



## wwPDB EM Validation Summary Report ⓘ

Jun 4, 2026 – 12:07 pm BST

PDB ID : 9TDM / pdb\_00009tdm  
EMDB ID : EMD-55802  
Title : Cryo-EM structure of AccA3/AccD4/AccD5/AccE5 in complex with Propionyl-CoA  
Authors : Mullapudi, E.; Thai, H.M.; de Carvalho, L.P.S.; Wilmanns, M.  
Deposited on : 2025-11-24  
Resolution : 2.40 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](mailto: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>.

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

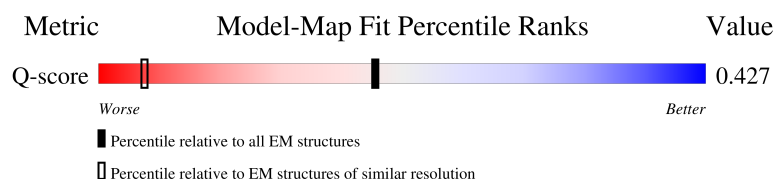
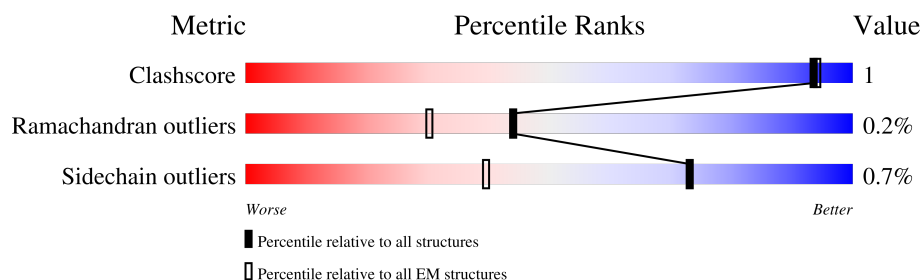
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.40 Å.

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





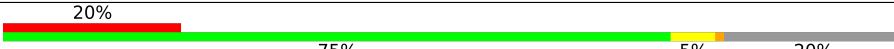
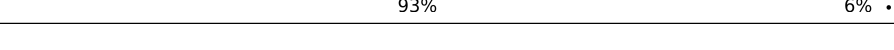
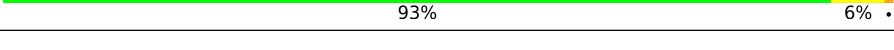
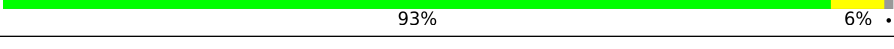
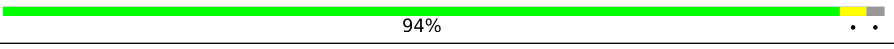
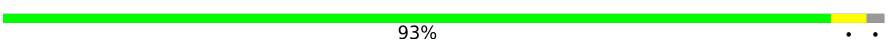
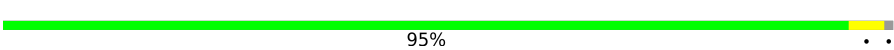

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5628 ( 1.90 - 2.90 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A3a	598	
1	A3b	598	
1	A3c	598	
1	A3d	598	

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Mol	Chain	Length	Quality of chain
1	A3e	598	 87% 9% .
1	A3f	598	 13% 88% . . 7%
1	A3g	598	 20% 75% 5% . 20%
1	A3h	598	 17% 88% . . 8%
2	D4a	517	 93% 6% .
2	D4b	517	 93% 6% .
3	D5a	542	 93% 6% .
3	D5b	542	 94% . .
3	D5c	542	 93% . .
3	D5d	542	 95% . .
4	E5a	94	 60% 6% 34%
4	E5b	94	 59% 7% 34%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 114486 atoms, of which 56504 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 Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A3a	574	Total	C	H	N	O	S	0	0
			8550	2712	4232	764	833	9		
1	A3b	555	Total	C	H	N	O	S	0	0
			8216	2612	4058	732	805	9		
1	A3c	481	Total	C	H	N	O	S	0	0
			7194	2297	3546	648	697	6		
1	A3d	553	Total	C	H	N	O	S	0	0
			8198	2603	4053	731	802	9		
1	A3e	576	Total	C	H	N	O	S	0	0
			8571	2719	4242	766	835	9		
1	A3f	555	Total	C	H	N	O	S	0	0
			8216	2612	4058	732	805	9		
1	A3g	481	Total	C	H	N	O	S	0	0
			7194	2297	3546	648	697	6		
1	A3h	553	Total	C	H	N	O	S	0	0
			8198	2603	4053	731	802	9		

- Molecule 2 is a protein called Propionyl-CoA carboxylase beta chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D4a	515	Total	C	H	N	O	S	0	0
			7817	2496	3878	689	738	16		
2	D4b	515	Total	C	H	N	O	S	0	0
			7817	2496	3878	689	738	16		

- Molecule 3 is a protein called Propionyl-CoA carboxylase beta chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D5a	538	Total	C	H	N	O	S	0	0
			8046	2577	3963	699	792	15		
3	D5b	530	Total	C	H	N	O	S	0	0
			7936	2541	3915	688	777	15		
3	D5c	530	Total	C	H	N	O	S	0	0
			7936	2541	3915	688	777	15		

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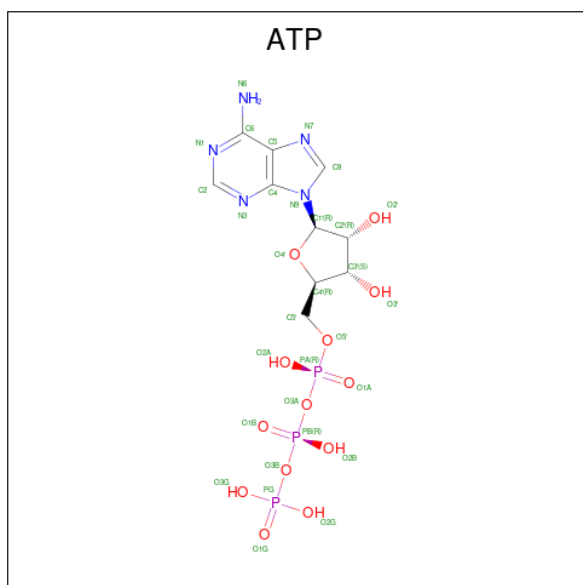
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Mol	Chain	Residues	Atoms						AltConf	Trace
3	D5d	538	Total	C	H	N	O	S	0	0
			8038	2575	3957	699	792	15		

- Molecule 4 is a protein called Acetyl-/propionyl-coenzyme A carboxylase AccE5.

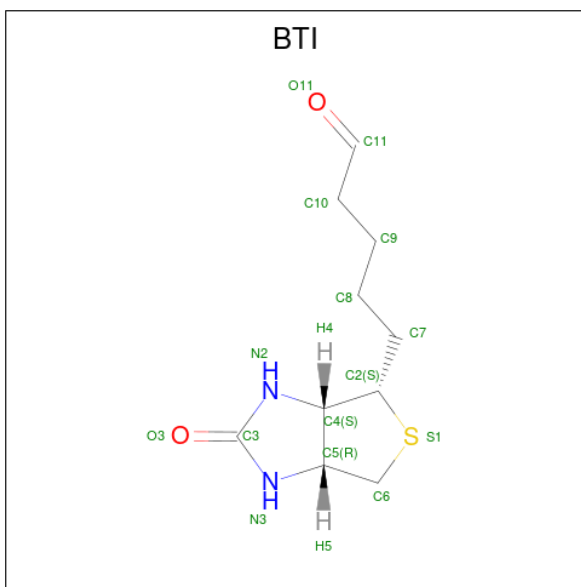
Mol	Chain	Residues	Atoms						AltConf	Trace
4	E5a	62	Total	C	H	N	O	S	0	0
			989	314	487	97	87	4		
4	E5b	62	Total	C	H	N	O	S	0	0
			989	314	487	97	87	4		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



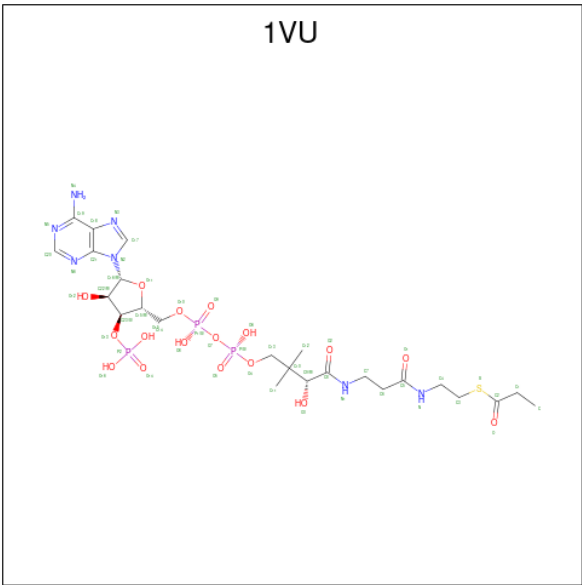
Mol	Chain	Residues	Atoms						AltConf
5	A3a	1	Total	C	H	N	O	P	0
			41	10	10	5	13	3	
5	A3e	1	Total	C	H	N	O	P	0
			41	10	10	5	13	3	

- Molecule 6 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (CCD ID: BTI) (formula:  $C_{10}H_{16}N_2O_2S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
6	A3a	1	Total 31	C 10	H 16	N 2	O 2	S 1	0
6	A3d	1	Total 31	C 10	H 16	N 2	O 2	S 1	0
6	A3e	1	Total 31	C 10	H 16	N 2	O 2	S 1	0
6	A3f	1	Total 31	C 10	H 16	N 2	O 2	S 1	0
6	A3h	1	Total 31	C 10	H 16	N 2	O 2	S 1	0

- Molecule 7 is propionyl Coenzyme A (CCD ID: 1VU) (formula:  $C_{24}H_{40}N_7O_{17}P_3S$ ) (labeled as "Ligand of Interest" by depositor).



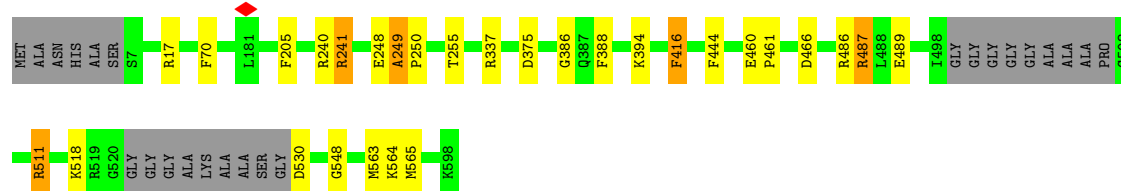
Mol	Chain	Residues	Atoms							AltConf
			Total	C	H	N	O	P	S	
7	D5a	1	86	24	34	7	17	3	1	0
7	D5b	1	86	24	34	7	17	3	1	0
7	D5c	1	86	24	34	7	17	3	1	0
7	D5d	1	86	24	34	7	17	3	1	0

### 3 Residue-property plots

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

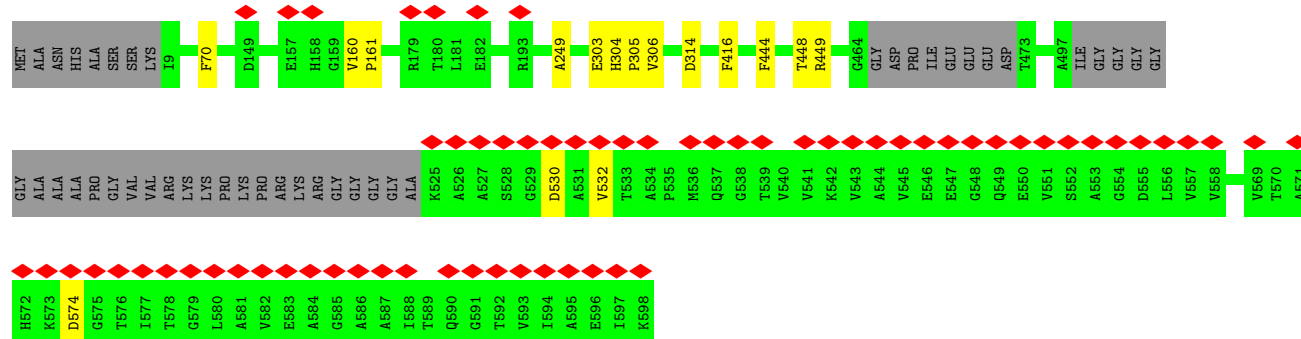
- Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

Chain A3a:  91%




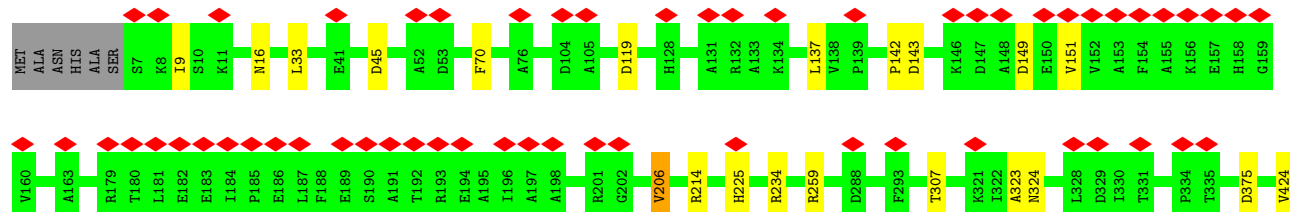
- Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

Chain A3b:  11% 90% 7%

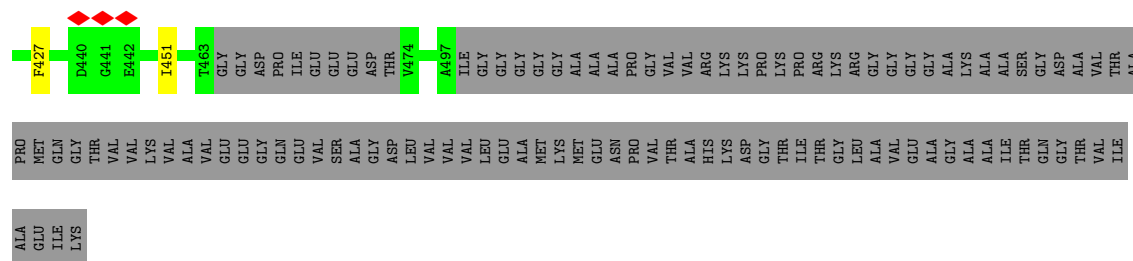


- Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

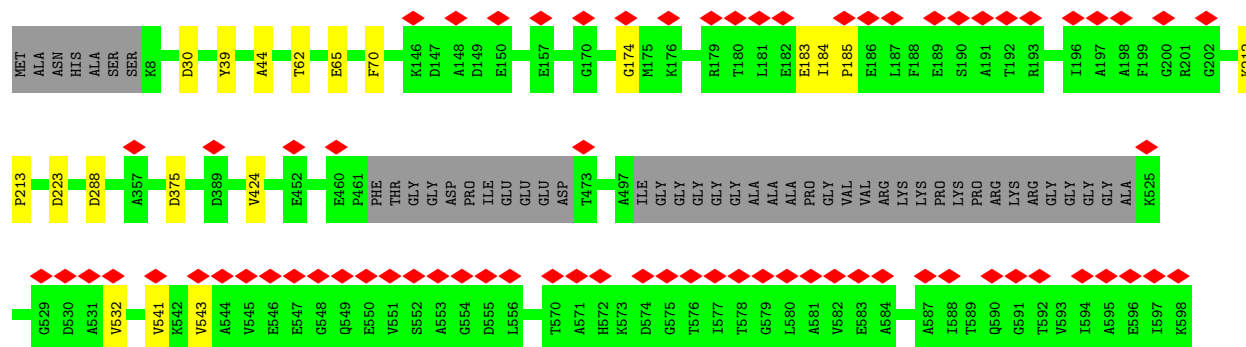
Chain A3c:  10% 77% 20%



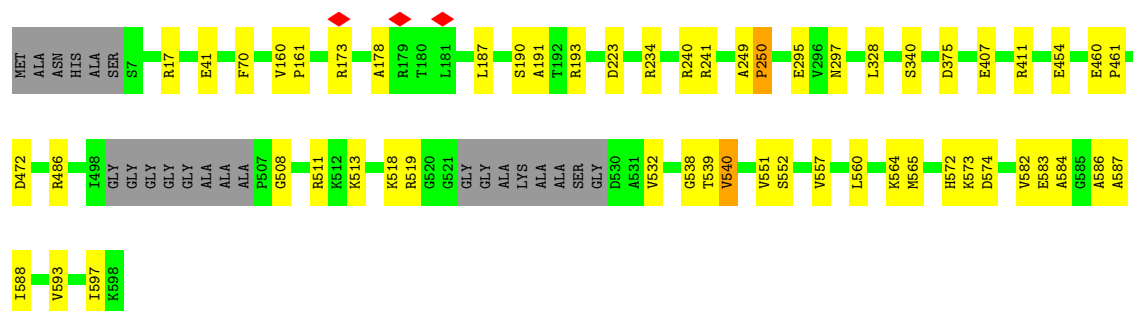




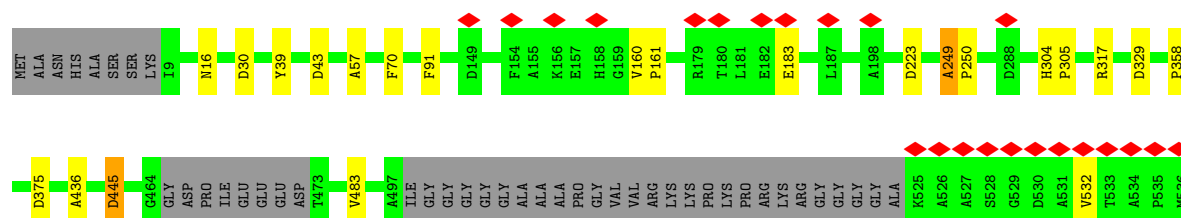
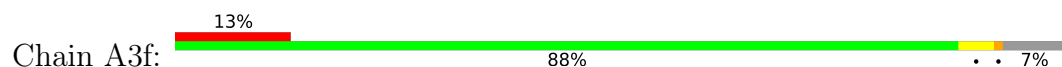
- Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

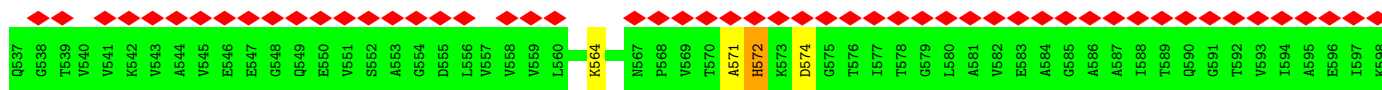


- Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

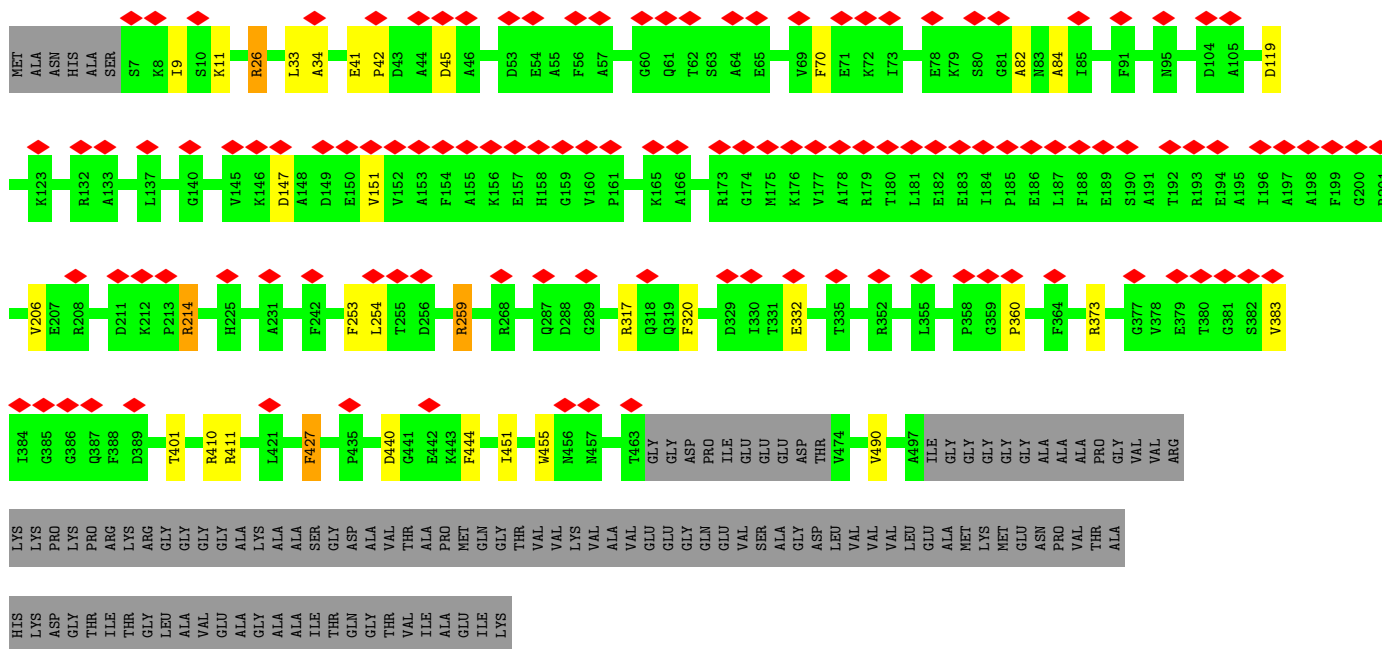
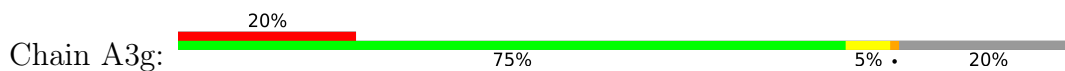


- Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit

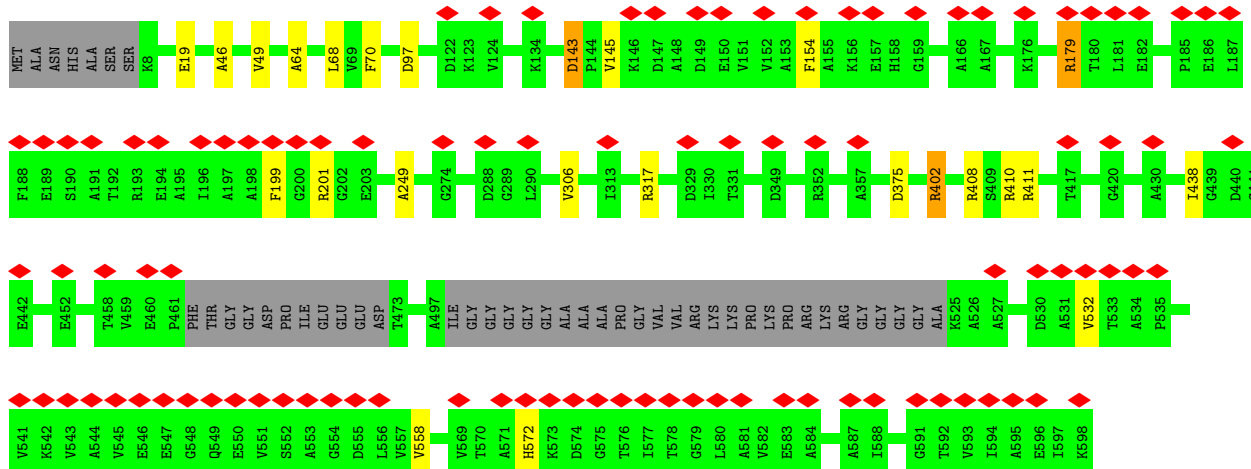
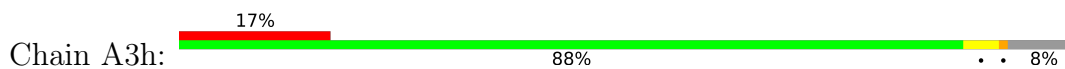




• Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit



• Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit



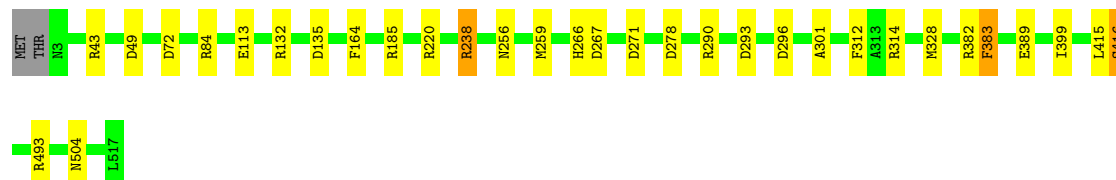
• Molecule 2: Propionyl-CoA carboxylase beta chain





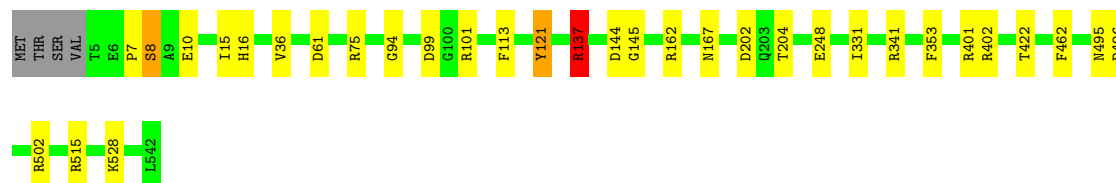
- Molecule 2: Propionyl-CoA carboxylase beta chain

Chain D4b: 93% 6% .



- Molecule 3: Propionyl-CoA carboxylase beta chain

Chain D5a: 93% 6% .



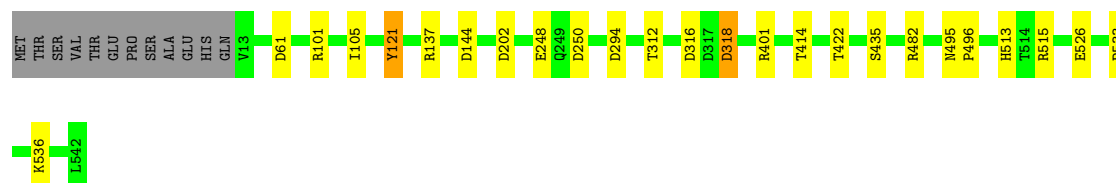
- Molecule 3: Propionyl-CoA carboxylase beta chain

Chain D5b: 94% . .



- Molecule 3: Propionyl-CoA carboxylase beta chain

Chain D5c: 93% . .

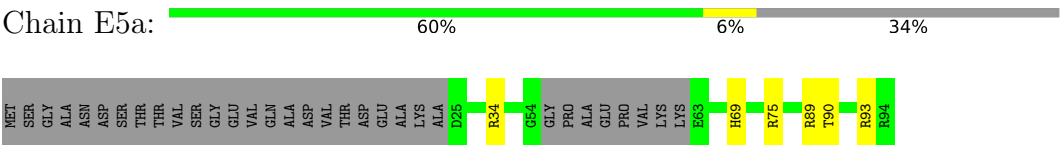


- Molecule 3: Propionyl-CoA carboxylase beta chain

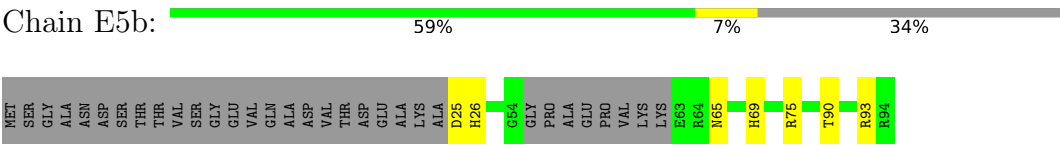
Chain D5d: 95% . .



● Molecule 4: Acetyl-/propionyl-coenzyme A carboxylase AccE5



● Molecule 4: Acetyl-/propionyl-coenzyme A carboxylase AccE5



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	52469	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	44.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2250	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.176	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	380.80002, 380.80002, 380.80002	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.68, 0.68, 0.68	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, BTI, 1VU

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	A3a	0.68	0/4396	1.16	10/5962 (0.2%)
1	A3b	0.65	0/4233	1.10	6/5744 (0.1%)
1	A3c	0.67	0/3721	1.15	9/5049 (0.2%)
1	A3d	0.68	0/4219	1.15	7/5724 (0.1%)
1	A3e	0.68	0/4408	1.14	5/5978 (0.1%)
1	A3f	0.65	0/4233	1.10	9/5744 (0.2%)
1	A3g	0.67	0/3721	1.13	9/5049 (0.2%)
1	A3h	0.67	0/4219	1.12	4/5724 (0.1%)
2	D4a	0.98	1/4020 (0.0%)	1.46	20/5449 (0.4%)
2	D4b	0.99	0/4020	1.49	26/5449 (0.5%)
3	D5a	0.98	0/4161	1.41	22/5655 (0.4%)
3	D5b	0.97	0/4097	1.40	16/5567 (0.3%)
3	D5c	0.98	0/4097	1.42	20/5567 (0.4%)
3	D5d	0.96	0/4159	1.42	15/5652 (0.3%)
4	E5a	0.84	0/513	1.32	3/690 (0.4%)
4	E5b	0.85	0/513	1.38	2/690 (0.3%)
All	All	0.81	1/58730 (0.0%)	1.27	183/79693 (0.2%)

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	A3a	0	9
1	A3c	0	2
1	A3e	0	8
1	A3f	0	1
1	A3g	0	6
1	A3h	0	5
2	D4a	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	D4b	0	4
3	D5a	0	5
3	D5b	0	2
3	D5c	0	2
3	D5d	0	3
4	E5a	0	2
4	E5b	0	2
All	All	0	60

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D4a	493	ARG	NE-CZ	5.07	1.38	1.33

The worst 5 of 183 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D5a	137	ARG	NE-CZ-NH2	9.06	127.35	119.20
3	D5c	533	PRO	N-CA-CB	8.42	107.60	103.22
2	D4a	383	PHE	CA-CB-CG	8.08	121.88	113.80
3	D5d	144	ASP	CA-CB-CG	8.07	120.67	112.60
2	D4b	383	PHE	CA-CB-CG	7.83	121.63	113.80

There are no chirality outliers.

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A3a	17	ARG	Peptide
1	A3a	240	ARG	Sidechain
1	A3a	241	ARG	Sidechain
1	A3a	337	ARG	Sidechain
1	A3a	486	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A3a	4318	4232	4306	18	0
1	A3b	4158	4058	4132	5	0
1	A3c	3648	3546	3611	10	0
1	A3d	4145	4053	4126	5	0
1	A3e	4329	4242	4317	33	0
1	A3f	4158	4058	4132	15	0
1	A3g	3648	3546	3611	23	0
1	A3h	4145	4053	4126	10	0
2	D4a	3939	3878	3939	4	0
2	D4b	3939	3878	3939	3	0
3	D5a	4083	3963	4055	10	0
3	D5b	4021	3915	4004	0	0
3	D5c	4021	3915	4004	2	0
3	D5d	4081	3957	4048	4	0
4	E5a	502	487	496	2	0
4	E5b	502	487	496	1	0
5	A3a	31	10	12	0	0
5	A3e	31	10	12	2	0
6	A3a	15	16	16	5	0
6	A3d	15	16	16	0	0
6	A3e	15	16	16	3	0
6	A3f	15	16	16	3	0
6	A3h	15	16	16	0	0
7	D5a	52	34	38	0	0
7	D5b	52	34	38	4	0
7	D5c	52	34	38	0	0
7	D5d	52	34	38	9	0
All	All	57982	56504	57598	144	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 1.

The worst 5 of 144 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:A3g:427:PHE:HE1	1:A3g:455:TRP:CE2	1.34	1.43
1:A3g:427:PHE:CE1	1:A3g:455:TRP:CE2	2.06	1.42
1:A3a:564:LYS:NZ	6:A3a:602:BTI:C11	1.98	1.25
1:A3e:295:GLU:OE2	5:A3e:601:ATP:O1B	1.53	1.19
1:A3g:427:PHE:CE1	1:A3g:455:TRP:CZ2	2.35	1.14

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A3a	568/598 (95%)	549 (97%)	18 (3%)	1 (0%)	43	58
1	A3b	549/598 (92%)	529 (96%)	19 (4%)	1 (0%)	43	58
1	A3c	477/598 (80%)	453 (95%)	24 (5%)	0	100	100
1	A3d	547/598 (92%)	520 (95%)	22 (4%)	5 (1%)	14	22
1	A3e	570/598 (95%)	548 (96%)	21 (4%)	1 (0%)	43	58
1	A3f	549/598 (92%)	529 (96%)	16 (3%)	4 (1%)	18	28
1	A3g	477/598 (80%)	459 (96%)	18 (4%)	0	100	100
1	A3h	547/598 (92%)	528 (96%)	17 (3%)	2 (0%)	30	43
2	D4a	513/517 (99%)	496 (97%)	17 (3%)	0	100	100
2	D4b	513/517 (99%)	500 (98%)	12 (2%)	1 (0%)	43	58
3	D5a	536/542 (99%)	523 (98%)	12 (2%)	1 (0%)	43	58
3	D5b	528/542 (97%)	517 (98%)	11 (2%)	0	100	100
3	D5c	528/542 (97%)	517 (98%)	11 (2%)	0	100	100
3	D5d	536/542 (99%)	525 (98%)	11 (2%)	0	100	100
4	E5a	58/94 (62%)	56 (97%)	2 (3%)	0	100	100
4	E5b	58/94 (62%)	57 (98%)	1 (2%)	0	100	100
All	All	7554/8174 (92%)	7306 (97%)	232 (3%)	16 (0%)	44	58

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A3a	249	ALA
1	A3f	249	ALA
3	D5a	8	SER
1	A3b	532	VAL
1	A3d	532	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A3a	446/453 (98%)	444 (100%)	2 (0%)	84	92
1	A3b	427/453 (94%)	427 (100%)	0	100	100
1	A3c	375/453 (83%)	373 (100%)	2 (0%)	81	91
1	A3d	426/453 (94%)	426 (100%)	0	100	100
1	A3e	447/453 (99%)	438 (98%)	9 (2%)	48	70
1	A3f	427/453 (94%)	425 (100%)	2 (0%)	81	91
1	A3g	375/453 (83%)	372 (99%)	3 (1%)	73	86
1	A3h	426/453 (94%)	421 (99%)	5 (1%)	63	81
2	D4a	410/412 (100%)	409 (100%)	1 (0%)	87	94
2	D4b	410/412 (100%)	408 (100%)	2 (0%)	81	91
3	D5a	432/436 (99%)	429 (99%)	3 (1%)	76	88
3	D5b	425/436 (98%)	421 (99%)	4 (1%)	70	85
3	D5c	425/436 (98%)	423 (100%)	2 (0%)	81	91
3	D5d	431/436 (99%)	425 (99%)	6 (1%)	59	79
4	E5a	52/76 (68%)	52 (100%)	0	100	100
4	E5b	52/76 (68%)	51 (98%)	1 (2%)	50	71
All	All	5986/6344 (94%)	5944 (99%)	42 (1%)	73	88

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D5a	331	ILE
3	D5d	12	GLN
3	D5b	121	TYR
3	D5b	513	HIS
3	D5d	307	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	1VU	D5b	601	-	49,54,54	0.51	0	69,80,80	1.06	3 (4%)
6	BTI	A3d	601	-	16,16,16	0.43	0	21,21,21	0.69	0
6	BTI	A3f	601	-	16,16,16	0.48	0	21,21,21	0.80	0
6	BTI	A3e	602	-	16,16,16	0.51	0	21,21,21	1.20	2 (9%)
5	ATP	A3a	601	-	29,33,33	0.47	0	44,52,52	0.63	0
6	BTI	A3a	602	-	16,16,16	0.40	0	21,21,21	1.35	3 (14%)
7	1VU	D5a	601	-	49,54,54	0.68	0	69,80,80	1.26	3 (4%)
5	ATP	A3e	601	-	29,33,33	0.49	0	44,52,52	0.67	0
6	BTI	A3h	601	-	16,16,16	0.53	0	21,21,21	0.97	1 (4%)
7	1VU	D5c	601	-	49,54,54	0.54	1 (2%)	69,80,80	1.52	8 (11%)
7	1VU	D5d	601	-	49,54,54	0.48	0	69,80,80	1.33	8 (11%)

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
7	1VU	D5b	601	-	-	14/53/69/69	0/3/3/3
6	BTI	A3d	601	-	-	1/5/27/27	0/2/2/2
6	BTI	A3f	601	-	-	2/5/27/27	0/2/2/2
6	BTI	A3e	602	-	-	2/5/27/27	0/2/2/2
5	ATP	A3a	601	-	-	10/22/38/38	0/3/3/3
6	BTI	A3a	602	-	-	4/5/27/27	0/2/2/2
7	1VU	D5a	601	-	-	15/53/69/69	0/3/3/3
5	ATP	A3e	601	-	-	0/22/38/38	0/3/3/3
6	BTI	A3h	601	-	-	0/5/27/27	0/2/2/2
7	1VU	D5c	601	-	-	21/53/69/69	0/3/3/3
7	1VU	D5d	601	-	-	15/53/69/69	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D5c	601	1VU	P2-O13	2.01	1.63	1.59

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D5c	601	1VU	C3-S-C2	7.18	124.23	101.87
7	D5d	601	1VU	C3-S-C2	5.68	119.56	101.87
7	D5c	601	1VU	C1-C2-S	5.29	120.18	113.63
7	D5a	601	1VU	C3-S-C2	5.05	117.60	101.87
7	D5a	601	1VU	C1-C2-S	4.74	119.49	113.63

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

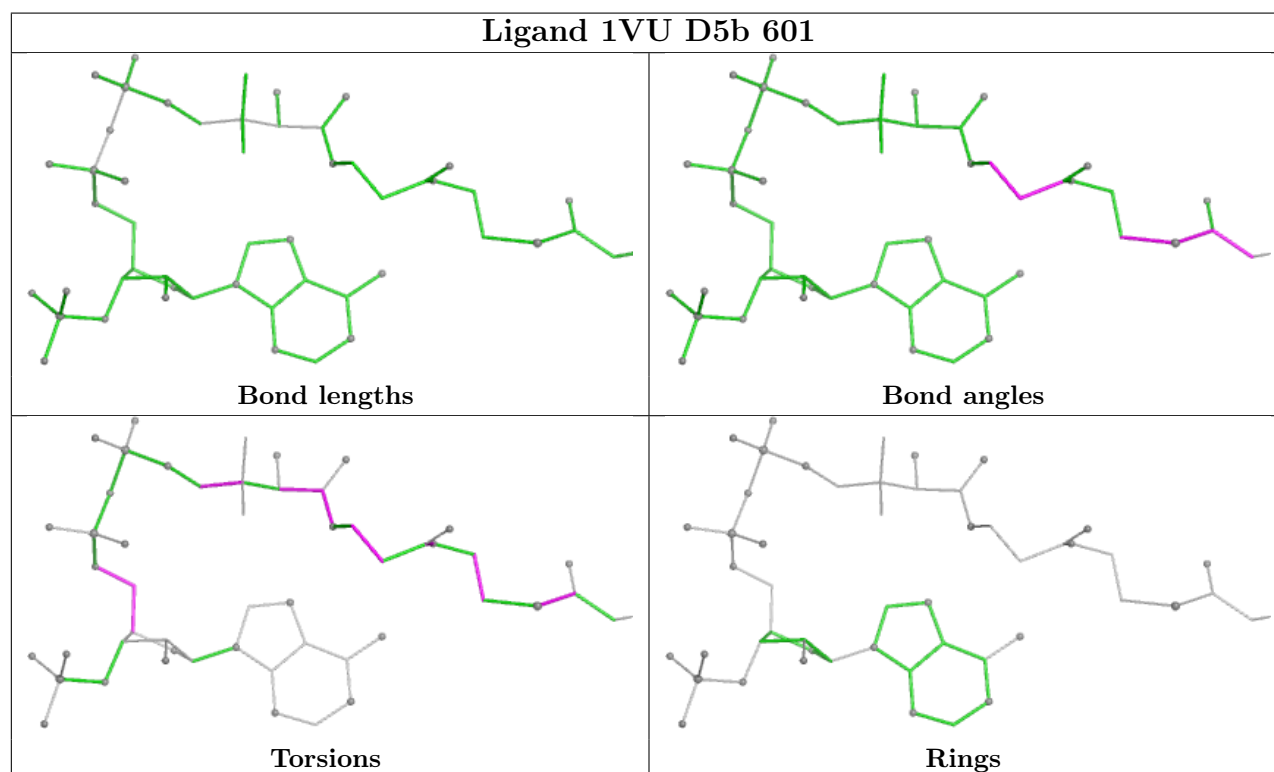
Mol	Chain	Res	Type	Atoms
5	A3a	601	ATP	PB-O3B-PG-O2G
5	A3a	601	ATP	C5'-O5'-PA-O1A
5	A3a	601	ATP	C5'-O5'-PA-O3A
6	A3a	602	BTI	C11-C10-C9-C8
6	A3a	602	BTI	C2-C7-C8-C9

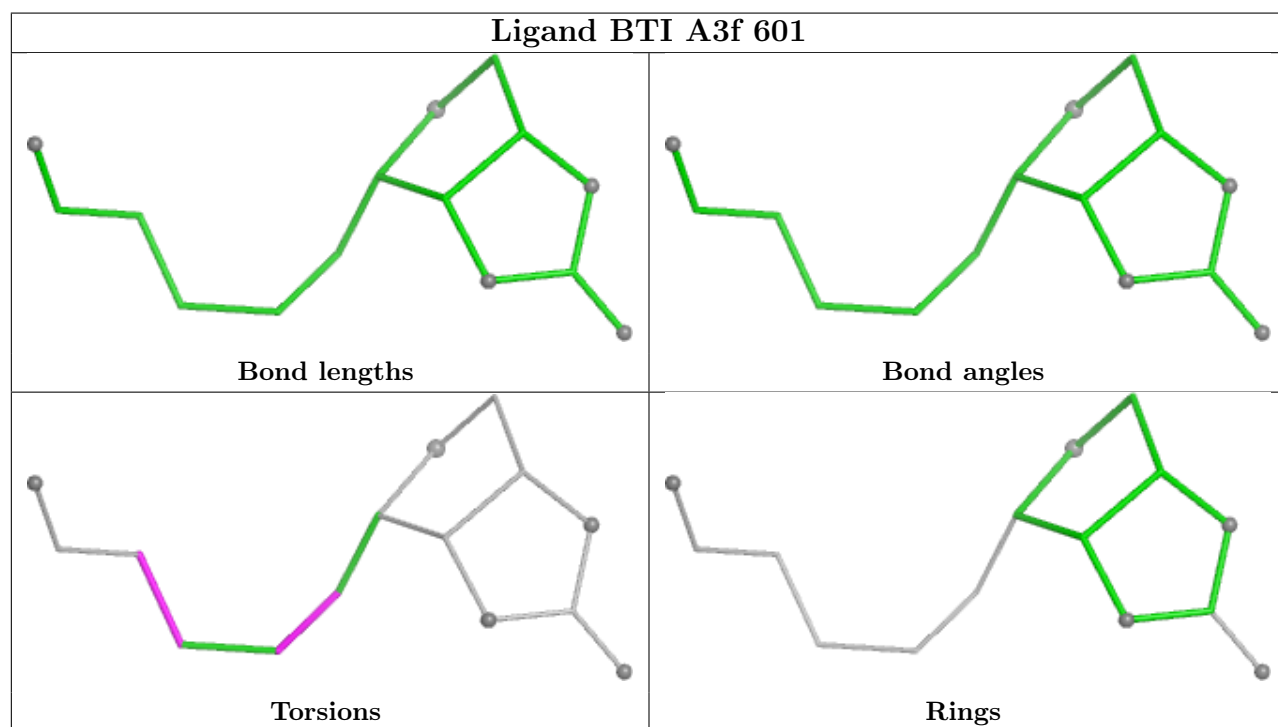
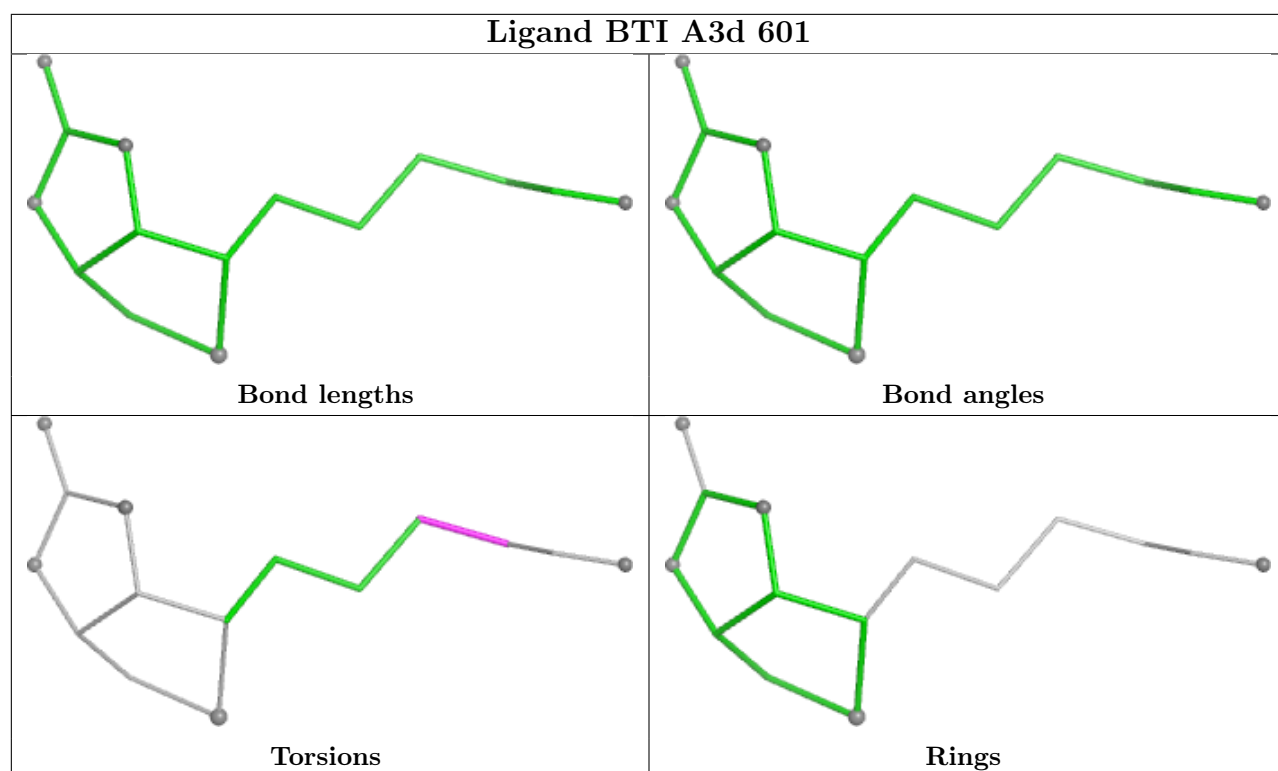
There are no ring outliers.

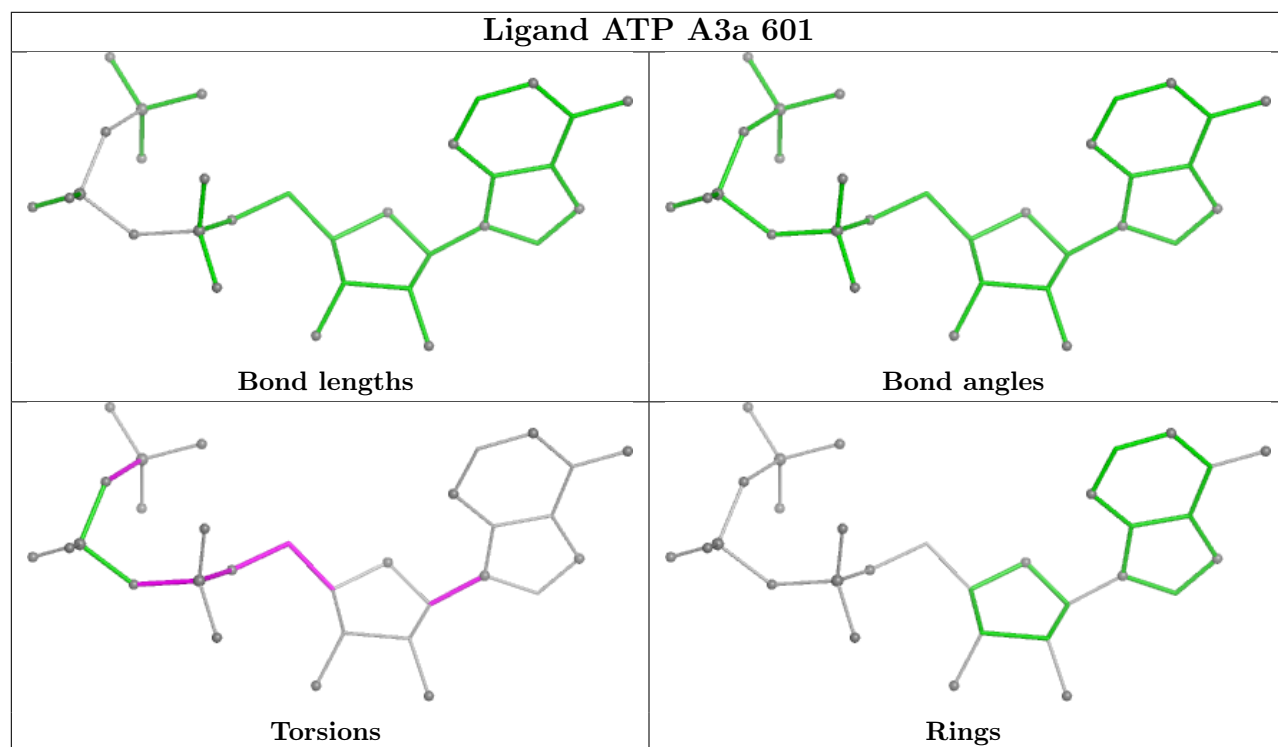
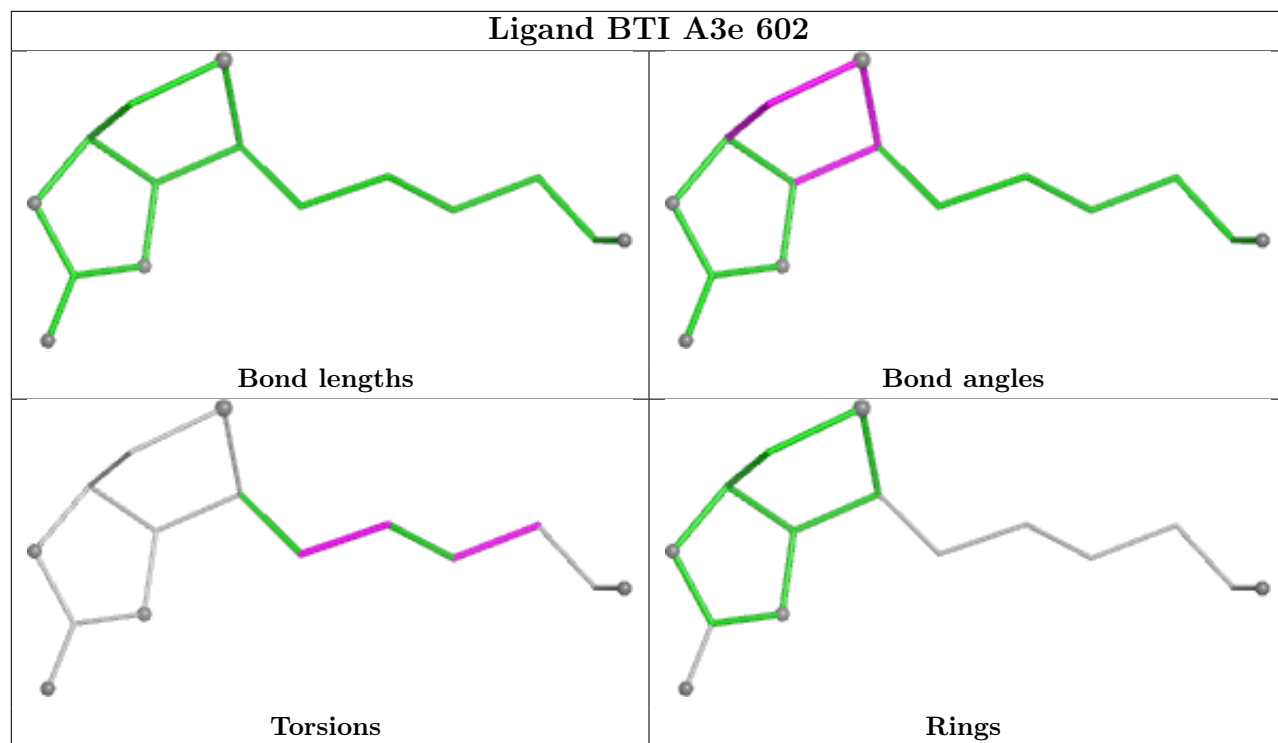
6 monomers are involved in 26 short contacts:

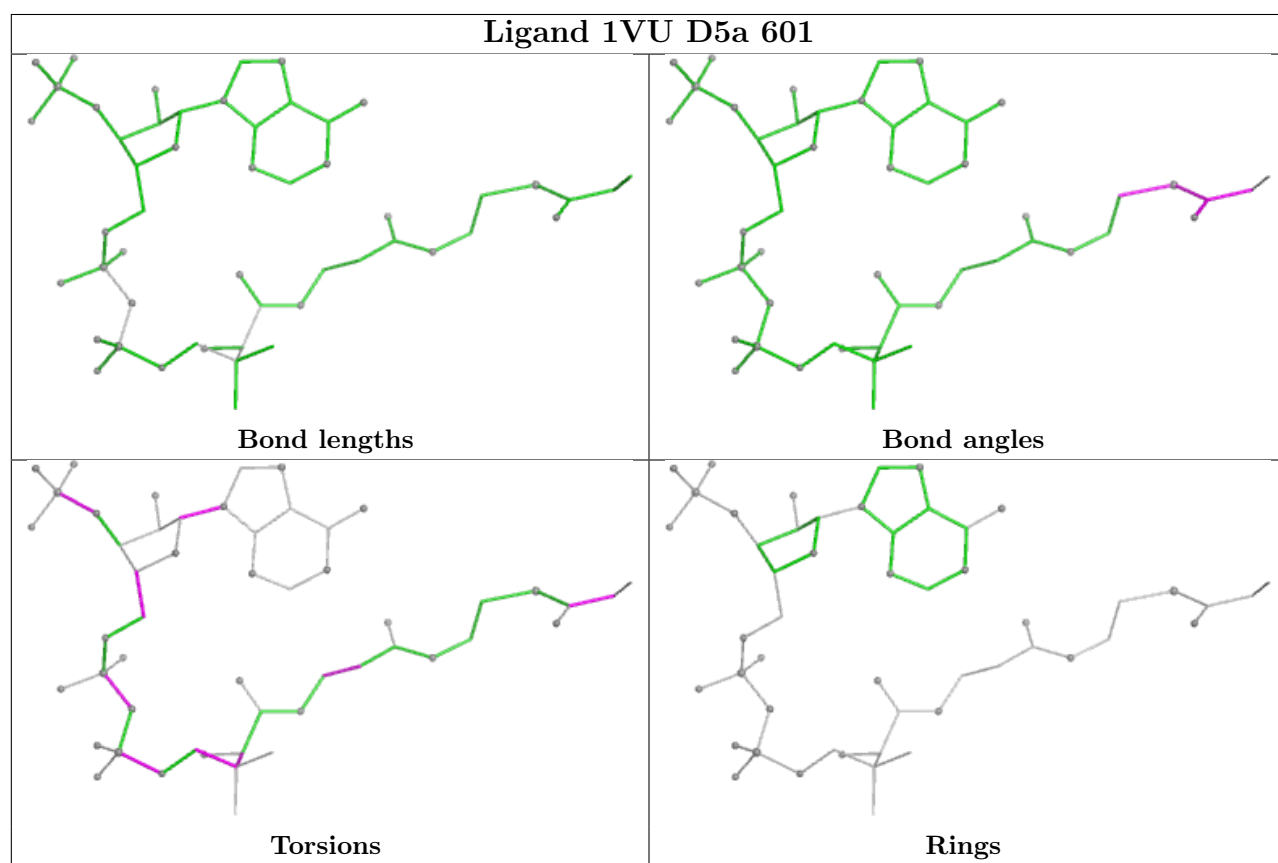
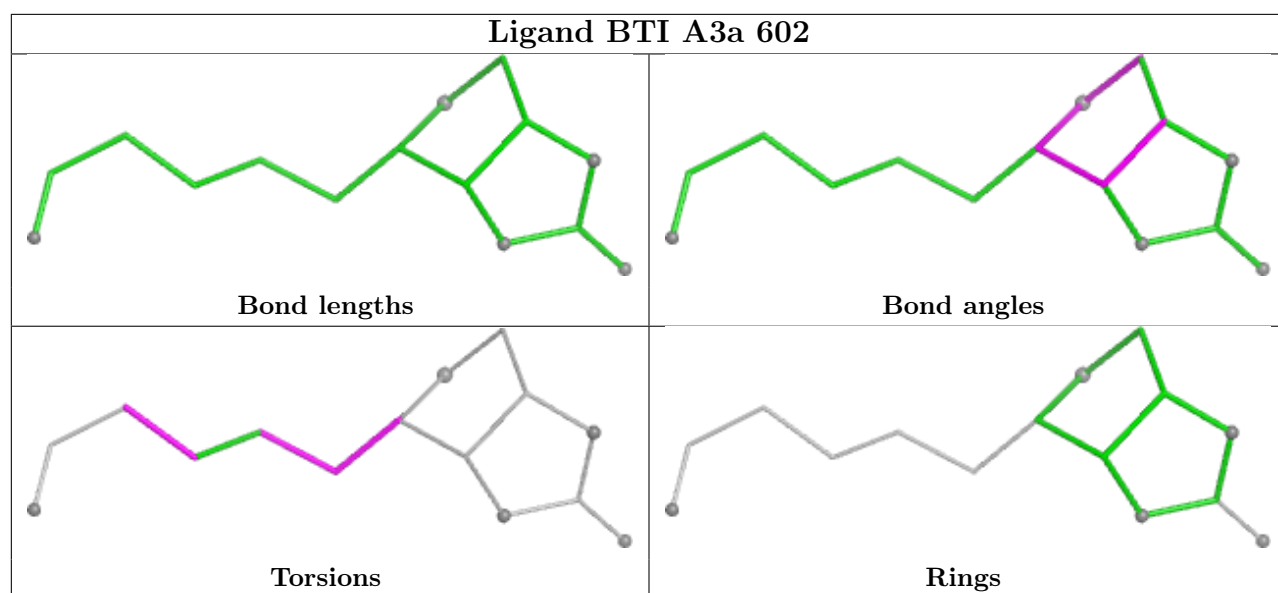
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D5b	601	1VU	4	0
6	A3f	601	BTI	3	0
6	A3e	602	BTI	3	0
6	A3a	602	BTI	5	0
5	A3e	601	ATP	2	0
7	D5d	601	1VU	9	0

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

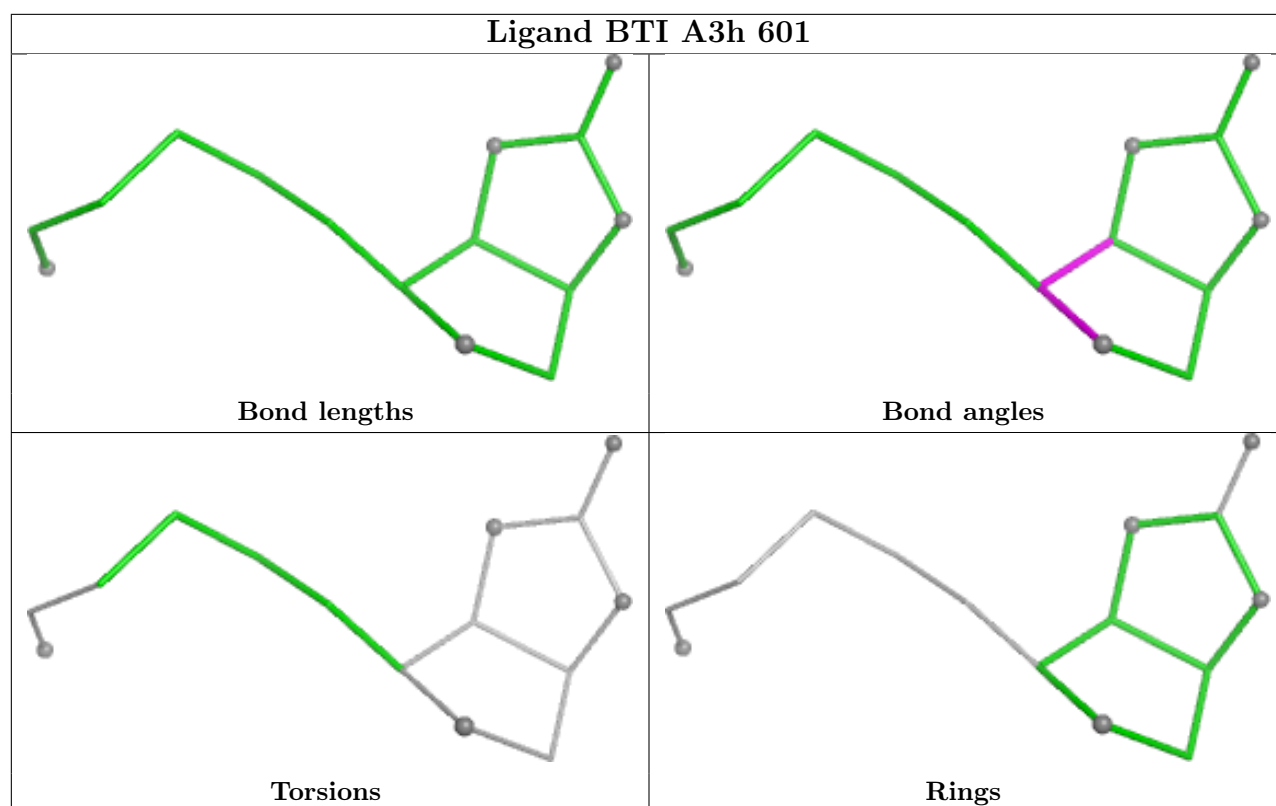
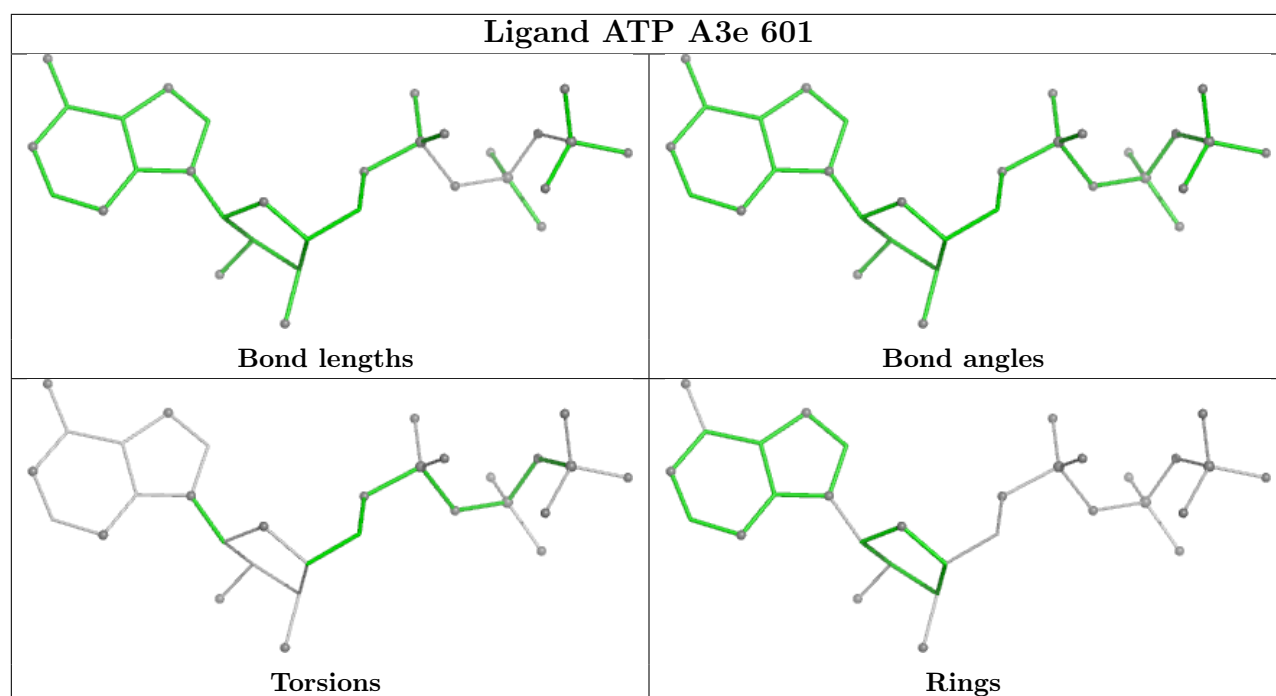




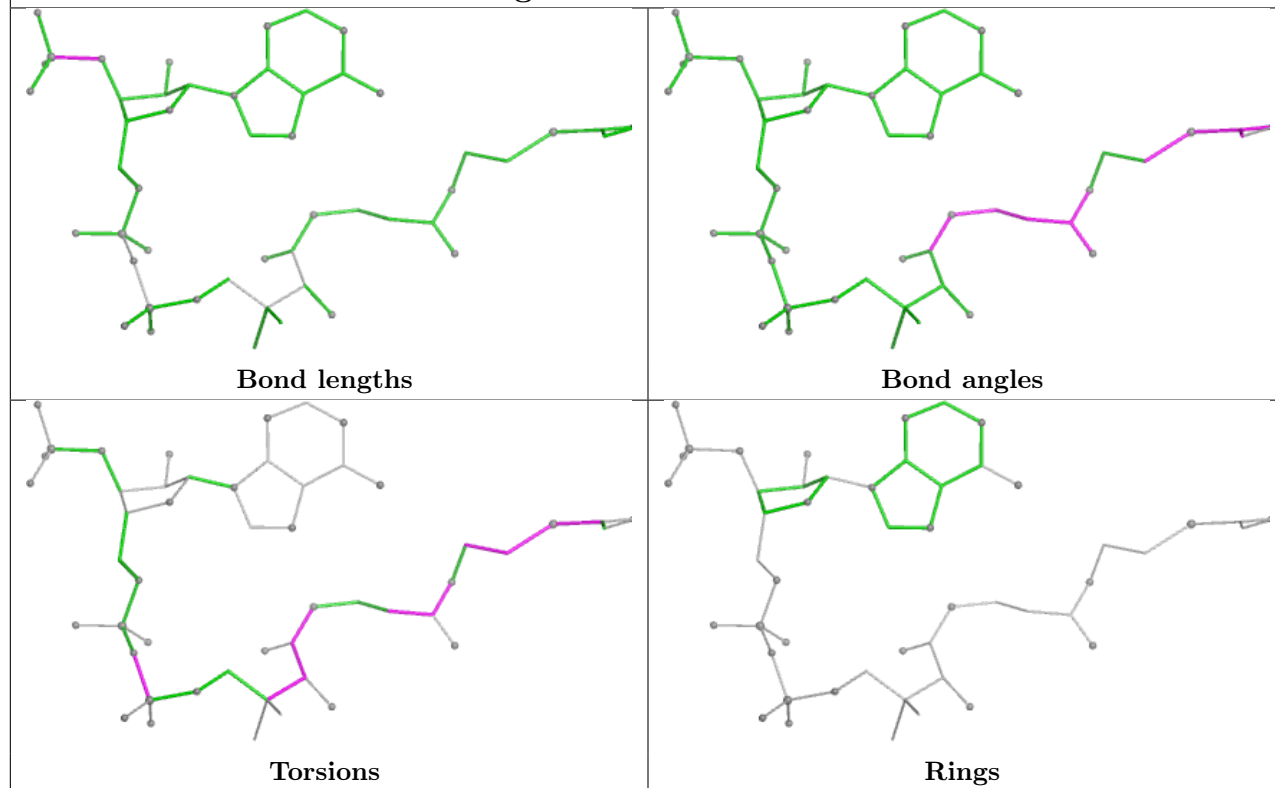




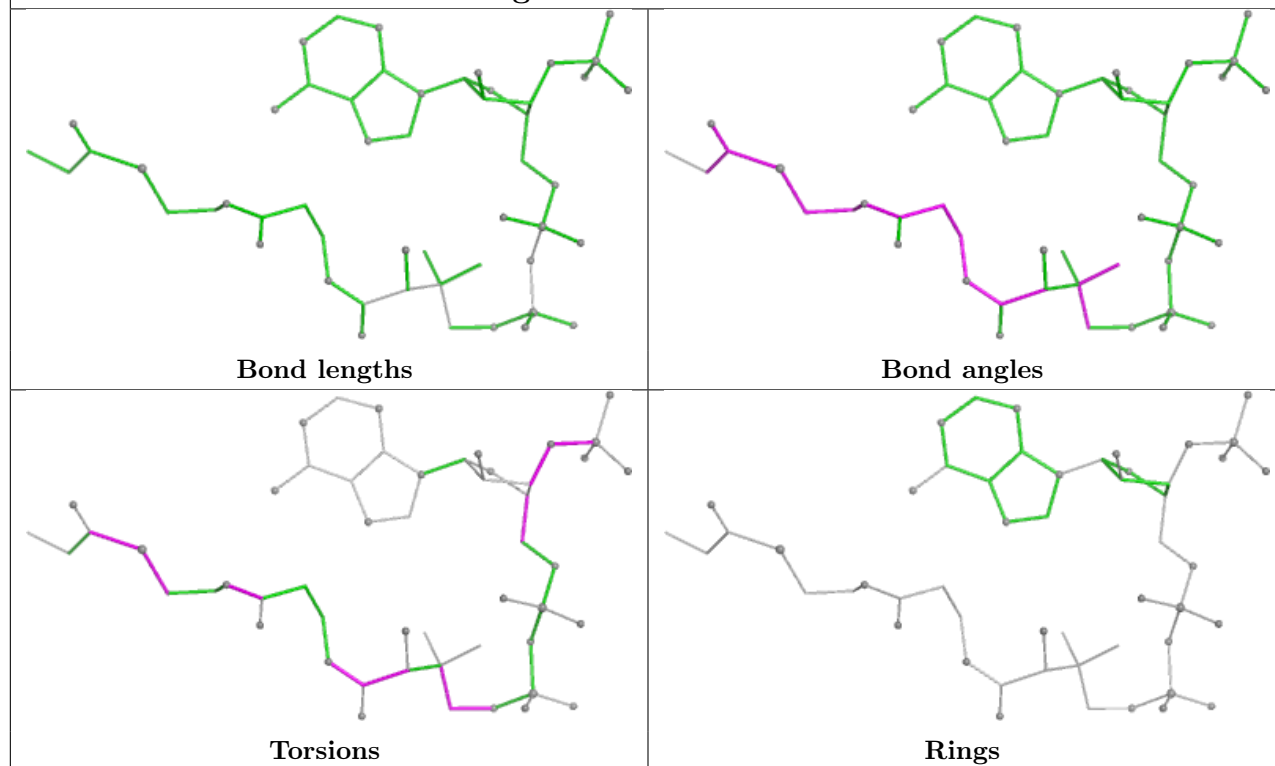




## Ligand 1VU D5c 601



## Ligand 1VU D5d 601



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

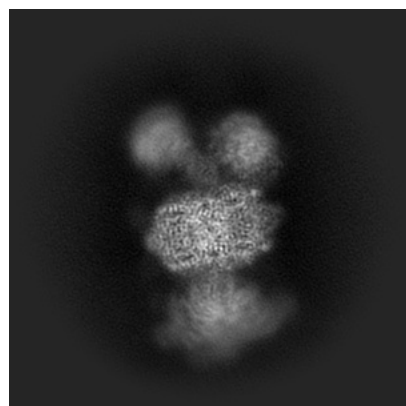
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55802. These allow visual inspection of the internal detail of the map and identification of artifacts.

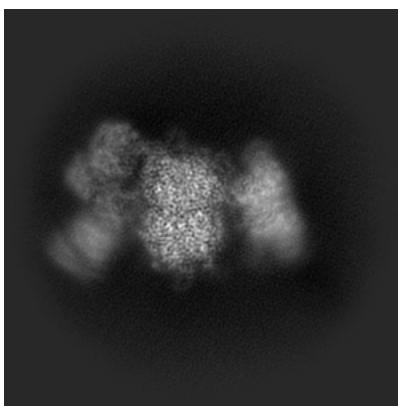
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

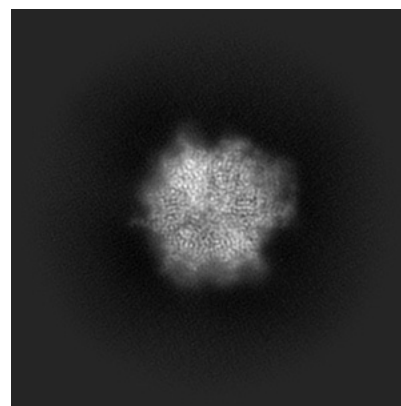
#### 6.1.1 Primary map



X

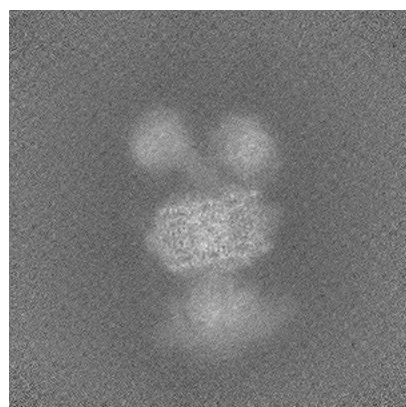


Y

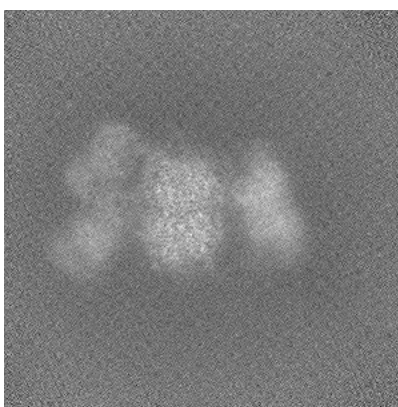


Z

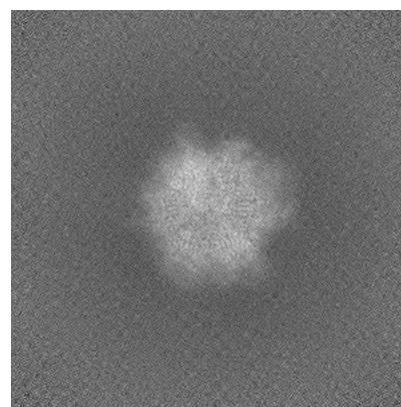
#### 6.1.2 Raw map



X



Y

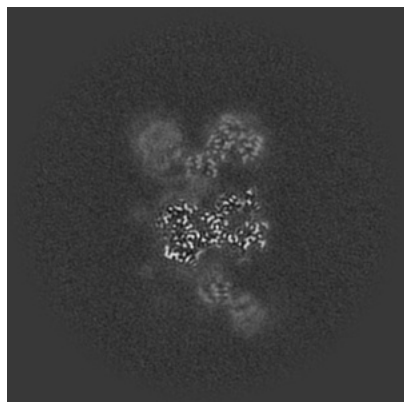


Z

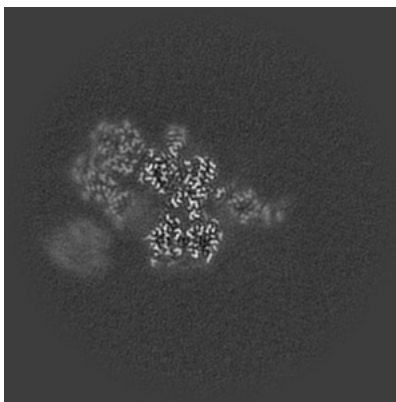
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

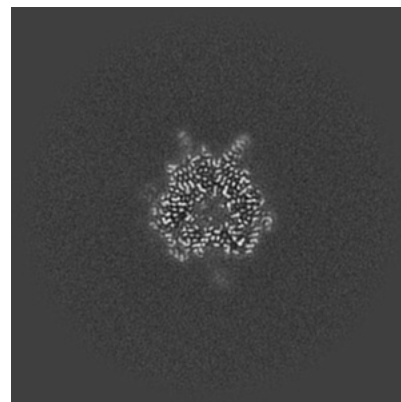
### 6.2.1 Primary map



X Index: 280

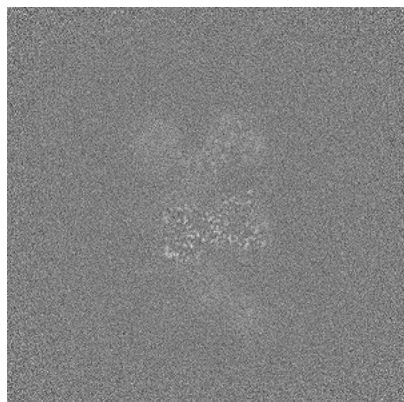


Y Index: 280

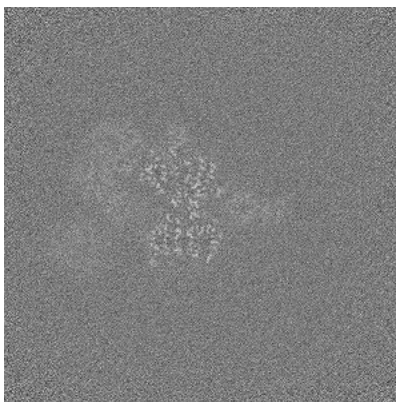


Z Index: 280

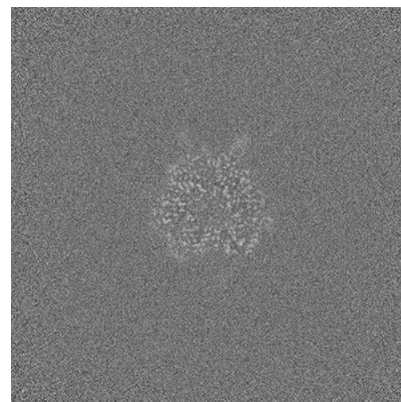
### 6.2.2 Raw map



X Index: 280



Y Index: 280



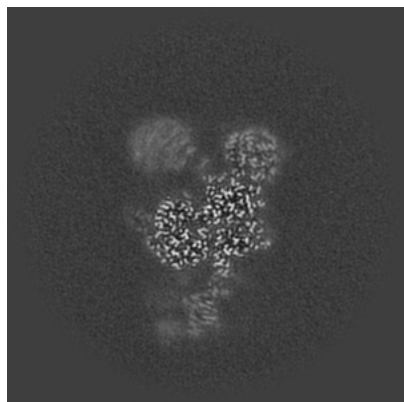
Z Index: 280

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

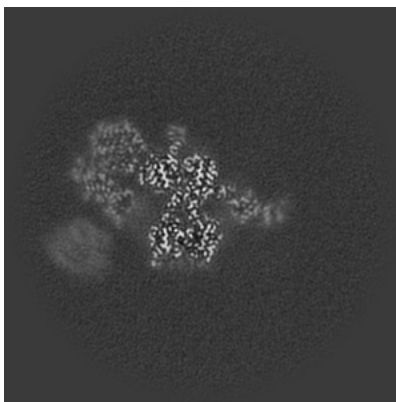


## 6.3 Largest variance slices [i](#)

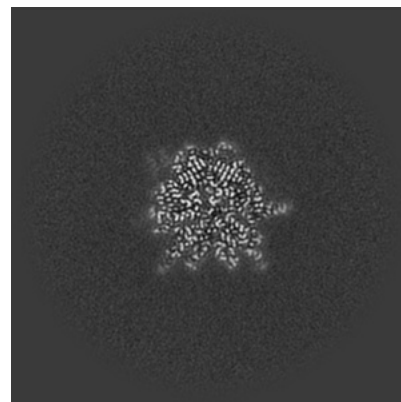
### 6.3.1 Primary map



X Index: 304

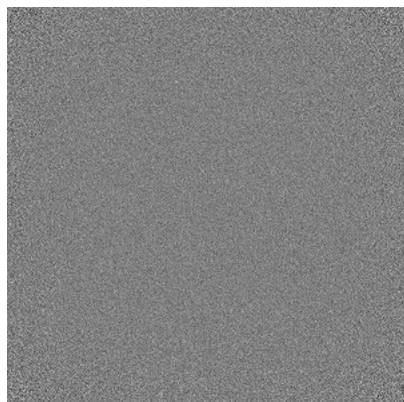


Y Index: 282

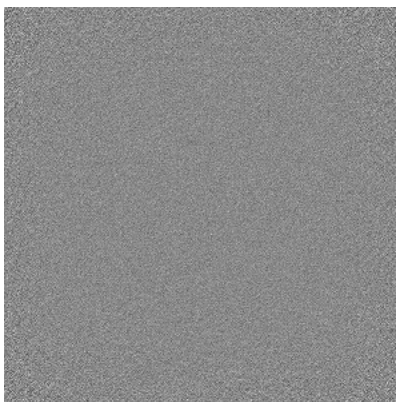


Z Index: 232

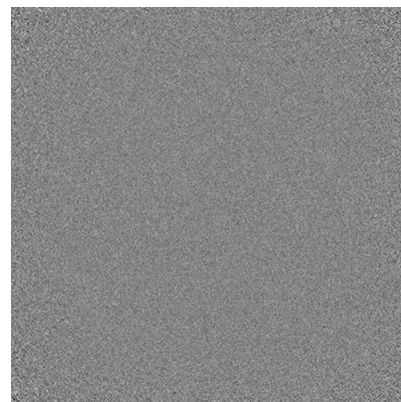
### 6.3.2 Raw map



X Index: 0



Y Index: 0

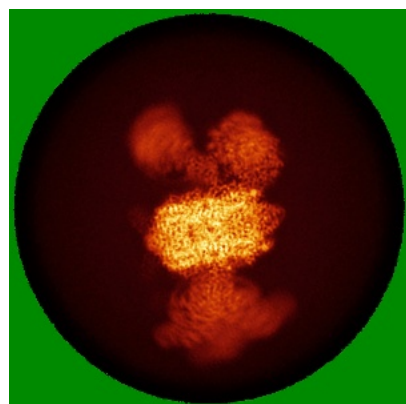


Z Index: 0

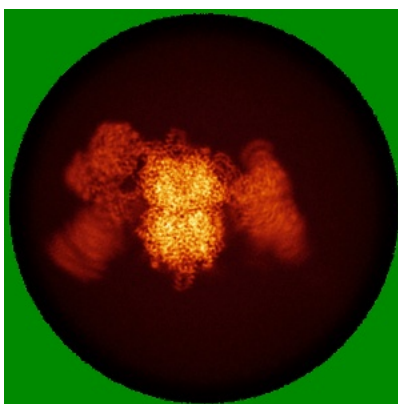
The images above show the largest variance slices of the map in three orthogonal directions.

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

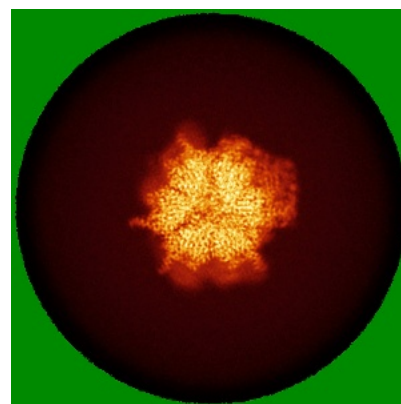
### 6.4.1 Primary map



X

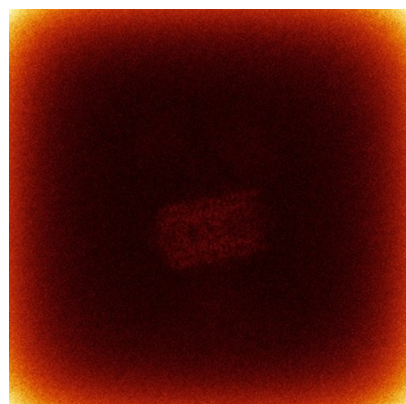


Y

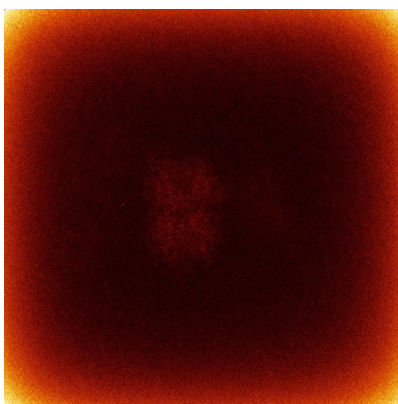


Z

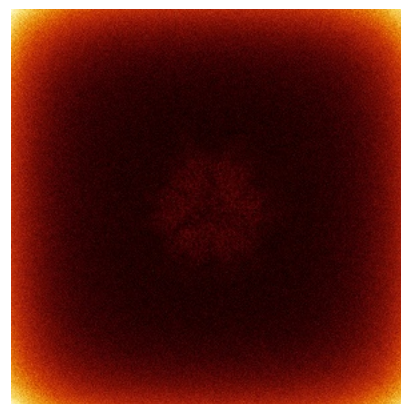
### 6.4.2 Raw map



X



Y

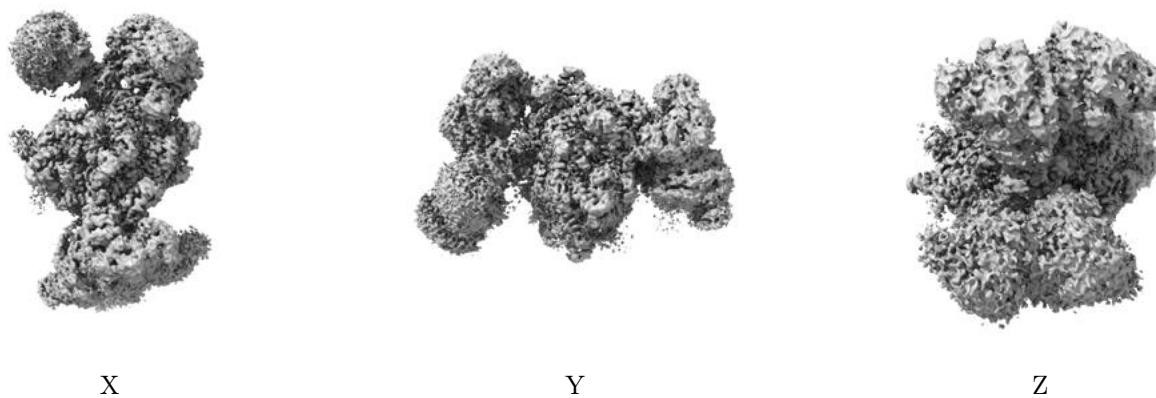


Z

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.

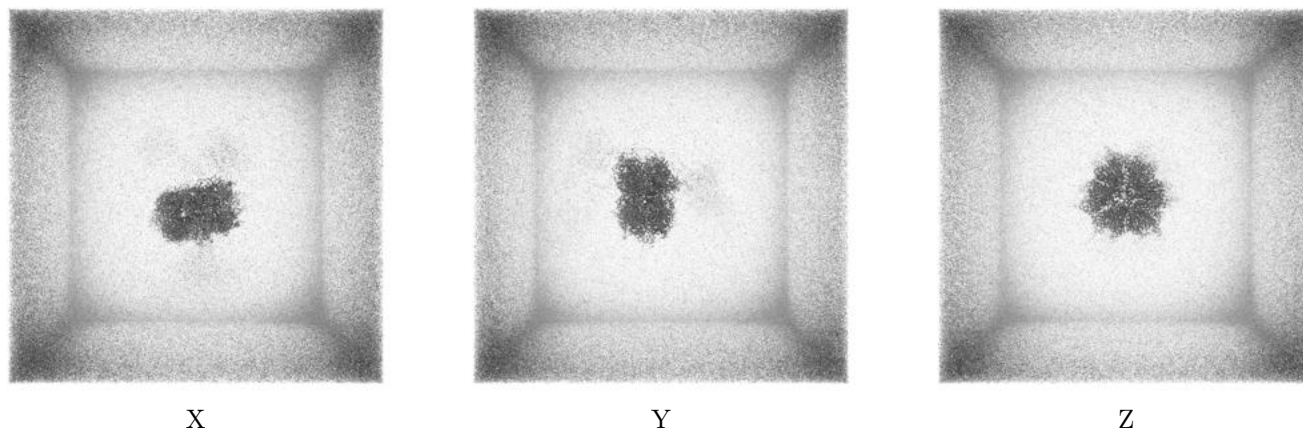
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation [i](#)

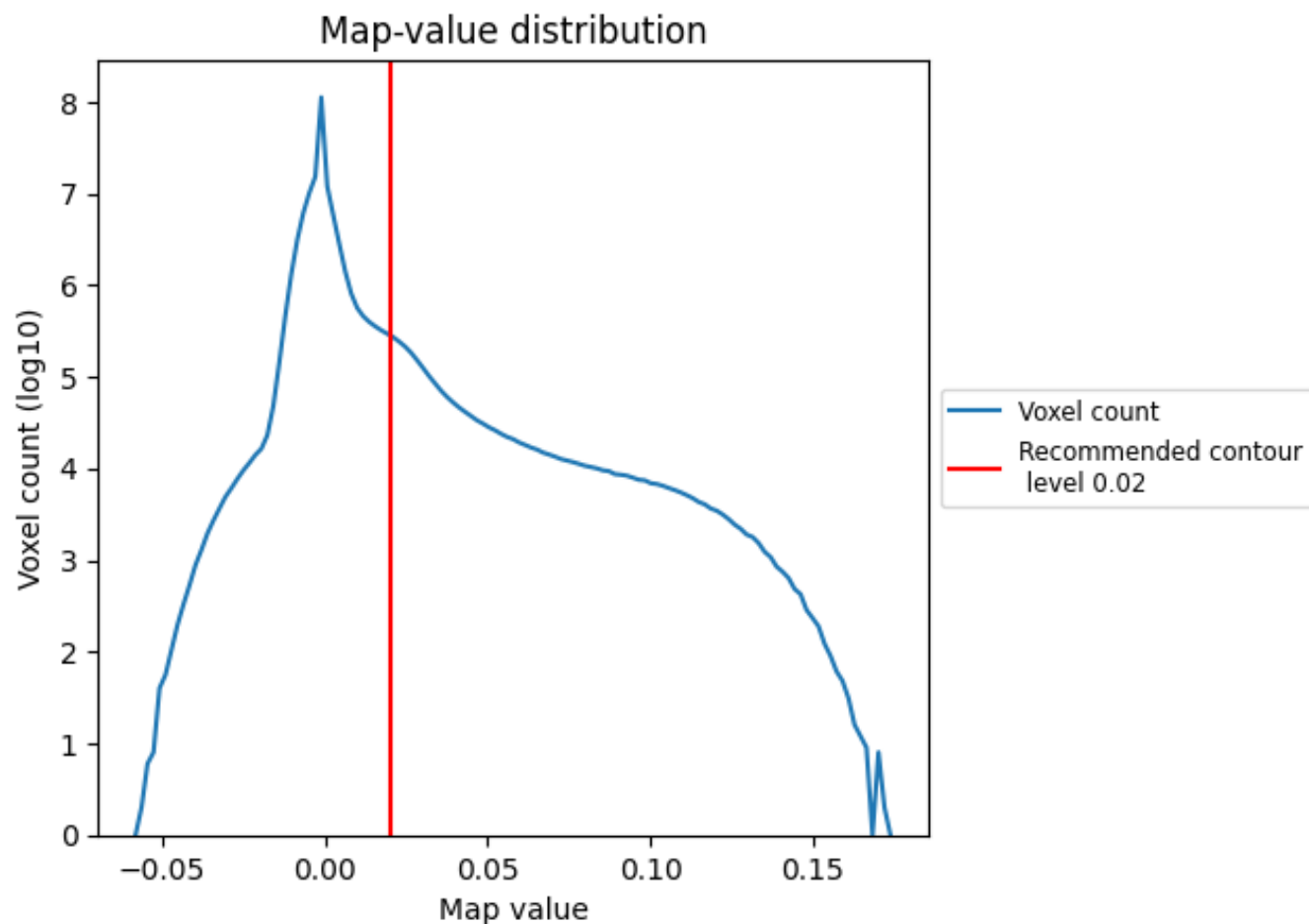
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

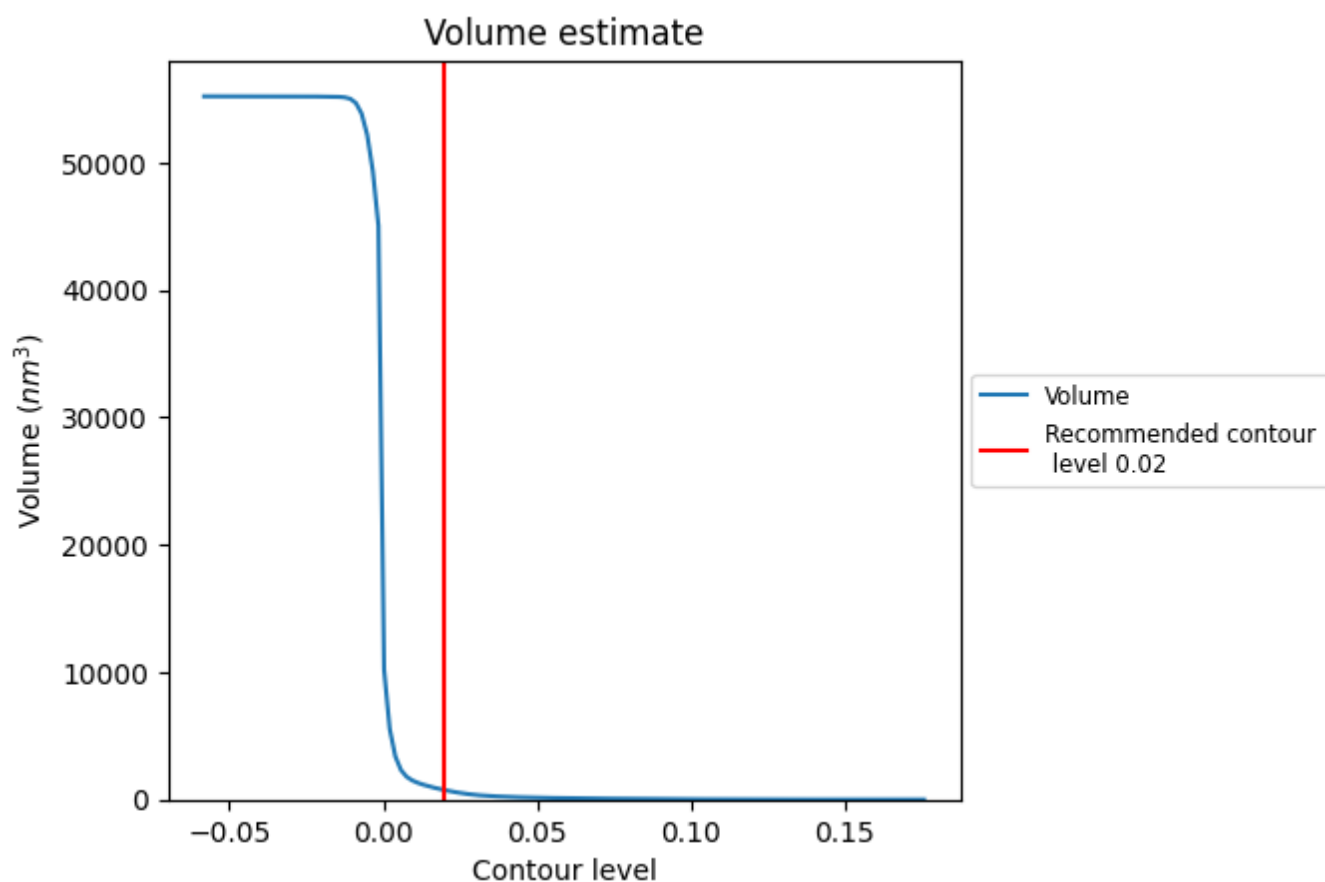
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

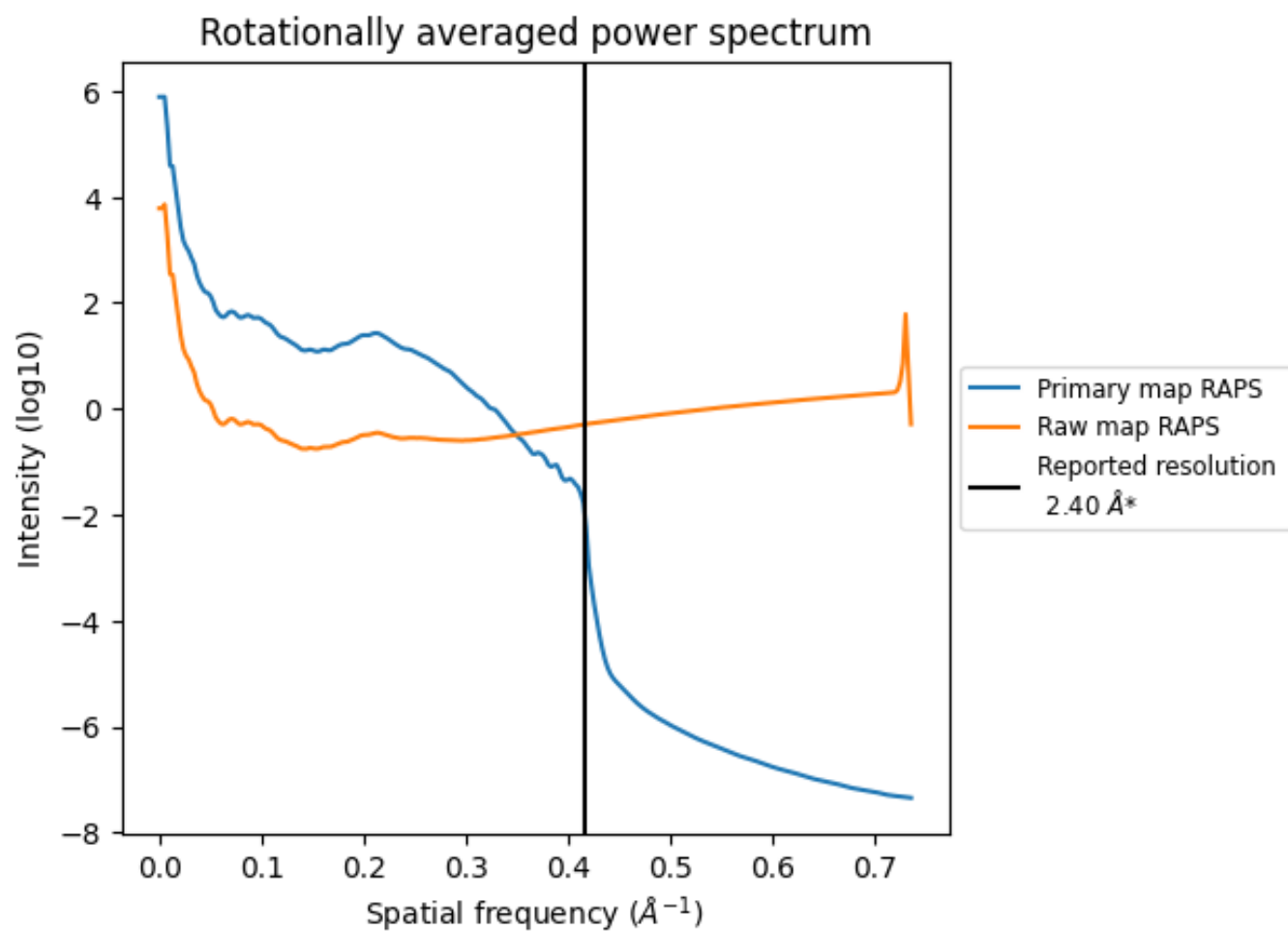
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 743  $\text{nm}^3$ ; this corresponds to an approximate mass of 671 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](#)

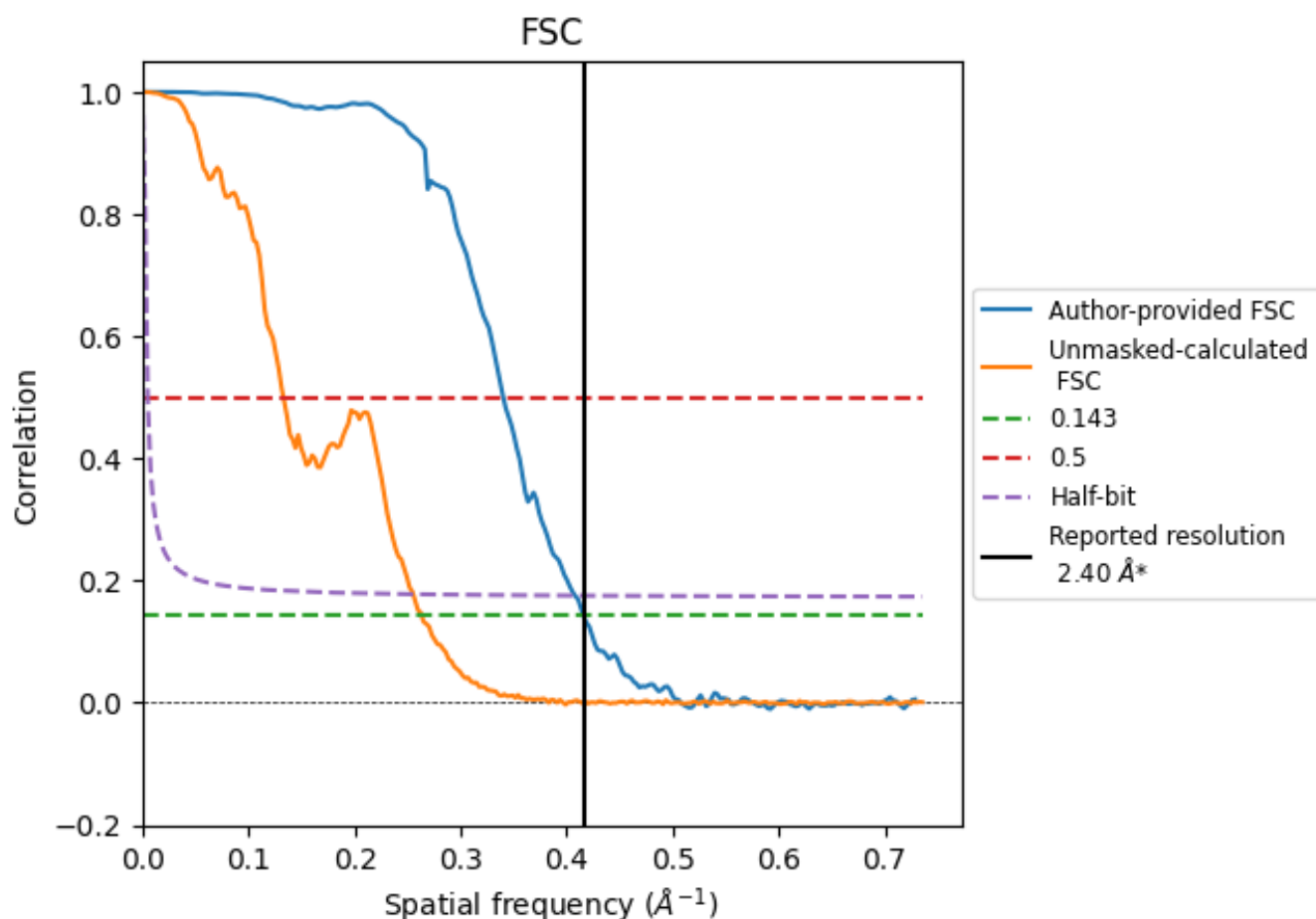


\*Reported resolution corresponds to spatial frequency of 0.417 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.417  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

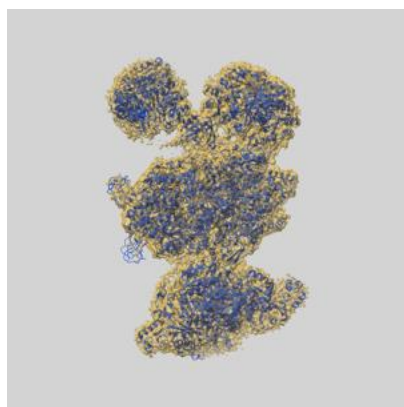
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.41	2.94	2.45
Unmasked-calculated*	3.80	7.51	3.92

\*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 3.80 differs from the reported value 2.4 by more than 10 %

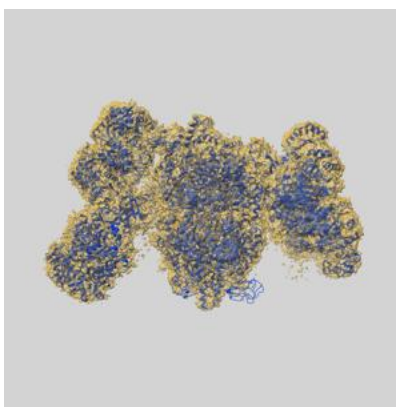
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55802 and PDB model 9TDM. Per-residue inclusion information can be found in section [3](#) on page [8](#).

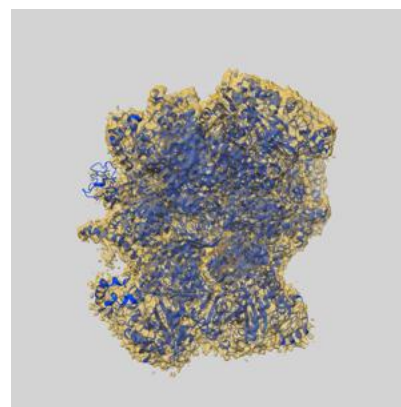
### 9.1 Map-model overlay [i](#)



X



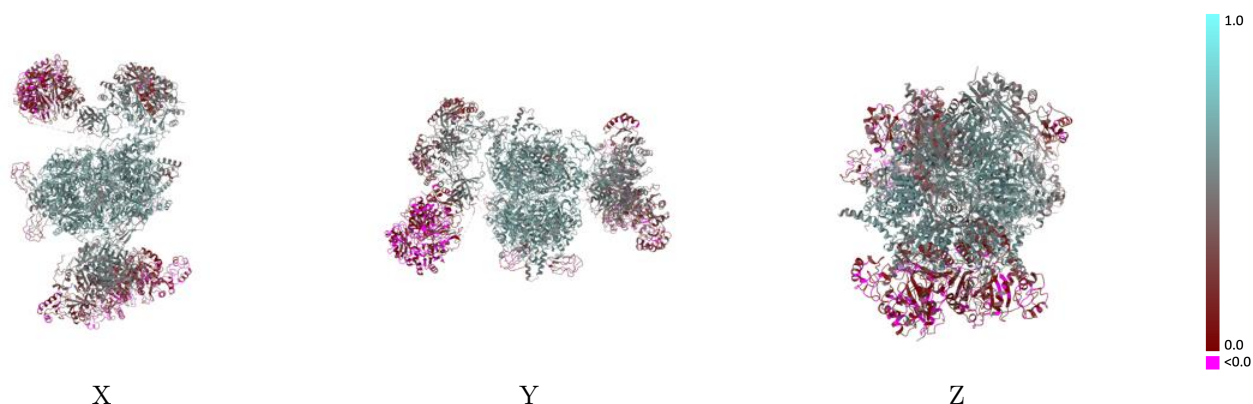
Y



Z

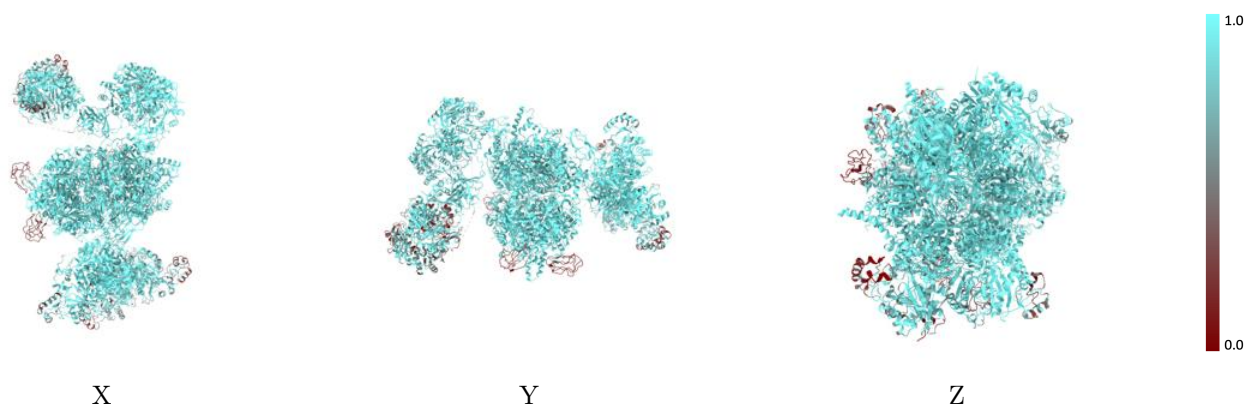
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



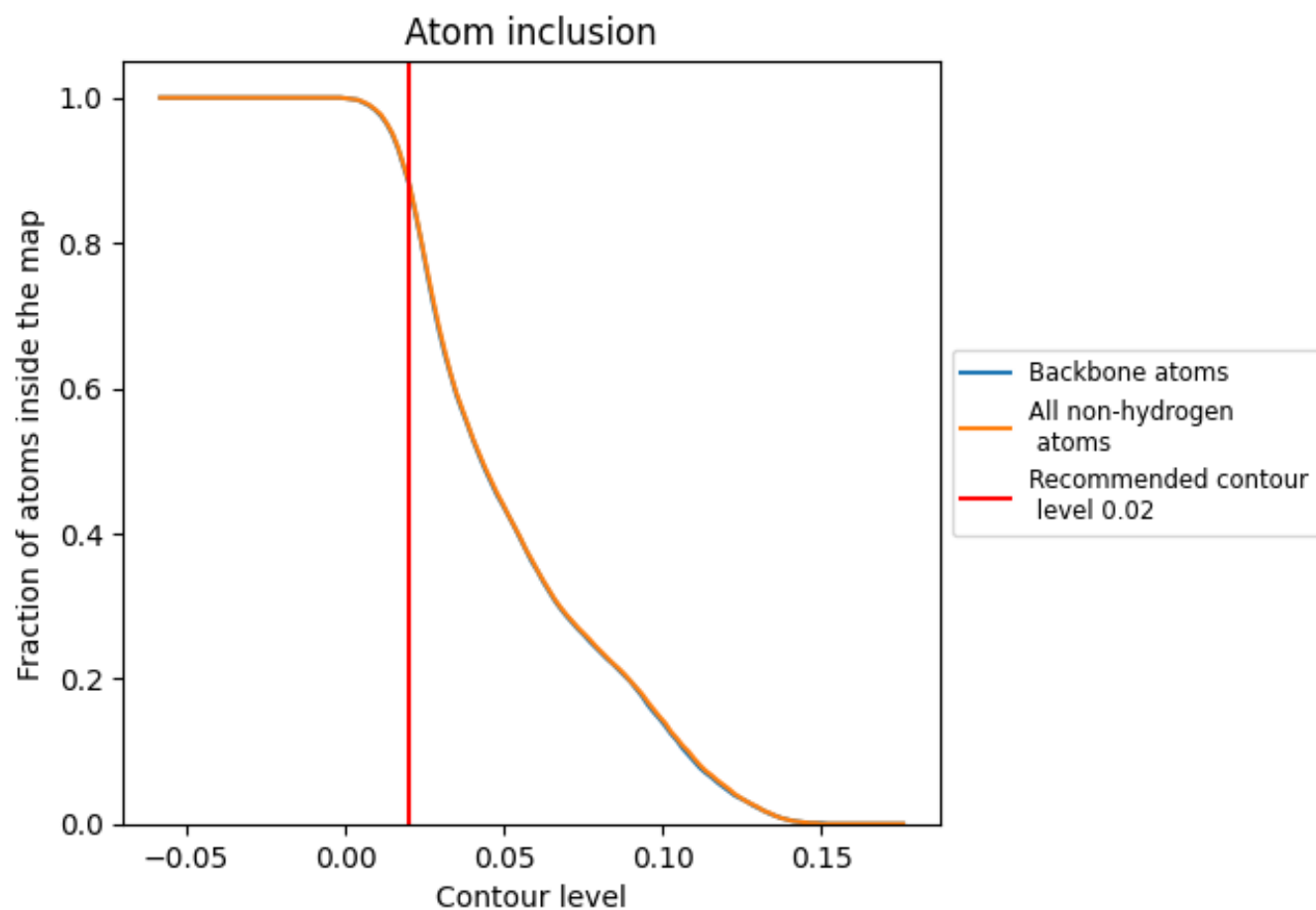
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

## 9.4 Atom inclusion [i](#)





































At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8850	 0.4270
A3a	 0.9600	 0.4870
A3b	 0.8290	 0.3610
A3c	 0.7610	 0.1780
A3d	 0.8060	 0.2110
A3e	 0.9250	 0.4490
A3f	 0.7920	 0.3270
A3g	 0.6460	 0.0830
A3h	 0.7130	 0.1550
D4a	 0.9850	 0.6050
D4b	 0.9830	 0.6060
D5a	 0.9900	 0.6100
D5b	 0.9910	 0.6110
D5c	 0.9880	 0.6120
D5d	 0.9870	 0.6080
E5a	 0.9840	 0.5670
E5b	 0.9590	 0.5570

