



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 01:41 AM UTC

PDB ID : 8UCO / pdb_00008uco
EMDB ID : EMD-42133
Title : CryoEM structure of Komagataella pastoris Cytochrome c oxidase (9 subunits)
in complex with human VMAT2 and Amphetamine
Authors : Ye, J.; Liu, B.; Li, W.
Deposited on : 2023-09-26
Resolution : 3.25 Å(reported)

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

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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

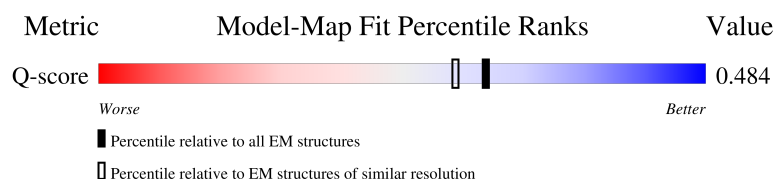
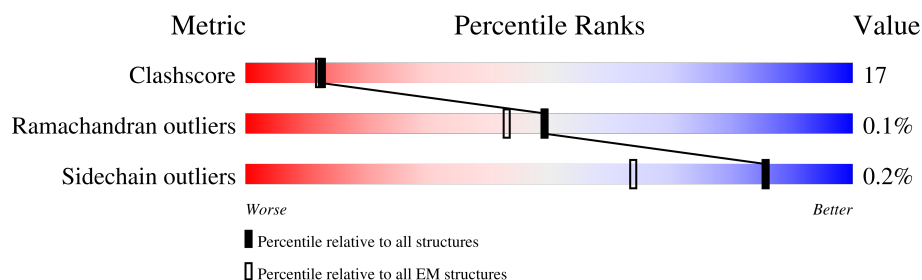
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.25 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	14599 (2.75 - 3.75)

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 $\leq 5\%$. 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	A	514	17% 34% 31% 34%
2	a	535	68% 32%
3	b	236	81% 19%
4	c	268	78% 22%

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Mol	Chain	Length	Quality of chain
5	d	117	 71%29%
6	e	124	 80%20%
7	f	100	 75%25%
8	g	58	 78%21%
9	h	48	 79%21%
10	i	56	 88%12%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 15154 atoms, of which 13 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 Synaptic vesicular amine transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	338	Total	C	N	O	S	0	0
			2508	1676	386	422	24		

- Molecule 2 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	535	Total	C	N	O	S	0	0
			4169	2788	646	717	18		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	4	ILE	MET	conflict	UNP F2R0K8
a	16	ILE	MET	conflict	UNP F2R0K8
a	22	ILE	MET	conflict	UNP F2R0K8
a	33	ILE	MET	conflict	UNP F2R0K8
a	37	ILE	MET	conflict	UNP F2R0K8
a	49	ILE	MET	conflict	UNP F2R0K8
a	78	ILE	MET	conflict	UNP F2R0K8
a	85	LEU	THR	conflict	UNP F2R0K8
a	90	ILE	MET	conflict	UNP F2R0K8
a	121	ILE	MET	conflict	UNP F2R0K8
a	150	ILE	MET	conflict	UNP F2R0K8
a	158	ILE	MET	conflict	UNP F2R0K8
a	165	ILE	MET	conflict	UNP F2R0K8
a	168	ILE	MET	conflict	UNP F2R0K8
a	177	ILE	MET	conflict	UNP F2R0K8
a	232	ILE	MET	conflict	UNP F2R0K8
a	237	LEU	THR	conflict	UNP F2R0K8
a	250	ILE	MET	conflict	UNP F2R0K8
a	256	ILE	MET	conflict	UNP F2R0K8
a	260	ILE	MET	conflict	UNP F2R0K8
a	273	ILE	MET	conflict	UNP F2R0K8

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Chain	Residue	Modelled	Actual	Comment	Reference
a	314	ILE	MET	conflict	UNP F2R0K8
a	320	ILE	MET	conflict	UNP F2R0K8
a	322	ILE	MET	conflict	UNP F2R0K8
a	334	ILE	MET	conflict	UNP F2R0K8
a	367	ILE	MET	conflict	UNP F2R0K8
a	401	LEU	THR	conflict	UNP F2R0K8
a	402	ILE	MET	conflict	UNP F2R0K8
a	421	ILE	MET	conflict	UNP F2R0K8
a	442	ILE	MET	conflict	UNP F2R0K8
a	455	ILE	MET	conflict	UNP F2R0K8
a	462	ILE	MET	conflict	UNP F2R0K8
a	464	ILE	MET	conflict	UNP F2R0K8
a	465	ILE	MET	conflict	UNP F2R0K8
a	510	ILE	MET	conflict	UNP F2R0K8
a	515	ILE	MET	conflict	UNP F2R0K8
a	524	LEU	THR	conflict	UNP F2R0K8

- Molecule 3 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	236	Total	C	N	O	S	0	0
			1896	1247	287	352	10		

- Molecule 4 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	c	268	Total	C	N	O	S	0	0
			2163	1460	337	354	12		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	45	ILE	MET	conflict	UNP F2R0J6
c	55	ILE	MET	conflict	UNP F2R0J6
c	62	ILE	MET	conflict	UNP F2R0J6
c	81	ILE	MET	conflict	UNP F2R0J6
c	89	ILE	MET	conflict	UNP F2R0J6
c	101	ILE	MET	conflict	UNP F2R0J6
c	120	ILE	MET	conflict	UNP F2R0J6
c	129	ILE	MET	conflict	UNP F2R0J6
c	132	ILE	MET	conflict	UNP F2R0J6
c	143	ILE	MET	conflict	UNP F2R0J6

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Chain	Residue	Modelled	Actual	Comment	Reference
c	247	ILE	MET	conflict	UNP F2R0J6
c	248	LEU	THR	conflict	UNP F2R0J6

- Molecule 5 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	117	Total	C	N	O	S	0	0
			910	576	147	183	4		

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	e	124	Total	C	N	O	S	0	0
			1027	659	176	191	1		

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f	100	Total	C	N	O	S	0	0
			835	531	134	168	2		

- Molecule 8 is a protein called Cytochrome c oxidase subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	g	58	Total	C	N	O	S	0	0
			465	309	74	81	1		

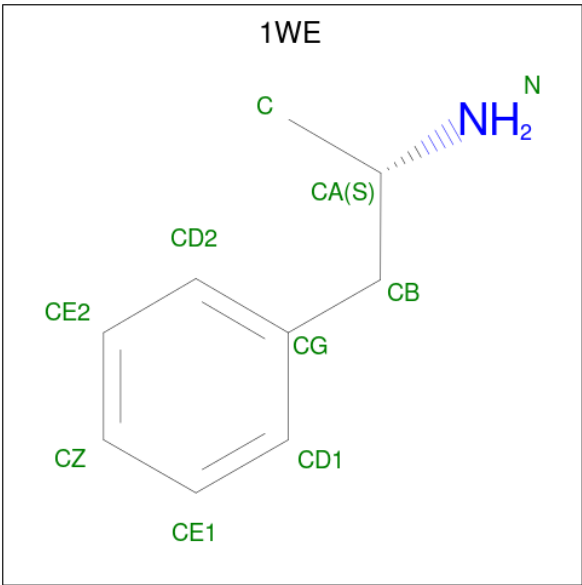
- Molecule 9 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	h	48	Total	C	N	O	S	0	0
			386	260	65	59	2		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	i	56	Total	C	N	O		0	0
			460	302	83	75			

- Molecule 11 is (2S)-1-phenylpropan-2-amine (CCD ID: 1WE) (formula: C₉H₁₃N) (labeled as "Ligand of Interest" by depositor).

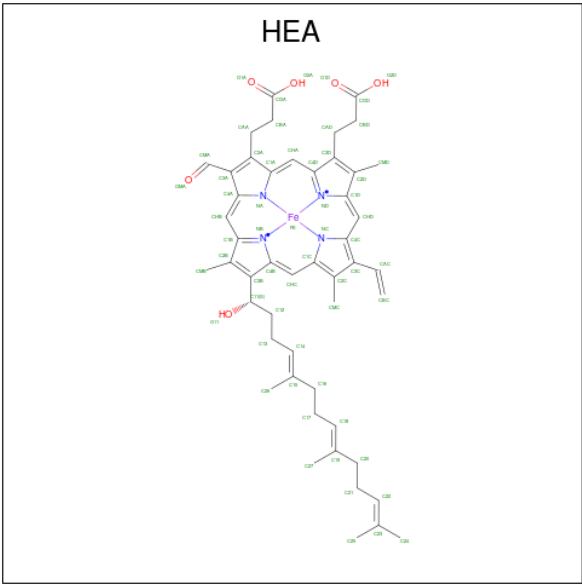


Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total	C	H	N	0
			23	9	13	1	

- Molecule 12 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

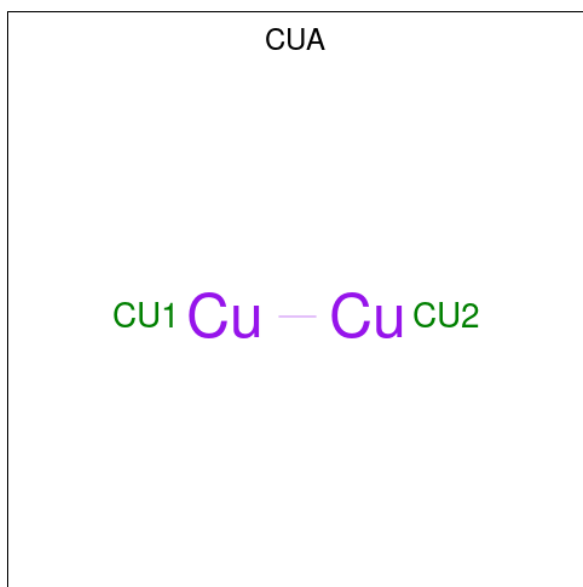
Mol	Chain	Residues	Atoms		AltConf
12	a	1	Total	Cu	0
			1	1	

- Molecule 13 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆) (labeled as "Ligand of Interest" by depositor).



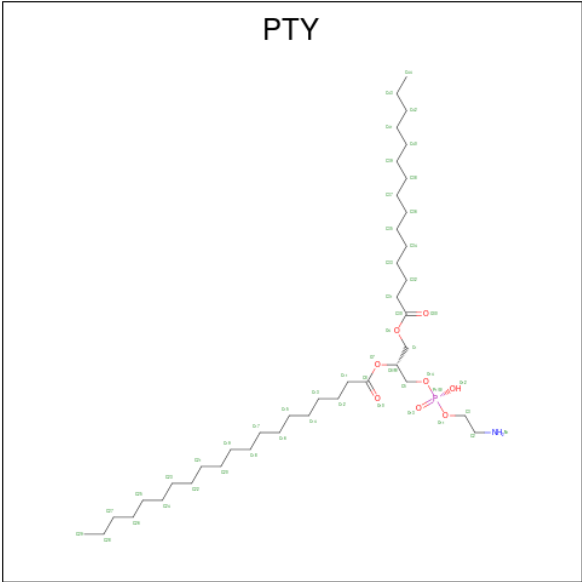
Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
13	a	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 14 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
14	b	1	Total	Cu	0
			2	2	

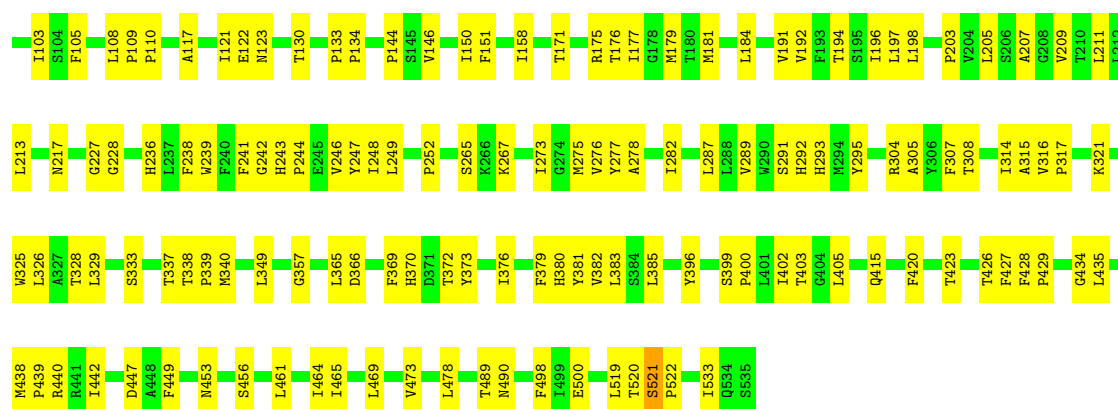
- Molecule 15 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $\text{C}_{40}\text{H}_{80}\text{NO}_8\text{P}$) (labeled as "Ligand of Interest" by depositor).



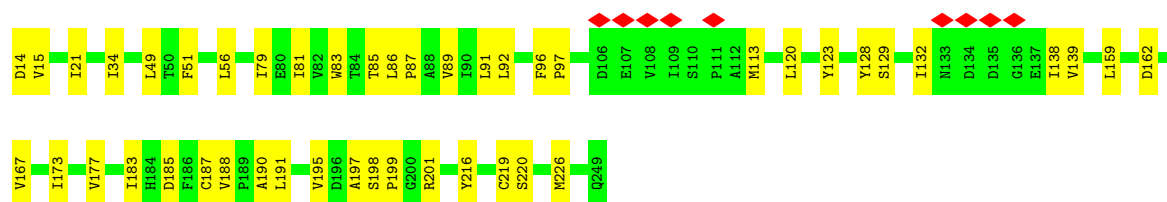
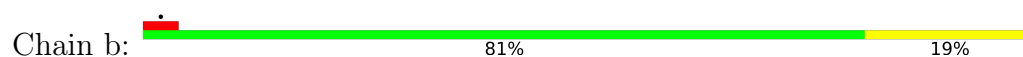
Mol	Chain	Residues	Atoms					AltConf
15	b	1	Total	C	N	O	P	0
			41	31	1	8	1	
15	c	1	Total	C	N	O	P	0
			34	24	1	8	1	
15	c	1	Total	C	N	O	P	0
			40	30	1	8	1	
15	e	1	Total	C	N	O	P	0
			33	23	1	8	1	
15	i	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

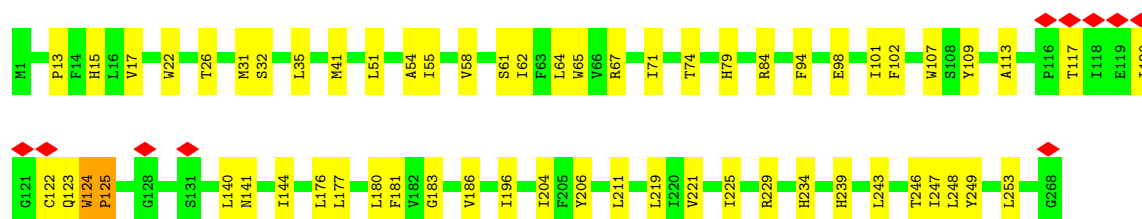
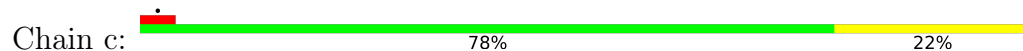
Mol	Chain	Residues	Atoms		AltConf
16	d	1	Total	Zn	0
			1	1	



• Molecule 3: Cytochrome c oxidase subunit 2



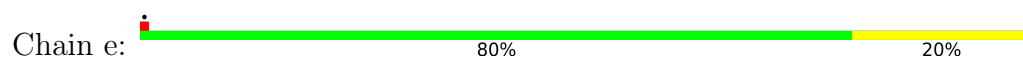
• Molecule 4: Cytochrome c oxidase subunit 3

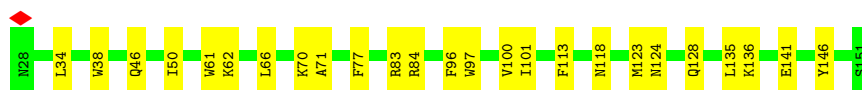


• Molecule 5: Cytochrome c oxidase subunit 4



• Molecule 6: Cytochrome c oxidase subunit 5

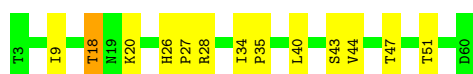
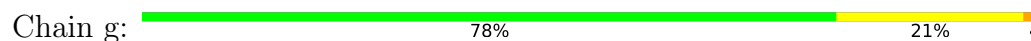




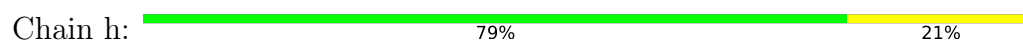
• Molecule 7: Cytochrome c oxidase subunit 6



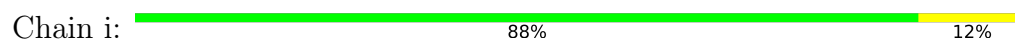
• Molecule 8: Cytochrome c oxidase subunit 7



• Molecule 9: Cytochrome c oxidase subunit 8



• Molecule 10: Cytochrome c oxidase subunit 9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	114678	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.881	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	352.0, 352.0, 352.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CU, 1WE, HEA, CUA, PTY

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/2564	0.48	2/3481 (0.1%)
2	a	0.27	0/4300	0.43	0/5878
3	b	0.25	0/1947	0.41	0/2664
4	c	0.26	0/2234	0.42	0/3057
5	d	0.25	0/928	0.50	0/1260
6	e	0.24	0/1055	0.47	0/1430
7	f	0.26	0/851	0.38	0/1148
8	g	0.24	0/478	0.39	0/647
9	h	0.24	0/400	0.39	0/541
10	i	0.22	0/473	0.42	0/638
All	All	0.27	0/15230	0.44	2/20744 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	a	0	2
4	c	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	THR	N-CA-C	-6.51	104.18	111.28
1	A	134	LEU	N-CA-C	-5.18	105.63	111.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	a	521	SER	Peptide
2	a	54	HIS	Peptide
4	c	124	TRP	Peptide

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	A	2508	0	2638	170	0
2	a	4169	0	4191	168	0
3	b	1896	0	1867	45	0
4	c	2163	0	2198	49	0
5	d	910	0	887	30	0
6	e	1027	0	1007	23	0
7	f	835	0	794	27	0
8	g	465	0	471	11	0
9	h	386	0	391	15	0
10	i	460	0	473	10	0
11	A	10	13	13	2	0
12	a	1	0	0	0	0
13	a	120	0	108	22	0
14	b	2	0	0	0	0
15	b	41	0	55	4	0
15	c	74	0	94	10	0
15	e	33	0	39	0	0
15	i	40	0	53	2	0
16	d	1	0	0	0	0
All	All	15141	13	15279	510	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 17.

The worst 5 of 510 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:A:306:MET:HG3	1:A:310:MET:HE2	1.42	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ILE:HG23	1:A:406:MET:HE1	1.42	0.99
3:b:132:ILE:HG12	3:b:138:ILE:HG12	1.49	0.94
1:A:412:LEU:HD13	1:A:473:PRO:HG2	1.51	0.91
2:a:45:PRO:HG2	6:e:123:MET:HE3	1.52	0.90

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	A	328/514 (64%)	315 (96%)	12 (4%)	1 (0%)	36	66
2	a	533/535 (100%)	501 (94%)	32 (6%)	0	100	100
3	b	234/236 (99%)	217 (93%)	17 (7%)	0	100	100
4	c	266/268 (99%)	247 (93%)	18 (7%)	1 (0%)	30	59
5	d	115/117 (98%)	101 (88%)	14 (12%)	0	100	100
6	e	122/124 (98%)	114 (93%)	8 (7%)	0	100	100
7	f	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
8	g	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
9	h	46/48 (96%)	43 (94%)	3 (6%)	0	100	100
10	i	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
All	All	1852/2056 (90%)	1738 (94%)	112 (6%)	2 (0%)	49	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
4	c	125	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	267/427 (62%)	265 (99%)	2 (1%)	76	79
2	a	452/452 (100%)	452 (100%)	0	100	100
3	b	212/212 (100%)	212 (100%)	0	100	100
4	c	234/234 (100%)	234 (100%)	0	100	100
5	d	99/99 (100%)	99 (100%)	0	100	100
6	e	110/110 (100%)	110 (100%)	0	100	100
7	f	90/90 (100%)	90 (100%)	0	100	100
8	g	48/48 (100%)	47 (98%)	1 (2%)	47	66
9	h	41/41 (100%)	41 (100%)	0	100	100
10	i	47/47 (100%)	47 (100%)	0	100	100
All	All	1600/1760 (91%)	1597 (100%)	3 (0%)	85	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	40	VAL
8	g	18	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
4	c	212	HIS
4	c	239	HIS
8	g	26	HIS
6	e	150	GLN
2	a	380	HIS

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 ⓘ

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	$\# Z > 2$
15	PTY	c	302	-	39,39,49	0.44	0	42,44,54	1.28	4 (9%)
15	PTY	i	101	-	39,39,49	0.45	0	42,44,54	1.29	4 (9%)
15	PTY	c	301	-	33,33,49	0.46	0	36,38,54	1.43	4 (11%)
13	HEA	a	603	-	67,67,67	1.05	5 (7%)	81,103,103	1.73	21 (25%)
13	HEA	a	602	2	67,67,67	1.01	4 (5%)	81,103,103	1.87	22 (27%)
15	PTY	e	201	-	32,32,49	0.48	0	35,37,54	1.35	4 (11%)
11	1WE	A	601	-	10,10,10	0.67	0	12,12,12	0.90	1 (8%)
14	CUA	b	301	-	0,1,1	-	-	-		
15	PTY	b	302	-	40,40,49	0.46	0	43,45,54	1.33	4 (9%)

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
15	PTY	c	302	-	-	10/43/43/53	-
15	PTY	i	101	-	-	11/43/43/53	-
15	PTY	c	301	-	-	15/37/37/53	-
13	HEA	a	603	-	-	14/36/76/76	-
13	HEA	a	602	2	-	23/36/76/76	-
15	PTY	e	201	-	-	8/36/36/53	-
11	1WE	A	601	-	-	2/4/4/4	0/1/1/1
15	PTY	b	302	-	-	15/44/44/53	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	603	HEA	C1A-C2A	-4.48	1.37	1.45
13	a	602	HEA	C1A-C2A	-4.06	1.38	1.45
13	a	603	HEA	C3A-C4A	-3.24	1.40	1.46
13	a	602	HEA	C3A-C4A	-3.20	1.40	1.46
13	a	603	HEA	C1C-C2C	-2.39	1.37	1.43

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	603	HEA	CHA-C1A-NA	-5.07	118.93	124.45
13	a	602	HEA	CHB-C4A-NA	-4.77	119.26	124.45
15	c	301	PTY	O7-C8-C11	4.63	121.49	111.48
13	a	602	HEA	CAD-C3D-C4D	4.58	132.68	124.70
15	b	302	PTY	O7-C8-C11	4.38	120.95	111.48

There are no chirality outliers.

5 of 98 torsion outliers are listed below:

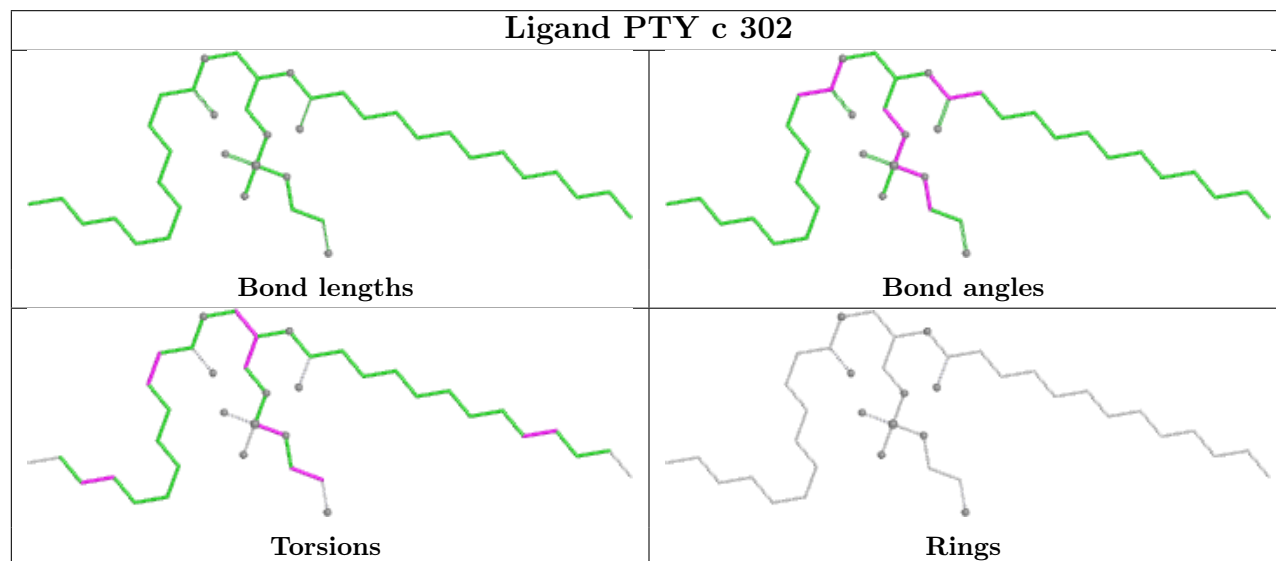
Mol	Chain	Res	Type	Atoms
11	A	601	1WE	C-CA-CB-CG
13	a	602	HEA	C2A-C3A-CMA-OMA
13	a	602	HEA	C12-C11-C3B-C2B
13	a	602	HEA	C12-C11-C3B-C4B
13	a	602	HEA	C2D-C3D-CAD-CBD

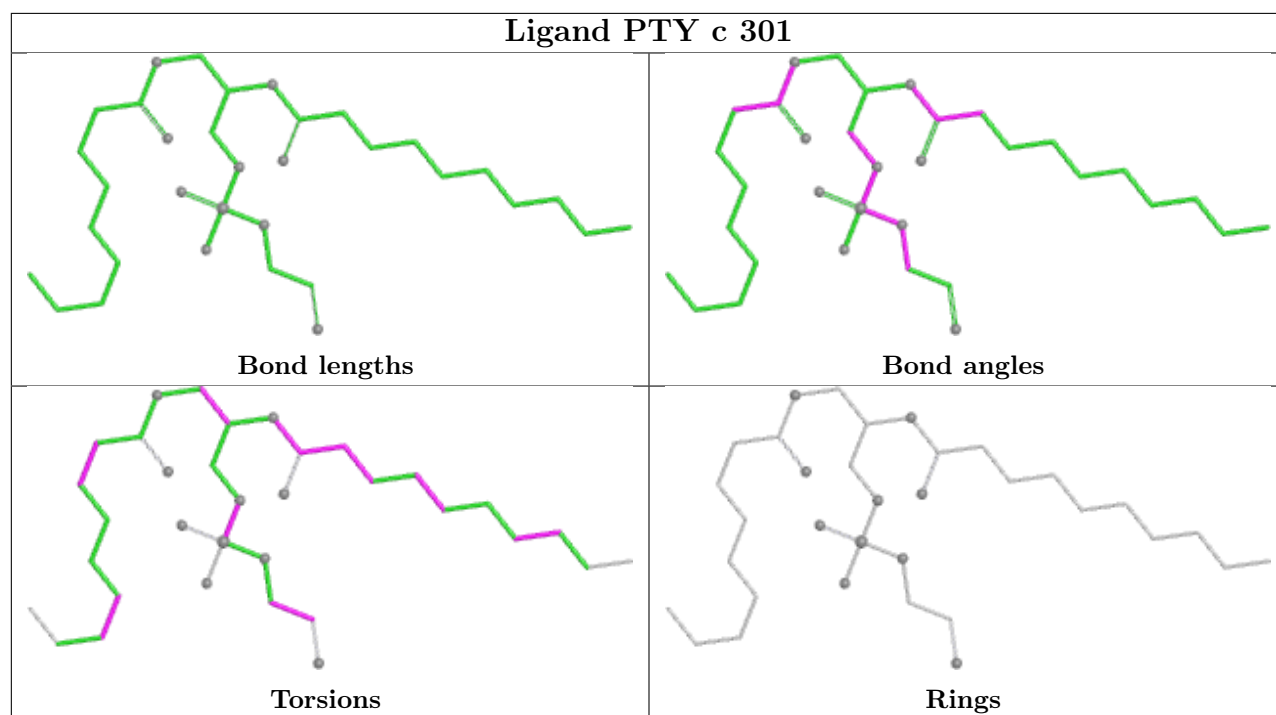
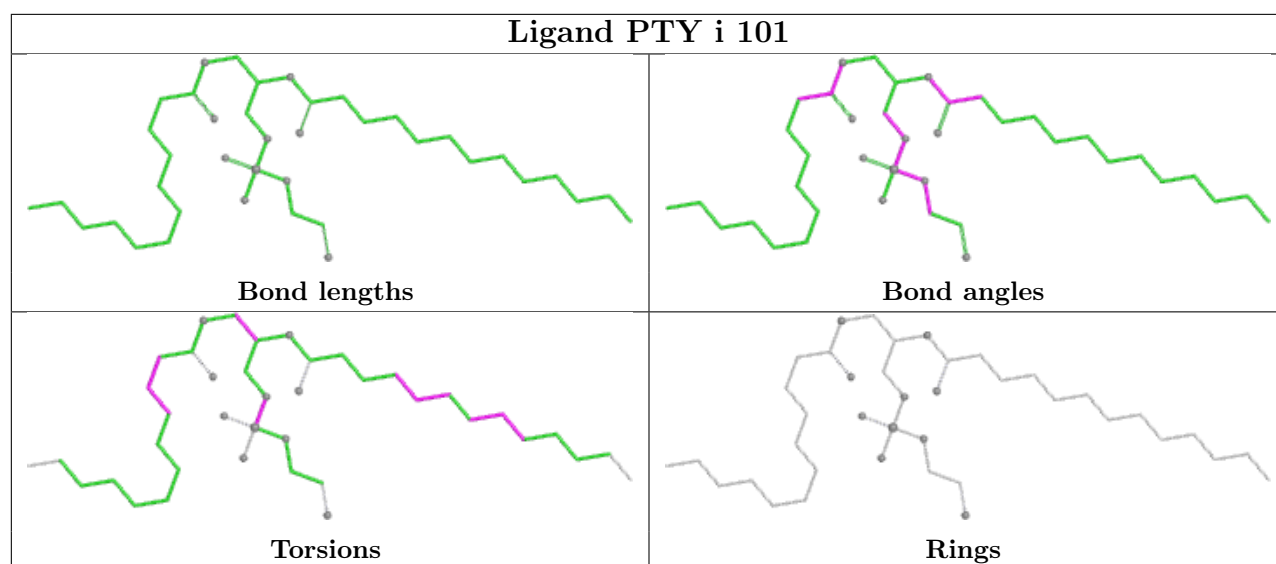
There are no ring outliers.

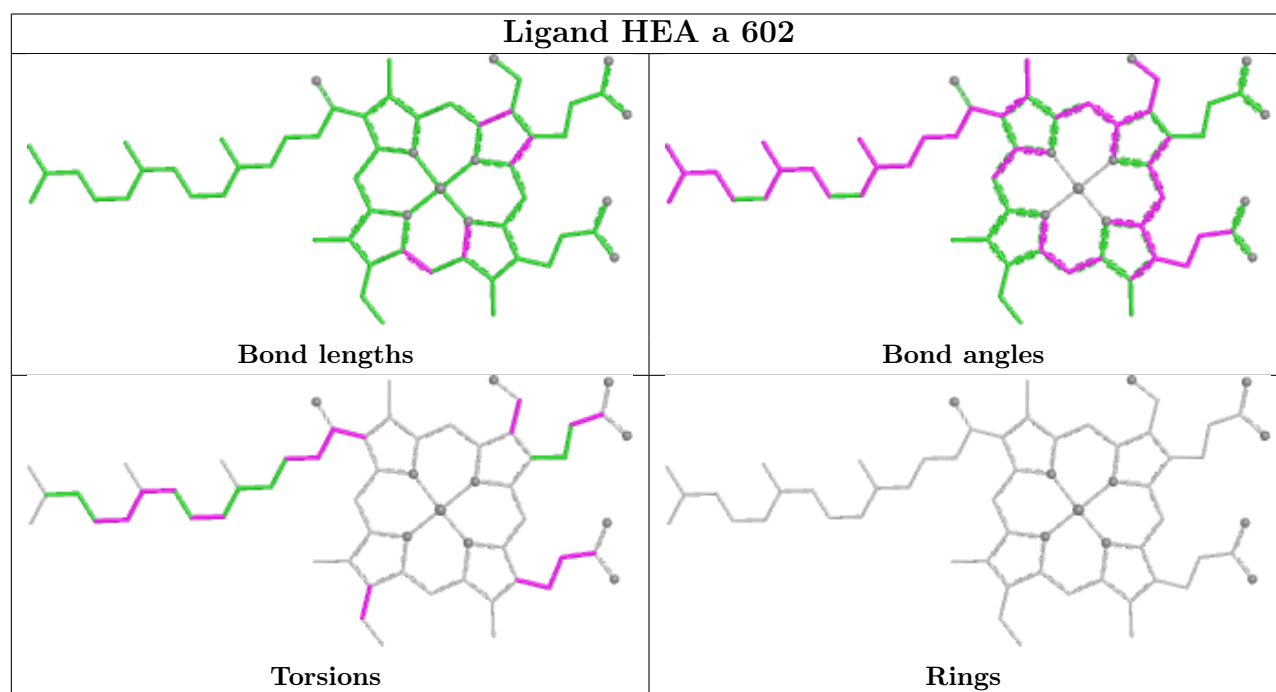
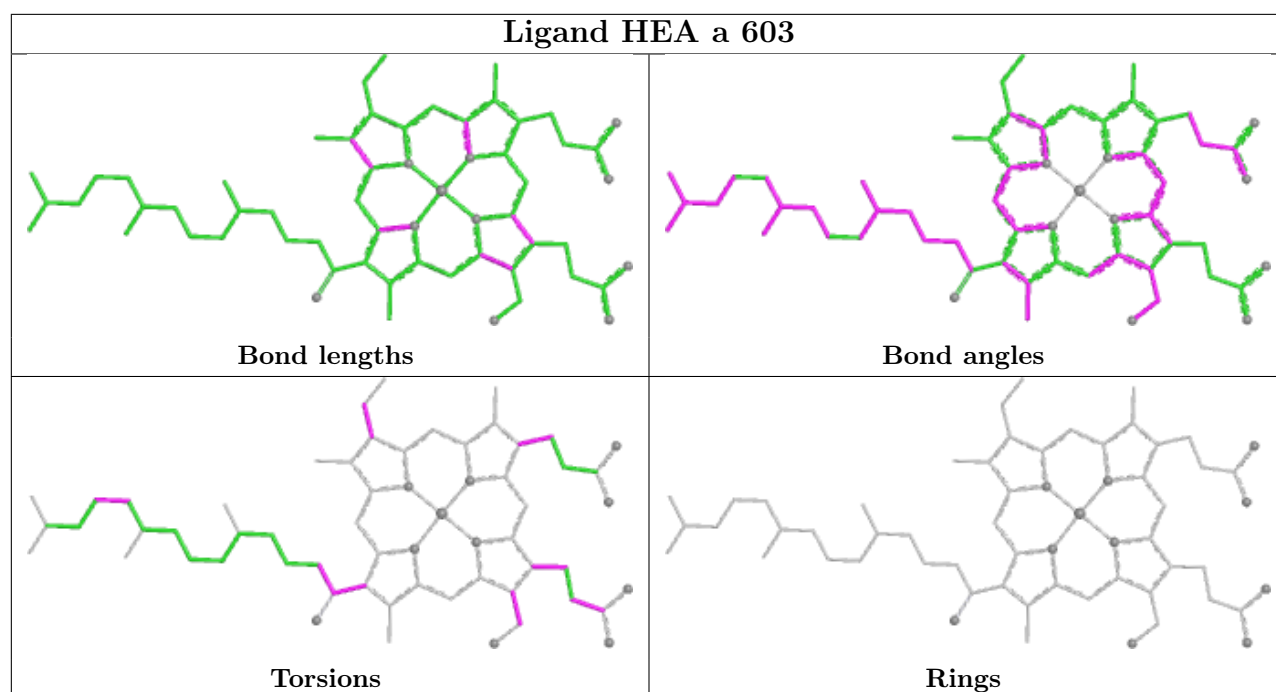
7 monomers are involved in 40 short contacts:

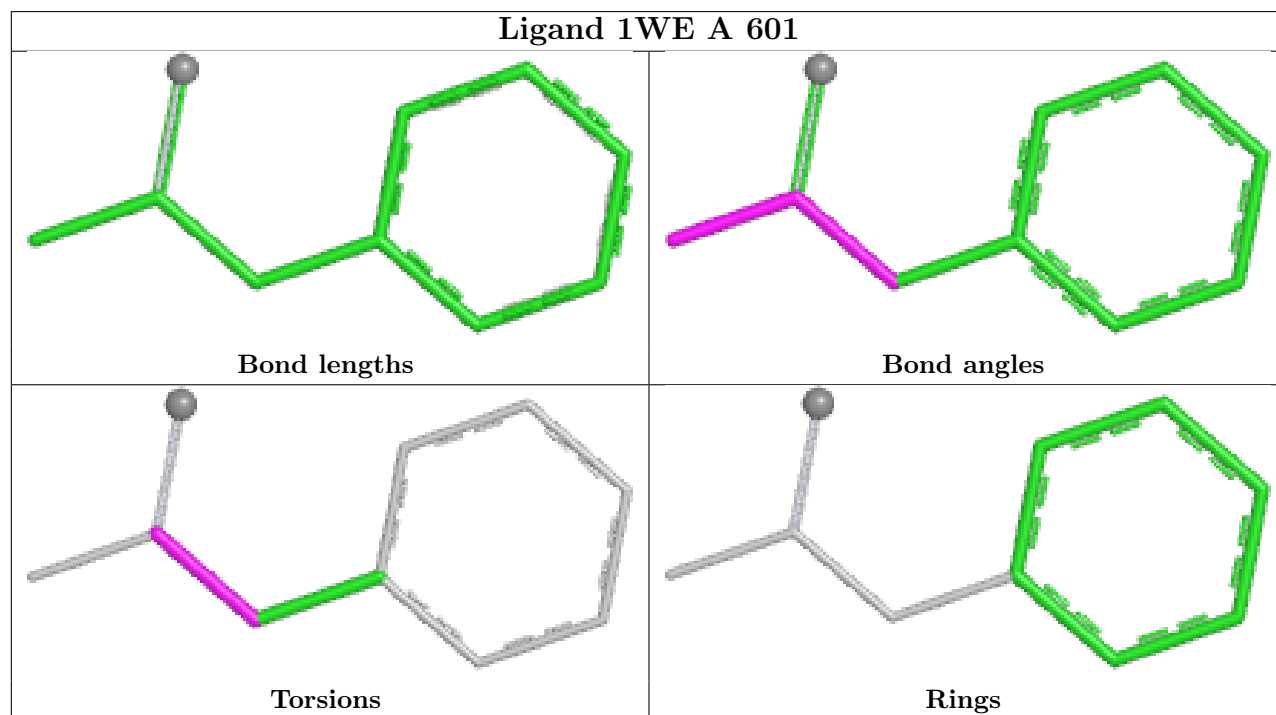
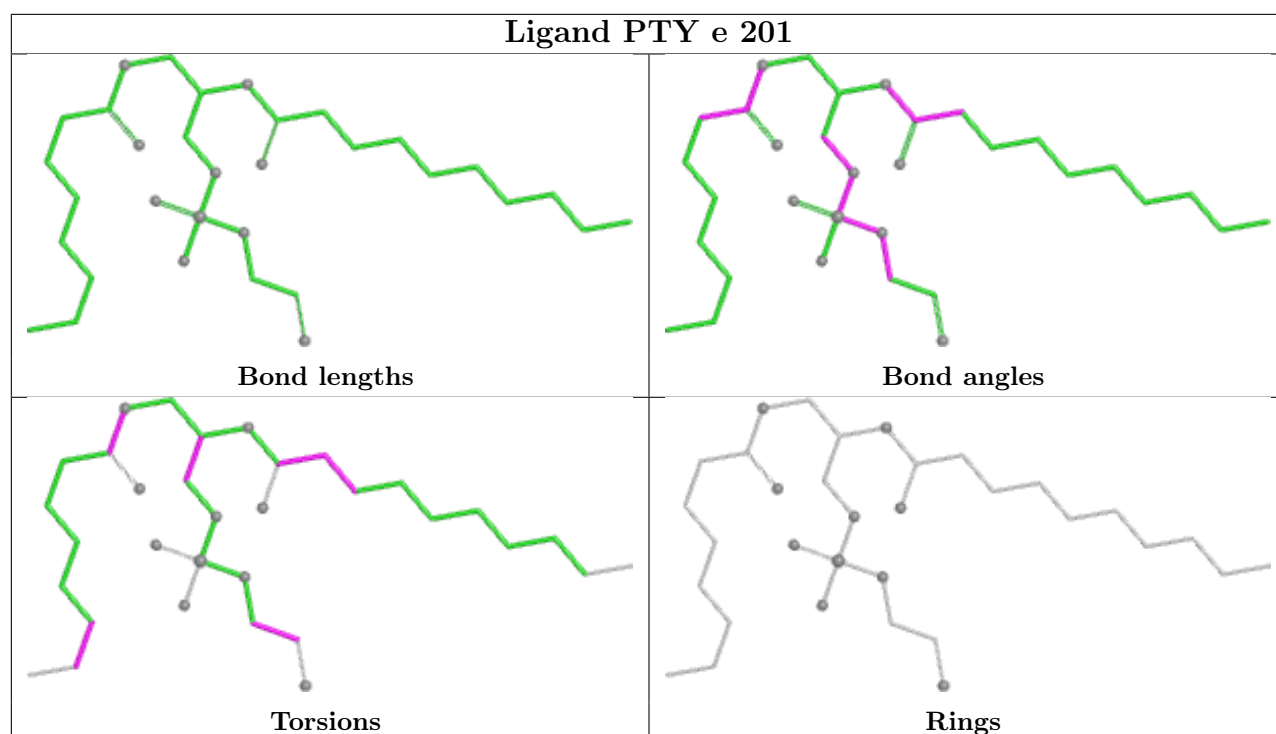
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	c	302	PTY	5	0
15	i	101	PTY	2	0
15	c	301	PTY	8	0
13	a	603	HEA	11	0
13	a	602	HEA	11	0
11	A	601	1WE	2	0
15	b	302	PTY	4	0

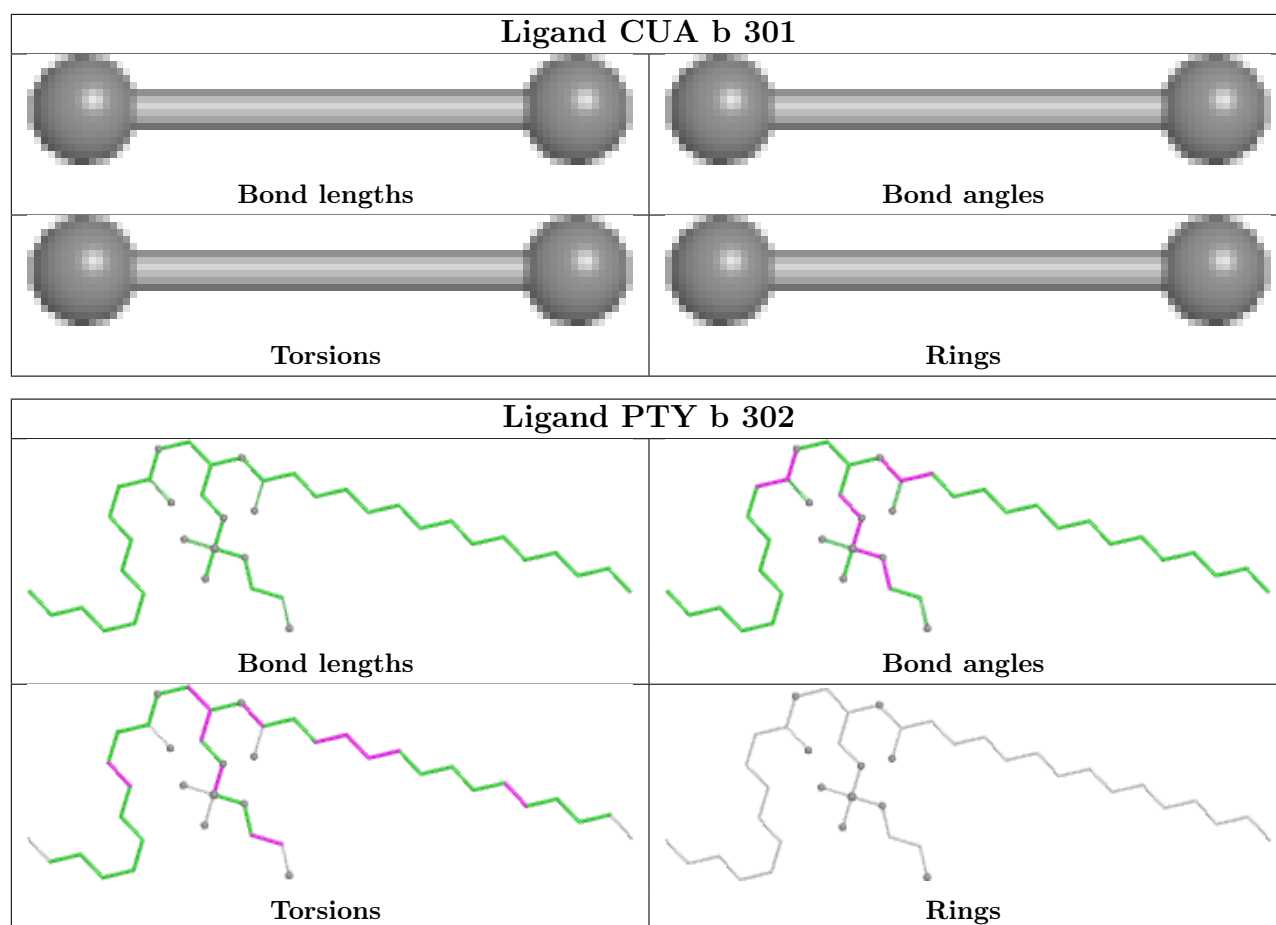
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

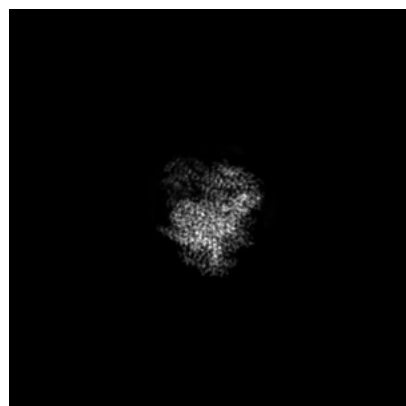
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42133. These allow visual inspection of the internal detail of the map and identification of artifacts.

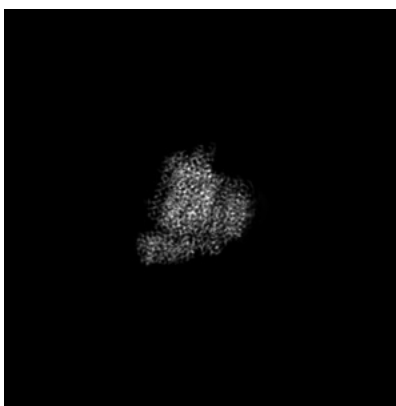
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

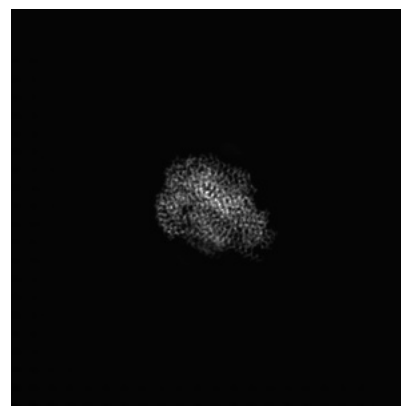
6.1.1 Primary map



X

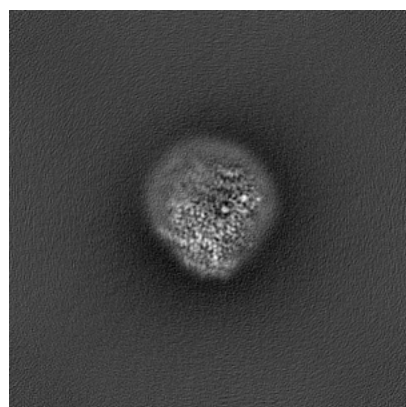


Y

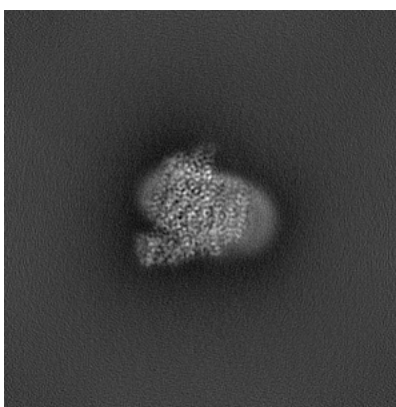


Z

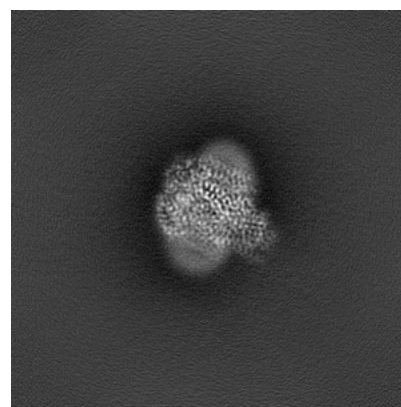
6.1.2 Raw map



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: 160

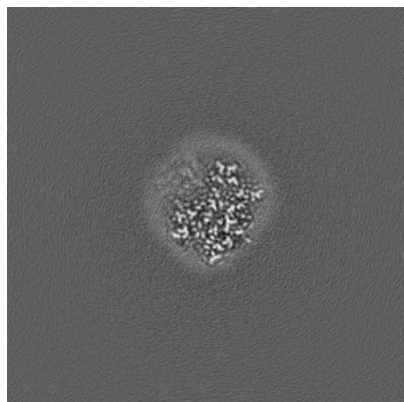


Y Index: 160

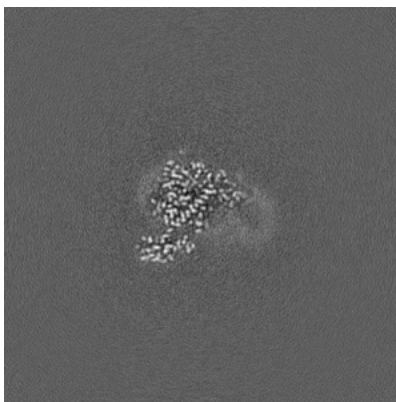


Z Index: 160

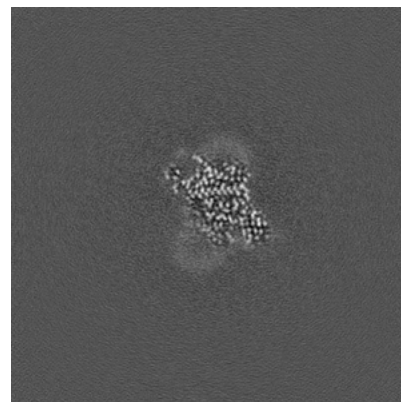
6.2.2 Raw map



X Index: 160



Y Index: 160

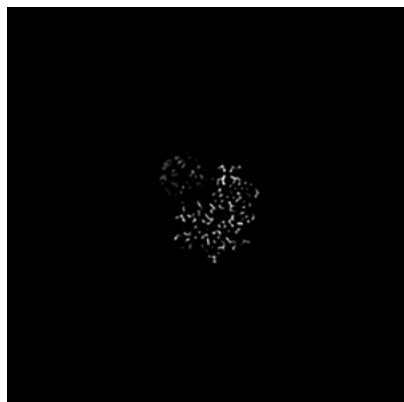


Z Index: 160

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 156

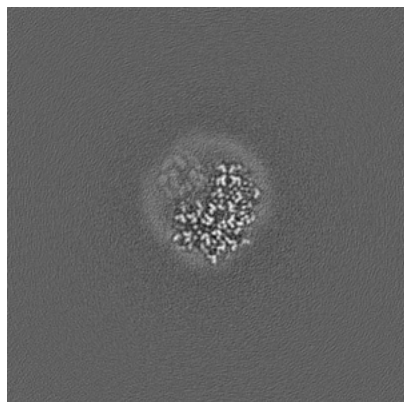


Y Index: 163

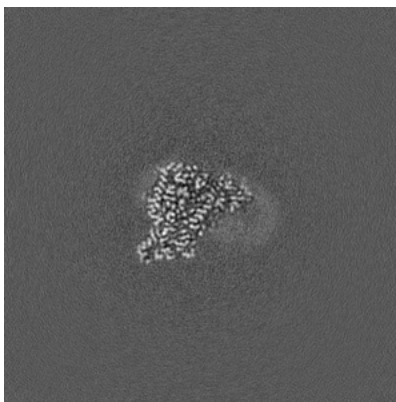


Z Index: 151

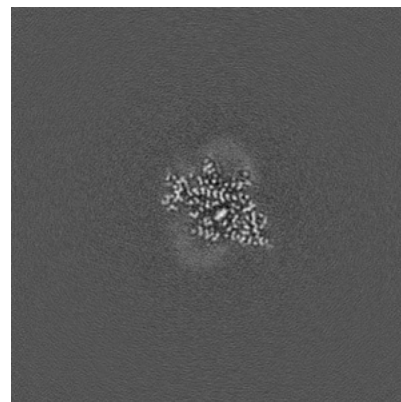
6.3.2 Raw map



X Index: 156



Y Index: 164

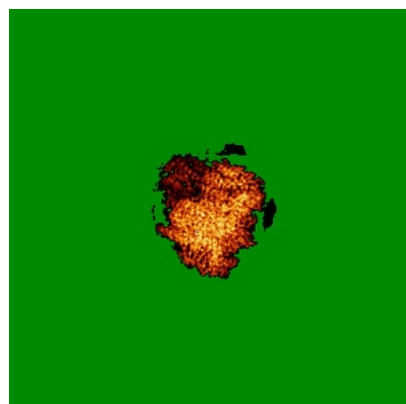


Z Index: 151

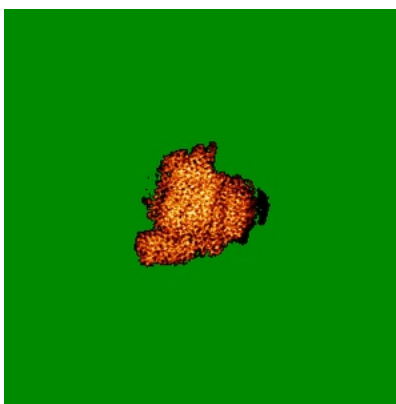
The images above show the largest variance slices of the map in three orthogonal directions.

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

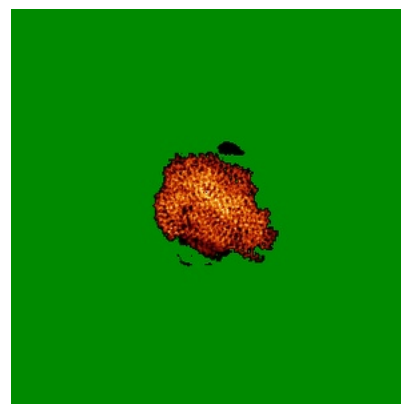
6.4.1 Primary map



X

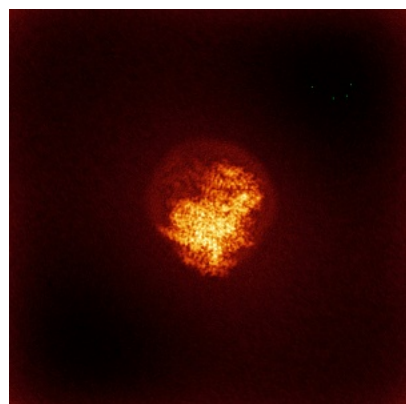


Y

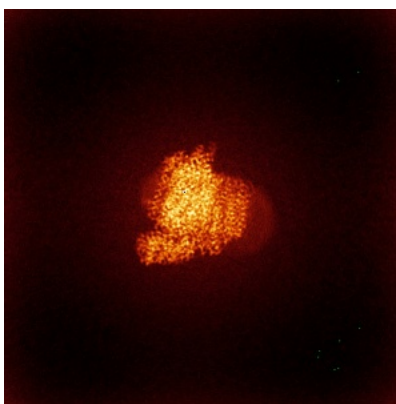


Z

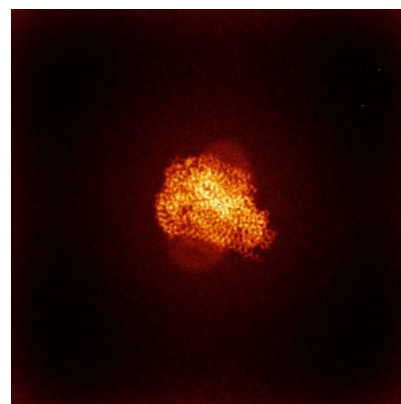
6.4.2 Raw map



X



Y

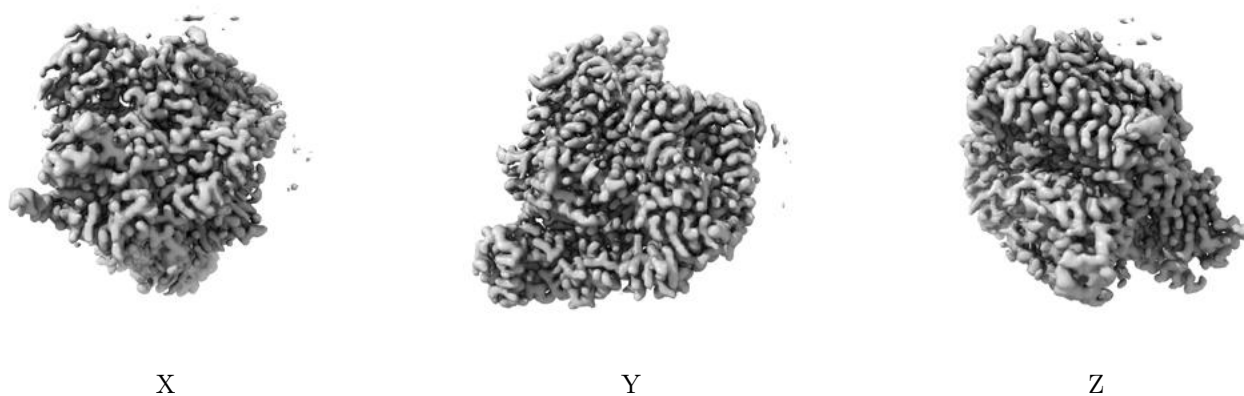


Z

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 0.03. 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



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.

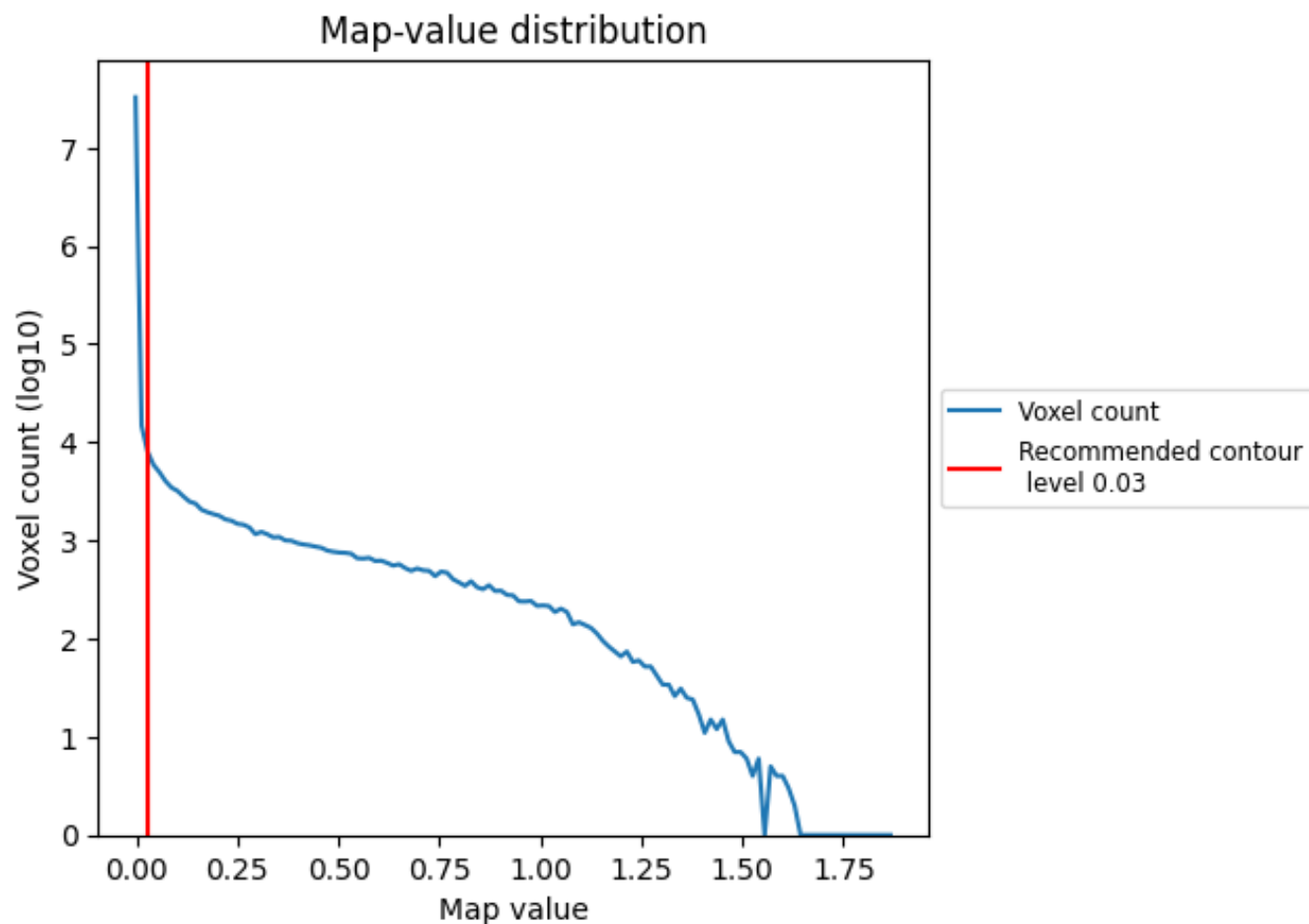
6.6 Mask visualisation [i](#)

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

7 Map analysis ⓘ

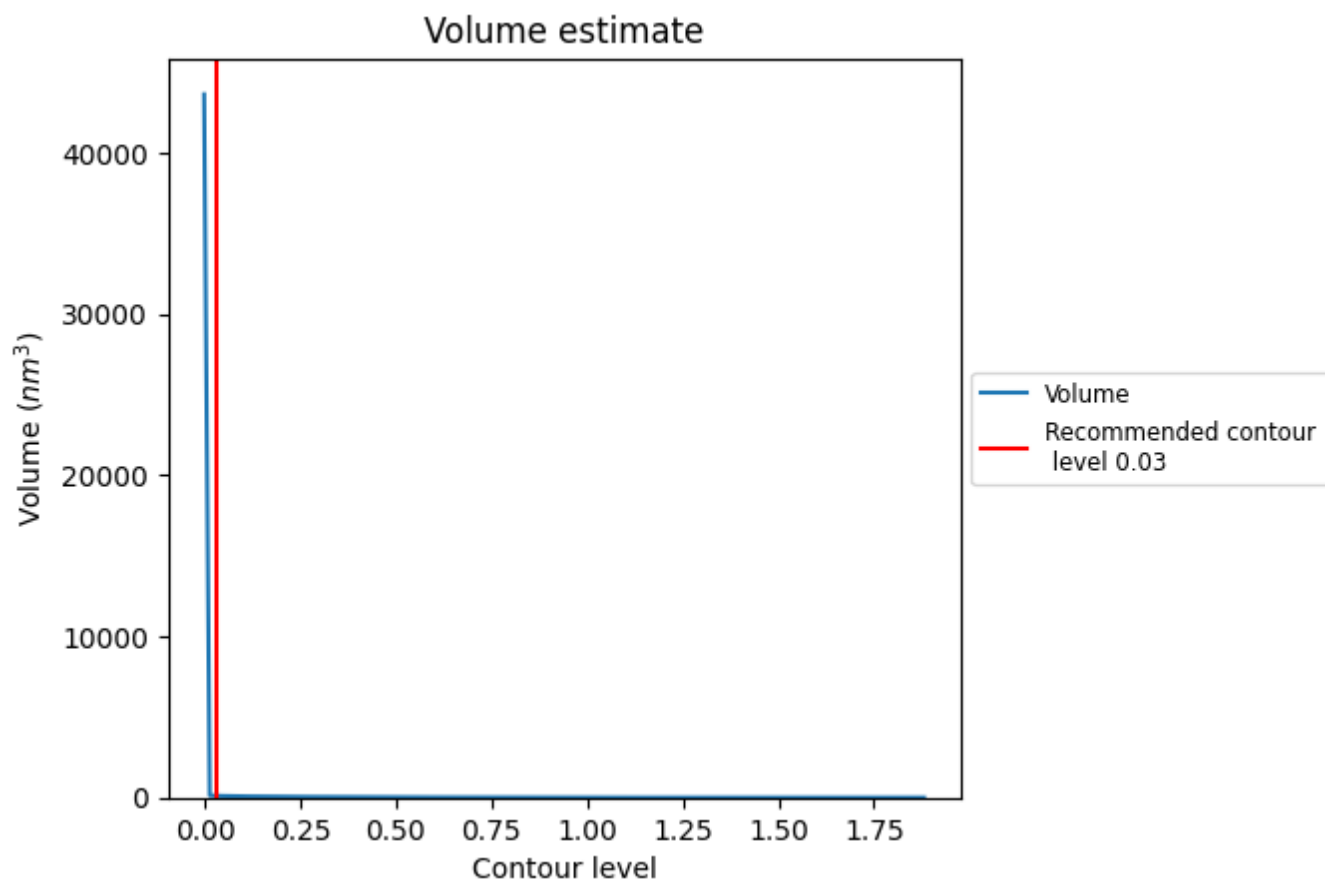
This section contains the results of statistical analysis of the map.

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.

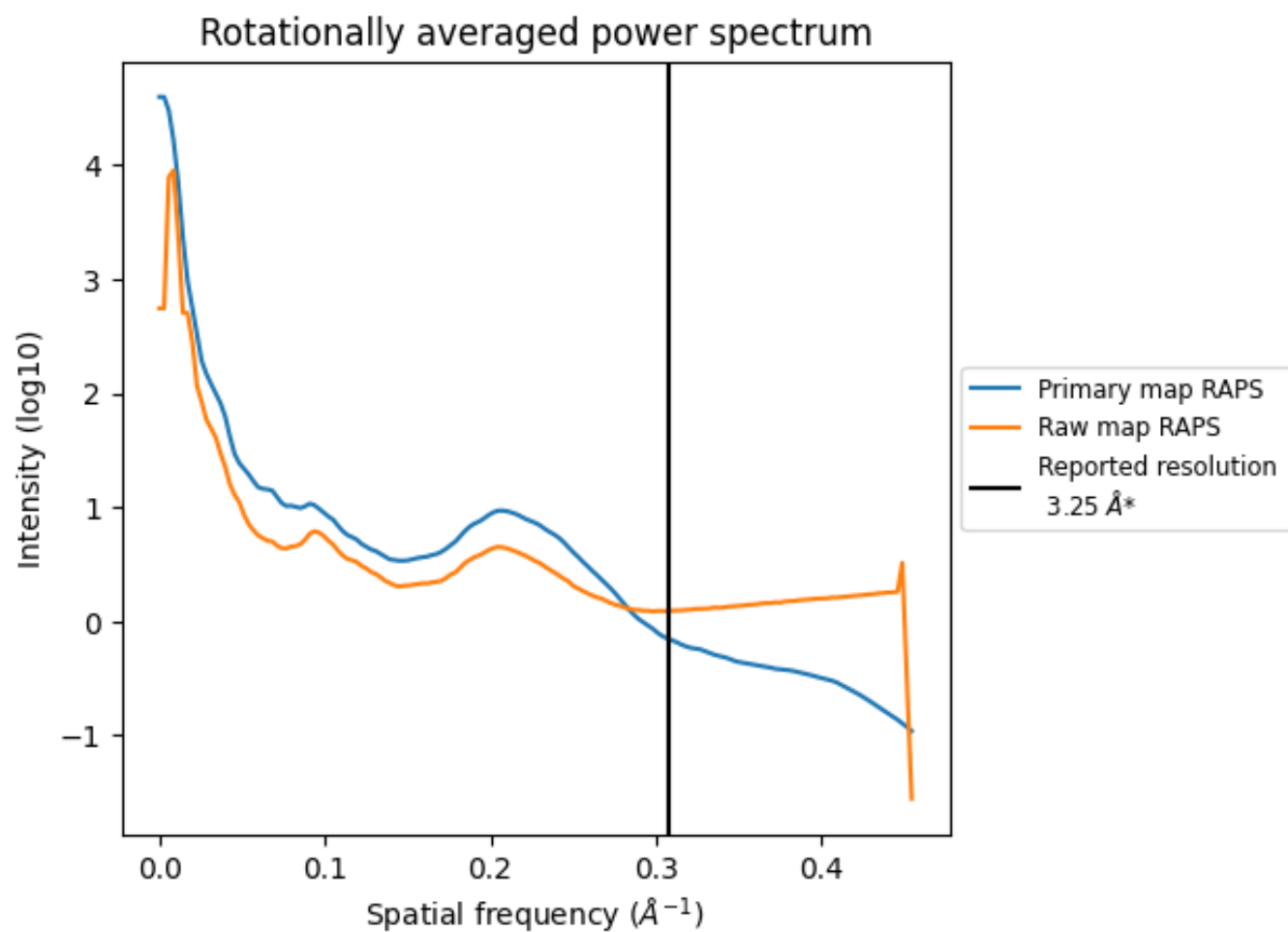
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 111 nm^3 ; this corresponds to an approximate mass of 100 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

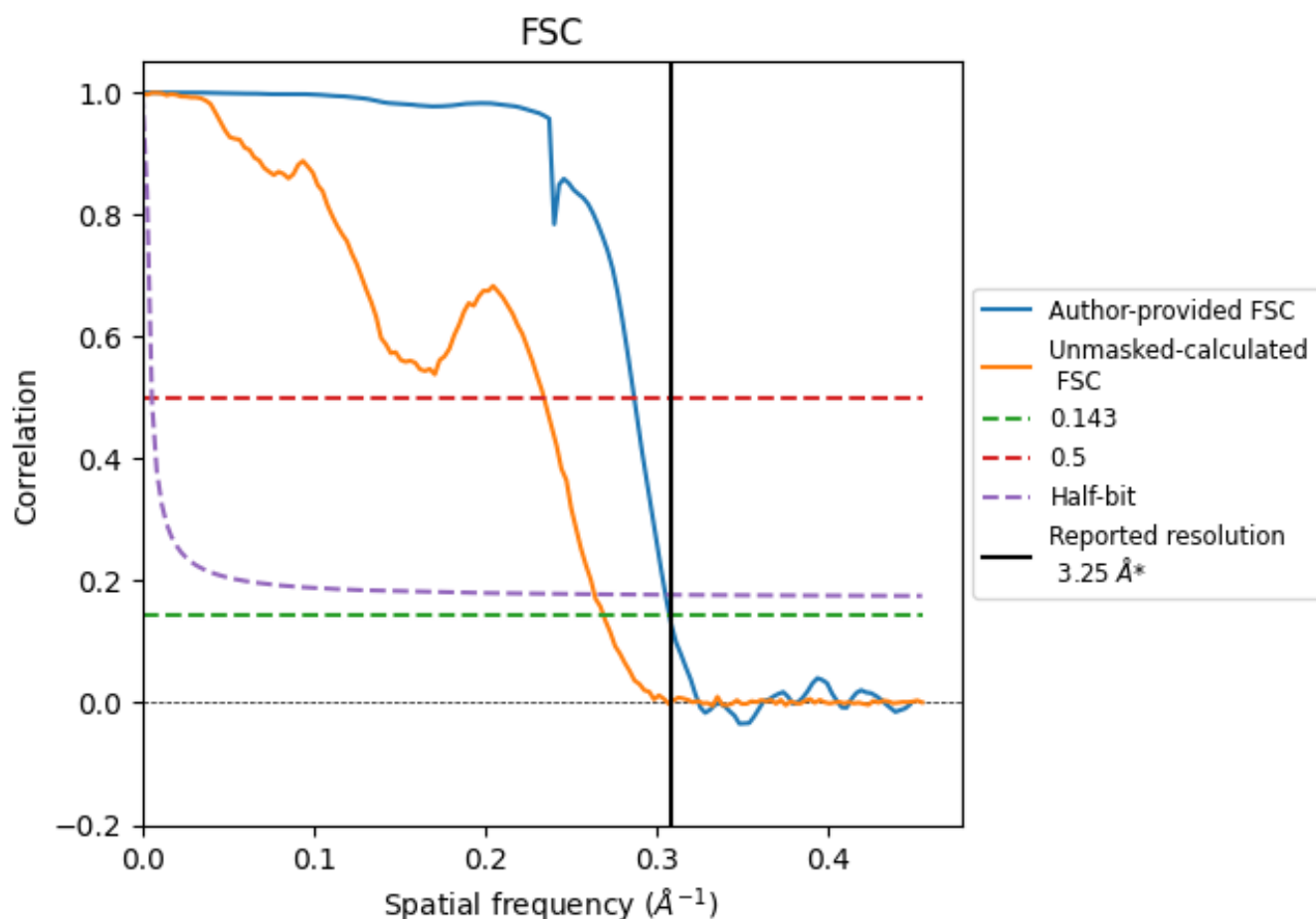


*Reported resolution corresponds to spatial frequency of 0.308 Å⁻¹

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 $0.308 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

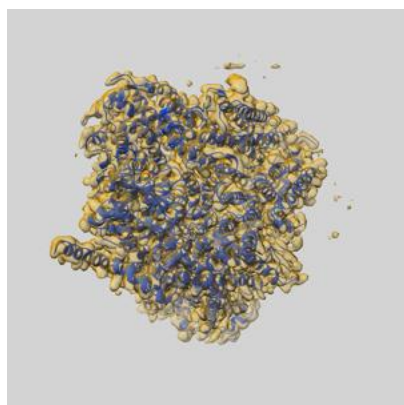
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.25	-	-
Author-provided FSC curve	3.25	3.49	3.28
Unmasked-calculated*	3.72	4.27	3.80

*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 3.72 differs from the reported value 3.25 by more than 10 %

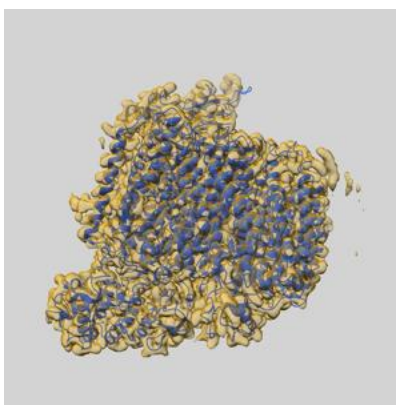
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42133 and PDB model 8UCO. Per-residue inclusion information can be found in section [3](#) on page [10](#).

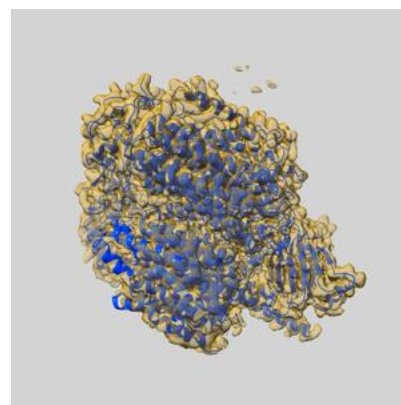
9.1 Map-model overlay [i](#)



X



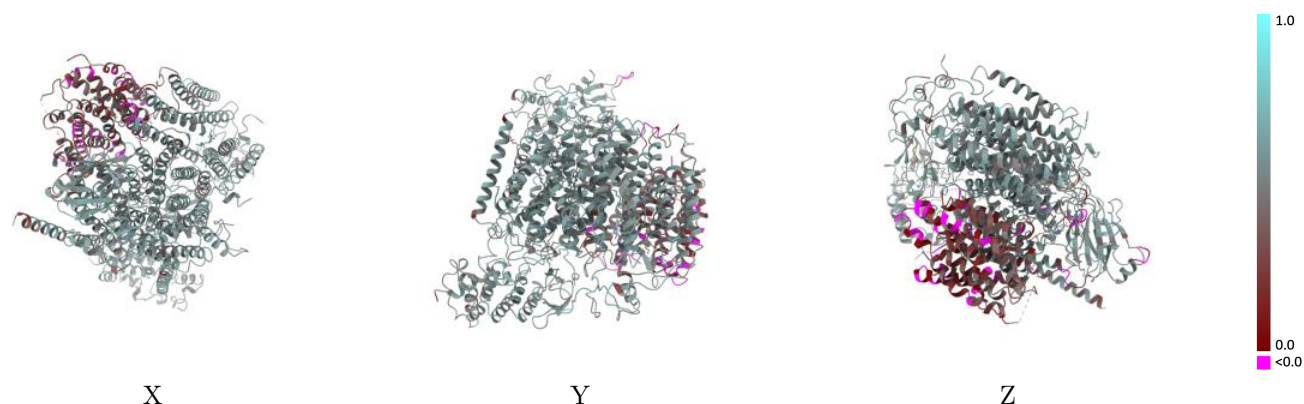
Y



Z

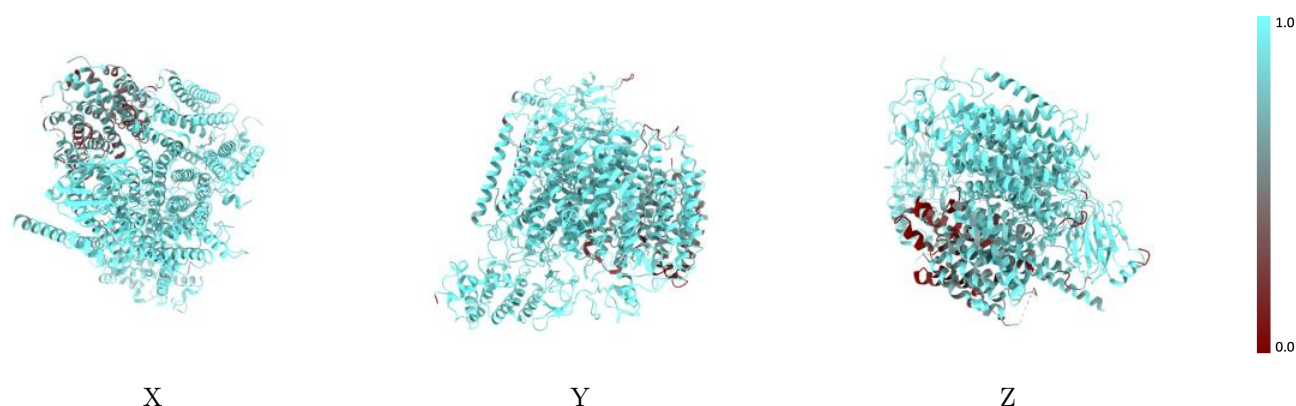
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



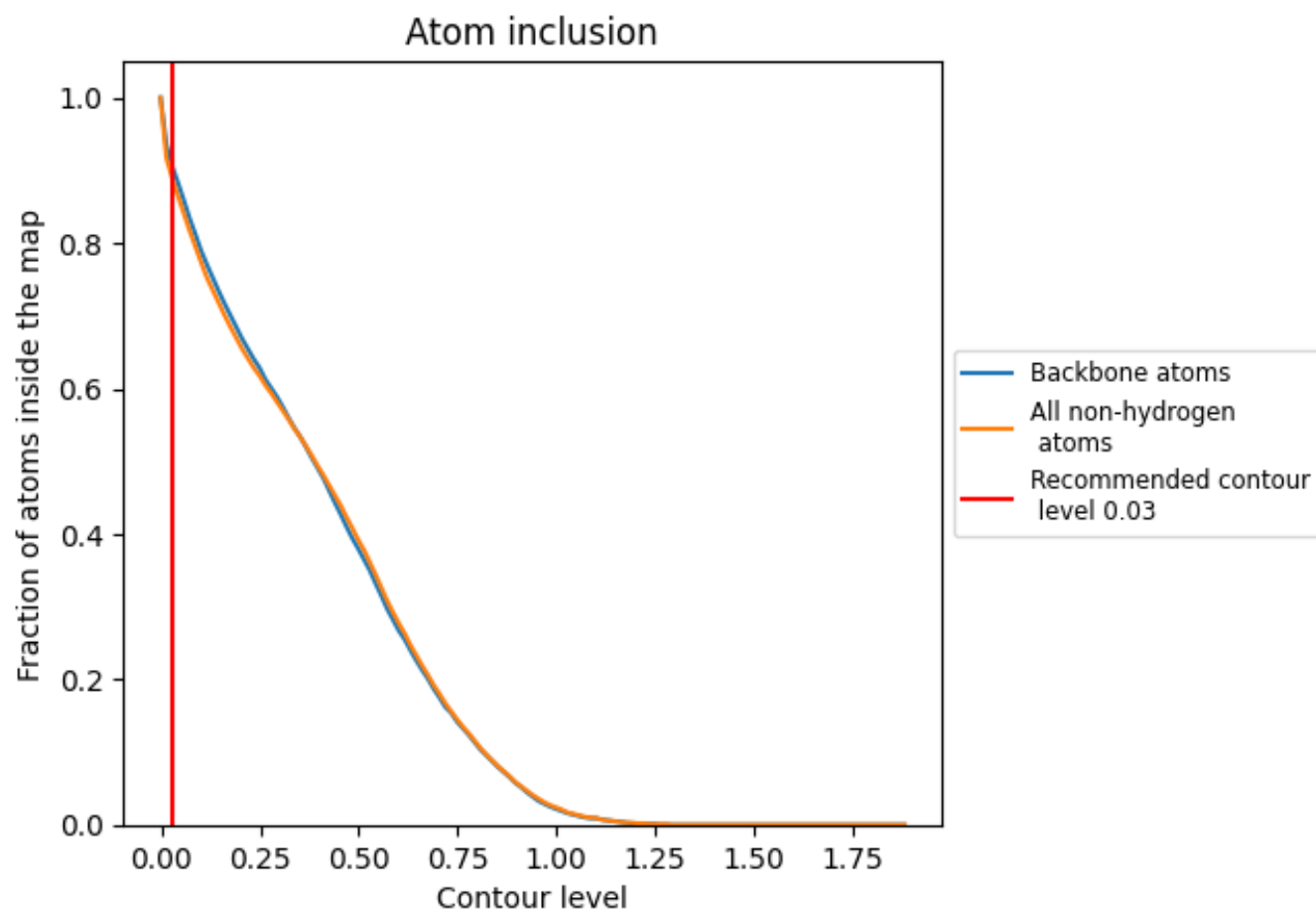
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8850	0.4840
A	0.5890	0.2440
a	0.9780	0.5540
b	0.9250	0.5140
c	0.9160	0.5140
d	0.9390	0.5260
e	0.9270	0.5190
f	0.9530	0.5410
g	0.9650	0.5400
h	0.9470	0.5420
i	0.9110	0.5160

1.0

0.0

<0.0