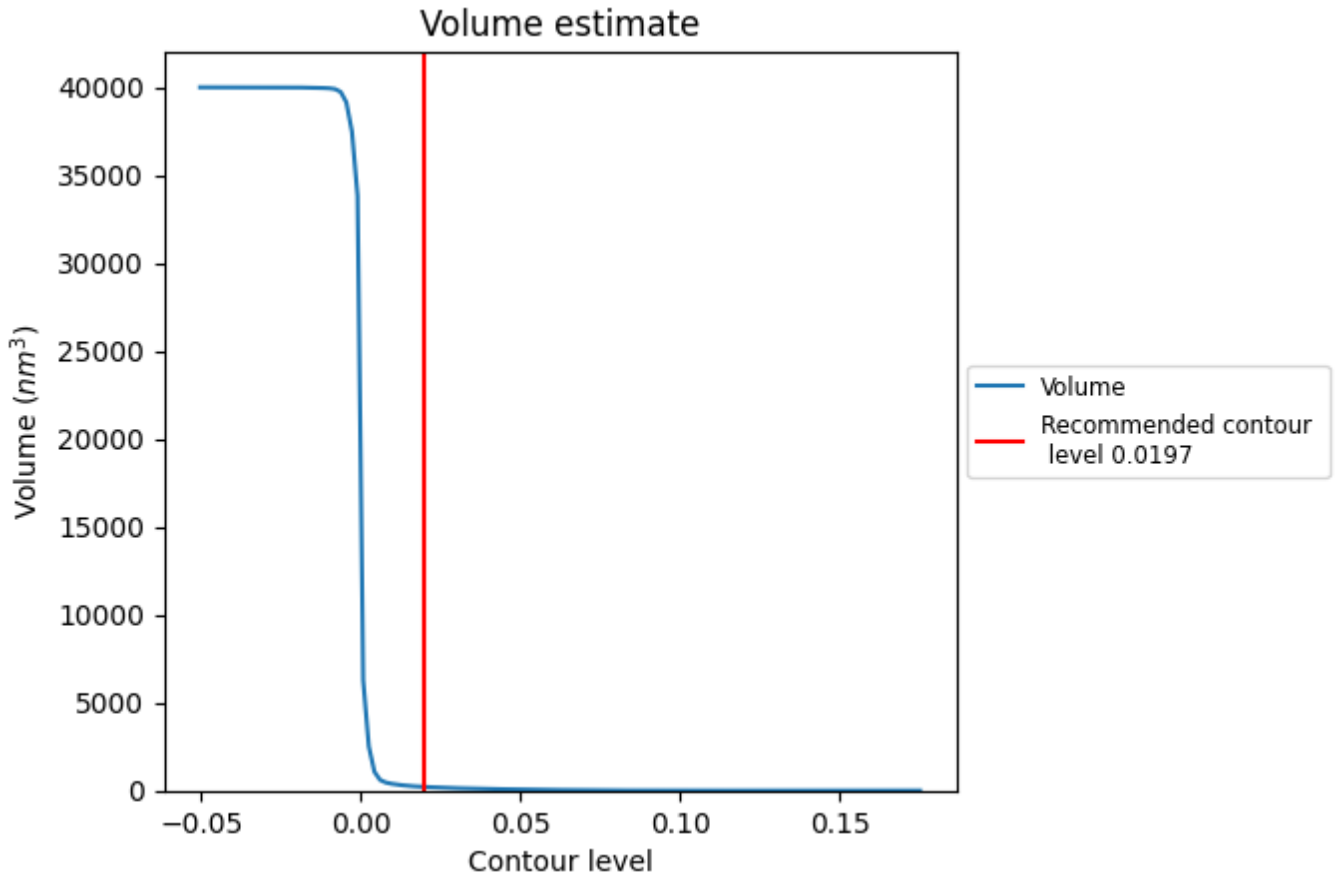
This section contains the results of statistical analysis of the map.

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.

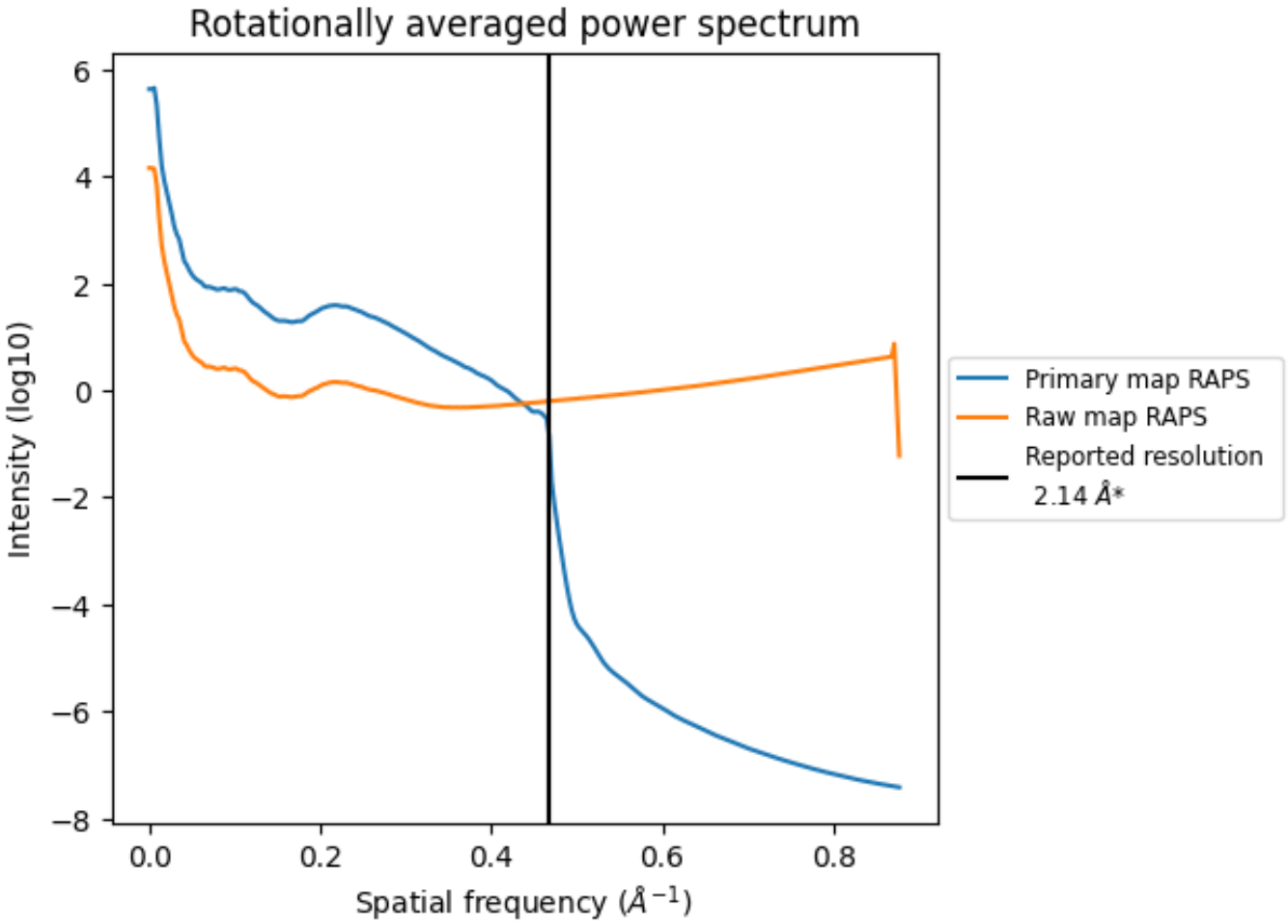
7.2 Volume estimate (i)



The volume at the recommended contour level is 209 nm^3; this corresponds to an approximate mass of 189 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)

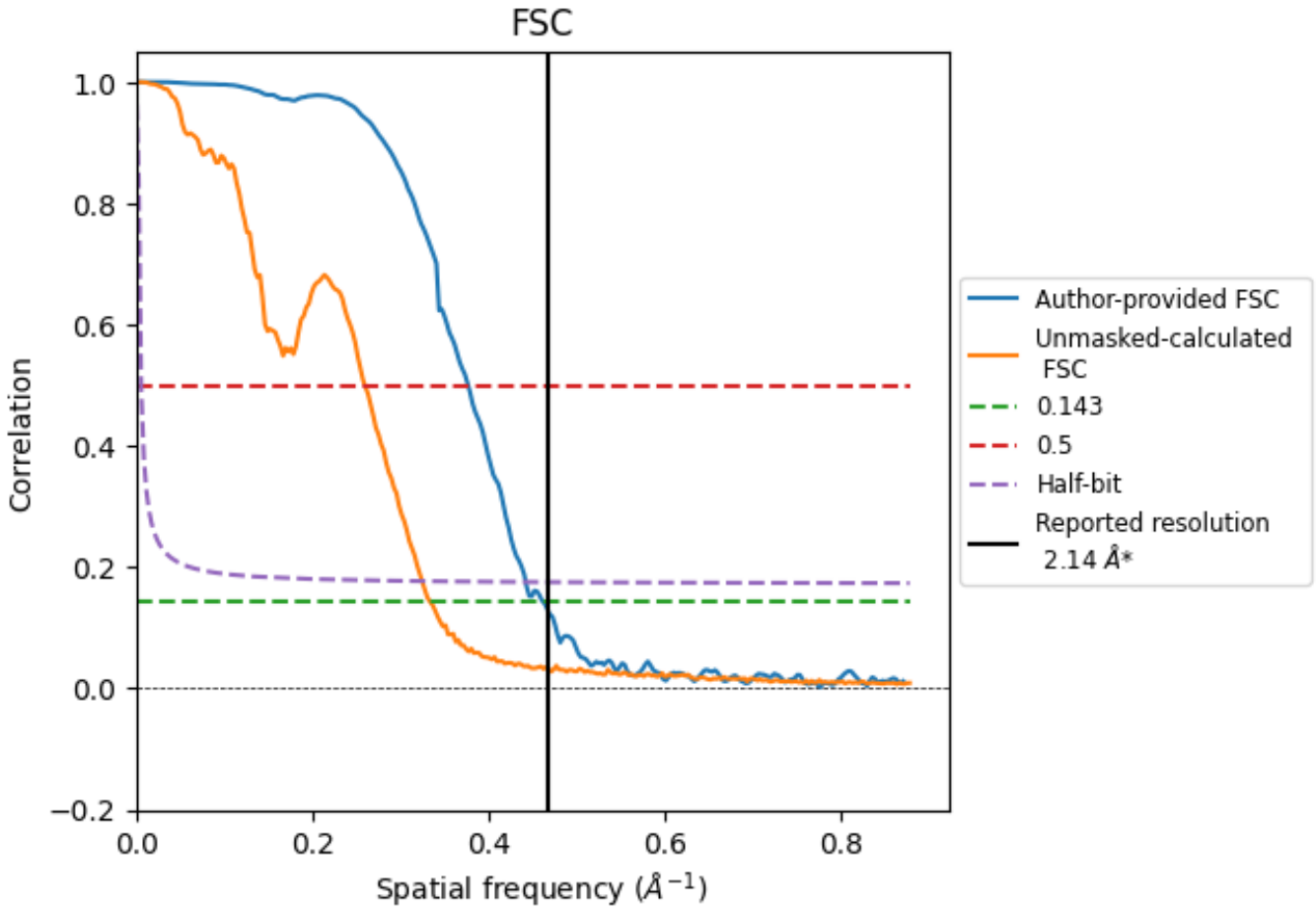


*Reported resolution corresponds to spatial frequency of 0.467 Å^{-1}

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 0.467 Å^{-1}

8.2 Resolution estimates (i)

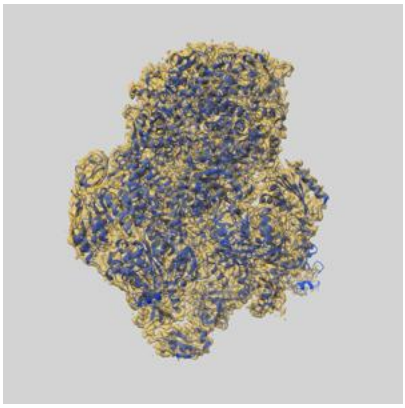
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.14	-	-
Author-provided FSC curve	2.17	2.66	2.26
Unmasked-calculated*	3.00	3.86	3.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.00 differs from the reported value 2.14 by more than 10 %

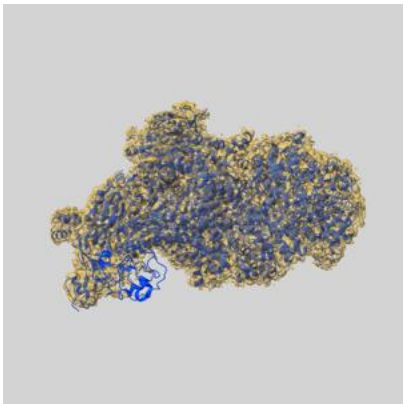
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51767 and PDB model 9H1L. Per-residue inclusion information can be found in section 3 on page 11.

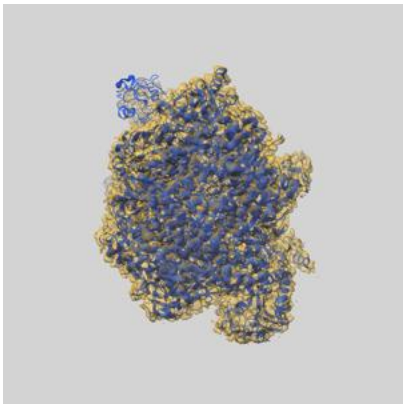
9.1 Map-model overlay



X



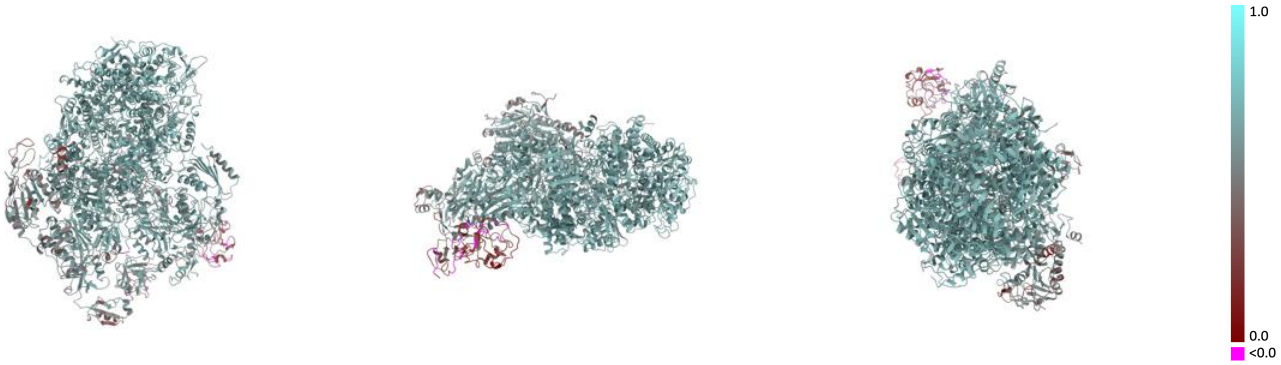
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0197 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.

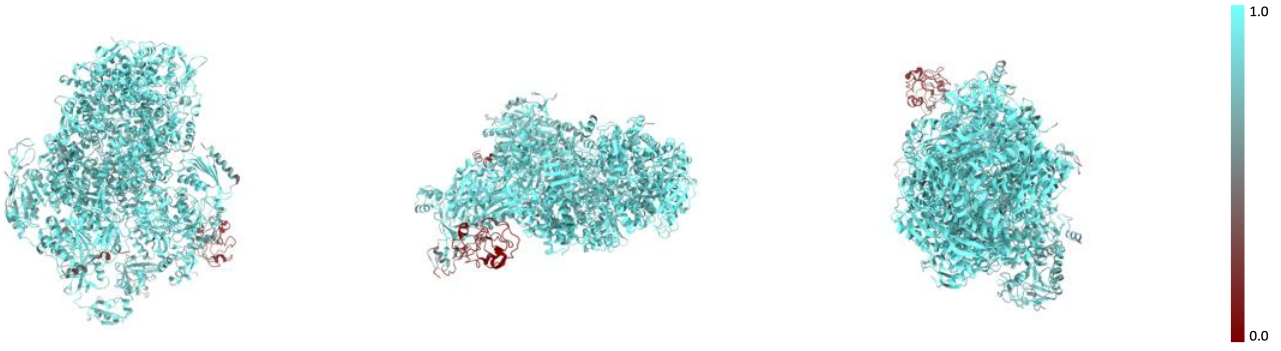
9.2 Q-score mapped to coordinate model



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.

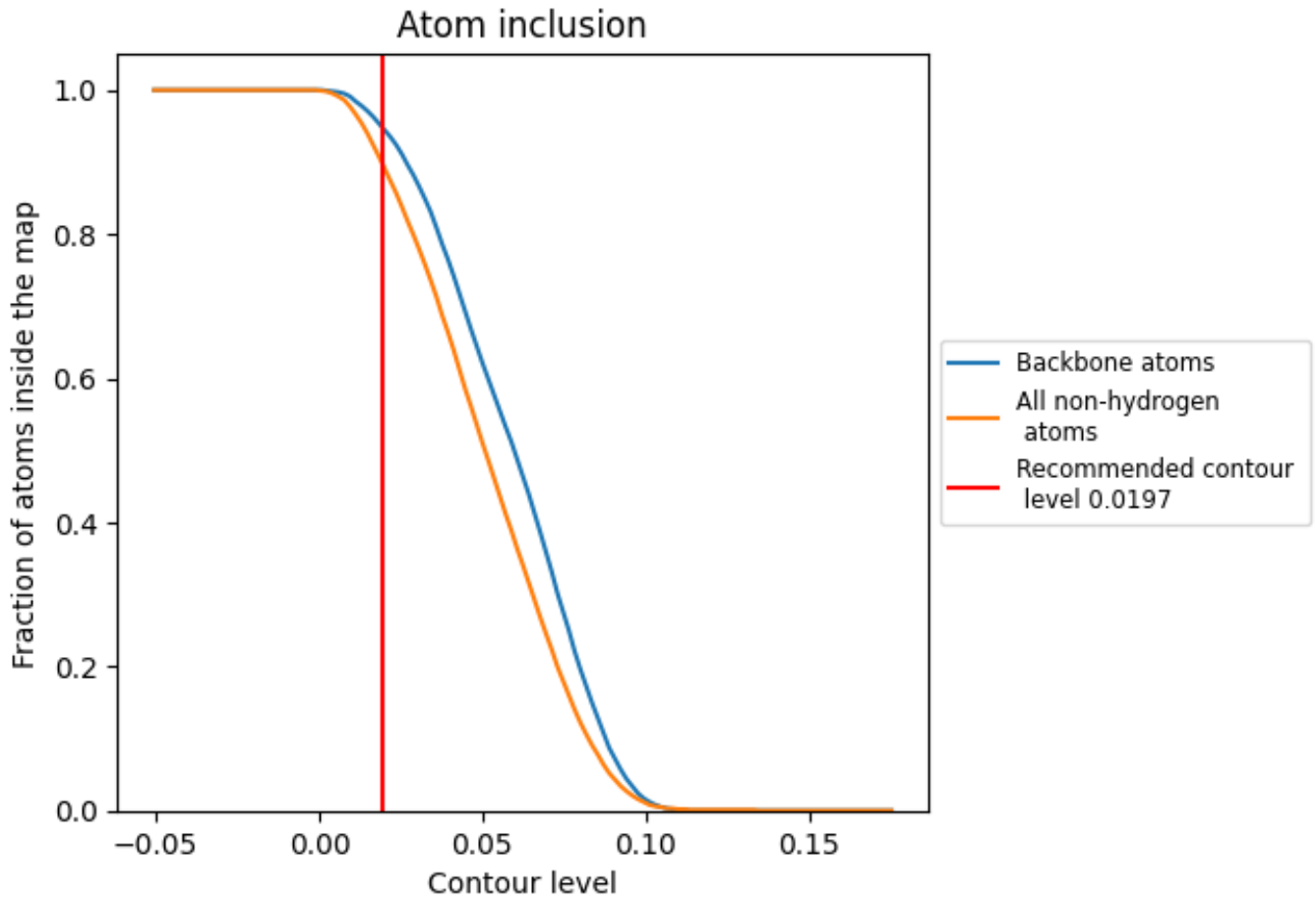
9.3 Atom inclusion mapped to coordinate model



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 (0.0197).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0197) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8950	0.5990
A	0.9520	0.6390
B	0.9640	0.6610
C	0.9530	0.6540
D	0.9690	0.6510
E	0.9650	0.6530
F	0.9370	0.6490
G	0.8790	0.6090
H	0.9200	0.6020
I	0.9340	0.6260
J	0.6300	0.4090
K	0.8570	0.5370
L	0.7400	0.4770