



## Full wwPDB EM Validation Report ⓘ

Jun 4, 2026 – 11:23 am BST

PDB ID : 9T97 / pdb\_00009t97  
EMDB ID : EMD-55718  
Title : cryo-EM structure of AccA3/AccD4/AccD5/AccE5 complex from Mycobacterium smegmatis  
Authors : Mullapudi, E.; Thai, H.M.; de Carvalho, L.P.S.; Wilmanns, M.  
Deposited on : 2025-11-14  
Resolution : 2.35 Å(reported)  
Based on initial model : .

This is a Full wwPDB EM Validation 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:

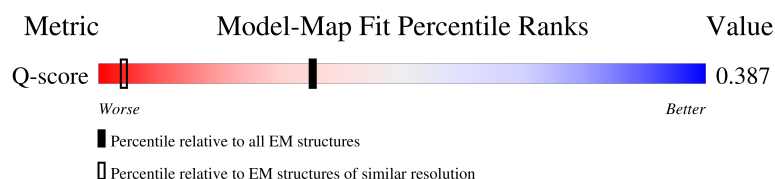
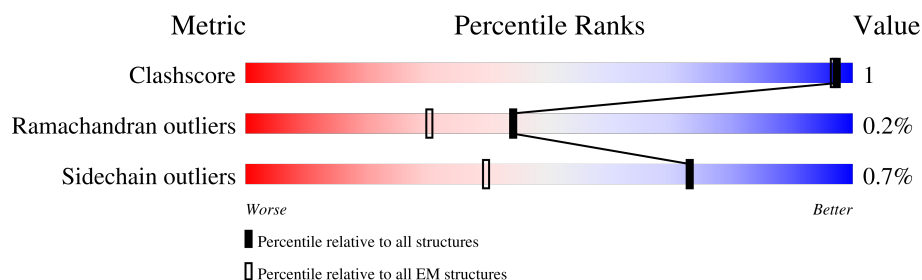
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using 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*

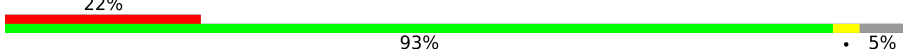


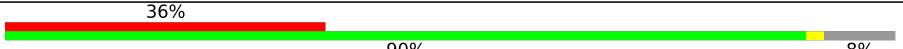
The reported resolution of this entry is 2.35 Å.

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	4607 ( 1.85 - 2.85 )

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	A3f	598	
1	A3g	598	
1	A3i	598	
2	D4a	517	
2	D4b	517	
3	D5a	542	
3	D5b	542	
3	D5c	542	
3	D5d	542	
4	E5a	94	
4	E5b	94	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 42207 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 Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A3a	571	Total	C	N	O	S	0	0
			4298	2698	762	829	9		
1	A3b	561	Total	C	N	O	S	0	0
			4210	2642	739	820	9		
1	A3c	483	Total	C	N	O	S	0	0
			3666	2304	649	707	6		
1	A3d	550	Total	C	N	O	S	0	0
			4127	2592	728	798	9		
1	A3f	74	Total	C	N	O	S	0	0
			514	318	85	108	3		
1	A3g	74	Total	C	N	O	S	0	0
			514	318	85	108	3		
1	A3i	13	Total	C	N	O		0	0
			105	66	26	13			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D4a	515	Total	C	N	O	S	0	0
			3939	2496	689	738	16		
2	D4b	515	Total	C	N	O	S	0	0
			3939	2496	689	738	16		

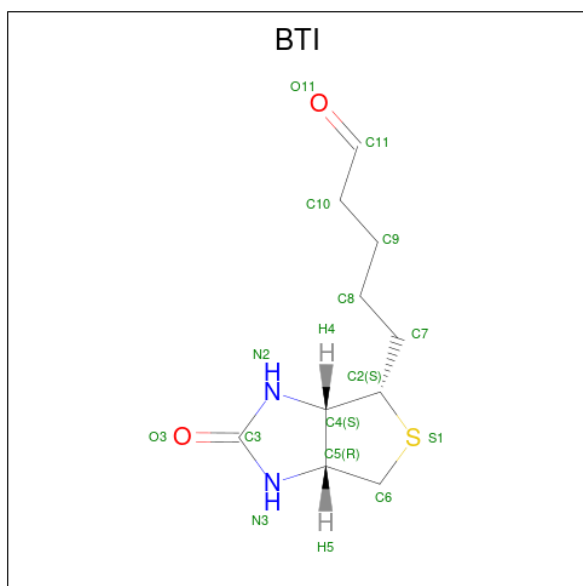
- Molecule 3 is a protein called Propionyl-CoA carboxylase beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D5a	529	Total	C	N	O	S	0	0
			4014	2536	687	776	15		
3	D5b	529	Total	C	N	O	S	0	0
			4014	2536	687	776	15		
3	D5c	529	Total	C	N	O	S	0	0
			4014	2536	687	776	15		
3	D5d	529	Total	C	N	O	S	0	0
			4014	2536	687	776	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E5a	59	Total	C	N	O	S	0	0
			476	299	92	81	4		
4	E5b	32	Total	C	N	O	S	0	0
			288	181	59	46	2		

- Molecule 5 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (CCD ID: BTI) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).

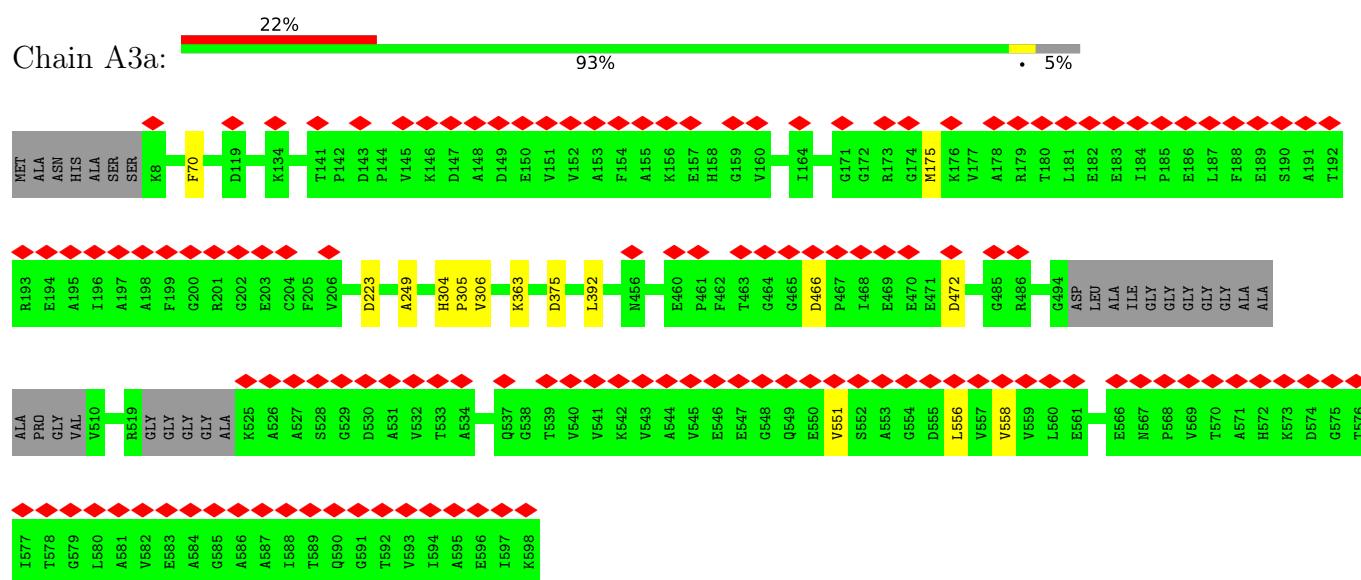


Mol	Chain	Residues	Atoms					AltConf
5	A3a	1	Total	C	N	O	S	0
			15	10	2	2	1	
5	A3b	1	Total	C	N	O	S	0
			15	10	2	2	1	
5	A3f	1	Total	C	N	O	S	0
			15	10	2	2	1	
5	D5a	1	Total	C	N	O	S	0
			15	10	2	2	1	
5	D5d	1	Total	C	N	O	S	0
			15	10	2	2	1	

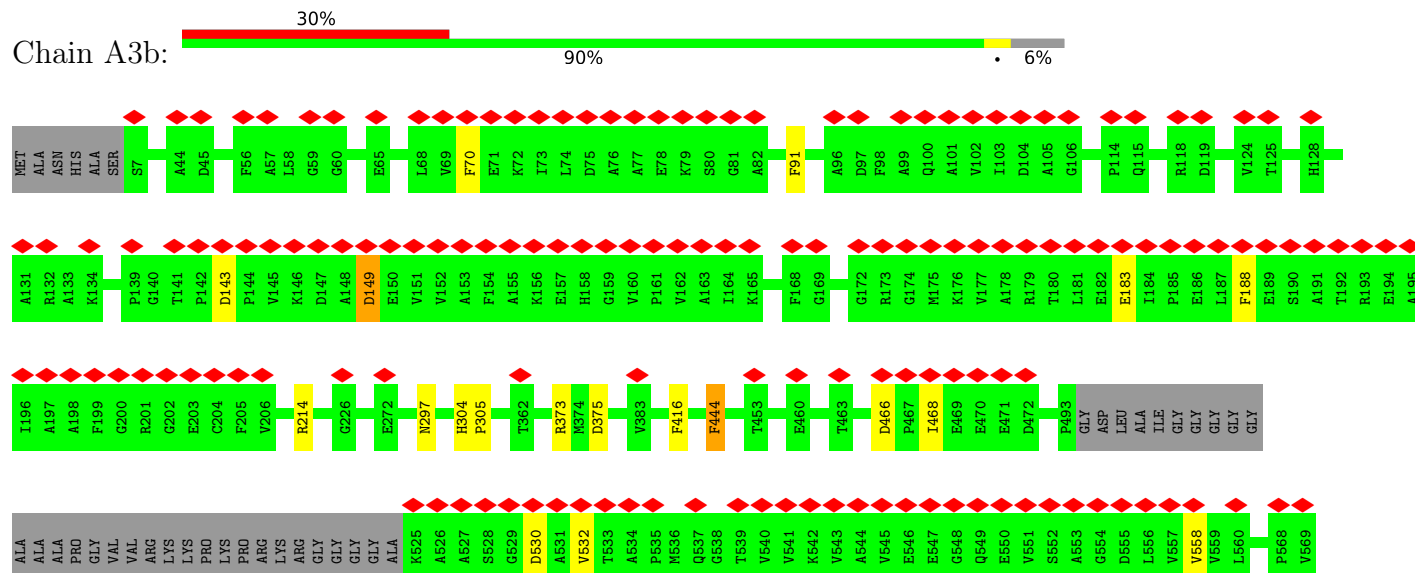
### 3 Residue-property plots

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



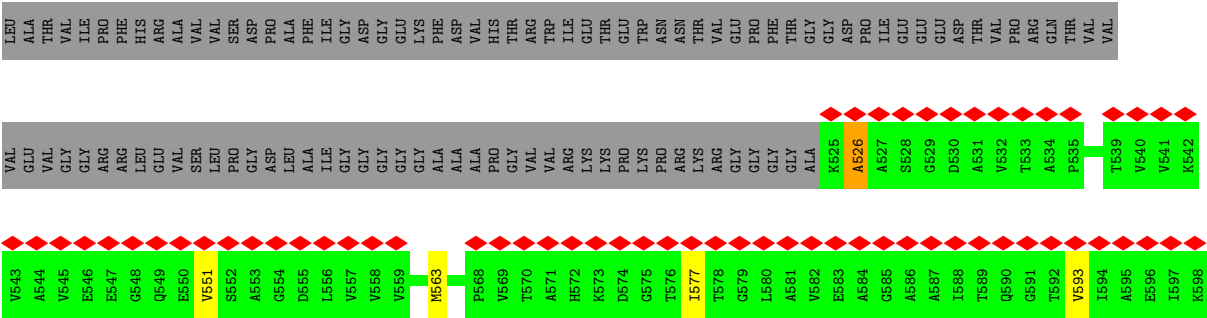
#### • Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit



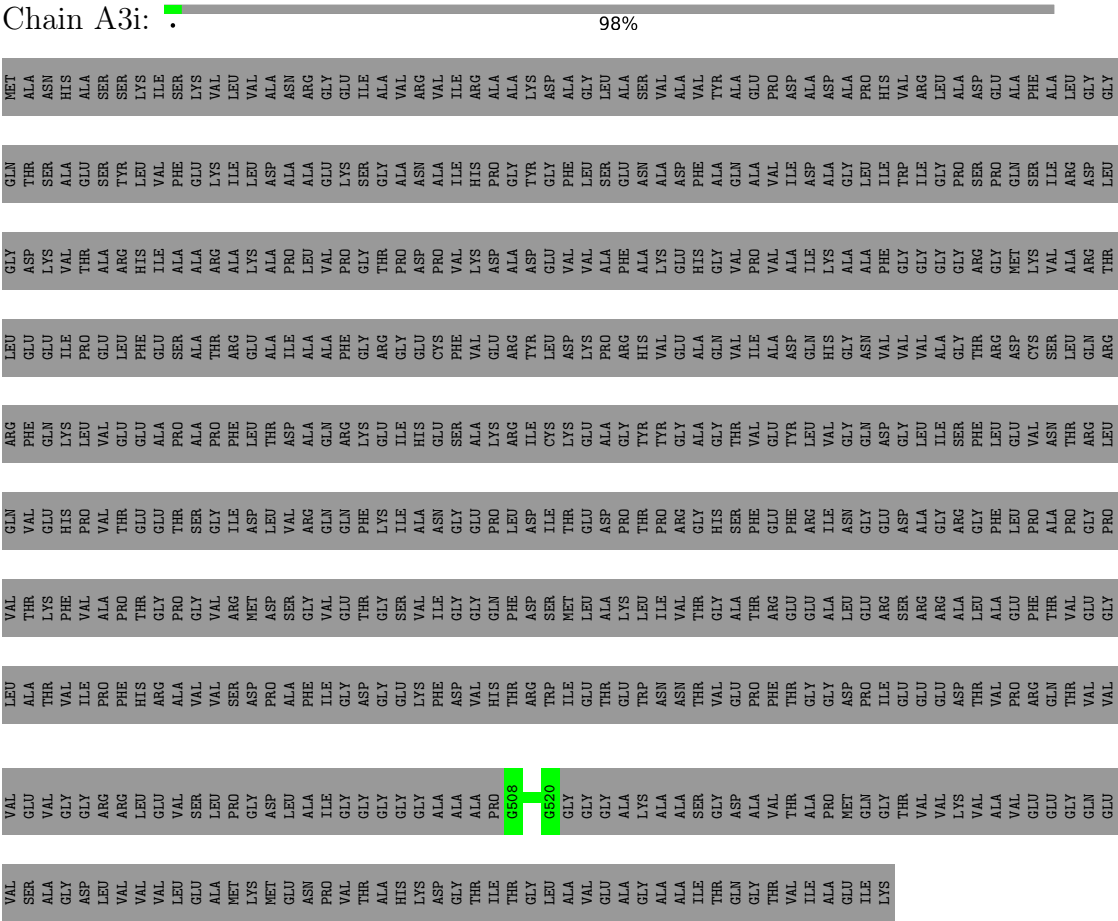




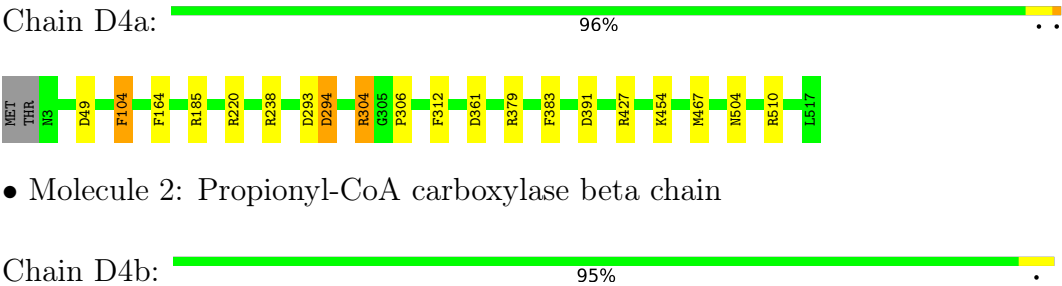




● Molecule 1: Biotin-dependent acyl-coenzyme A carboxylase alpha3 subunit



● Molecule 2: Propionyl-CoA carboxylase beta chain



● Molecule 2: Propionyl-CoA carboxylase beta chain



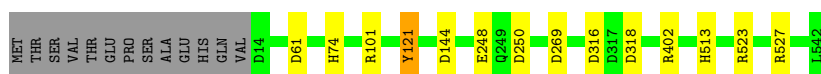
- Molecule 3: Propionyl-CoA carboxylase beta chain

Chain D5a: 94%



- Molecule 3: Propionyl-CoA carboxylase beta chain

Chain D5b: 95%



- Molecule 3: Propionyl-CoA carboxylase beta chain

Chain D5c: 95%



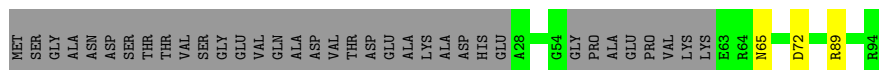
- Molecule 3: Propionyl-CoA carboxylase beta chain

Chain D5d: 95%



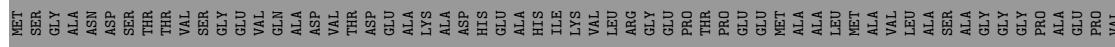
- Molecule 4: Acetyl-/propionyl-coenzyme A carboxylase AccE5

Chain E5a: 60% 37%



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

Chain E5b: 32% 66%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	251974	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	0.470	Depositor
Minimum map value	-0.176	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.03	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: BTI

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	0.66	0/4376	1.04	5/5932 (0.1%)
1	A3b	0.66	0/4287	1.05	10/5818 (0.2%)
1	A3c	0.65	0/3740	1.07	2/5077 (0.0%)
1	A3d	0.66	0/4201	1.08	4/5697 (0.1%)
1	A3f	0.81	0/516	1.20	1/699 (0.1%)
1	A3g	0.78	0/516	1.13	0/699
1	A3i	0.68	0/106	1.10	0/137
2	D4a	0.84	0/4020	1.30	14/5449 (0.3%)
2	D4b	0.87	1/4020 (0.0%)	1.32	16/5449 (0.3%)
3	D5a	0.85	0/4090	1.28	10/5557 (0.2%)
3	D5b	0.86	0/4090	1.28	10/5557 (0.2%)
3	D5c	0.87	0/4090	1.30	9/5557 (0.2%)
3	D5d	0.86	0/4090	1.30	11/5557 (0.2%)
4	E5a	0.73	0/486	1.07	1/652 (0.2%)
4	E5b	0.77	0/296	1.14	1/396 (0.3%)
All	All	0.78	1/42924 (0.0%)	1.20	94/58233 (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	A3b	0	2
1	A3c	0	1
1	A3g	0	1
2	D4a	0	6
2	D4b	0	3
3	D5a	0	2
3	D5b	0	3
3	D5c	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	E5a	0	1
All	All	0	20

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D4b	157	VAL	C-O	-5.04	1.20	1.24

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D5a	144	ASP	CA-CB-CG	10.01	122.61	112.60
3	D5c	250	ASP	CA-CB-CG	9.76	122.36	112.60
3	D5d	144	ASP	CA-CB-CG	9.00	121.60	112.60
3	D5b	250	ASP	CA-CB-CG	7.65	120.25	112.60
3	D5b	144	ASP	CA-CB-CG	7.20	119.80	112.60
2	D4a	104	PHE	CA-CB-CG	7.09	120.89	113.80
2	D4b	306	PRO	N-CA-C	7.00	122.60	114.20
2	D4b	84	ARG	NE-CZ-NH2	6.93	125.44	119.20
2	D4a	306	PRO	N-CA-C	6.88	122.45	114.20
2	D4a	49	ASP	CA-CB-CG	6.84	119.44	112.60
3	D5c	144	ASP	CA-CB-CG	6.77	119.37	112.60
3	D5a	61	ASP	CA-CB-CG	6.72	119.32	112.60
1	A3b	183	GLU	CA-C-N	6.61	124.41	120.24
1	A3b	183	GLU	C-N-CA	6.61	124.41	120.24
3	D5c	61	ASP	CA-CB-CG	6.55	119.15	112.60
2	D4a	379	ARG	NE-CZ-NH2	6.51	125.06	119.20
3	D5b	316	ASP	CA-CB-CG	6.49	119.09	112.60
3	D5b	61	ASP	CA-CB-CG	6.44	119.04	112.60
2	D4b	85	PRO	N-CA-C	6.38	121.21	111.19
3	D5a	318	ASP	CA-CB-CG	6.35	118.95	112.60
3	D5d	121	TYR	CA-CB-CG	6.33	125.30	113.90
1	A3a	375	ASP	CA-CB-CG	6.32	118.92	112.60
3	D5c	101	ARG	NE-CZ-NH2	6.32	124.88	119.20
3	D5b	318	ASP	CA-CB-CG	6.31	118.91	112.60
1	A3d	375	ASP	CA-CB-CG	6.27	118.87	112.60
3	D5d	61	ASP	CA-CB-CG	6.25	118.85	112.60
2	D4a	238	ARG	NE-CZ-NH2	6.25	124.82	119.20
3	D5c	318	ASP	CA-CB-CG	6.23	118.83	112.60
2	D4b	104	PHE	CA-CB-CG	6.14	119.94	113.80
3	D5c	316	ASP	CA-CB-CG	6.10	118.70	112.60
2	D4b	399	ILE	O-C-N	-6.07	116.76	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D4a	164	PHE	CA-CB-CG	6.00	119.80	113.80
3	D5b	101	ARG	NE-CZ-NH2	5.97	124.58	119.20
1	A3a	466	ASP	CA-CB-CG	5.97	118.57	112.60
3	D5d	402	ARG	NE-CZ-NH2	5.94	124.55	119.20
1	A3f	530	ASP	CA-CB-CG	5.86	118.46	112.60
2	D4b	294	ASP	CA-CB-CG	5.83	118.43	112.60
1	A3c	143	ASP	CA-CB-CG	5.80	118.40	112.60
2	D4b	49	ASP	CA-CB-CG	5.80	118.40	112.60
3	D5b	121	TYR	CA-CB-CG	5.79	124.32	113.90
2	D4b	383	PHE	CA-CB-CG	5.76	119.56	113.80
1	A3b	143	ASP	CA-CB-CG	5.71	118.31	112.60
1	A3b	91	PHE	CA-CB-CG	5.69	119.49	113.80
1	A3d	444	PHE	CA-CB-CG	5.66	119.46	113.80
3	D5d	316	ASP	CA-CB-CG	5.65	118.25	112.60
3	D5a	316	ASP	CA-CB-CG	5.61	118.21	112.60
1	A3b	444	PHE	CA-CB-CG	5.61	119.41	113.80
3	D5c	121	TYR	CA-CB-CG	5.60	123.98	113.90
4	E5a	72	ASP	CA-CB-CG	5.56	118.16	112.60
1	A3d	205	PHE	CA-CB-CG	5.55	119.35	113.80
2	D4a	304	ARG	NE-CZ-NH2	5.53	124.17	119.20
2	D4a	383	PHE	CA-CB-CG	5.50	119.31	113.80
2	D4b	127	ASP	CA-CB-CG	5.50	118.10	112.60
3	D5d	74	HIS	CA-CB-CG	5.46	119.27	113.80
1	A3a	223	ASP	CA-CB-CG	5.45	118.05	112.60
2	D4a	312	PHE	CA-CB-CG	5.44	119.24	113.80
3	D5a	266	ASN	CA-CB-CG	5.41	118.01	112.60
2	D4b	400	ARG	N-CA-C	5.38	116.50	108.31
3	D5a	74	HIS	CA-CB-CG	5.36	119.16	113.80
1	A3b	375	ASP	CA-CB-CG	5.35	117.95	112.60
4	E5b	72	ASP	CA-CB-CG	5.34	117.94	112.60
2	D4a	293	ASP	CA-CB-CG	5.34	117.94	112.60
3	D5b	74	HIS	CA-CB-CG	5.34	119.14	113.80
2	D4b	150	HIS	CB-CG-CD2	-5.30	124.31	131.20
3	D5a	121	TYR	CA-CB-CG	5.30	123.43	113.90
1	A3a	70	PHE	CA-CB-CG	5.29	119.09	113.80
1	A3b	149	ASP	CA-CB-CG	5.28	117.88	112.60
3	D5a	423	ARG	CB-CA-C	5.27	120.90	110.42
2	D4b	43	ARG	NE-CZ-NH2	5.23	123.91	119.20
3	D5d	167	ASN	OD1-CG-ND2	-5.22	117.38	122.60
1	A3b	530	ASP	CA-CB-CG	5.21	117.81	112.60
1	A3b	70	PHE	CA-CB-CG	5.19	118.99	113.80
1	A3c	466	ASP	CA-CB-CG	5.19	117.79	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D4b	267	ASP	CA-CB-CG	5.18	117.78	112.60
1	A3a	472	ASP	CA-CB-CG	5.17	117.77	112.60
2	D4a	304	ARG	NE-CZ-NH1	-5.15	116.35	121.50
3	D5d	202	ASP	N-CA-C	5.15	117.63	111.71
2	D4a	361	ASP	CA-CB-CG	5.15	117.75	112.60
3	D5d	202	ASP	CA-CB-CG	5.14	117.74	112.60
3	D5d	318	ASP	CA-CB-CG	5.14	117.74	112.60
3	D5c	164	PHE	CA-CB-CG	5.13	118.93	113.80
3	D5b	269	ASP	CA-CB-CG	5.11	117.71	112.60
2	D4b	366	MET	CB-CA-C	-5.10	101.76	109.26
3	D5d	101	ARG	NE-CZ-NH2	5.10	123.79	119.20
3	D5a	290	ASP	CA-CB-CG	5.10	117.70	112.60
2	D4b	276	ASP	CA-CB-CG	5.08	117.68	112.60
2	D4b	335	ASP	CA-CB-CG	5.07	117.67	112.60
1	A3d	75	ASP	CB-CA-C	5.05	119.44	110.85
3	D5b	248	GLU	CB-CG-CD	5.05	121.19	112.60
2	D4a	391	ASP	CA-CB-CG	5.05	117.65	112.60
2	D4a	238	ARG	CD-NE-CZ	5.04	131.46	124.40
1	A3b	466	ASP	CA-CB-CG	5.04	117.64	112.60
3	D5c	212	PRO	N-CA-C	5.01	120.42	113.65
3	D5a	412	GLU	CB-CG-CD	5.01	121.11	112.60

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A3b	214	ARG	Sidechain
1	A3b	373	ARG	Sidechain
1	A3c	373	ARG	Sidechain
1	A3g	526	ALA	Peptide
2	D4a	185	ARG	Sidechain
2	D4a	294	ASP	Peptide
2	D4a	304	ARG	Sidechain
2	D4a	427	ARG	Sidechain
2	D4a	504	ASN	Peptide
2	D4a	510	ARG	Sidechain
2	D4b	293	ASP	Peptide
2	D4b	304	ARG	Sidechain
2	D4b	379	ARG	Sidechain
3	D5a	341	ARG	Sidechain
3	D5a	401	ARG	Sidechain
3	D5b	402	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	D5b	523	ARG	Sidechain
3	D5b	527	ARG	Sidechain
3	D5c	515	ARG	Sidechain
4	E5a	89	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	4298	0	4286	4	0
1	A3b	4210	0	4175	1	0
1	A3c	3666	0	3610	11	0
1	A3d	4127	0	4104	14	0
1	A3f	514	0	529	0	0
1	A3g	514	0	529	10	0
1	A3i	105	0	128	0	0
2	D4a	3939	0	3939	1	0
2	D4b	3939	0	3939	2	0
3	D5a	4014	0	3995	3	0
3	D5b	4014	0	3995	0	0
3	D5c	4014	0	3995	1	0
3	D5d	4014	0	3995	2	0
4	E5a	476	0	479	0	0
4	E5b	288	0	284	2	0
5	A3a	15	0	16	0	0
5	A3b	15	0	16	0	0
5	A3f	15	0	16	0	0
5	D5a	15	0	16	0	0
5	D5d	15	0	16	1	0
All	All	42207	0	42062	48	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.

All (48) 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:551:VAL:CG1	1:A3g:577:ILE:HD12	1.69	1.20
1:A3d:38:VAL:CG1	1:A3d:58:LEU:HG	1.81	1.10
1:A3g:551:VAL:HG12	1:A3g:577:ILE:HD12	1.08	1.05
1:A3g:526:ALA:HA	1:A3g:593:VAL:HG23	1.42	1.01
1:A3d:38:VAL:HG11	1:A3d:58:LEU:HD11	1.42	1.00
1:A3c:253:PHE:HD2	1:A3c:444:PHE:CD2	1.83	0.97
1:A3d:38:VAL:HG13	1:A3d:58:LEU:HG	1.45	0.95
1:A3c:253:PHE:CD2	1:A3c:444:PHE:CD2	2.54	0.94
1:A3c:253:PHE:CD2	1:A3c:444:PHE:HD2	1.85	0.94
1:A3d:38:VAL:HG11	1:A3d:58:LEU:CD1	1.97	0.93
1:A3g:551:VAL:HG12	1:A3g:577:ILE:CD1	1.99	0.92
1:A3d:38:VAL:CG1	1:A3d:58:LEU:CG	2.46	0.92
1:A3g:551:VAL:CG1	1:A3g:577:ILE:CD1	2.49	0.90
1:A3c:249:ALA:HB3	1:A3c:306:VAL:HG12	1.59	0.84
1:A3d:38:VAL:CG1	1:A3d:58:LEU:CD1	2.55	0.84
1:A3g:526:ALA:HA	1:A3g:593:VAL:CG2	2.13	0.79
1:A3d:38:VAL:HG11	1:A3d:58:LEU:CG	2.13	0.73
1:A3c:253:PHE:HD2	1:A3c:444:PHE:CE2	2.14	0.65
1:A3c:249:ALA:CB	1:A3c:306:VAL:HG12	2.30	0.61
1:A3d:38:VAL:CG1	1:A3d:58:LEU:HD11	2.23	0.61
1:A3c:249:ALA:HB3	1:A3c:306:VAL:CG1	2.33	0.55
2:D4b:336:ASN:ND2	2:D4b:371:GLU:OE1	2.41	0.54
1:A3d:556:LEU:H	1:A3d:556:LEU:HD23	1.73	0.54
1:A3d:249:ALA:HB1	1:A3d:250:PRO:HD2	1.90	0.53
1:A3g:563:MET:HE2	5:D5d:601:BTI:S1	2.48	0.53
1:A3c:444:PHE:HD1	1:A3c:446:VAL:HG22	1.74	0.52
1:A3d:38:VAL:HG12	1:A3d:58:LEU:CD1	2.40	0.51
3:D5d:529:ILE:HD12	4:E5b:67:TRP:CE2	2.45	0.51
3:D5a:495:ASN:HB2	3:D5a:496:PRO:HD2	1.93	0.50
1:A3d:249:ALA:HB1	1:A3d:250:PRO:CD	2.43	0.49
3:D5c:495:ASN:HB2	3:D5c:496:PRO:HD2	1.96	0.48
1:A3a:249:ALA:HB3	1:A3a:306:VAL:HG12	1.96	0.47
1:A3g:526:ALA:C	1:A3g:593:VAL:HG21	2.39	0.47
1:A3c:19:GLU:OE2	1:A3c:375:ASP:HB3	2.16	0.46
3:D5a:36:VAL:HG12	3:D5a:36:VAL:O	2.17	0.45
1:A3b:304:HIS:N	1:A3b:305:PRO:CD	2.81	0.44
1:A3a:304:HIS:N	1:A3a:305:PRO:CD	2.81	0.44
1:A3d:492:LEU:HB3	1:A3d:493:PRO:CD	2.49	0.43
1:A3c:304:HIS:N	1:A3c:305:PRO:HD2	2.34	0.43
3:D5a:36:VAL:O	3:D5a:36:VAL:CG1	2.67	0.42
1:A3a:551:VAL:HG23	1:A3a:556:LEU:HA	2.01	0.42
1:A3g:526:ALA:CA	1:A3g:593:VAL:CG2	2.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A3a:551:VAL:O	1:A3a:551:VAL:HG22	2.20	0.41
1:A3c:350:ALA:HB2	1:A3c:354:PHE:CE1	2.55	0.41
3:D5d:529:ILE:HD12	4:E5b:67:TRP:CZ2	2.56	0.41
2:D4a:220:ARG:NH1	2:D4b:373:LYS:HE2	2.36	0.41
1:A3g:526:ALA:C	1:A3g:593:VAL:CG2	2.94	0.40
1:A3d:249:ALA:O	1:A3d:250:PRO:C	2.64	0.40

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	A3a	565/598 (94%)	533 (94%)	31 (6%)	1 (0%)	43	52
1	A3b	557/598 (93%)	531 (95%)	22 (4%)	4 (1%)	18	20
1	A3c	481/598 (80%)	467 (97%)	14 (3%)	0	100	100
1	A3d	544/598 (91%)	522 (96%)	20 (4%)	2 (0%)	30	34
1	A3f	72/598 (12%)	64 (89%)	6 (8%)	2 (3%)	4	2
1	A3g	72/598 (12%)	65 (90%)	7 (10%)	0	100	100
1	A3i	11/598 (2%)	10 (91%)	1 (9%)	0	100	100
2	D4a	513/517 (99%)	499 (97%)	14 (3%)	0	100	100
2	D4b	513/517 (99%)	502 (98%)	11 (2%)	0	100	100
3	D5a	527/542 (97%)	515 (98%)	12 (2%)	0	100	100
3	D5b	527/542 (97%)	515 (98%)	12 (2%)	0	100	100
3	D5c	527/542 (97%)	514 (98%)	13 (2%)	0	100	100
3	D5d	527/542 (97%)	516 (98%)	11 (2%)	0	100	100
4	E5a	55/94 (58%)	53 (96%)	2 (4%)	0	100	100
4	E5b	30/94 (32%)	30 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5521/7576 (73%)	5336 (97%)	176 (3%)	9 (0%)	44	52

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A3b	468	ILE
1	A3f	532	VAL
1	A3b	532	VAL
1	A3f	558	VAL
1	A3a	558	VAL
1	A3b	594	ILE
1	A3b	558	VAL
1	A3d	250	PRO
1	A3d	597	ILE

### 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	443/453 (98%)	440 (99%)	3 (1%)	76	86
1	A3b	434/453 (96%)	428 (99%)	6 (1%)	59	73
1	A3c	377/453 (83%)	376 (100%)	1 (0%)	86	92
1	A3d	424/453 (94%)	423 (100%)	1 (0%)	87	94
1	A3f	53/453 (12%)	52 (98%)	1 (2%)	50	65
1	A3g	53/453 (12%)	53 (100%)	0	100	100
1	A3i	11/453 (2%)	11 (100%)	0	100	100
2	D4a	410/412 (100%)	406 (99%)	4 (1%)	68	81
2	D4b	410/412 (100%)	410 (100%)	0	100	100
3	D5a	424/436 (97%)	420 (99%)	4 (1%)	70	82
3	D5b	424/436 (97%)	422 (100%)	2 (0%)	81	89
3	D5c	424/436 (97%)	421 (99%)	3 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D5d	424/436 (97%)	420 (99%)	4 (1%)	70	82
4	E5a	49/76 (64%)	48 (98%)	1 (2%)	48	63
4	E5b	31/76 (41%)	31 (100%)	0	100	100
All	All	4391/5891 (74%)	4361 (99%)	30 (1%)	73	86

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A3a	175	MET
1	A3a	363	LYS
1	A3a	392	LEU
1	A3b	149	ASP
1	A3b	188	PHE
1	A3b	297	ASN
1	A3b	416	PHE
1	A3b	444	PHE
1	A3b	598	LYS
1	A3c	373	ARG
1	A3d	416	PHE
1	A3f	537	GLN
2	D4a	104	PHE
2	D4a	294	ASP
2	D4a	454	LYS
2	D4a	467	MET
3	D5a	121	TYR
3	D5a	137	ARG
3	D5a	144	ASP
3	D5a	513	HIS
3	D5b	121	TYR
3	D5b	513	HIS
3	D5c	121	TYR
3	D5c	307	MET
3	D5c	513	HIS
3	D5d	121	TYR
3	D5d	144	ASP
3	D5d	469	LYS
3	D5d	513	HIS
4	E5a	65	ASN

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 ⓘ

5 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	$\# Z  > 2$
5	BTI	A3a	1001	-	16,16,16	0.53	0	21,21,21	1.27	3 (14%)
5	BTI	A3b	601	-	16,16,16	0.51	0	21,21,21	0.49	0
5	BTI	A3f	601	-	16,16,16	0.53	0	21,21,21	0.33	0
5	BTI	D5a	601	-	16,16,16	0.52	0	21,21,21	0.42	0
5	BTI	D5d	601	-	16,16,16	0.47	0	21,21,21	0.69	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
5	BTI	A3a	1001	-	-	2/5/27/27	0/2/2/2
5	BTI	A3b	601	-	-	1/5/27/27	0/2/2/2
5	BTI	A3f	601	-	-	1/5/27/27	0/2/2/2
5	BTI	D5a	601	-	-	0/5/27/27	0/2/2/2
5	BTI	D5d	601	-	-	4/5/27/27	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A3a	1001	BTI	C6-S1-C2	-3.22	83.28	89.89
5	A3a	1001	BTI	C6-C5-C4	-2.54	106.45	108.66
5	A3a	1001	BTI	C2-C4-C5	-2.49	106.05	108.94

There are no chirality outliers.

All (8) torsion outliers are listed below:

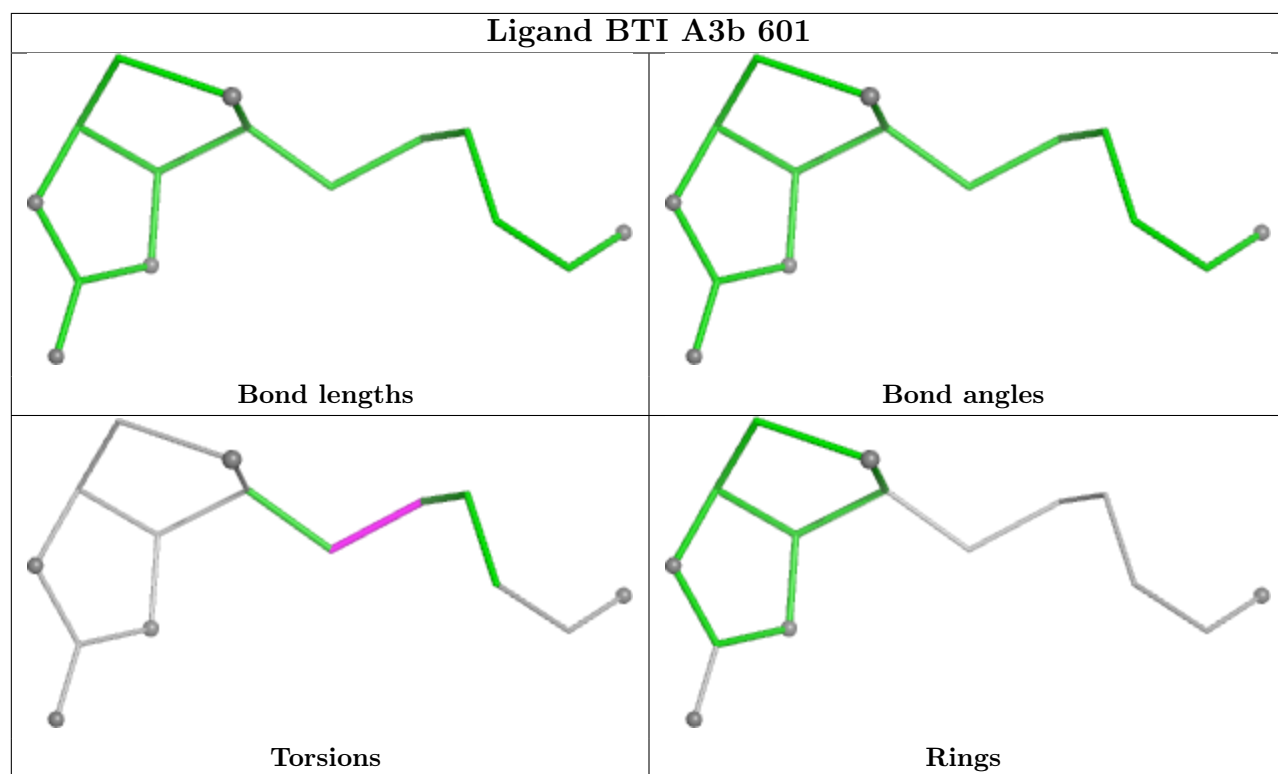
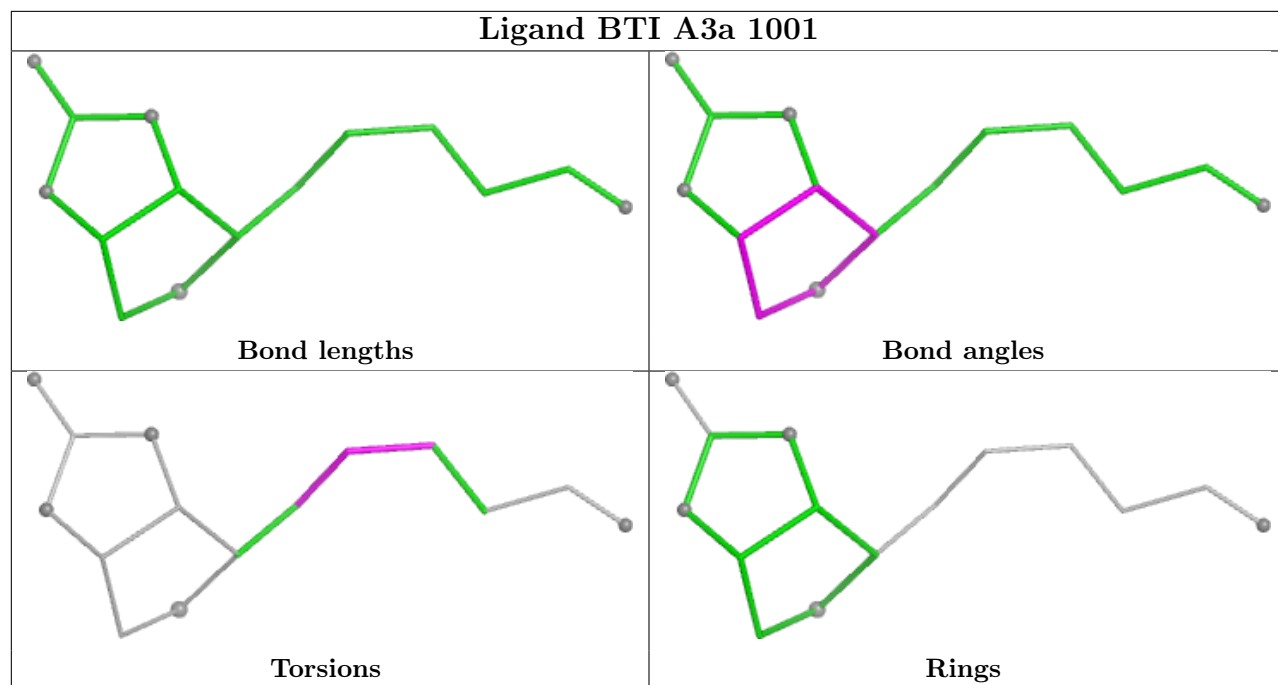
Mol	Chain	Res	Type	Atoms
5	D5d	601	BTI	S1-C2-C7-C8
5	A3f	601	BTI	C2-C7-C8-C9
5	A3a	1001	BTI	C2-C7-C8-C9
5	A3b	601	BTI	C2-C7-C8-C9
5	D5d	601	BTI	C2-C7-C8-C9
5	D5d	601	BTI	C4-C2-C7-C8
5	A3a	1001	BTI	C7-C8-C9-C10
5	D5d	601	BTI	C7-C8-C9-C10

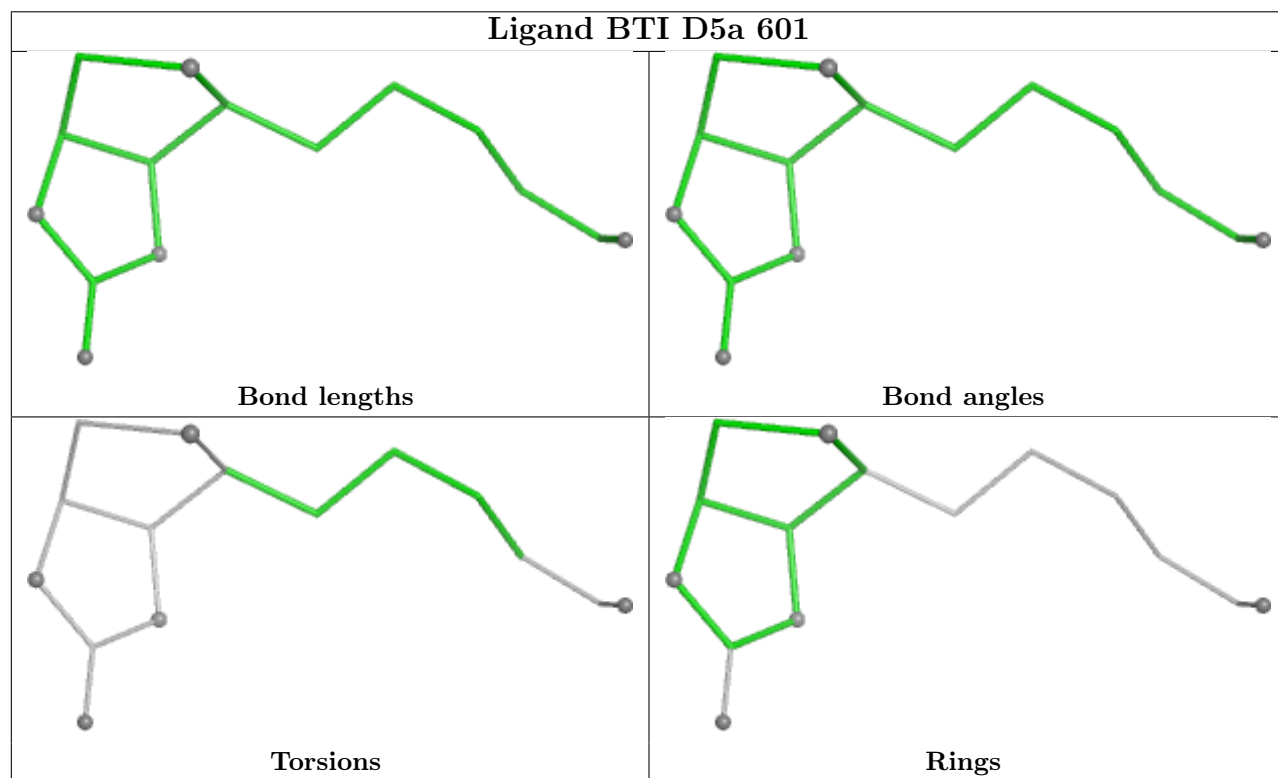
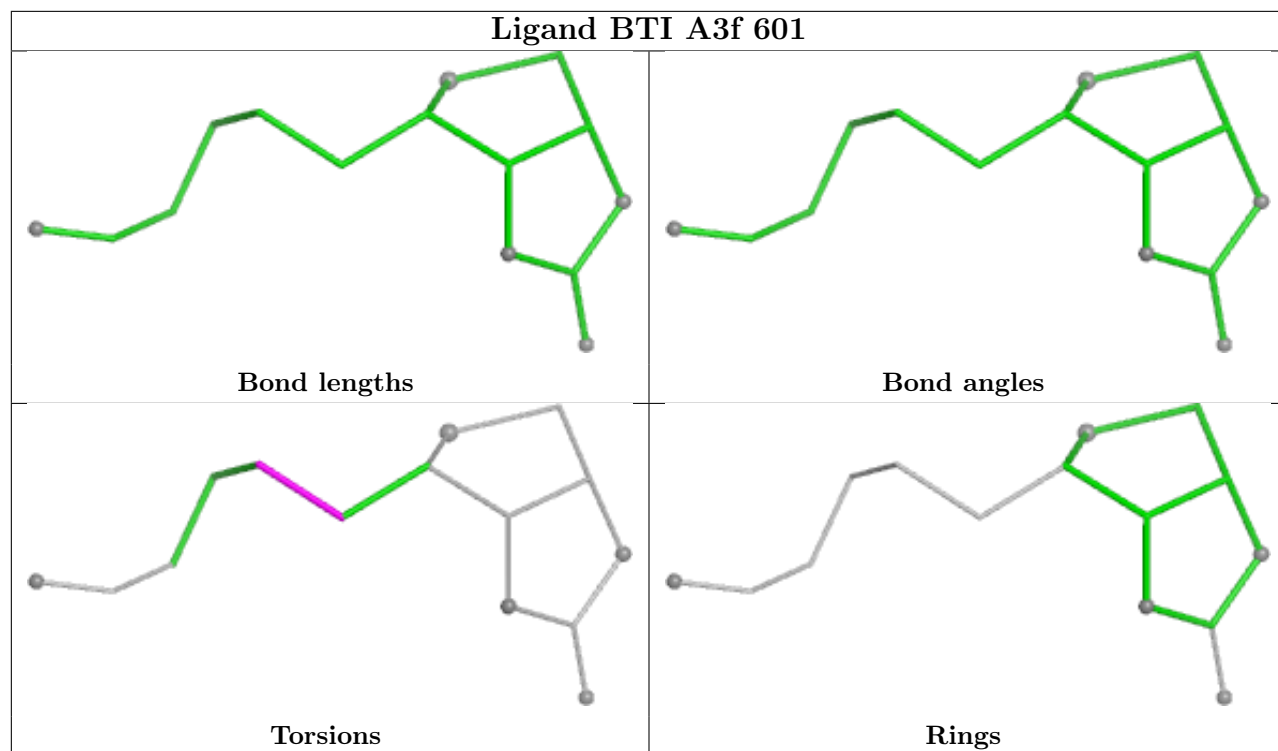
There are no ring outliers.

1 monomer is involved in 1 short contact:

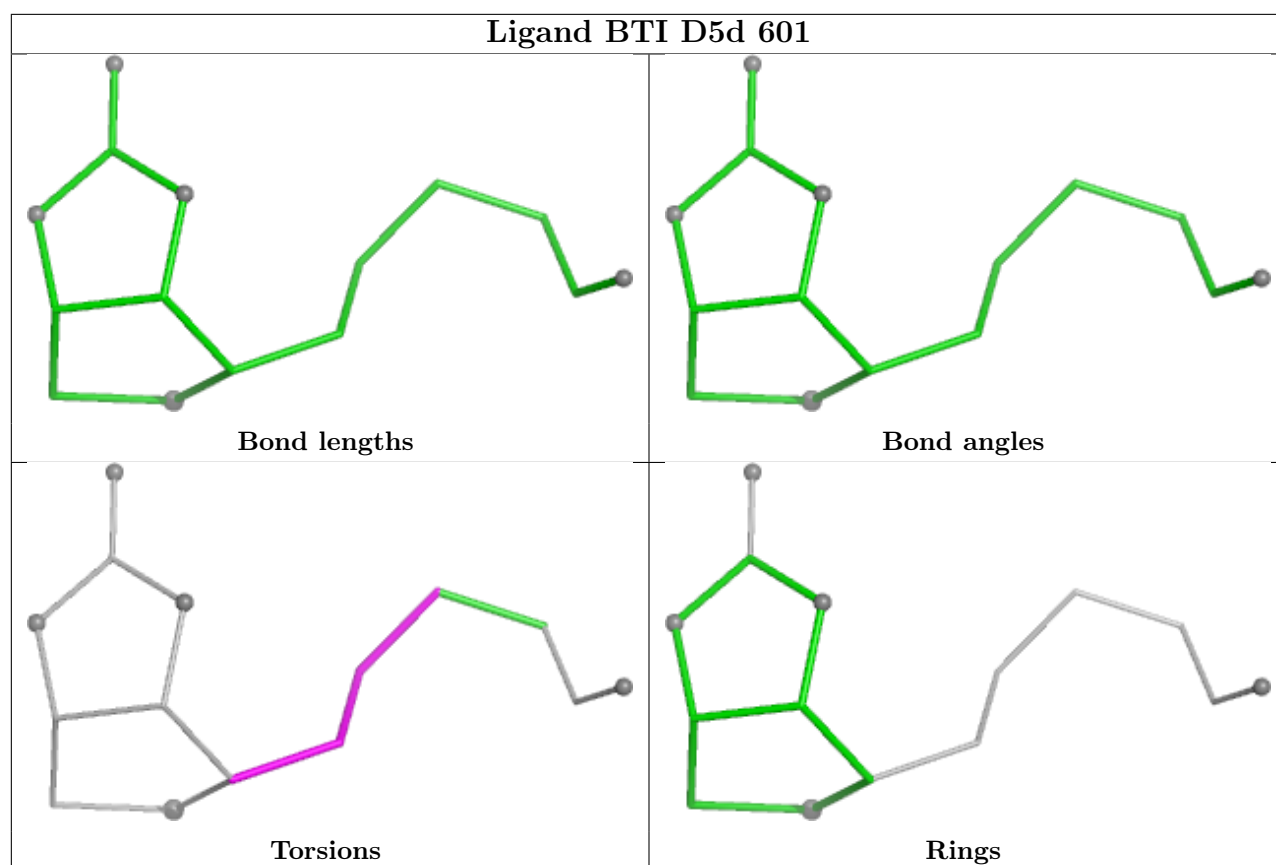
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D5d	601	BTI	1	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

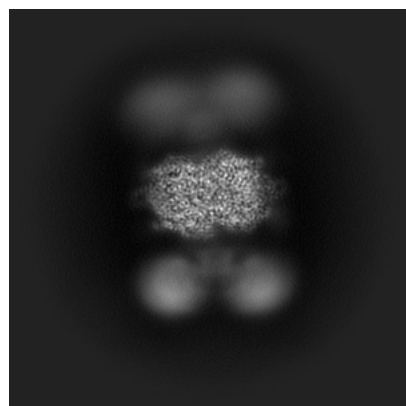
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55718. These allow visual inspection of the internal detail of the map and identification of artifacts.

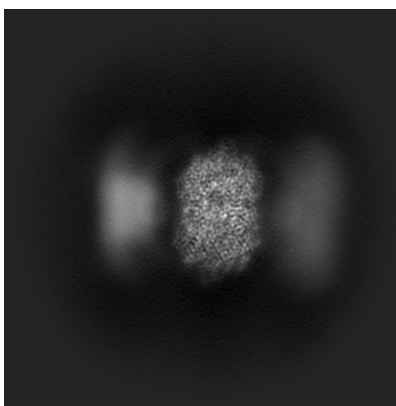
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

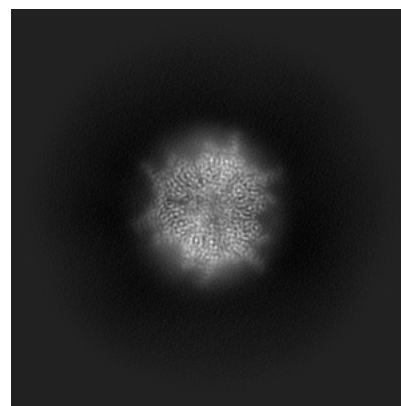
#### 6.1.1 Primary map



X

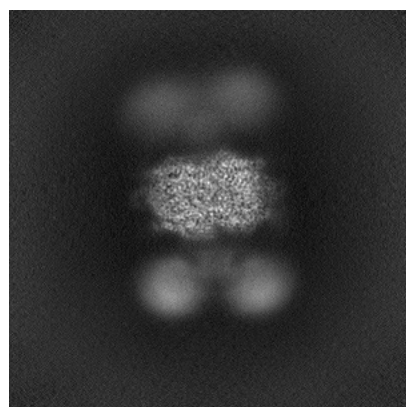


Y

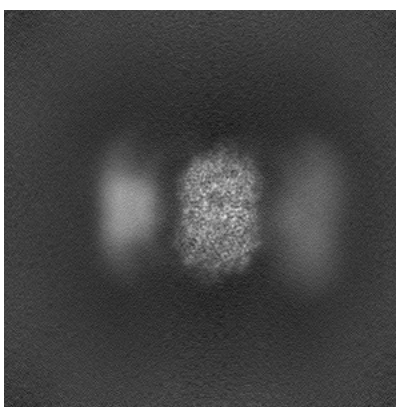


Z

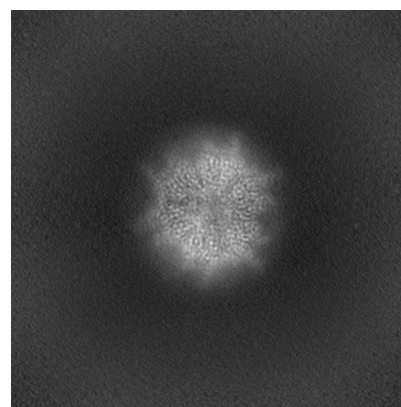
#### 6.1.2 Raw map



X



Y

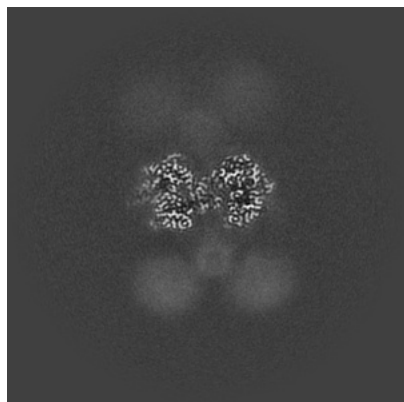


Z

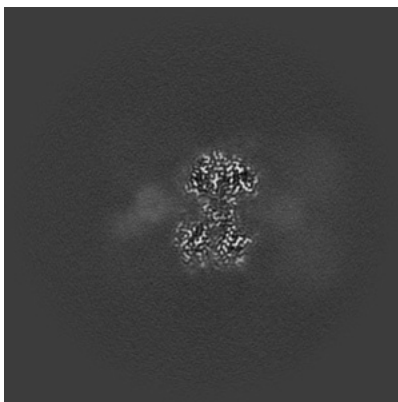
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

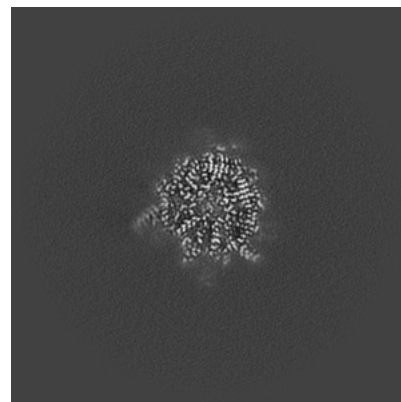
### 6.2.1 Primary map



X Index: 280

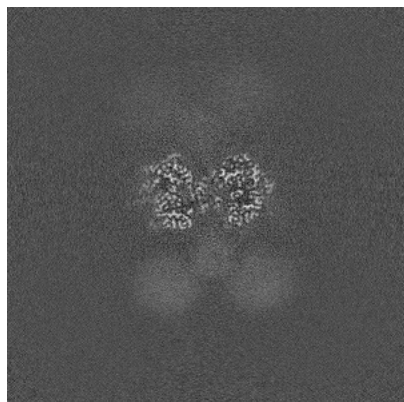


Y Index: 280

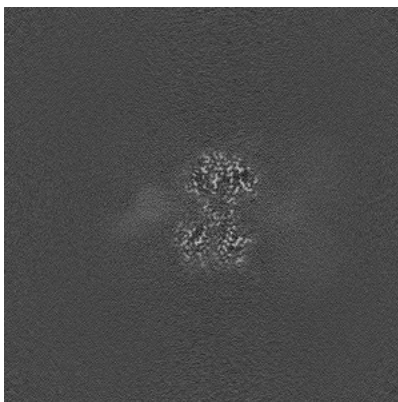


Z Index: 280

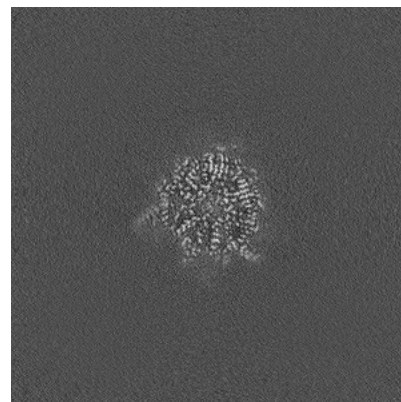
### 6.2.2 Raw map



X Index: 280



Y Index: 280

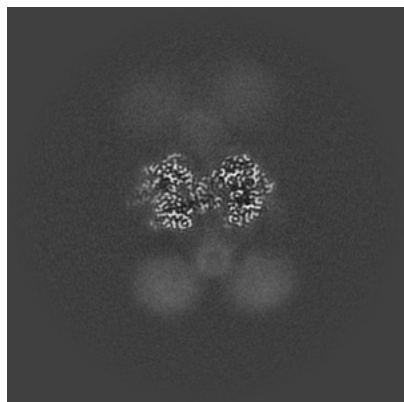


Z Index: 280

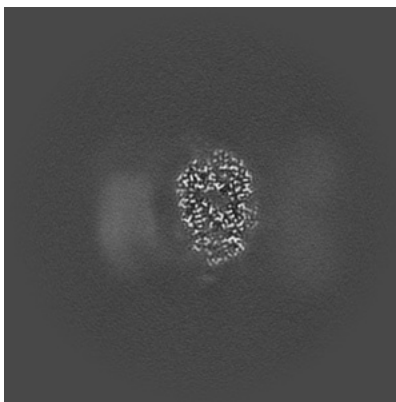
The images above show central slices of the map in three orthogonal directions.

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

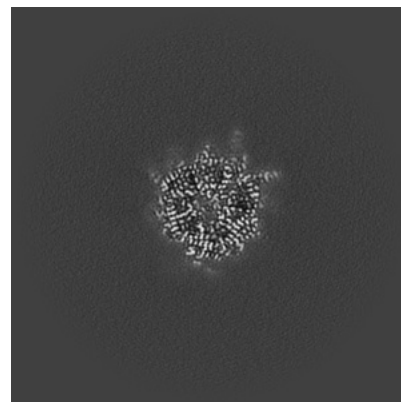
### 6.3.1 Primary map



X Index: 280

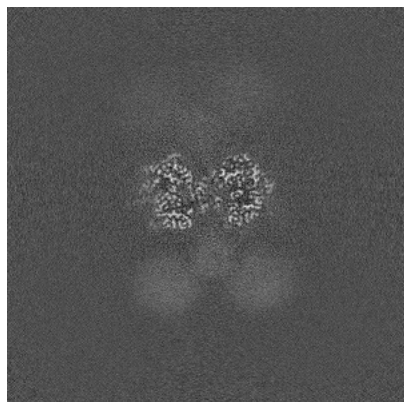


Y Index: 243

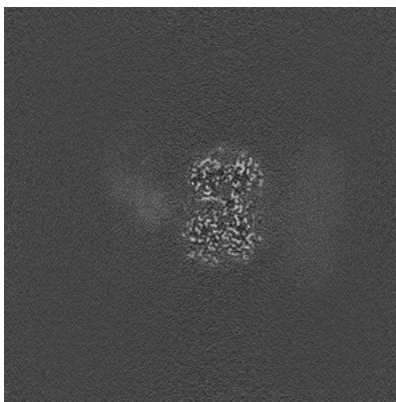


Z Index: 322

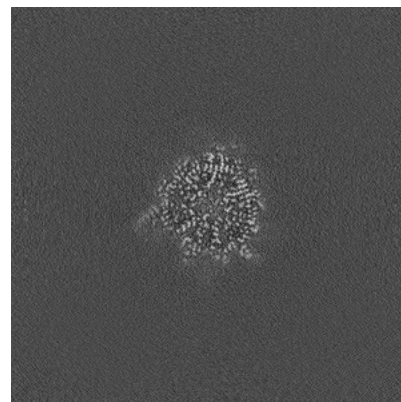
### 6.3.2 Raw map



X Index: 280



Y Index: 302



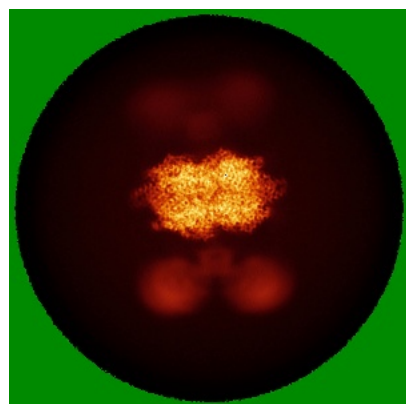
Z Index: 279

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

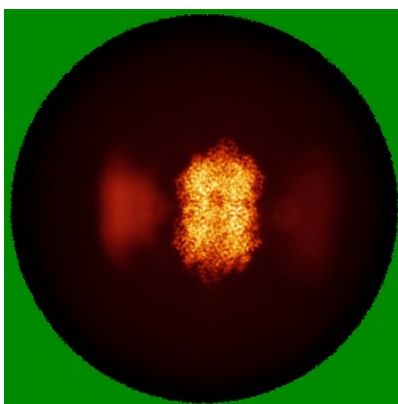


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

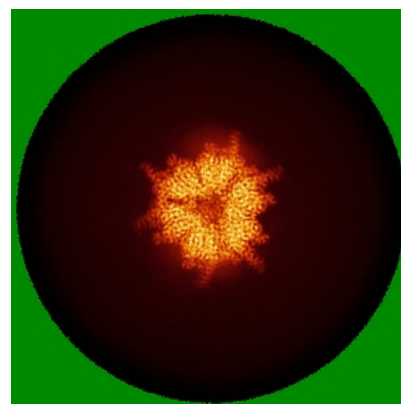
### 6.4.1 Primary map



X

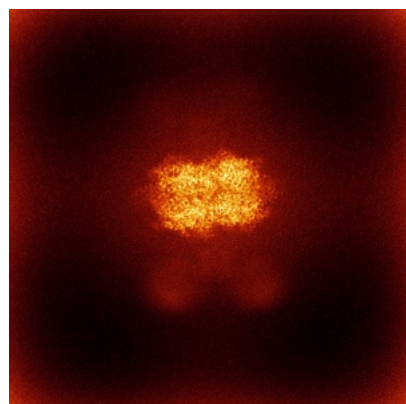


Y

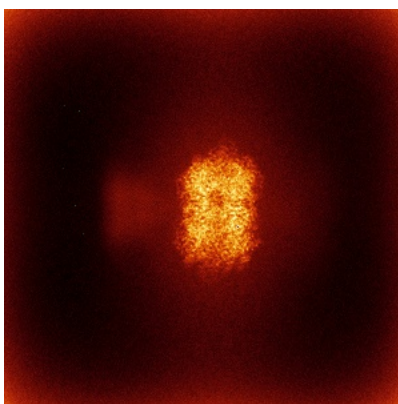


Z

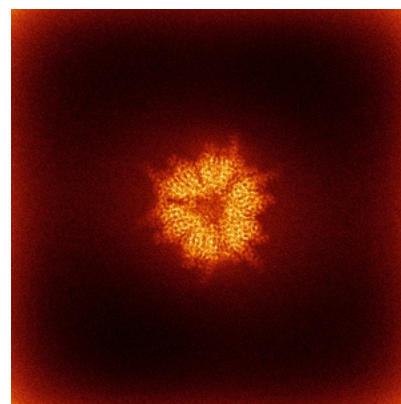
### 6.4.2 Raw map



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



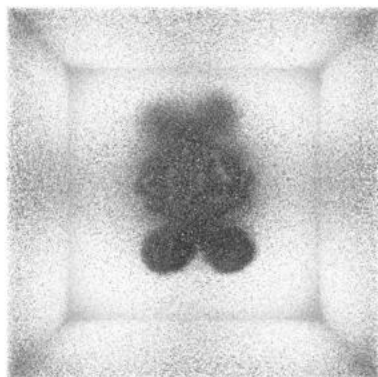
Y



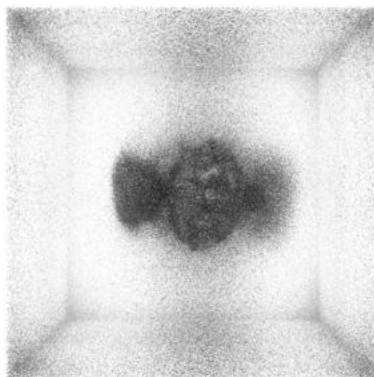
Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

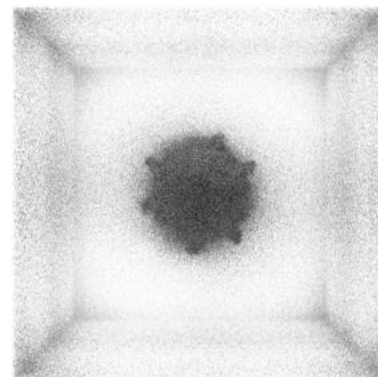
### 6.5.2 Raw map



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.

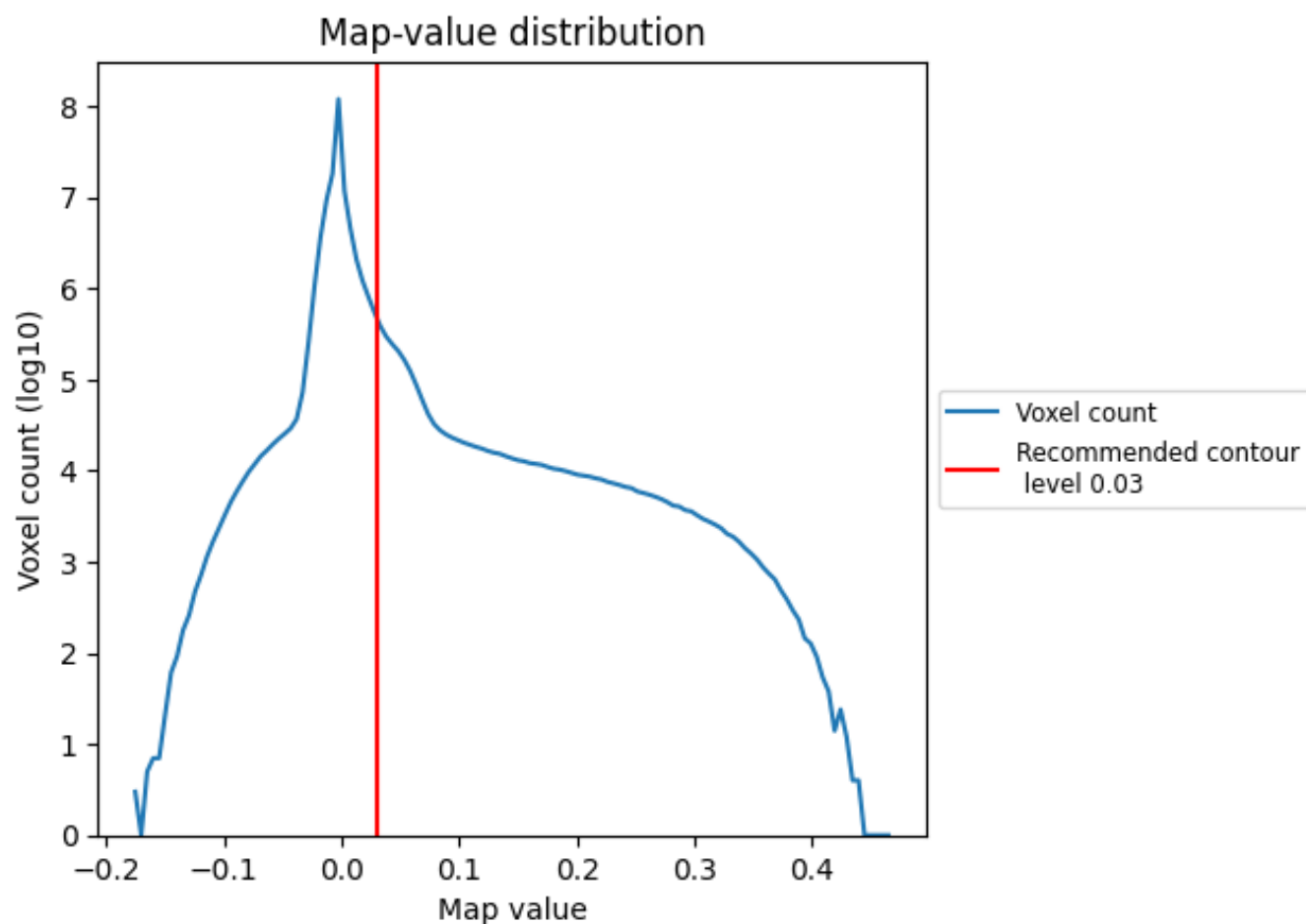
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

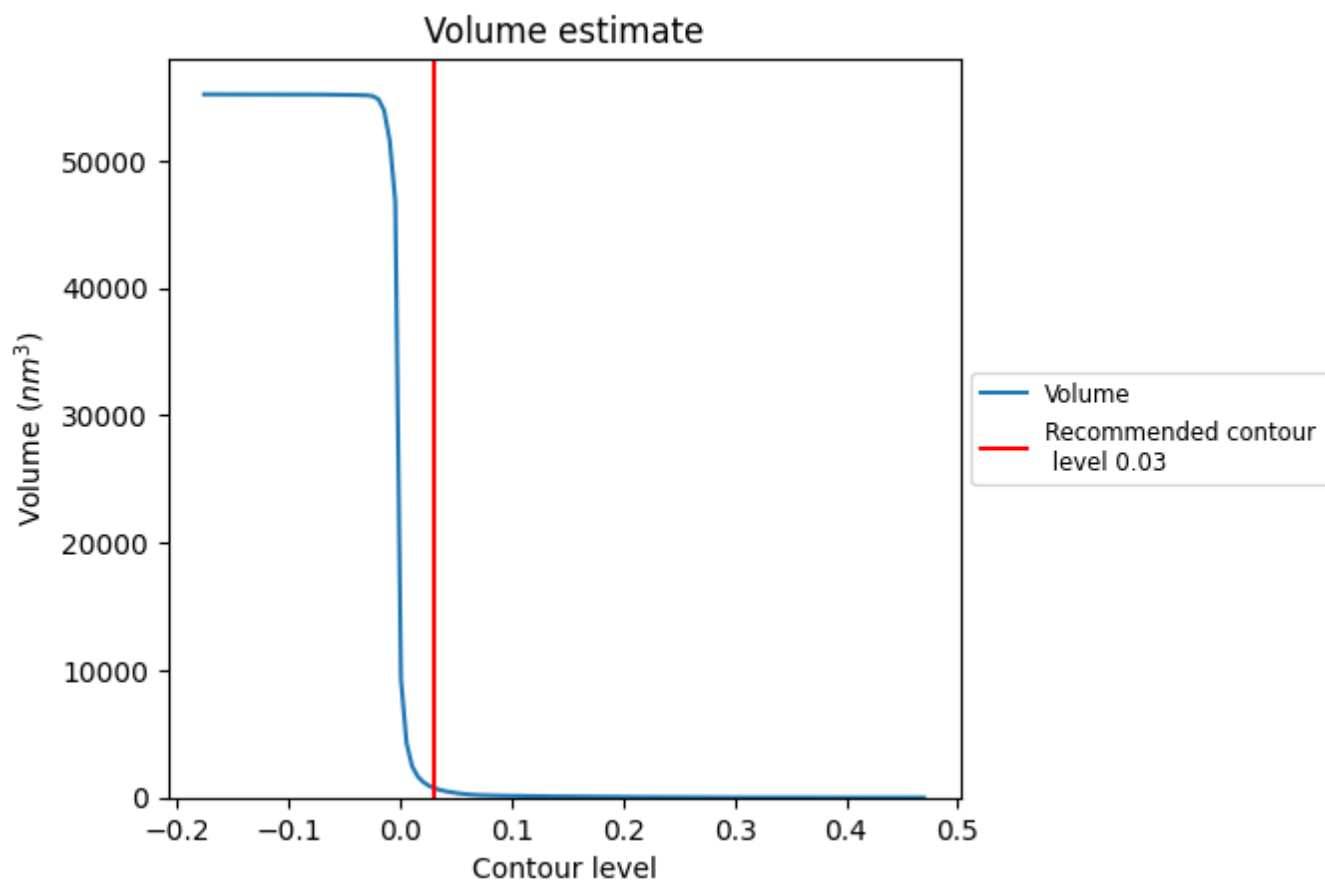
This section contains the results of statistical analysis of the map.

### 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](#)

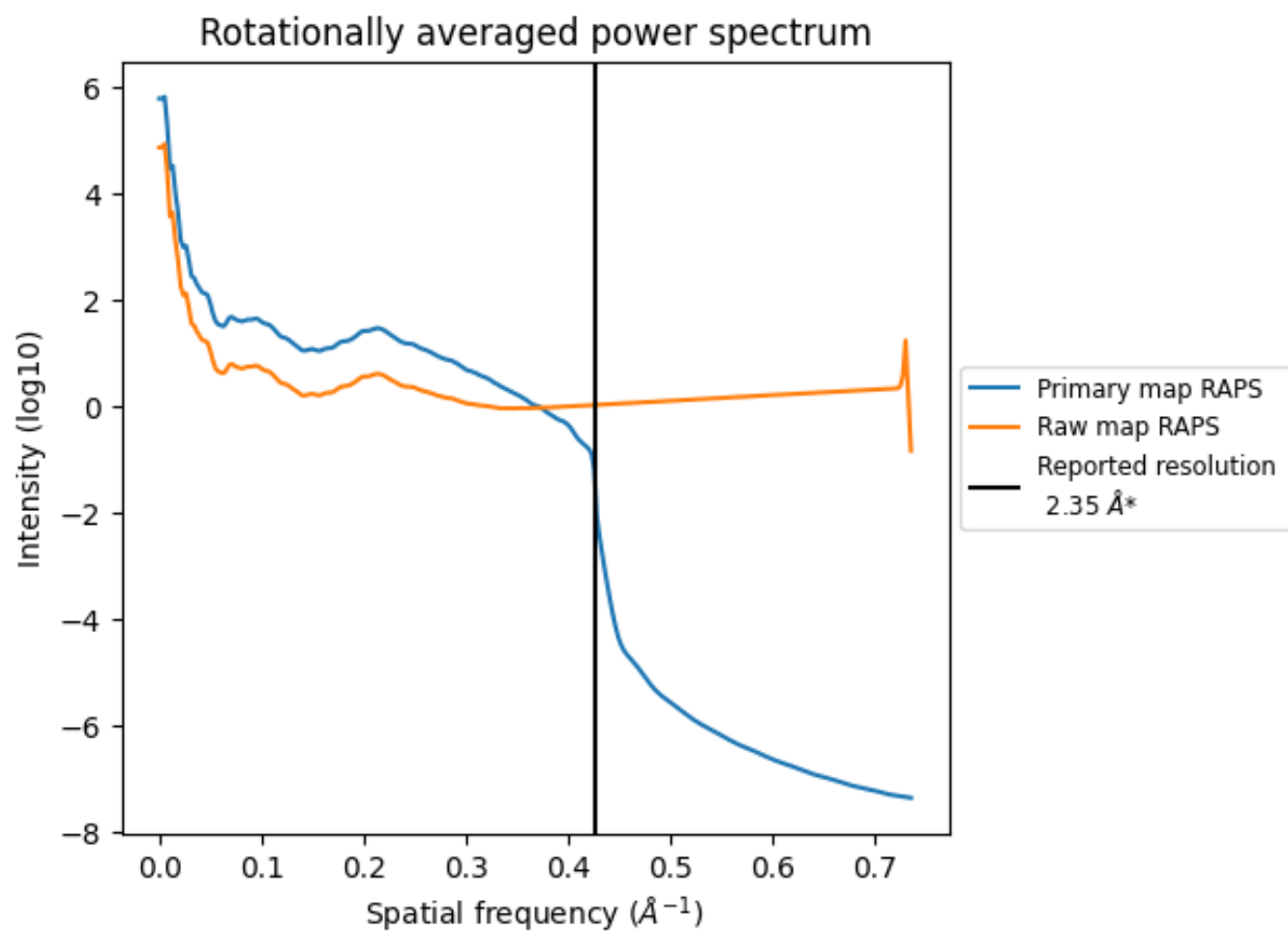


The volume at the recommended contour level is 771  $\text{nm}^3$ ; this corresponds to an approximate mass of 697 kDa.

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](#)

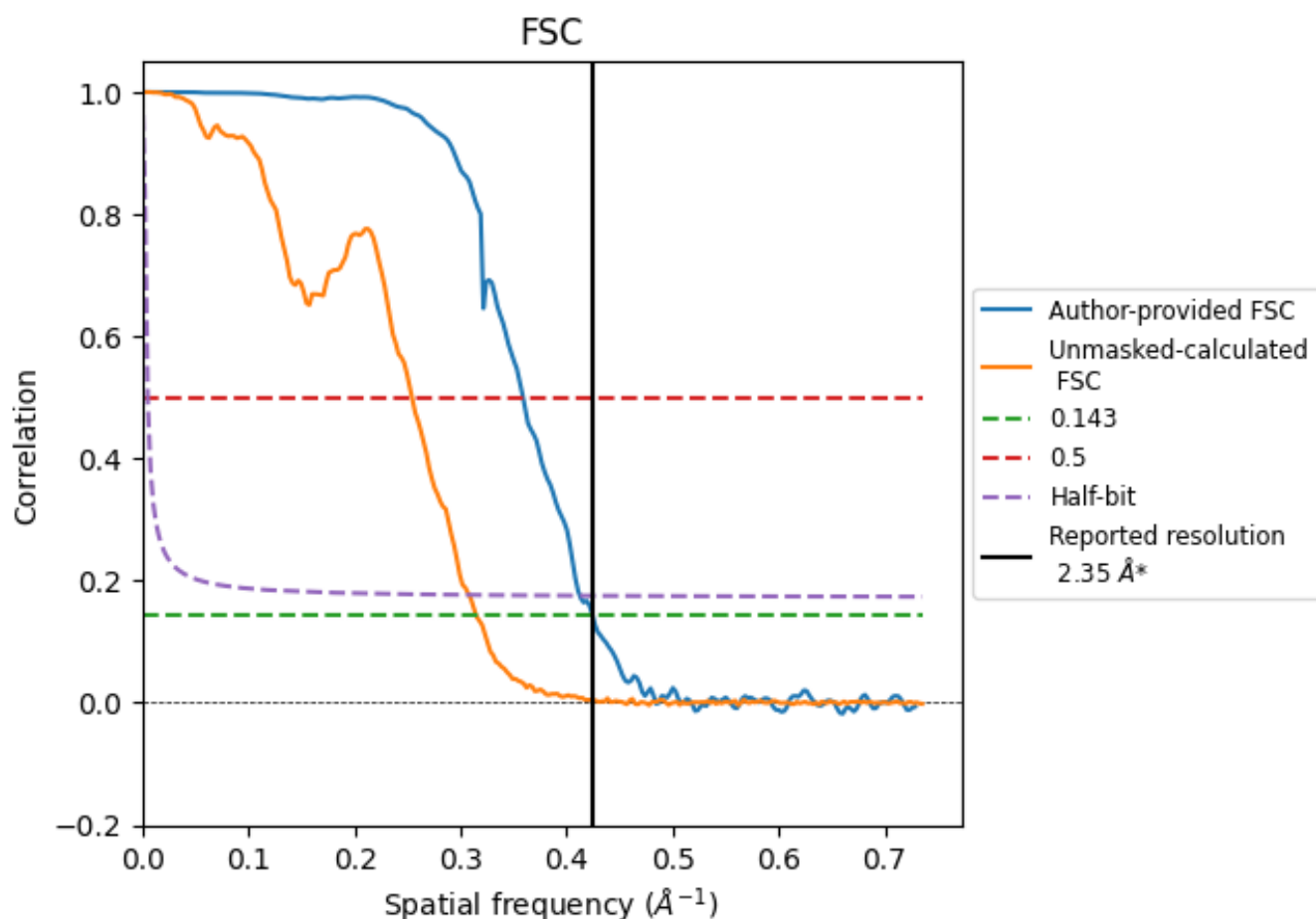


\*Reported resolution corresponds to spatial frequency of 0.426 Å<sup>-1</sup>

## 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  $0.426 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

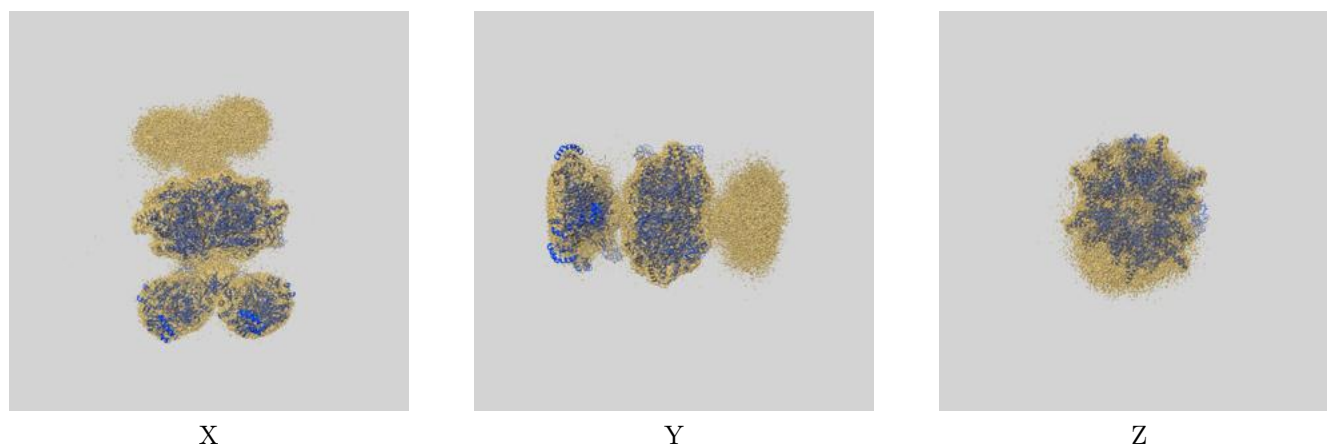
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.35	-	-
Author-provided FSC curve	2.36	2.79	2.42
Unmasked-calculated*	3.18	3.93	3.25

\*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 3.18 differs from the reported value 2.35 by more than 10 %

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

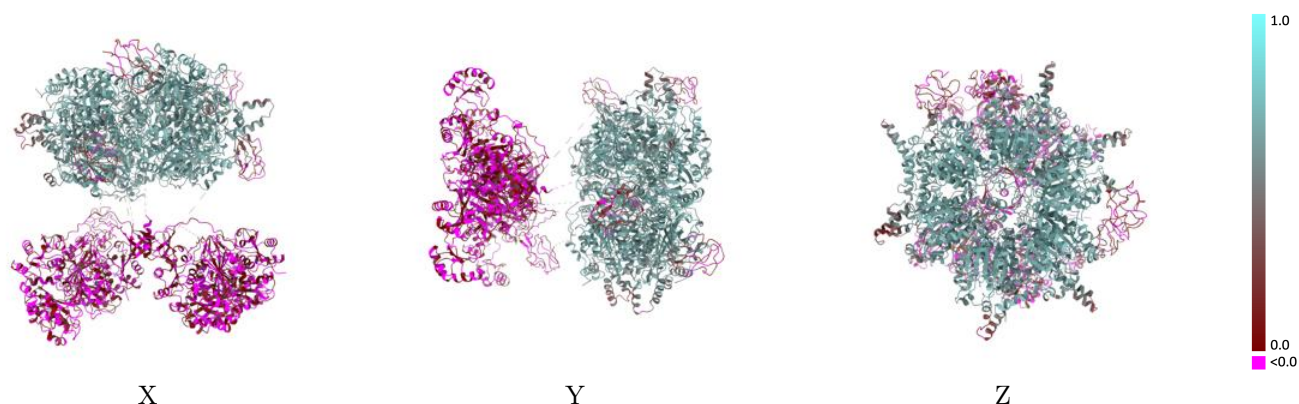
This section contains information regarding the fit between EMDB map EMD-55718 and PDB model 9T97. Per-residue inclusion information can be found in section [3](#) on page [6](#).

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



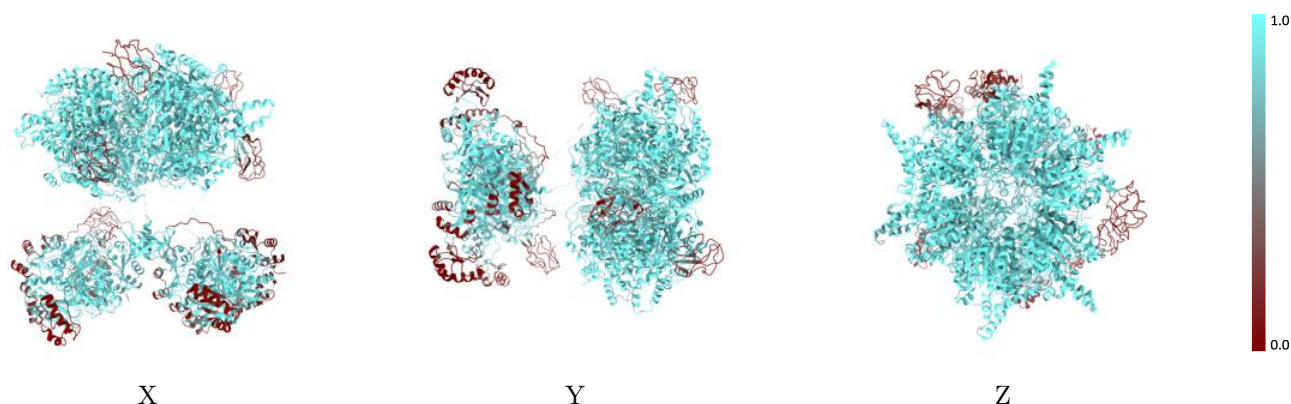
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



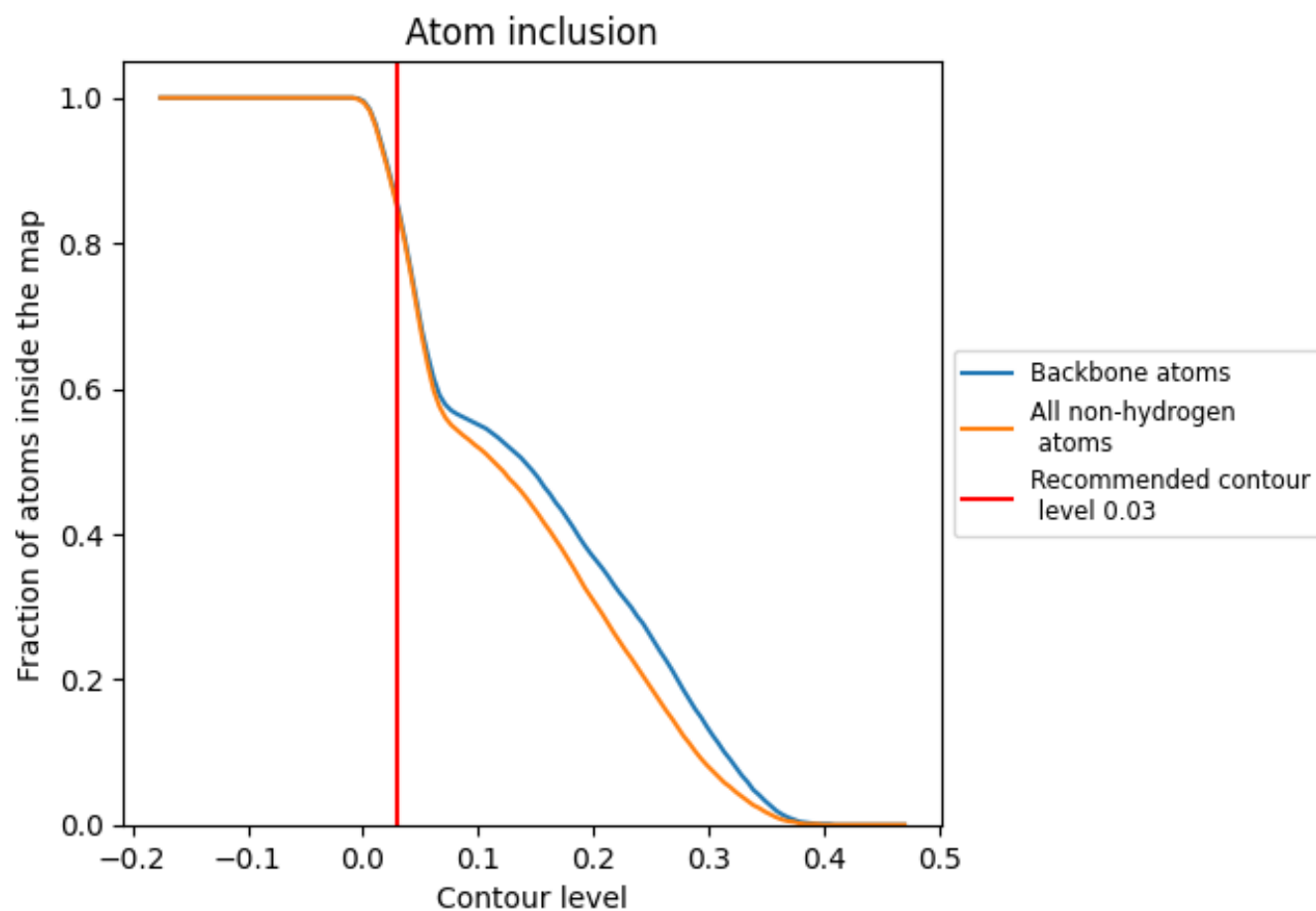
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8480	 0.3870
A3a	 0.7390	 0.0510
A3b	 0.6440	 0.0390
A3c	 0.7310	 0.0290
A3d	 0.5880	 0.0340
A3f	 0.2080	 0.1740
A3g	 0.1480	 0.1260
A3i	 0.9500	 0.5290
D4a	 0.9850	 0.6120
D4b	 0.9880	 0.6110
D5a	 0.9940	 0.6390
D5b	 0.9930	 0.6400
D5c	 0.9940	 0.6420
D5d	 0.9930	 0.6410
E5a	 0.9670	 0.4070
E5b	 0.9960	 0.6460

