



wwPDB EM Validation Summary Report ⓘ

Apr 16, 2026 – 04:39 pm BST

PDB ID : 9T94 / pdb_00009t94
EMDB ID : EMD-55716
Title : cryo-EM structure of AKT phosphorylated mTOR complex 2, focused on a single protomer
Authors : Hay, I.M.; Anandapadamanaban, M.; Williams, R.L.
Deposited on : 2025-11-13
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

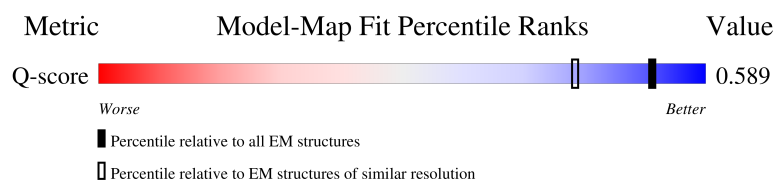
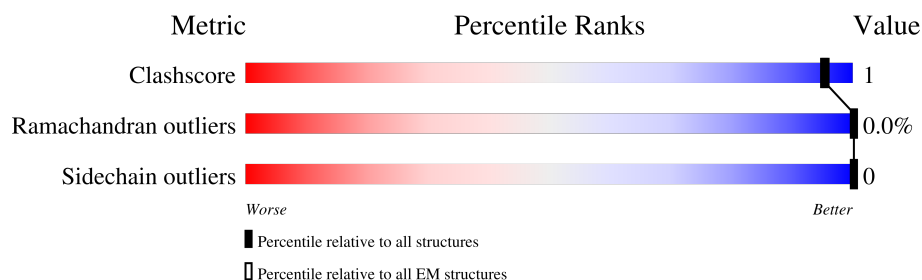
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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	8728 (2.10 - 3.10)

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	2590	
2	C	326	
3	E	1734	
4	G	522	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24959 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 Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1573	Total	C	N	O	S	0	0
			12757	8153	2230	2286	88		

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-40	MET	-	initiating methionine	UNP P42345
A	-39	ALA	-	expression tag	UNP P42345
A	-38	SER	-	expression tag	UNP P42345
A	-37	TRP	-	expression tag	UNP P42345
A	-36	SER	-	expression tag	UNP P42345
A	-35	HIS	-	expression tag	UNP P42345
A	-34	PRO	-	expression tag	UNP P42345
A	-33	GLN	-	expression tag	UNP P42345
A	-32	PHE	-	expression tag	UNP P42345
A	-31	GLU	-	expression tag	UNP P42345
A	-30	LYS	-	expression tag	UNP P42345
A	-29	GLY	-	expression tag	UNP P42345
A	-28	GLY	-	expression tag	UNP P42345
A	-27	GLY	-	expression tag	UNP P42345
A	-26	ALA	-	expression tag	UNP P42345
A	-25	ARG	-	expression tag	UNP P42345
A	-24	GLY	-	expression tag	UNP P42345
A	-23	GLY	-	expression tag	UNP P42345
A	-22	SER	-	expression tag	UNP P42345
A	-21	GLY	-	expression tag	UNP P42345
A	-20	GLY	-	expression tag	UNP P42345
A	-19	GLY	-	expression tag	UNP P42345
A	-18	SER	-	expression tag	UNP P42345
A	-17	TRP	-	expression tag	UNP P42345
A	-16	SER	-	expression tag	UNP P42345
A	-15	HIS	-	expression tag	UNP P42345
A	-14	PRO	-	expression tag	UNP P42345

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	GLN	-	expression tag	UNP P42345
A	-12	PHE	-	expression tag	UNP P42345
A	-11	GLU	-	expression tag	UNP P42345
A	-10	LYS	-	expression tag	UNP P42345
A	-9	GLY	-	expression tag	UNP P42345
A	-8	GLU	-	expression tag	UNP P42345
A	-7	ASN	-	expression tag	UNP P42345
A	-6	LEU	-	expression tag	UNP P42345
A	-5	TYR	-	expression tag	UNP P42345
A	-4	PHE	-	expression tag	UNP P42345
A	-3	GLN	-	expression tag	UNP P42345
A	-2	GLY	-	expression tag	UNP P42345
A	-1	GLY	-	expression tag	UNP P42345
A	0	THR	-	expression tag	UNP P42345

- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	315	Total	C	N	O	S	0	0
			2443	1518	434	473	18		

- Molecule 3 is a protein called Rapamycin-insensitive companion of mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	1119	Total	C	N	O	S	0	0
			8990	5732	1584	1625	49		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-25	MET	-	initiating methionine	UNP Q6R327
E	-24	ALA	-	expression tag	UNP Q6R327
E	-23	ASP	-	expression tag	UNP Q6R327
E	-22	TYR	-	expression tag	UNP Q6R327
E	-21	LYS	-	expression tag	UNP Q6R327
E	-20	ASP	-	expression tag	UNP Q6R327
E	-19	HIS	-	expression tag	UNP Q6R327
E	-18	ASP	-	expression tag	UNP Q6R327
E	-17	GLY	-	expression tag	UNP Q6R327
E	-16	ASP	-	expression tag	UNP Q6R327
E	-15	TYR	-	expression tag	UNP Q6R327
E	-14	LYS	-	expression tag	UNP Q6R327

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-13	ASP	-	expression tag	UNP Q6R327
E	-12	HIS	-	expression tag	UNP Q6R327
E	-11	ASP	-	expression tag	UNP Q6R327
E	-10	ILE	-	expression tag	UNP Q6R327
E	-9	ASP	-	expression tag	UNP Q6R327
E	-8	TYR	-	expression tag	UNP Q6R327
E	-7	LYS	-	expression tag	UNP Q6R327
E	-6	ASP	-	expression tag	UNP Q6R327
E	-5	ASP	-	expression tag	UNP Q6R327
E	-4	ASP	-	expression tag	UNP Q6R327
E	-3	ASP	-	expression tag	UNP Q6R327
E	-2	LYS	-	expression tag	UNP Q6R327
E	-1	GLY	-	expression tag	UNP Q6R327
E	0	THR	-	expression tag	UNP Q6R327

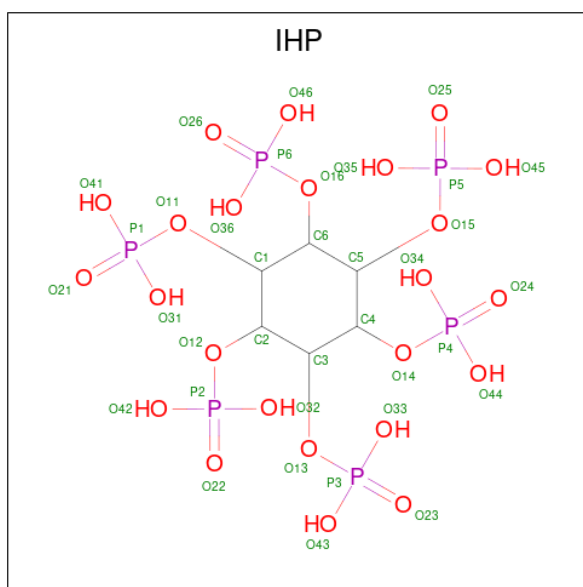
- Molecule 4 is a protein called Target of rapamycin complex 2 subunit MAPKAP1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	G	84	Total	C	N	O	P	S	0	0
			674	418	115	136	1	4		

There is a discrepancy between the modelled and reference sequences:

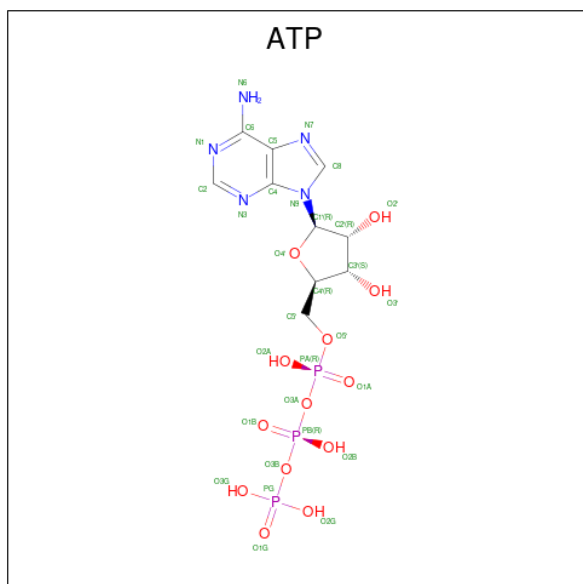
Chain	Residue	Modelled	Actual	Comment	Reference
G	1	ACE	-	acetylation	UNP Q9BPZ7

- Molecule 5 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 6 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
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

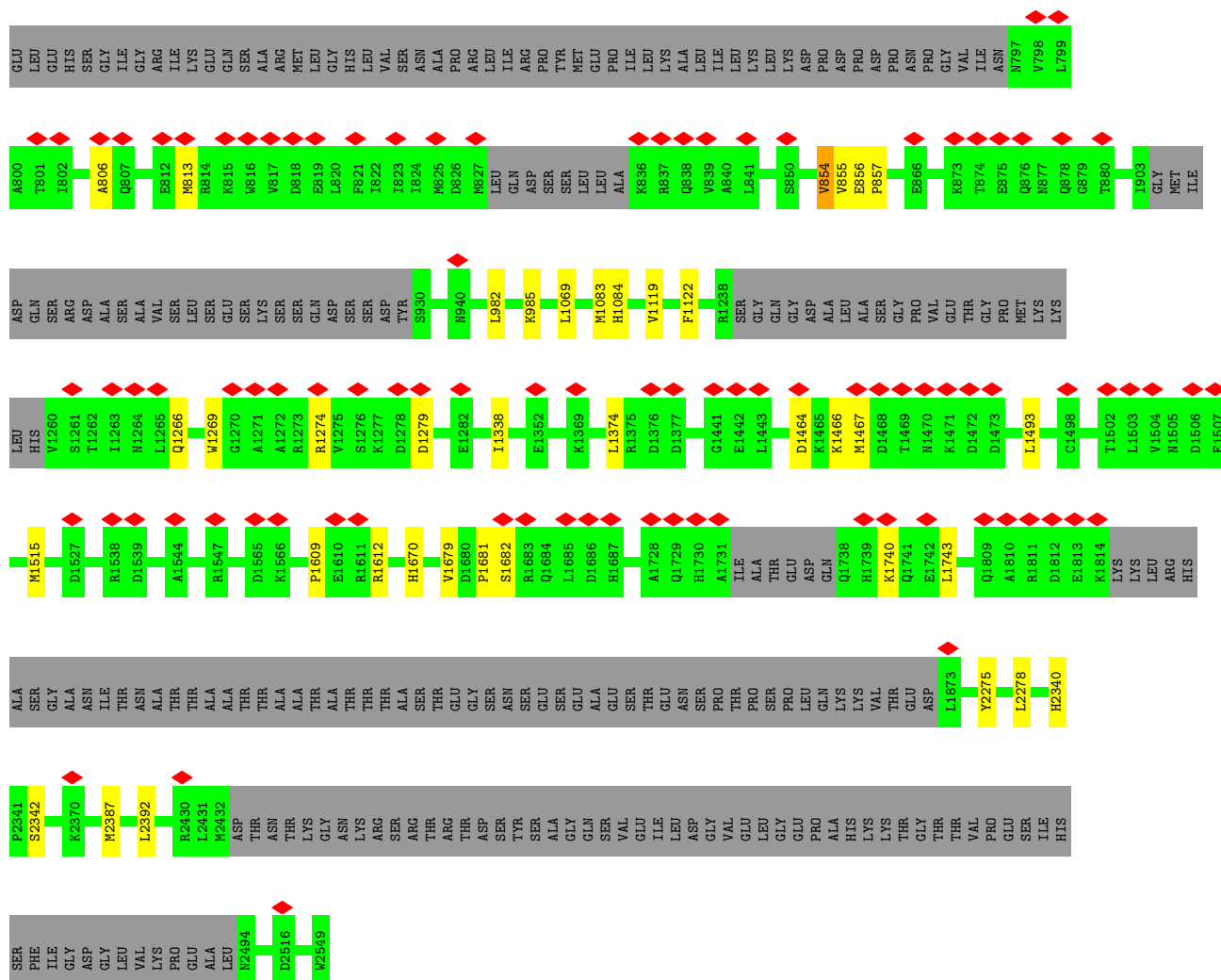
- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



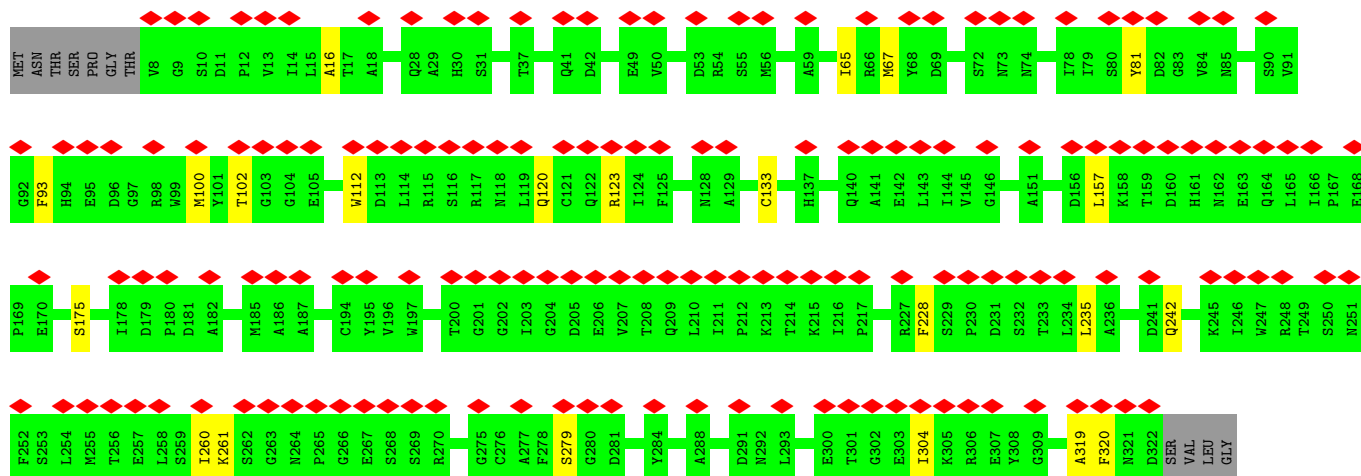
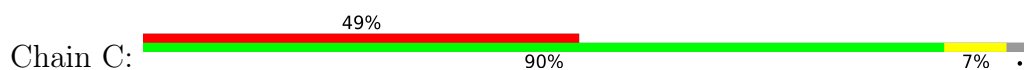
Mol	Chain	Residues	Atoms					AltConf
7	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	E	1	Total	Zn	0
			1	1	

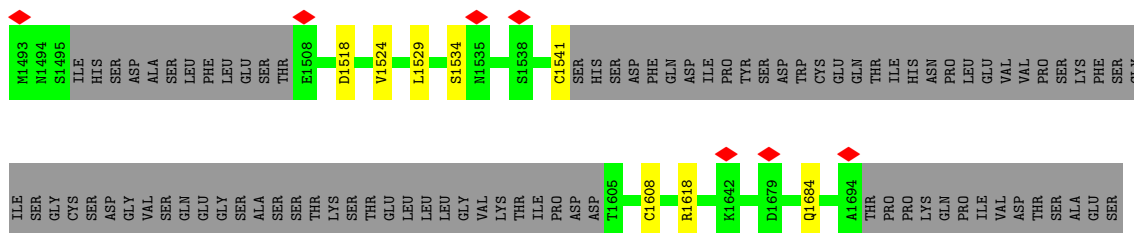


• Molecule 2: Target of rapamycin complex subunit LST8

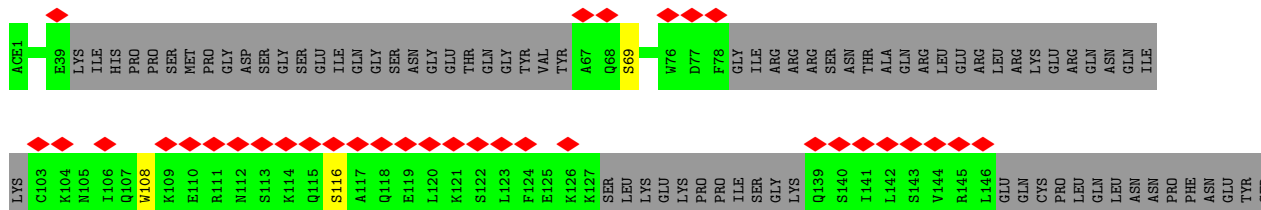


• Molecule 3: Rapamycin-insensitive companion of mTOR

Opinion	Percentage
Doing a good job	63%
Doing a bad job	35%



- Chain G:  7% 16% 84%



GLN	ASP	LEU	GLU	ARG	LYS	LYS
	TTR	ILE	SER	ILE	LEU	PHE
	LYS	ILE	GLN	ASN	ASN	ASP
	HIS	SER	SER	ALA	ASP	GLY
	LEU	GLY	ALA	ALA	ASN	GLY
	TTR	ASP	TRP	HIS	VAL	GLY
	PHE	LYS	GLU	GLY	SER	HIS
	GLU	VAL	PHE	PHE	ALA	VAL
	SER	GLU	CYS	LEU	GLY	GLY
	ASP	ILE	LEU	SER	CYS	TTR
	ALA	PRO	ARG	GLN	LEU	THR
	ALA	VAL	GLU	VAL	HIS	ALA
	THR	VAL	GLU	VAL	ILE	THR
	VAL	THR	ASN	ASP	ALA	LYS
	ASN	ASN	SER	ASN	GLU	LYS
	GLU	GLN	SER	THR	ASP	ILE
	ILE	LYS	ARG	LYS	ASP	ASP
	VAL	ALA	ALA	VAL	GLY	VAL
	LEU	SER	ASP	THR	GLU	TYR
	LYS	THR	GLY	MET	VAL	LEU
	VAL	PHE	VAL	LYS	ASP	PRO
	ASN	ASN	PHE	GLU	THR	LEU
	TTR	TRP	GLU	ILE	ASP	HIS
	ILE	ILE	GLU	LEU	PHE	SER
	LEU	LYS	ASP	LEU	PRO	SER
	GLU	GLN	SER	LYS	PRO	GLN
	SER	LYS	SER	ALA	ASP	ARG
	ARG	PRO	ILE	VAL	SER	LEU
	ALA	ILE	ASP	LYS	SER	LEU
	SER	SER	ILE	ARG	ASN	LEU
	THR	ILE	ALA	ARG	GLU	PRO
	ALA	ASP	THR	LYS	PRO	MET
	ARG	SER	VAL	GLY	ILE	THR
	ALA	ASP	GLN	SER	HIS	VAL
	ASP	LEU	ASP	GLN	LYS	VAL
	TTR	CYS	MET	LYS	PHE	THR
	PHE	LEU	LEU	VAL	GLY	MET
	ALA	ALA	SER	SER	PHE	ALA
	GLN	CYS	SER	GLY	SER	ALA
	LYS	ASP	HIS	PRO	THR	ALA
	GLN	LEU	HIS	GLN	LEU	ARG
	ARG	ALA	TYR	TYR	ALA	VAL
	LYS	GLU	LYS	ARG	LEU	GLN
	LEU	GLU	SER	LEU	VAL	ASP
	ASN	LYS	PHE	GLU	GLU	LYS
	ARG	SER	LYS	LYS	LYS	ILE
	ARG	PRO	VAL	GLN	TYR	GLY
	THR	SER	SER	SER	SER	LEU
	SER	HIS	MET	GLU	SER	ILE
	PHE	ALA	ILE	PRO	CYS	ILE
	SER	ILE	HIS	ASN	GLY	TRP
	PHE	PHE	ARG	VAL	LEU	GLN
	GLN	LYS	LEU	ALA	THR	TYR
	LYS	LEU	ARG	VAL	SER	THR
	GLU	THR	PHE	ASP	LYS	SER
	LYS	TYR	THR	LEU	GLU	GLY
	LYS	LEU	THR	ASP	SER	ARG
	SER	SER	ASP	SER	LEU	ARG
	GLN	ASN	VAL	THR	PHE	GLU
	GLY	HIS	GLN	LEU	VAL	PRO

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	210421	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.041	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	488.96, 488.96, 488.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.955, 0.955, 0.955	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP, ZN, IHP, ACE, SEP

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	0.13	0/13039	0.38	0/17658
2	C	0.13	0/2501	0.42	0/3408
3	E	0.13	0/9154	0.37	0/12384
4	G	0.13	0/668	0.42	0/895
All	All	0.13	0/25362	0.38	0/34345

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
3	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	997	ARG	Sidechain

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	12757	0	12860	22	0
2	C	2443	0	2327	13	0
3	E	8990	0	9187	14	0
4	G	674	0	657	2	0
5	A	36	0	6	0	0
6	A	31	0	12	0	0
7	E	27	0	12	0	0
8	E	1	0	0	0	0
All	All	24959	0	25061	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.

The worst 5 of 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:A:854:VAL:HG13	1:A:855:VAL:H	1.54	0.72
2:C:242:GLN:HB3	2:C:260:ILE:HB	1.71	0.71
1:A:1274:ARG:HD3	1:A:1279:ASP:HB3	1.74	0.70
1:A:2340:HIS:CE1	1:A:2342:SER:HB2	2.37	0.59
3:E:746:PHE:HB3	3:E:749:ASN:HD21	1.67	0.58

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	A	1559/2590 (60%)	1528 (98%)	30 (2%)	1 (0%)	48	70
2	C	313/326 (96%)	301 (96%)	12 (4%)	0	100	100
3	E	1103/1734 (64%)	1080 (98%)	23 (2%)	0	100	100
4	G	75/522 (14%)	66 (88%)	9 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3050/5172 (59%)	2975 (98%)	74 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	854	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	A	1394/2248 (62%)	1394 (100%)	0	100	100
2	C	267/276 (97%)	267 (100%)	0	100	100
3	E	1005/1562 (64%)	1005 (100%)	0	100	100
4	G	77/469 (16%)	77 (100%)	0	100	100
All	All	2743/4555 (60%)	2743 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	561	ASN
3	E	1485	GLN
3	E	590	ASN
3	E	827	GLN
3	E	1632	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SEP	G	69	4	8,9,10	1.50	1 (12%)	8,12,14	1.64	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SEP	G	69	4	-	1/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	69	SEP	P-O1P	3.32	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	69	SEP	P-OG-CB	-3.17	109.55	118.30
4	G	69	SEP	OG-CB-CA	2.84	110.90	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	69	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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
5	IHP	A	2601	-	36,36,36	1.91	6 (16%)	54,60,60	1.00	2 (3%)
6	ATP	A	2602	-	29,33,33	0.28	0	44,52,52	0.53	1 (2%)
7	ADP	E	1801	-	27,29,29	1.36	4 (14%)	42,45,45	1.93	9 (21%)

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	IHP	A	2601	-	-	4/30/54/54	0/1/1/1
6	ATP	A	2602	-	-	2/22/38/38	0/3/3/3
7	ADP	E	1801	-	-	6/16/32/32	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	1801	ADP	C5-C4	4.62	1.47	1.39
5	A	2601	IHP	P2-O12	4.61	1.68	1.59
5	A	2601	IHP	P5-O15	4.44	1.67	1.59
5	A	2601	IHP	P6-O16	4.29	1.67	1.59
5	A	2601	IHP	P4-O14	4.26	1.67	1.59

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	1801	ADP	C5-C4-N3	-6.62	118.11	126.75
7	E	1801	ADP	N3-C4-N9	5.21	135.66	127.08
7	E	1801	ADP	C2-N3-C4	3.94	121.07	111.75
5	A	2601	IHP	C5-C4-C3	-3.58	102.58	110.41
7	E	1801	ADP	C4-C5-N7	-3.10	106.84	110.62

There are no chirality outliers.

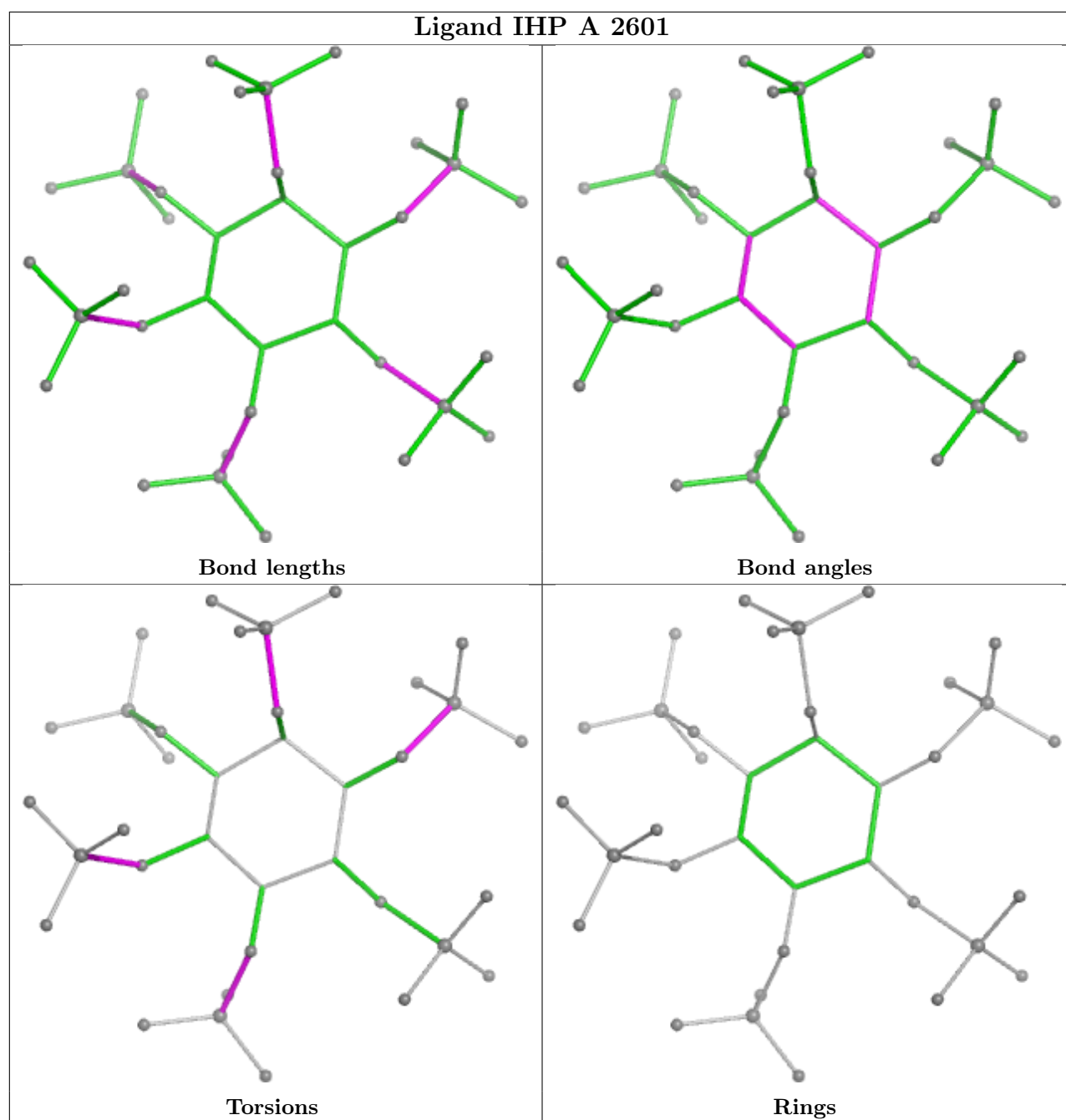
5 of 12 torsion outliers are listed below:

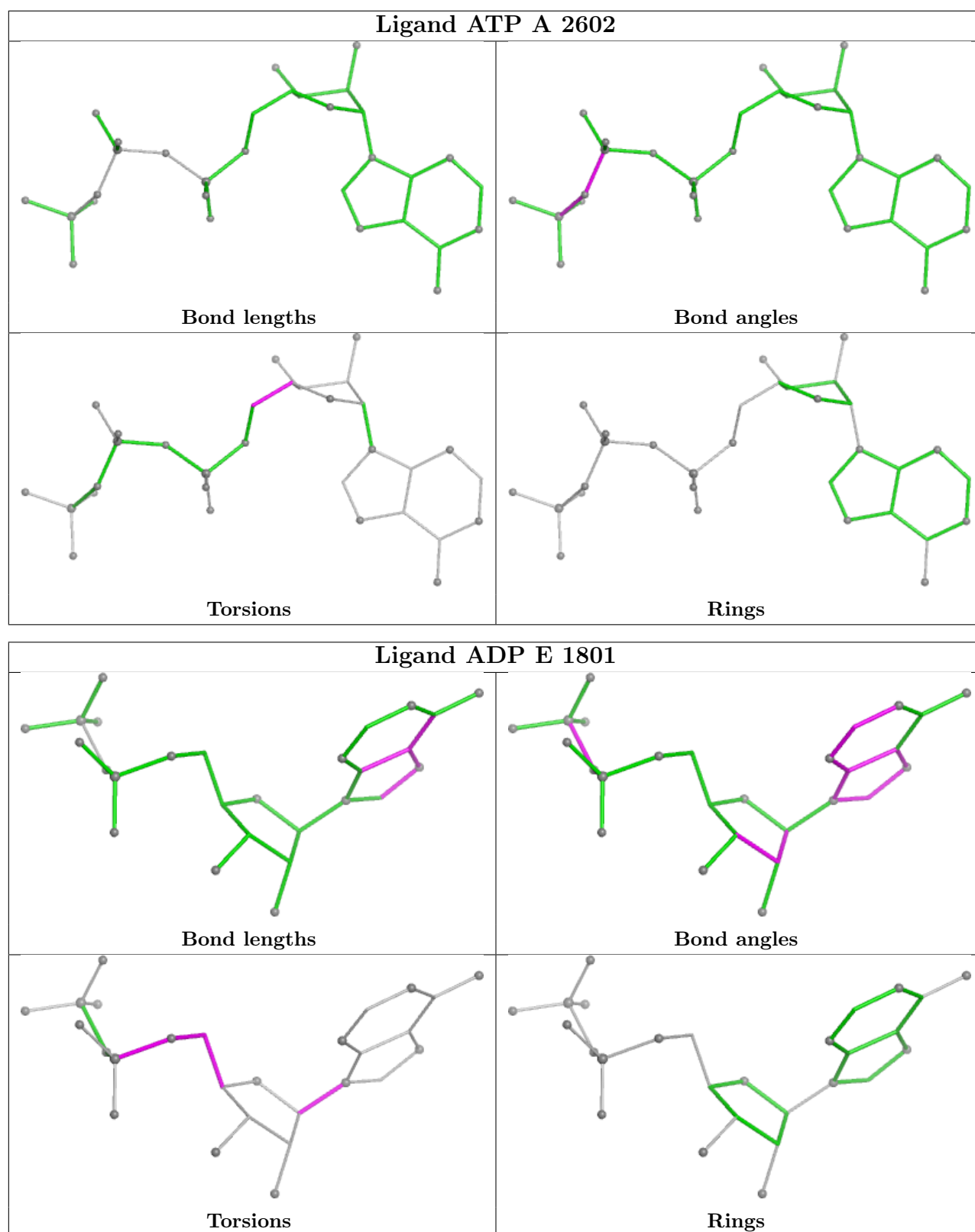
Mol	Chain	Res	Type	Atoms
5	A	2601	IHP	C2-O12-P2-O42
7	E	1801	ADP	C5'-O5'-PA-O1A
7	E	1801	ADP	C5'-O5'-PA-O2A
7	E	1801	ADP	C5'-O5'-PA-O3A
7	E	1801	ADP	C4'-C5'-O5'-PA

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

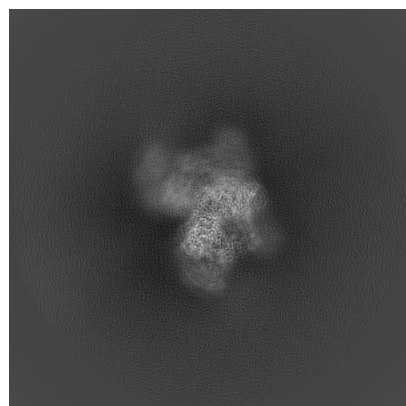
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55716. These allow visual inspection of the internal detail of the map and identification of artifacts.

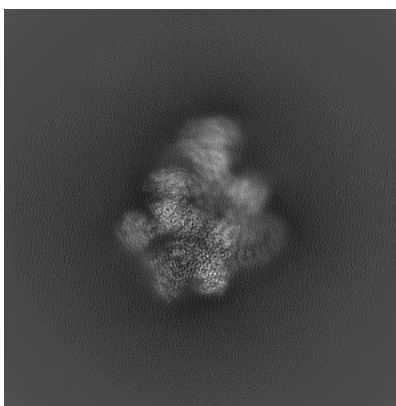
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

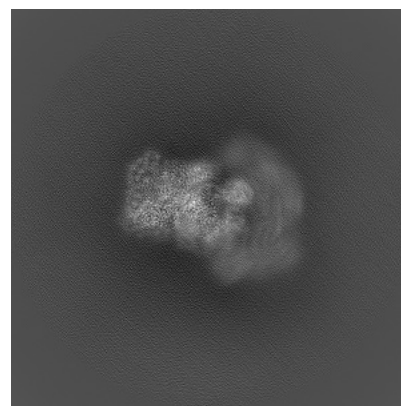
6.1.1 Primary map



X

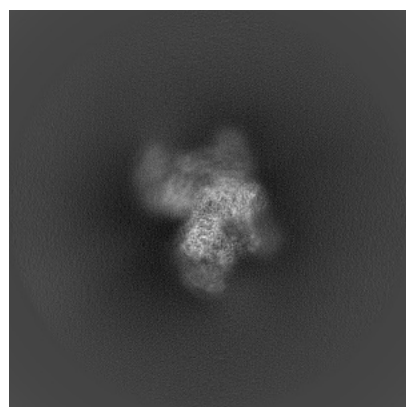


Y

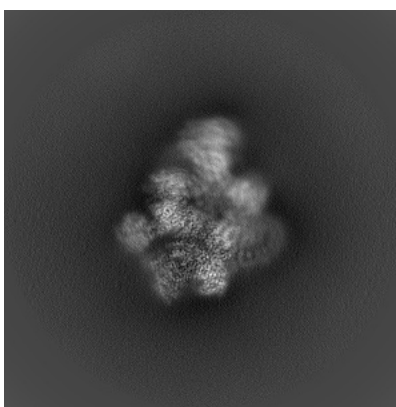


Z

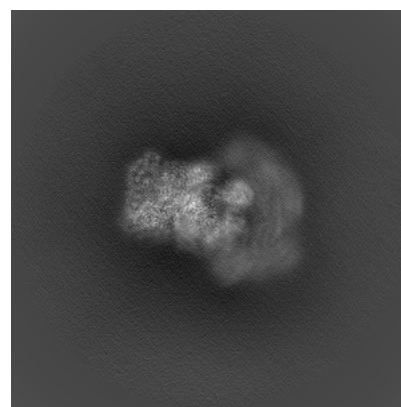
6.1.2 Raw map



X



Y

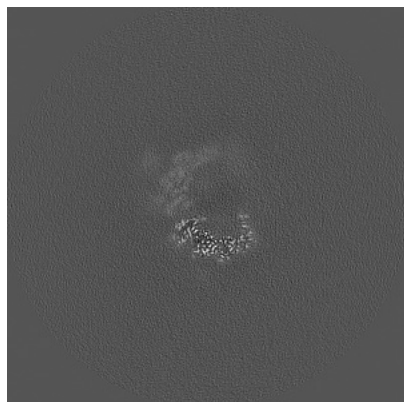


Z

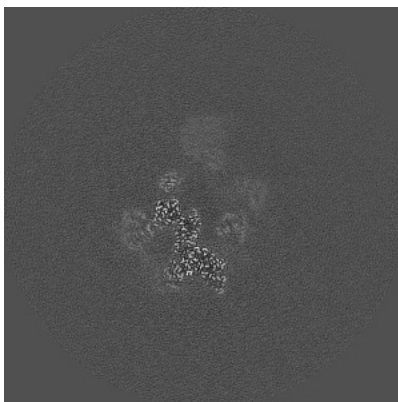
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

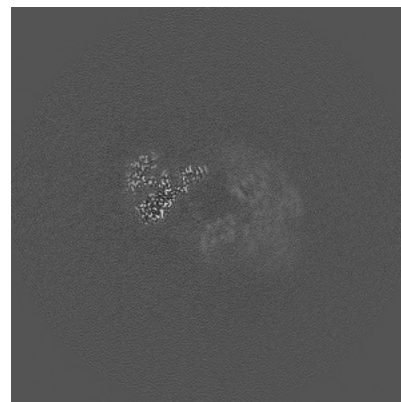
6.2.1 Primary map



X Index: 256

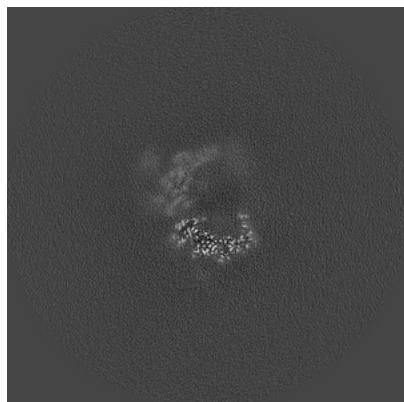


Y Index: 256

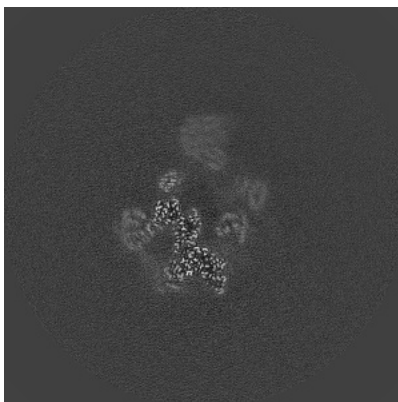


Z Index: 256

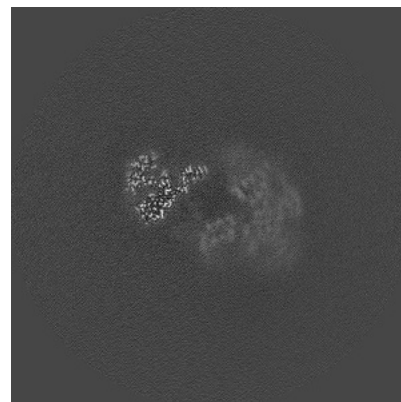
6.2.2 Raw map



X Index: 256



Y Index: 256

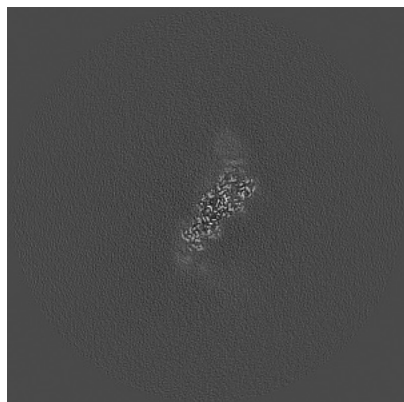


Z Index: 256

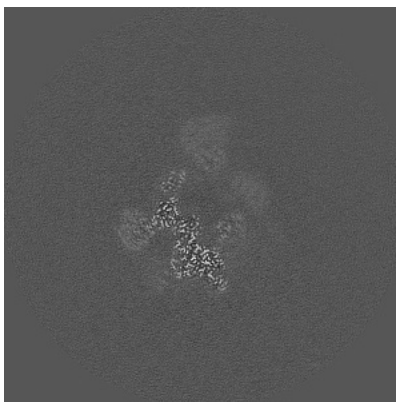
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

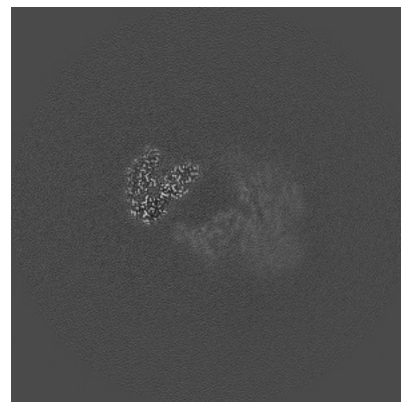
6.3.1 Primary map



X Index: 197

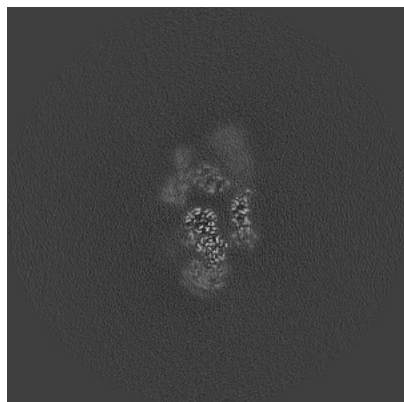


Y Index: 260

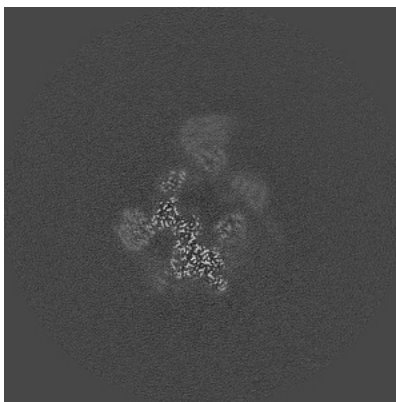


Z Index: 264

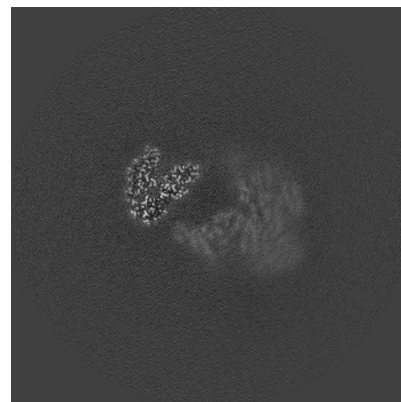
6.3.2 Raw map



X Index: 235



Y Index: 260

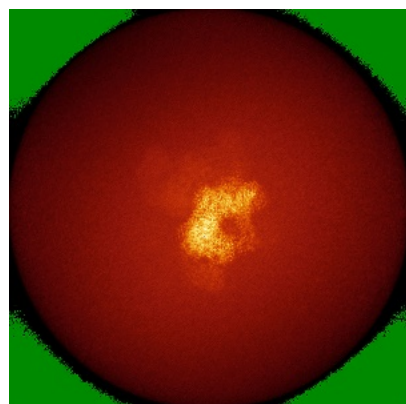


Z Index: 264

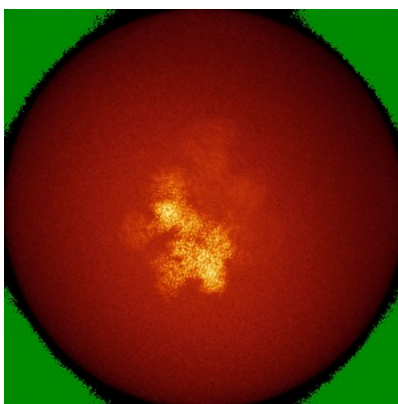
The images above show the largest variance slices of the map in three orthogonal directions.

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

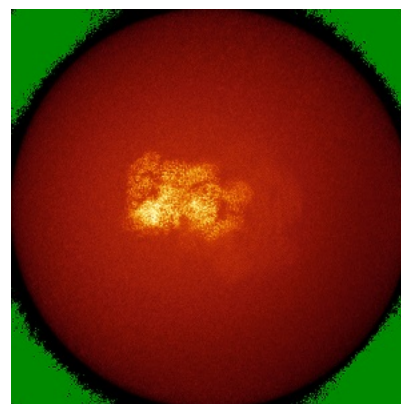
6.4.1 Primary map



X

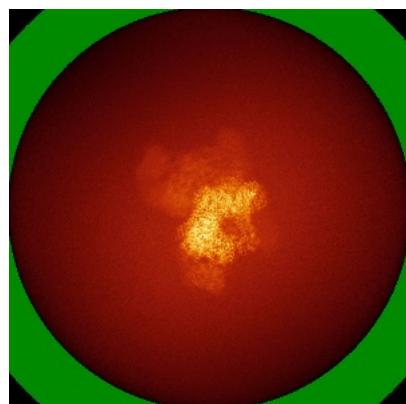


Y

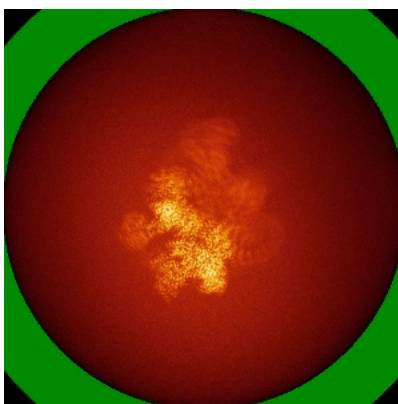


Z

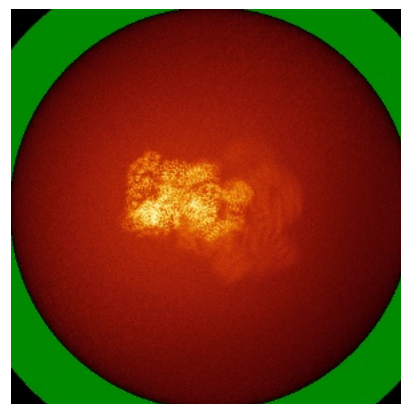
6.4.2 Raw map



X



Y

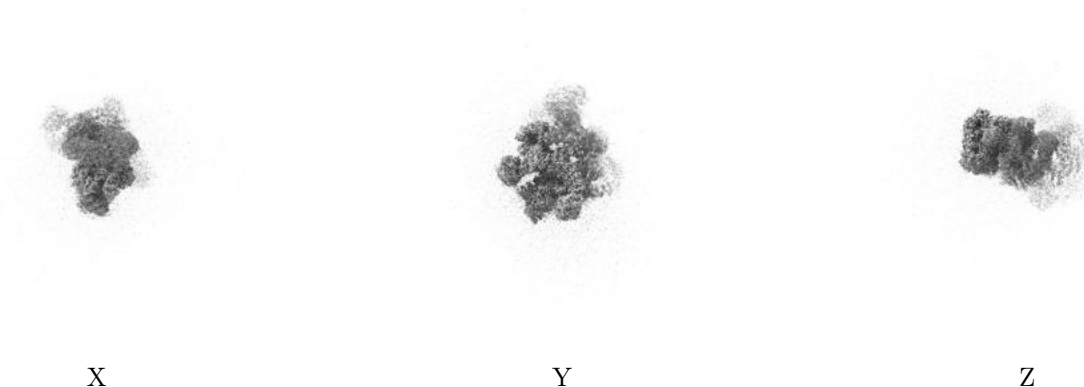


Z

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.

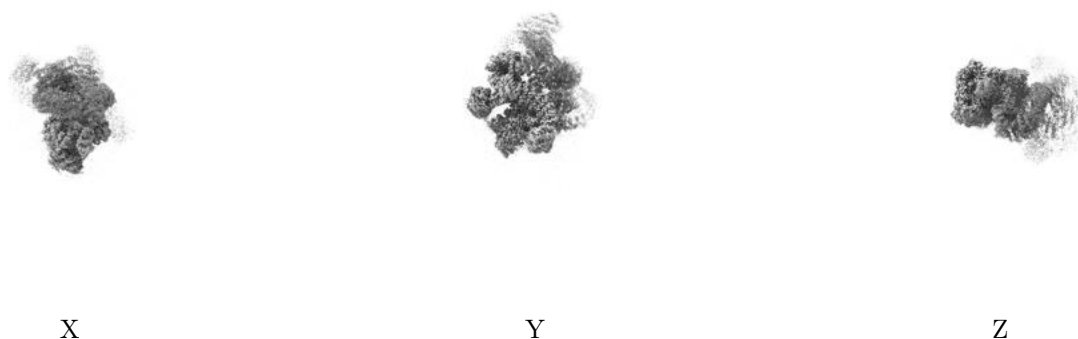
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

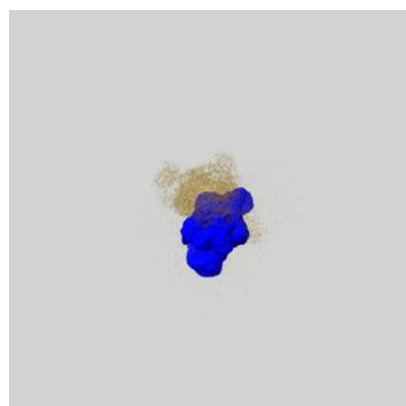
6.6 Mask visualisation [i](#)

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

A mask typically either:

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

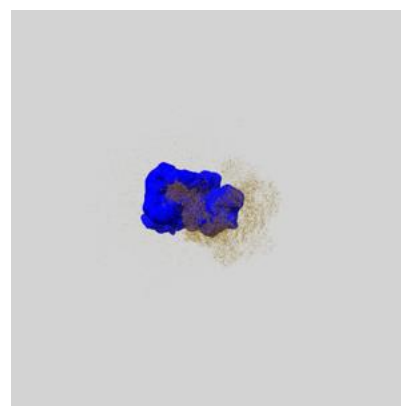
6.6.1 emd_55716_msk_1.map [i](#)



X



Y

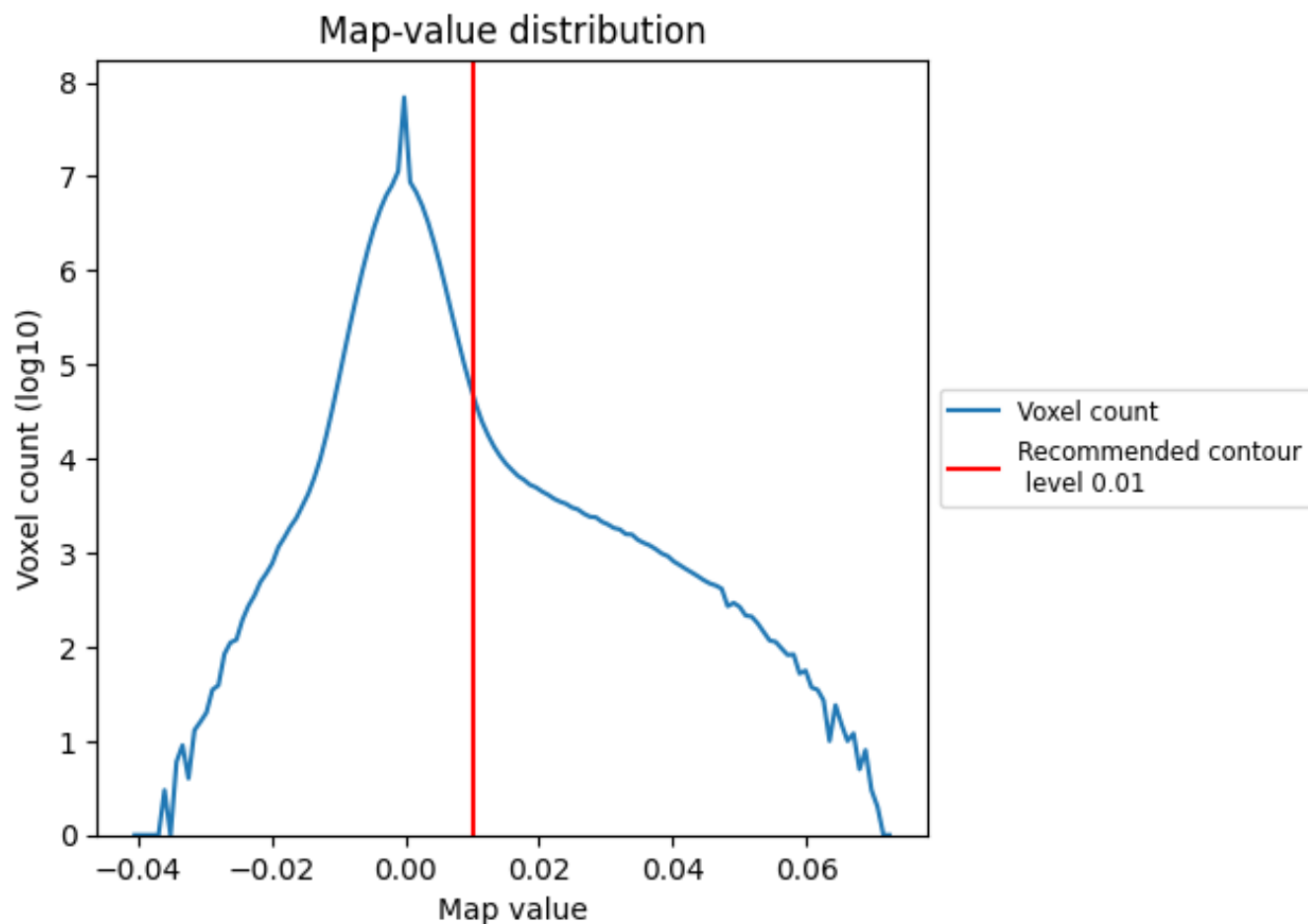


Z

7 Map analysis [i](#)

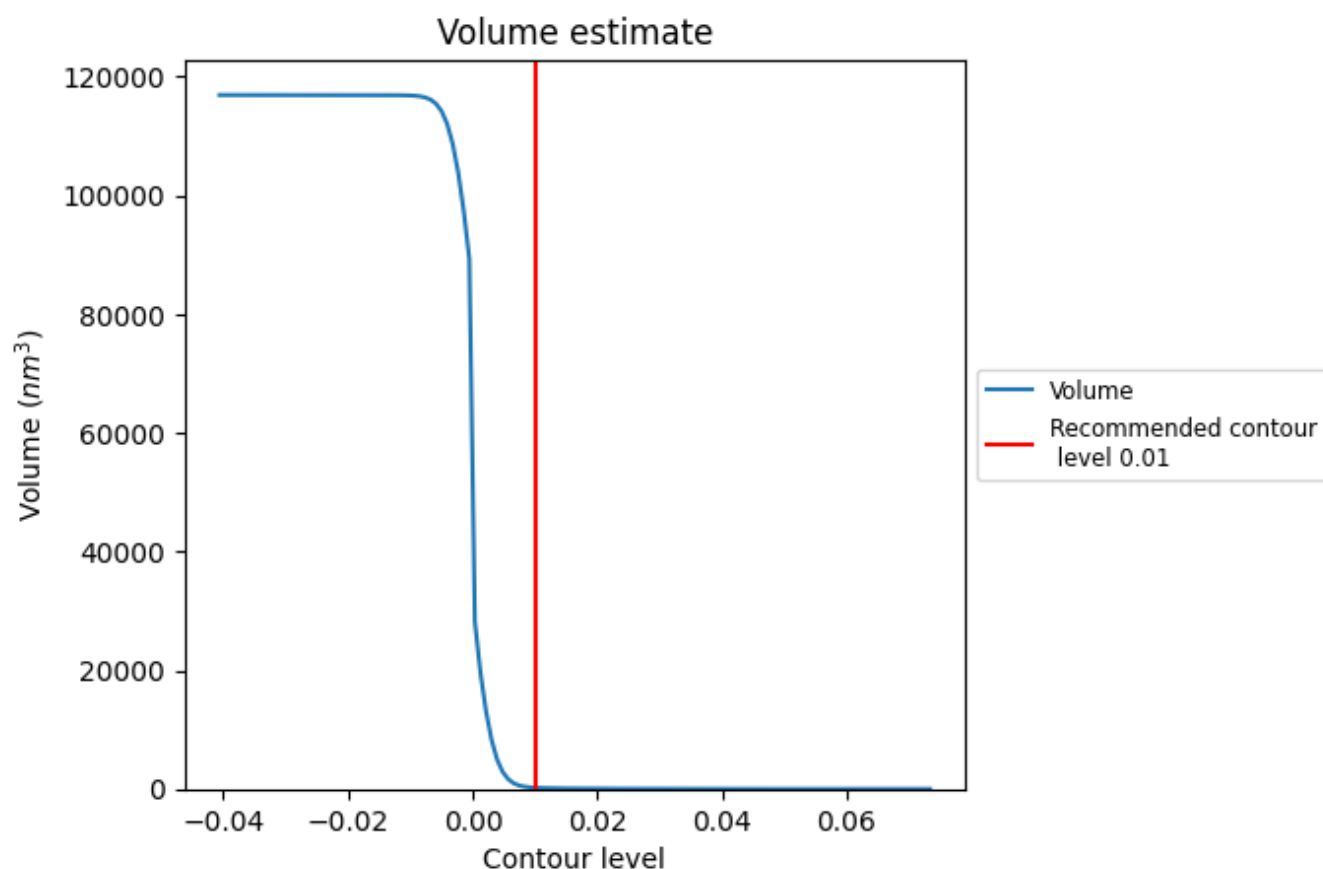
This section contains the results of statistical analysis of the map.

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.

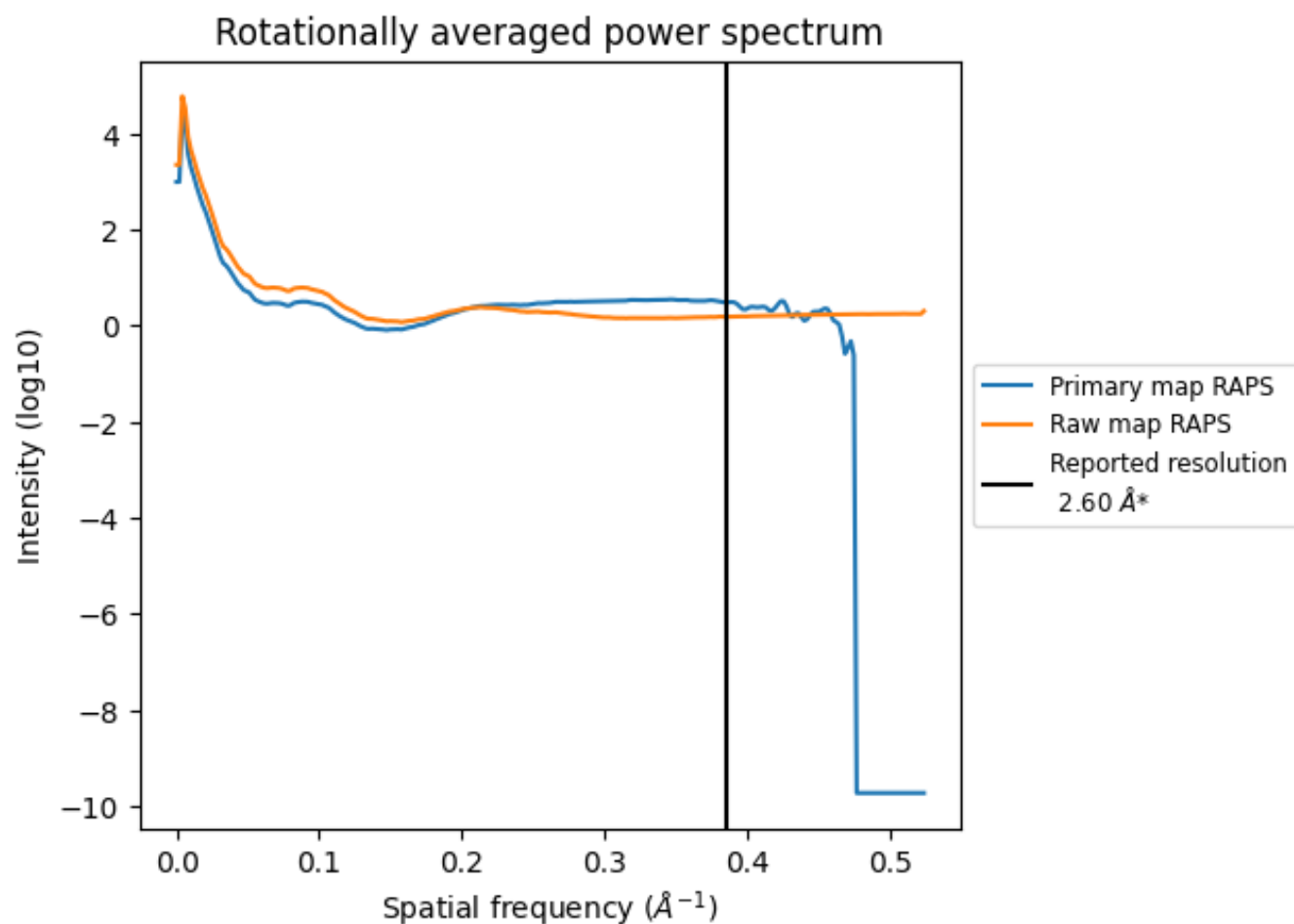
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 207 nm³; this corresponds to an approximate mass of 187 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 ⓘ

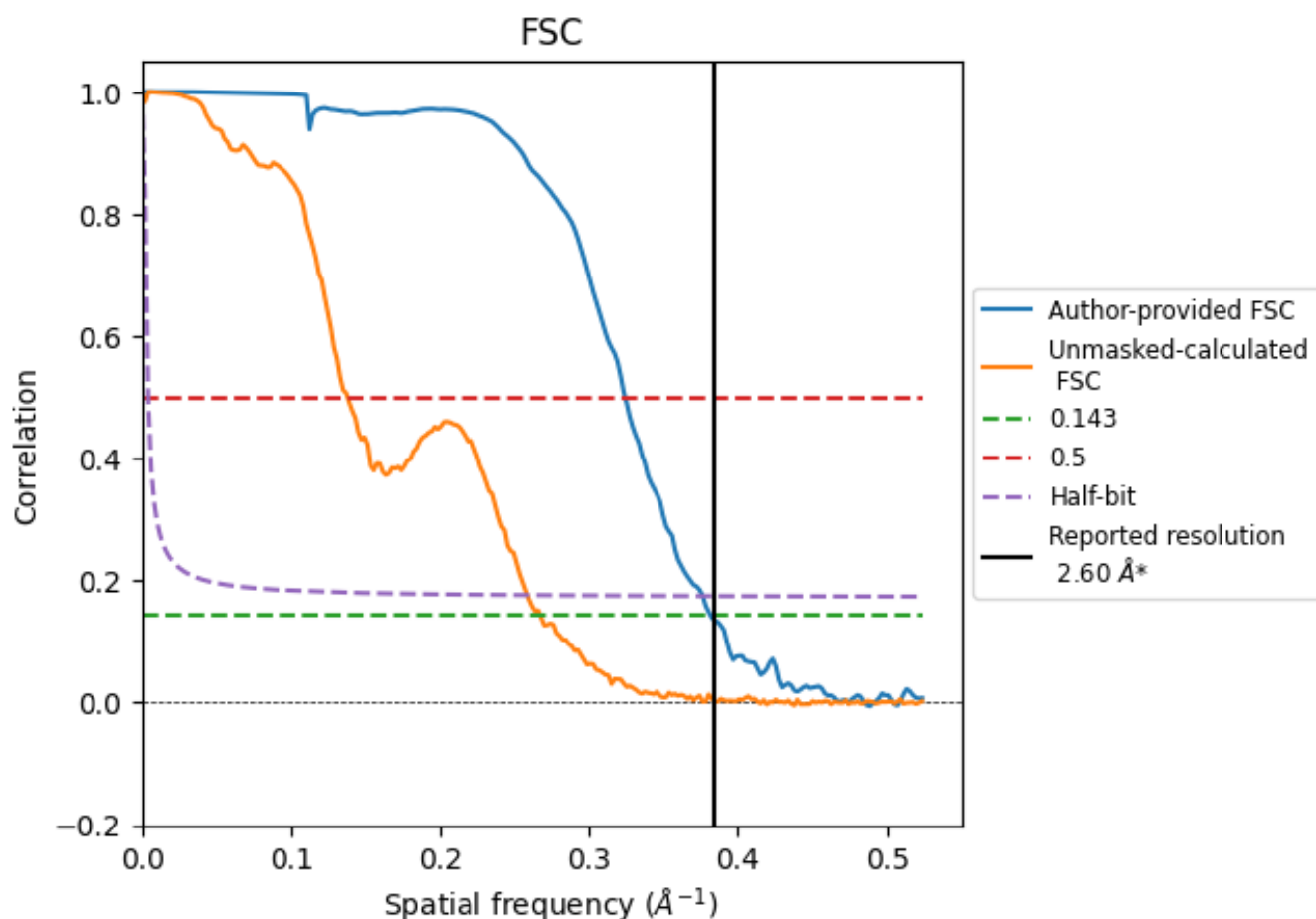


*Reported resolution corresponds to spatial frequency of 0.385 \AA^{-1}

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 0.385 \AA^{-1}

8.2 Resolution estimates [i](#)

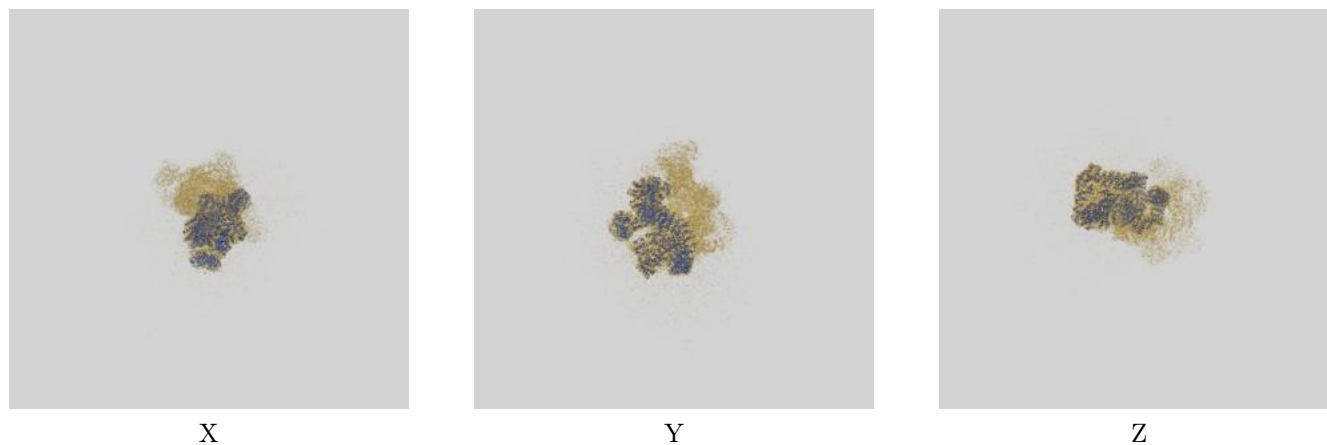
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.62	3.09	2.66
Unmasked-calculated*	3.74	7.25	3.87

*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 3.74 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

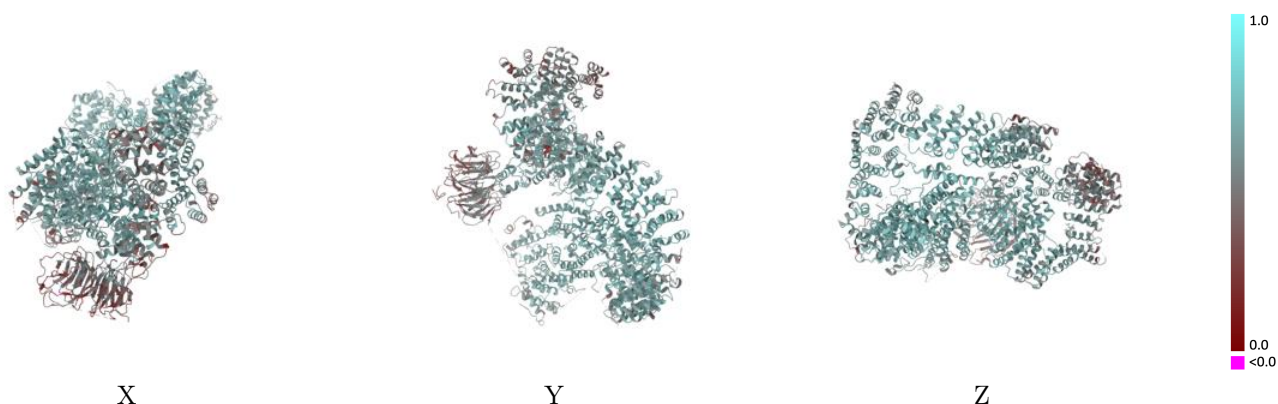
This section contains information regarding the fit between EMDB map EMD-55716 and PDB model 9T94. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



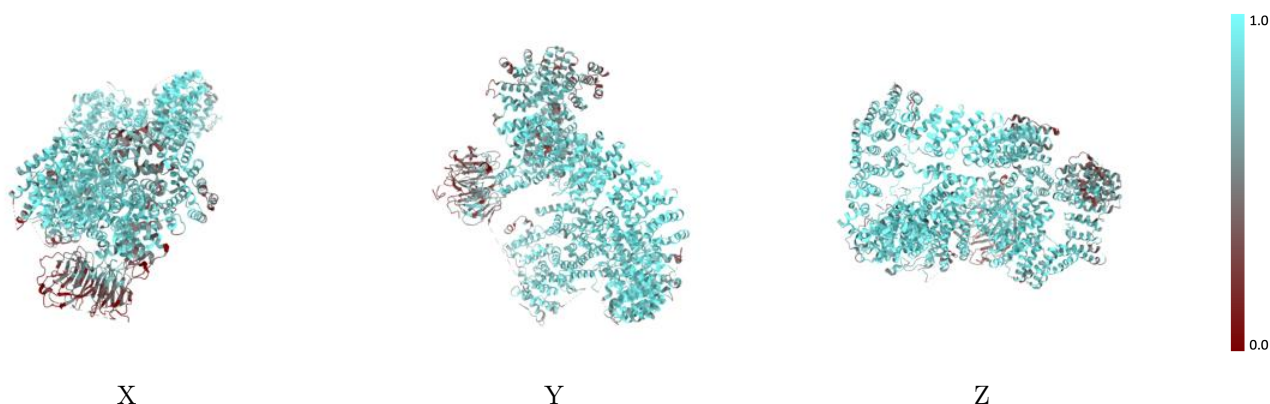
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



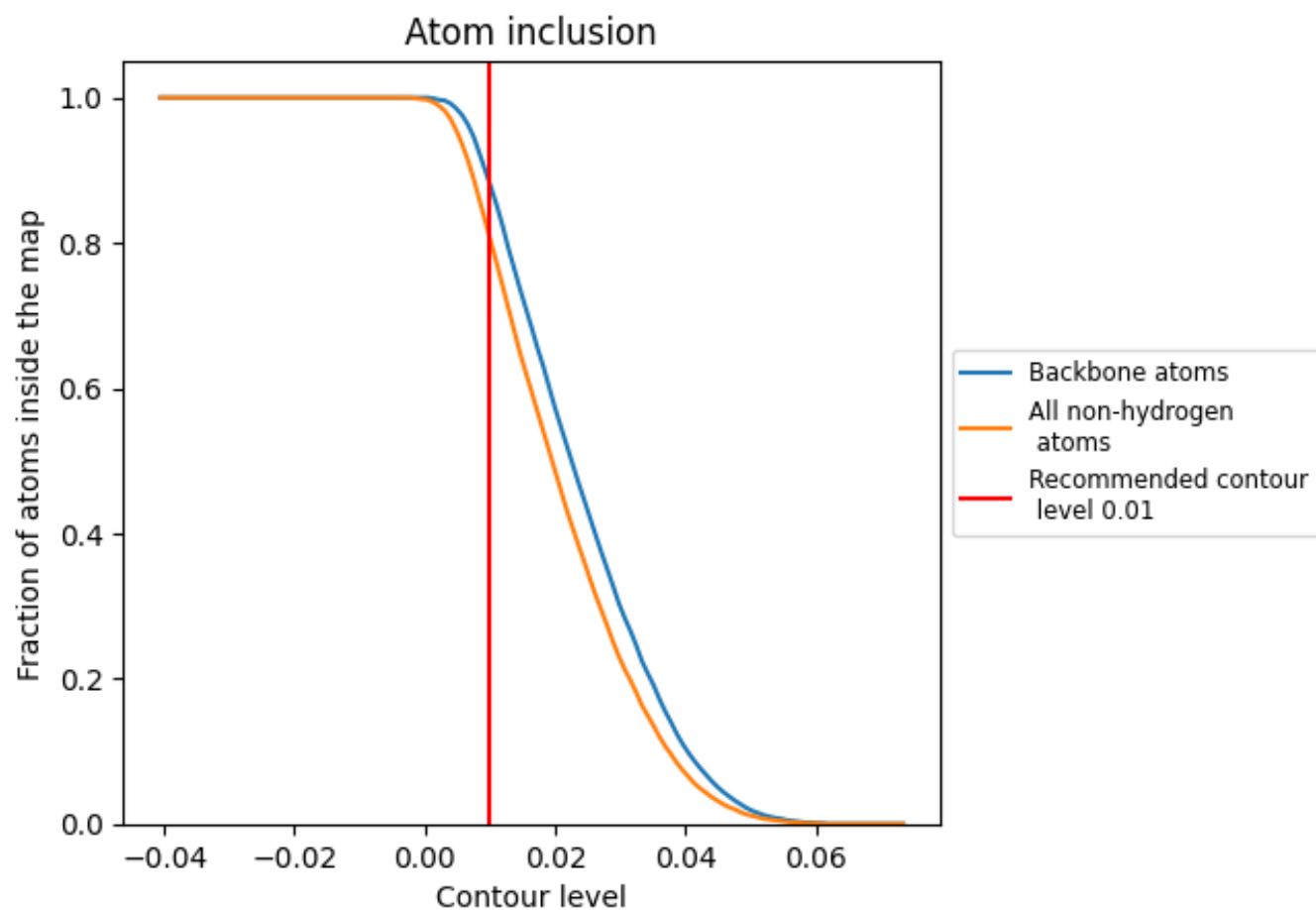
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8050	<div></div> 0.5890
A	<div></div> 0.8400	<div></div> 0.6000
C	<div></div> 0.4170	<div></div> 0.3830
E	<div></div> 0.8770	<div></div> 0.6340
G	<div></div> 0.5580	<div></div> 0.4960

