



## wwPDB EM Validation Summary Report ⓘ

Mar 30, 2025 – 12:39 AM JST

PDB ID : 8ZIR  
EMDB ID : EMD-60127  
Title : DUF4297-HerA complex  
Authors : Yu, Y.; Chen, Q.  
Deposited on : 2024-05-14  
Resolution : 3.08 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](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.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.4

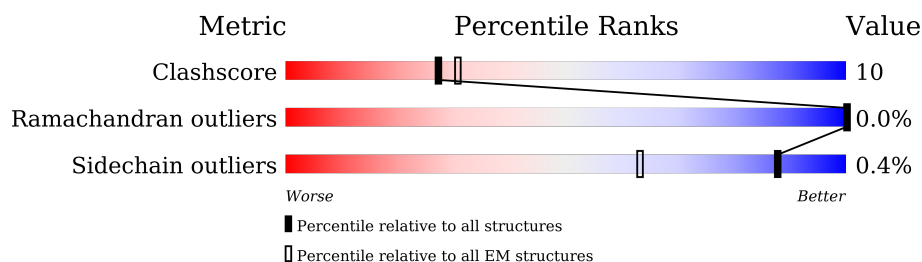
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.08 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	397	
1	B	397	
1	C	397	
1	D	397	
1	E	397	
1	F	397	
1	G	397	
1	H	397	

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Mol	Chain	Length	Quality of chain
1	I	397	
1	J	397	
1	K	397	
1	L	397	
2	M	617	
2	N	617	
2	O	617	
2	P	617	
2	Q	617	
2	R	617	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 102988 atoms, of which 50586 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 DUF4297.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	388	Total	C	H	N	O	S	0	0
			5985	2005	2851	545	576	8		
1	B	167	Total	C	H	N	O	S	0	0
			2789	889	1400	251	245	4		
1	C	386	Total	C	H	N	O	S	0	0
			6002	1990	2890	541	573	8		
1	D	169	Total	C	H	N	O	S	0	0
			2827	902	1418	253	250	4		
1	E	387	Total	C	H	N	O	S	0	0
			5977	1993	2859	544	573	8		
1	F	167	Total	C	H	N	O	S	0	0
			2794	889	1405	251	245	4		
1	G	380	Total	C	H	N	O	S	0	0
			5931	1965	2856	537	565	8		
1	H	168	Total	C	H	N	O	S	0	0
			2806	893	1409	252	248	4		
1	I	385	Total	C	H	N	O	S	0	0
			5959	1988	2851	542	570	8		
1	J	169	Total	C	H	N	O	S	0	0
			2827	902	1418	253	250	4		
1	K	384	Total	C	H	N	O	S	0	0
			5948	1985	2846	541	568	8		
1	L	168	Total	C	H	N	O	S	0	0
			2806	893	1409	252	248	4		

- Molecule 2 is a protein called HerA.

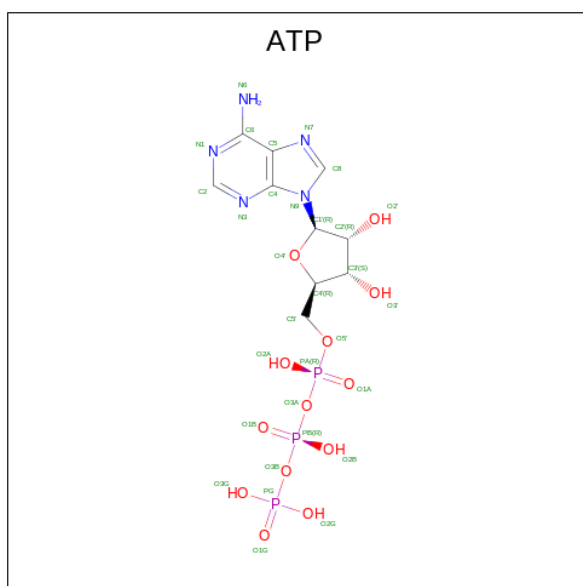
Mol	Chain	Residues	Atoms						AltConf	Trace
2	M	546	Total	C	H	N	O	S	0	0
			8430	2709	4189	713	806	13		
2	N	531	Total	C	H	N	O	S	0	0
			8172	2619	4065	694	781	13		
2	O	543	Total	C	H	N	O	S	0	0
			8390	2697	4168	710	802	13		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	P	553	Total	C	H	N	O	S	0	0
			8479	2719	4211	724	812	13		
2	Q	546	Total	C	H	N	O	S	0	0
			8401	2703	4168	708	809	13		
2	R	543	Total	C	H	N	O	S	0	0
			8333	2675	4137	707	801	13		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).

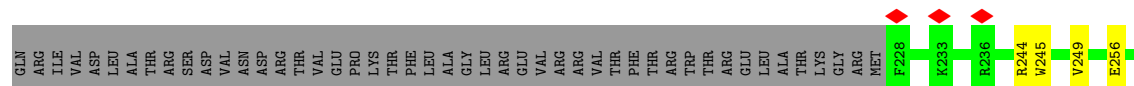
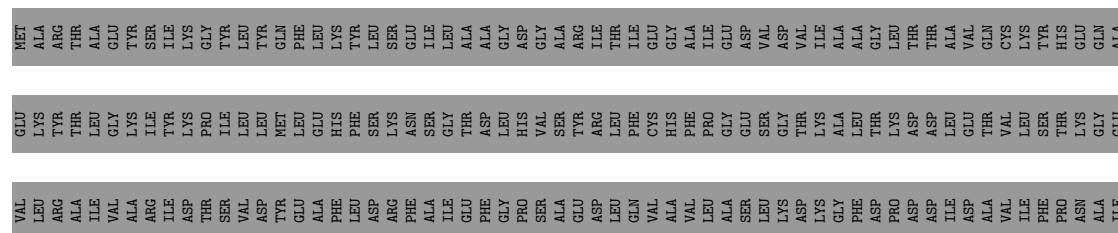




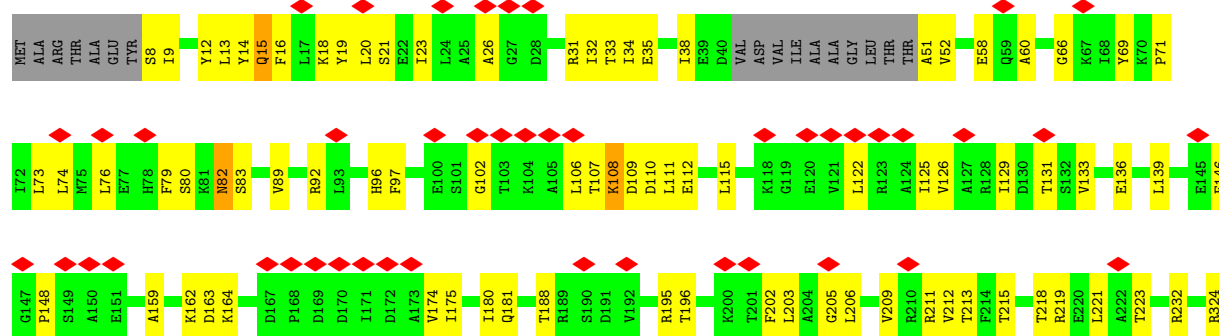
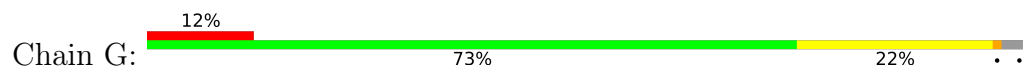




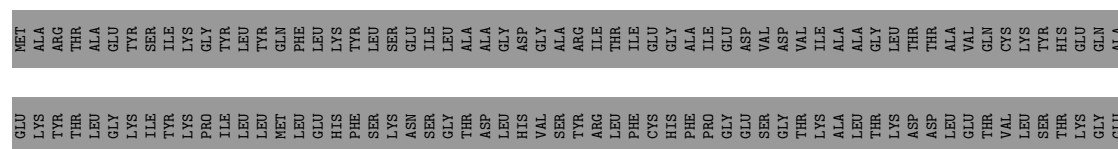
• Molecule 1: DUF4297



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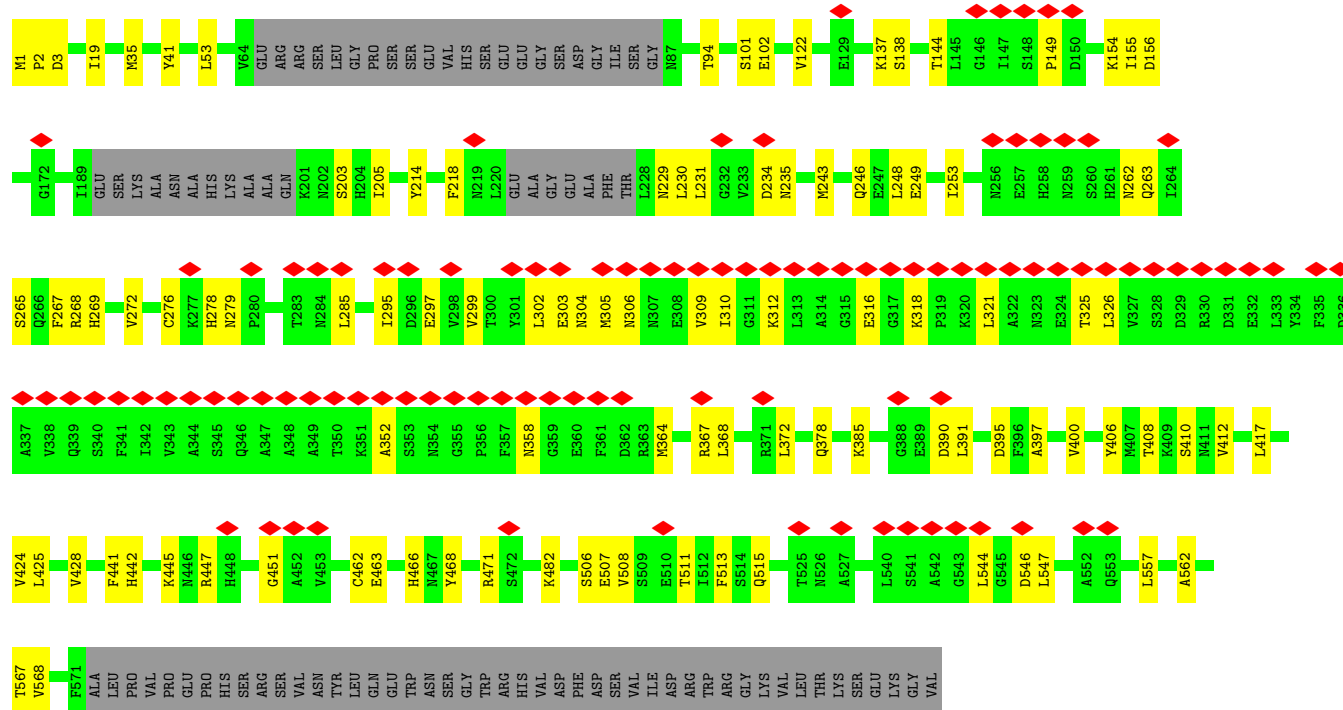




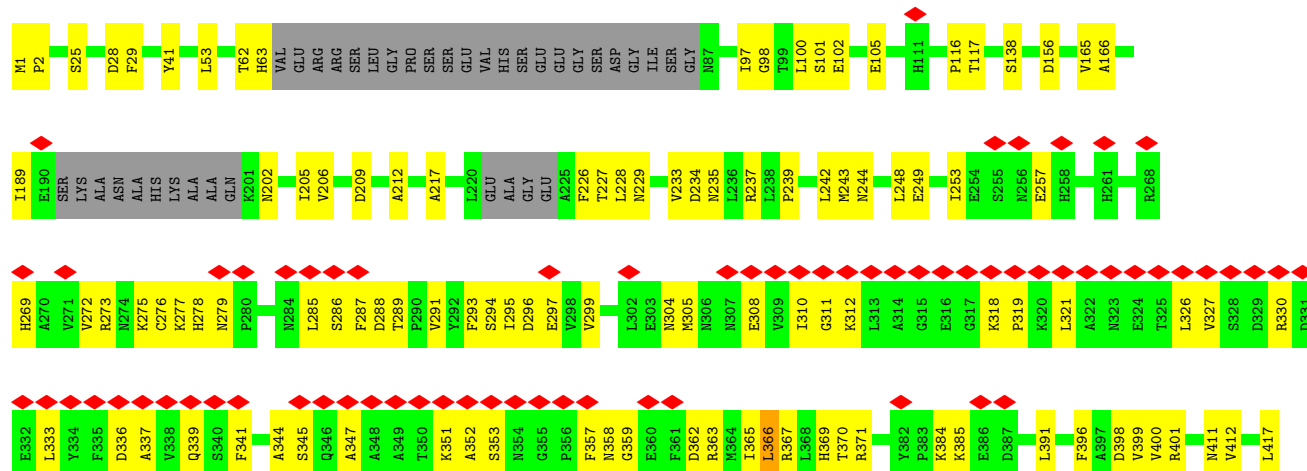


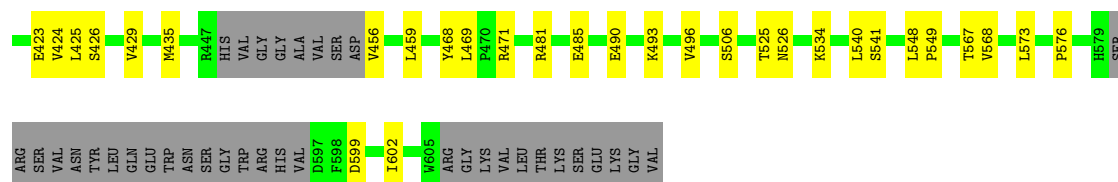


- Molecule 2: HerA

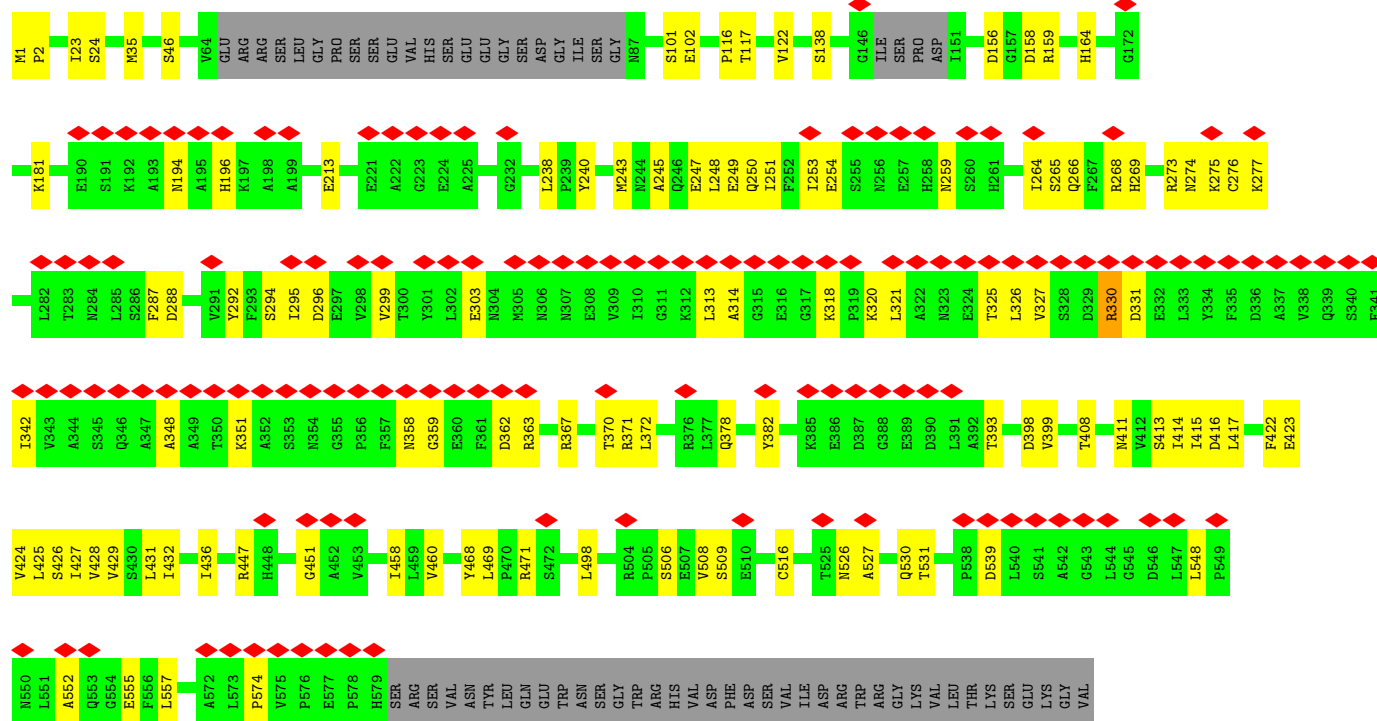


- Molecule 2: HerA

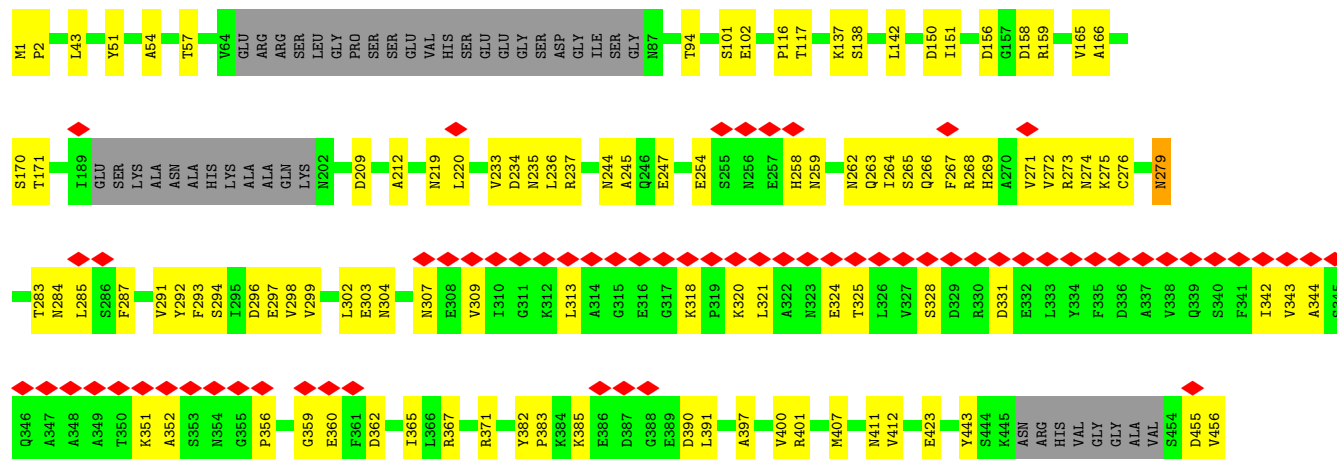


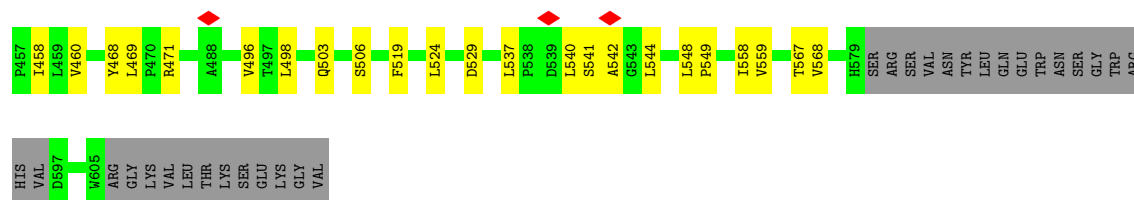


• Molecule 2: HerA

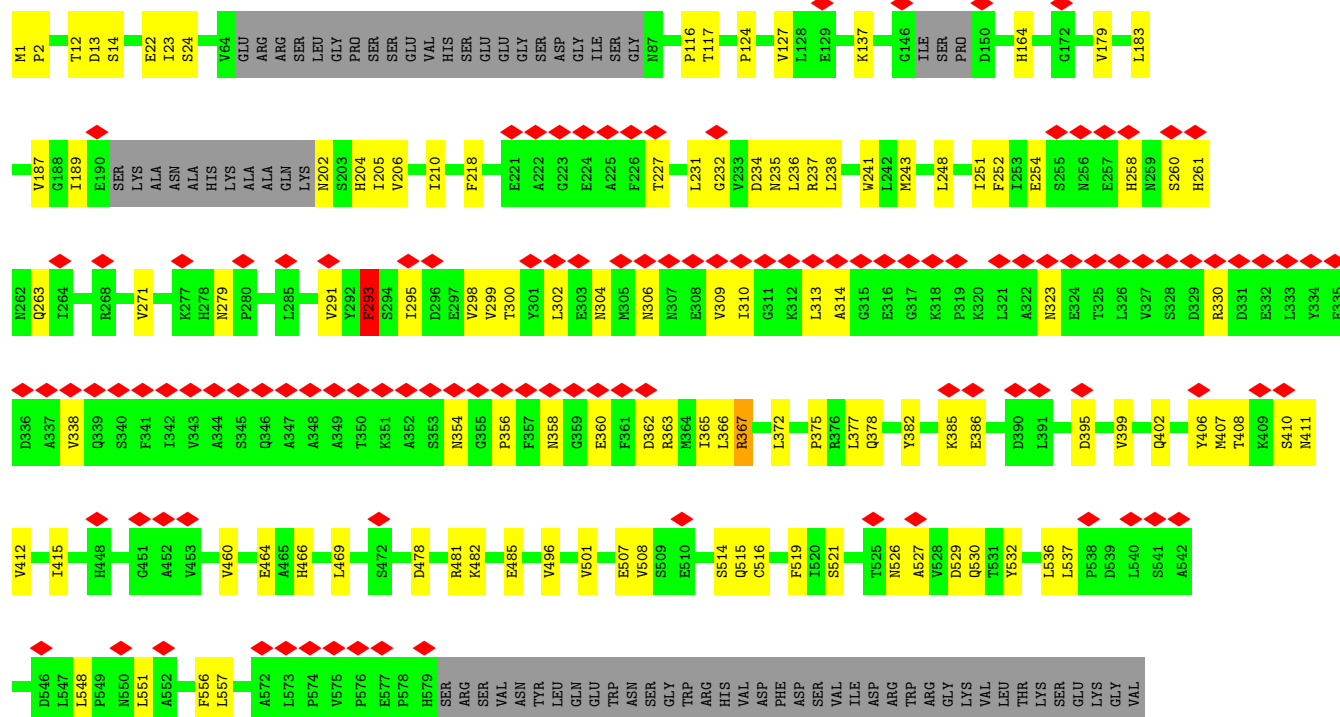


• Molecule 2: HerA





• Molecule 2: HerA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	158570	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	65.58	Depositor
Minimum defocus (nm)	328	Depositor
Maximum defocus (nm)	5899	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.780	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.05	Depositor
Map size ( $\text{\AA}$ )	484.0, 484.0, 484.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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: ATP, MG

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	0.51	0/3196	0.52	0/4316
1	B	0.65	0/1419	0.52	0/1912
1	C	0.52	0/3172	0.56	2/4280 (0.0%)
1	D	0.65	0/1440	0.55	0/1941
1	E	0.52	0/3179	0.51	0/4292
1	F	0.66	0/1419	0.53	0/1912
1	G	0.52	0/3136	0.58	3/4232 (0.1%)
1	H	0.65	0/1427	0.54	0/1923
1	I	0.52	0/3169	0.53	0/4279
1	J	0.65	0/1440	0.54	1/1941 (0.1%)
1	K	0.52	0/3163	0.54	0/4272
1	L	0.67	0/1427	0.54	0/1923
2	M	0.50	0/4331	0.51	1/5875 (0.0%)
2	N	0.46	0/4192	0.52	0/5684
2	O	0.49	0/4312	0.51	0/5848
2	P	0.44	0/4359	0.53	2/5913 (0.0%)
2	Q	0.49	0/4324	0.50	0/5868
2	R	0.45	0/4285	0.54	2/5814 (0.0%)
All	All	0.52	0/53390	0.53	11/72225 (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
1	E	0	1
1	I	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	330	ARG	NE-CZ-NH2	-8.52	116.04	120.30
2	R	293	PHE	CB-CG-CD1	-6.50	116.25	120.80
2	P	330	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	G	79	PHE	CB-CG-CD2	-6.26	116.42	120.80
2	R	293	PHE	CB-CG-CD2	5.93	124.95	120.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	113	THR	Peptide
1	I	47	GLY	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	3134	2851	3150	66	0
1	B	1389	1400	1404	8	0
1	C	3112	2890	3128	76	0
1	D	1409	1418	1417	10	0
1	E	3118	2859	3138	82	0
1	F	1389	1405	1404	11	0
1	G	3075	2856	3089	63	0
1	H	1397	1409	1408	8	0
1	I	3108	2851	3130	80	0
1	J	1409	1418	1417	14	0
1	K	3102	2846	3125	81	0
1	L	1397	1409	1408	18	0
2	M	4241	4189	4201	87	0
2	N	4107	4065	4082	73	0
2	O	4222	4168	4181	94	0
2	P	4268	4211	4234	77	0
2	Q	4233	4168	4181	88	0
2	R	4196	4137	4152	82	0
3	M	31	12	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	31	12	12	1	0
3	Q	31	12	12	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
4	Q	1	0	0	0	0
All	All	52402	50586	52285	1007	0

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

The worst 5 of 1007 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:G:107:THR:OG1	1:G:109:ASP:OD2	1.80	0.97
1:K:38:ILE:HB	1:K:51:ALA:HB1	1.44	0.96
1:A:14:TYR:OH	1:A:148:PRO:O	1.84	0.95
1:B:322:LEU:O	1:B:340:ARG:NH1	2.00	0.95
1:I:117:THR:O	1:I:123:ARG:NH1	2.00	0.94

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	384/397 (97%)	364 (95%)	20 (5%)	0	100	100
1	B	165/397 (42%)	161 (98%)	4 (2%)	0	100	100
1	C	380/397 (96%)	358 (94%)	22 (6%)	0	100	100
1	D	167/397 (42%)	160 (96%)	7 (4%)	0	100	100
1	E	383/397 (96%)	372 (97%)	10 (3%)	1 (0%)	37	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	165/397 (42%)	158 (96%)	7 (4%)	0	100	100
1	G	376/397 (95%)	360 (96%)	16 (4%)	0	100	100
1	H	166/397 (42%)	157 (95%)	9 (5%)	0	100	100
1	I	381/397 (96%)	363 (95%)	17 (4%)	1 (0%)	37	66
1	J	167/397 (42%)	160 (96%)	7 (4%)	0	100	100
1	K	380/397 (96%)	365 (96%)	15 (4%)	0	100	100
1	L	166/397 (42%)	161 (97%)	5 (3%)	0	100	100
2	M	534/617 (86%)	506 (95%)	28 (5%)	0	100	100
2	N	523/617 (85%)	500 (96%)	23 (4%)	0	100	100
2	O	531/617 (86%)	505 (95%)	26 (5%)	0	100	100
2	P	547/617 (89%)	518 (95%)	29 (5%)	0	100	100
2	Q	536/617 (87%)	508 (95%)	28 (5%)	0	100	100
2	R	535/617 (87%)	512 (96%)	22 (4%)	1 (0%)	44	72
All	All	6486/8466 (77%)	6188 (95%)	295 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	46	ALA
1	E	114	VAL
2	R	356	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	337/346 (97%)	337 (100%)	0	100	100
1	B	154/346 (44%)	154 (100%)	0	100	100
1	C	334/346 (96%)	330 (99%)	4 (1%)	67	82
1	D	156/346 (45%)	156 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	336/346 (97%)	335 (100%)	1 (0%)	91	94
1	F	154/346 (44%)	154 (100%)	0	100	100
1	G	332/346 (96%)	329 (99%)	3 (1%)	75	86
1	H	155/346 (45%)	155 (100%)	0	100	100
1	I	335/346 (97%)	332 (99%)	3 (1%)	75	86
1	J	156/346 (45%)	156 (100%)	0	100	100
1	K	335/346 (97%)	335 (100%)	0	100	100
1	L	155/346 (45%)	153 (99%)	2 (1%)	65	80
2	M	470/525 (90%)	469 (100%)	1 (0%)	92	96
2	N	454/525 (86%)	453 (100%)	1 (0%)	92	96
2	O	467/525 (89%)	465 (100%)	2 (0%)	89	93
2	P	468/525 (89%)	468 (100%)	0	100	100
2	Q	468/525 (89%)	466 (100%)	2 (0%)	89	93
2	R	462/525 (88%)	460 (100%)	2 (0%)	89	93
All	All	5728/7302 (78%)	5707 (100%)	21 (0%)	88	93

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	482	LYS
2	Q	279	ASN
2	R	367	ARG
2	Q	313	LEU
2	O	384	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
2	P	442	HIS
2	R	262	ASN
2	P	570	HIS
2	Q	503	GLN
2	R	284	ASN

### 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 6 ligands modelled in this entry, 3 are 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$
3	ATP	O	1501	4	26,33,33	0.98	2 (7%)	31,52,52	1.51	4 (12%)
3	ATP	Q	1501	4	26,33,33	0.95	2 (7%)	31,52,52	1.54	5 (16%)
3	ATP	M	1501	-	26,33,33	0.96	2 (7%)	31,52,52	1.66	6 (19%)

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
3	ATP	O	1501	4	-	3/18/38/38	0/3/3/3
3	ATP	Q	1501	4	-	5/18/38/38	0/3/3/3
3	ATP	M	1501	-	-	7/18/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	1501	ATP	C5-C4	2.33	1.47	1.40
3	Q	1501	ATP	C5-C4	2.32	1.47	1.40
3	O	1501	ATP	C5-C4	2.29	1.47	1.40
3	O	1501	ATP	O4'-C1'	2.22	1.44	1.41
3	M	1501	ATP	O4'-C1'	2.04	1.43	1.41

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	1501	ATP	PB-O3B-PG	-4.17	118.50	132.83
3	O	1501	ATP	PB-O3B-PG	-3.89	119.46	132.83
3	Q	1501	ATP	PB-O3B-PG	-3.64	120.34	132.83
3	O	1501	ATP	N3-C2-N1	-3.63	123.00	128.68
3	Q	1501	ATP	PA-O3A-PB	-3.61	120.43	132.83

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	1501	ATP	C5'-O5'-PA-O3A
3	M	1501	ATP	C4'-C5'-O5'-PA
3	O	1501	ATP	C5'-O5'-PA-O2A
3	O	1501	ATP	C5'-O5'-PA-O3A
3	Q	1501	ATP	C5'-O5'-PA-O3A

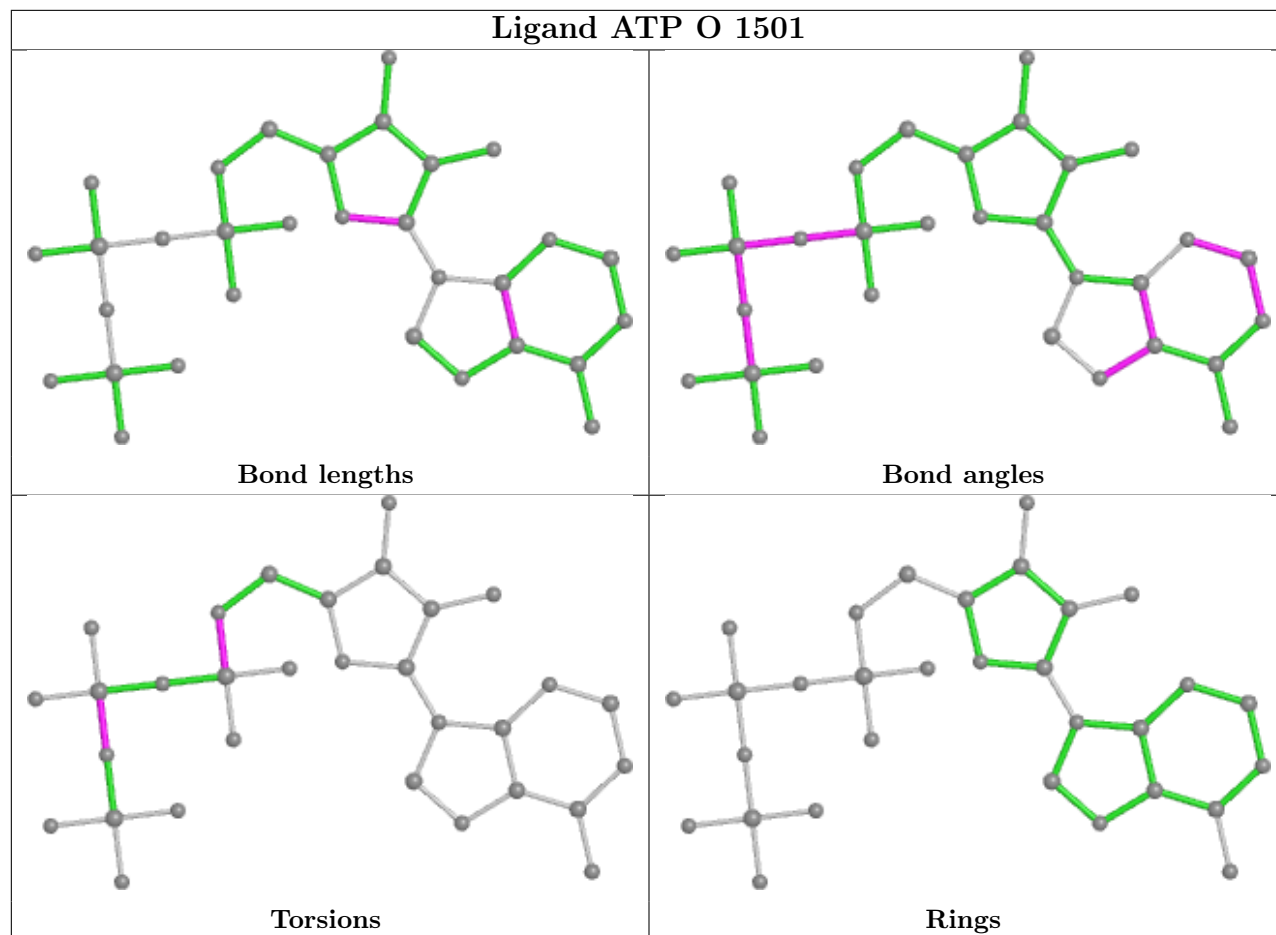
There are no ring outliers.

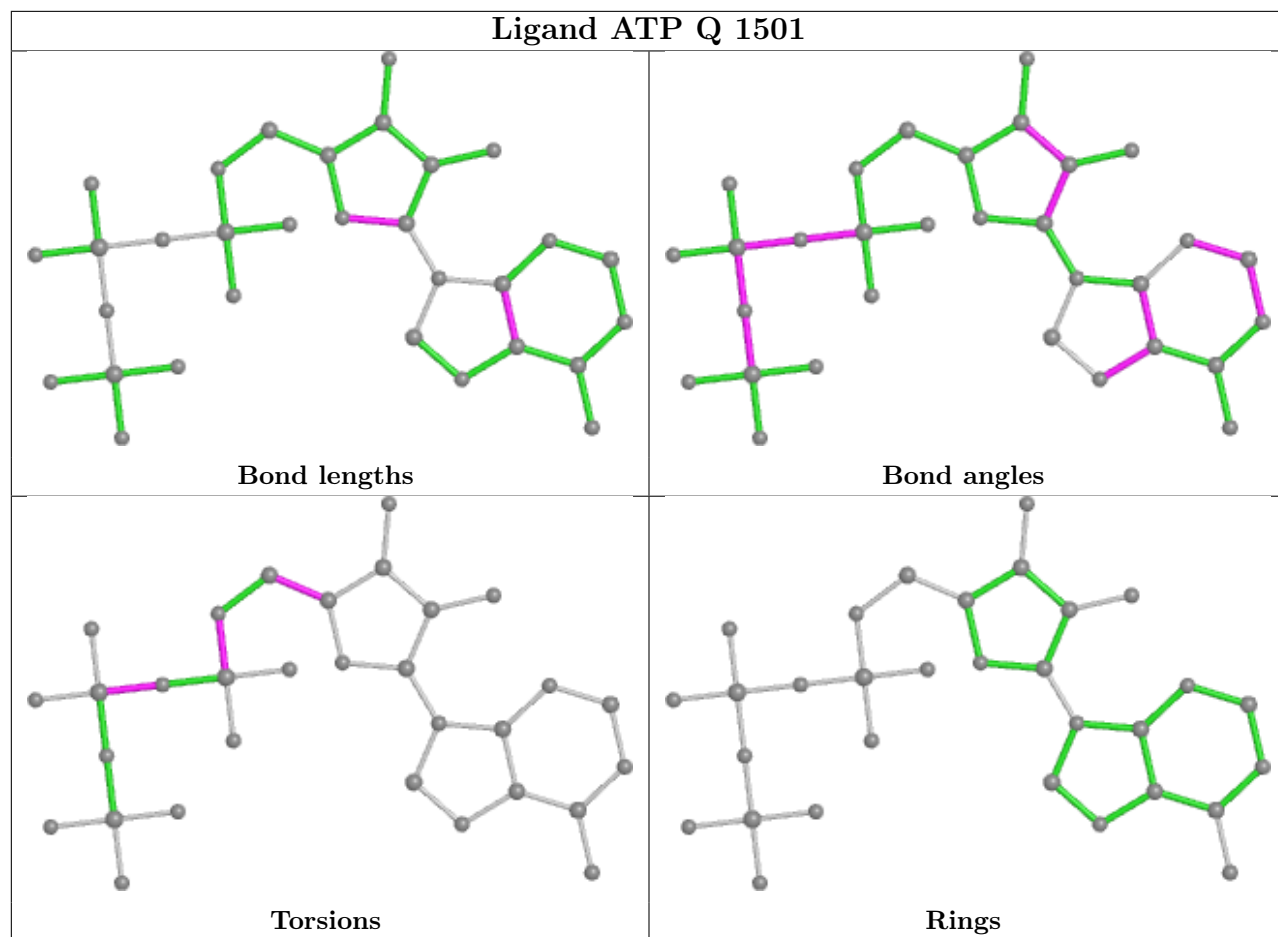
2 monomers are involved in 3 short contacts:

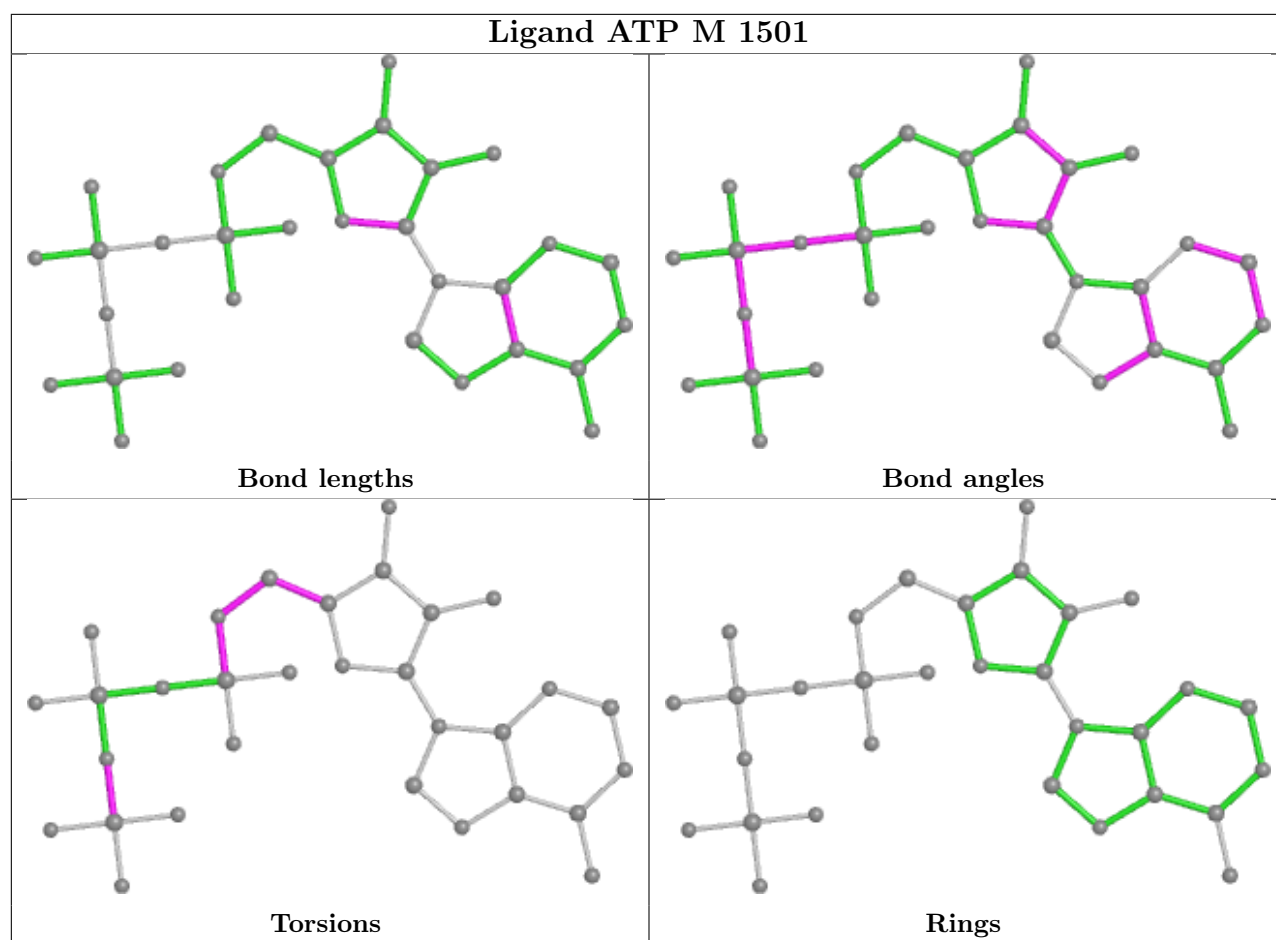
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	1501	ATP	1	0
3	M	1501	ATP	2	0

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.



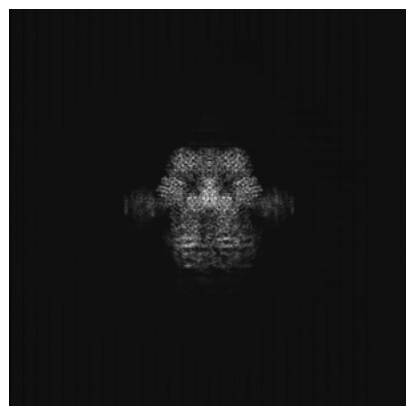
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60127. These allow visual inspection of the internal detail of the map and identification of artifacts.

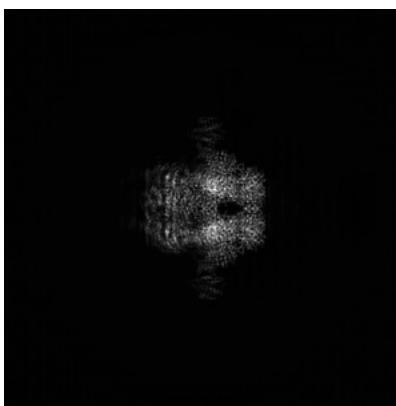
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

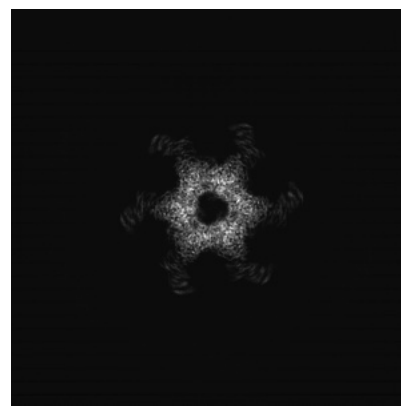
#### 6.1.1 Primary map



X

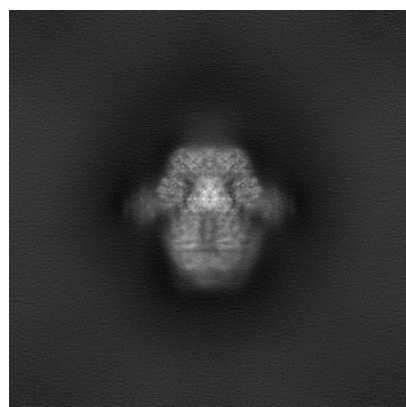


Y

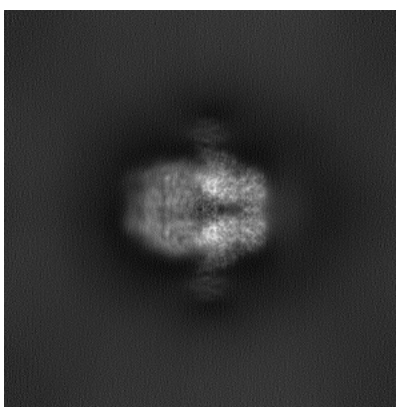


Z

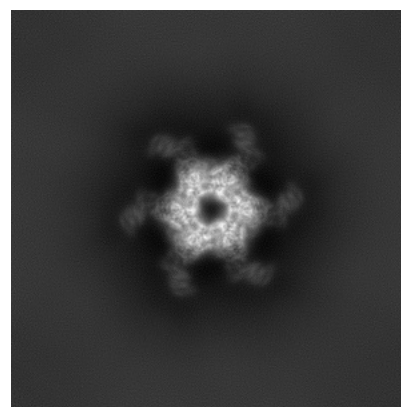
#### 6.1.2 Raw map



X



Y

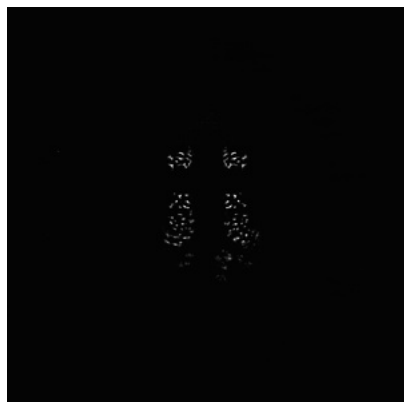


Z

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

## 6.2 Central slices [i](#)

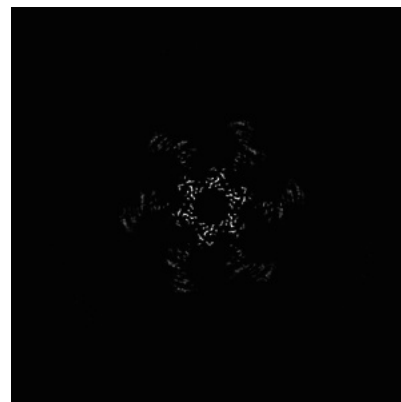
### 6.2.1 Primary map



X Index: 220

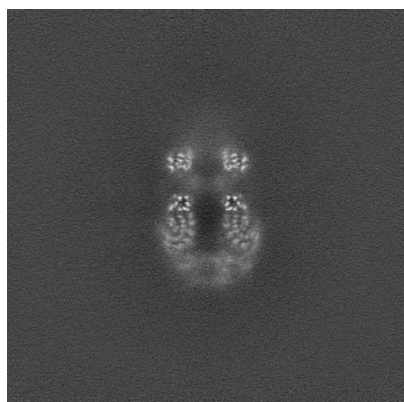


Y Index: 220

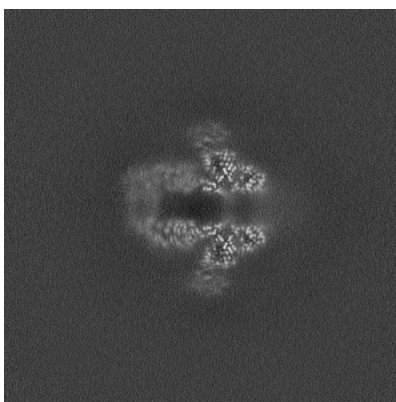


Z Index: 220

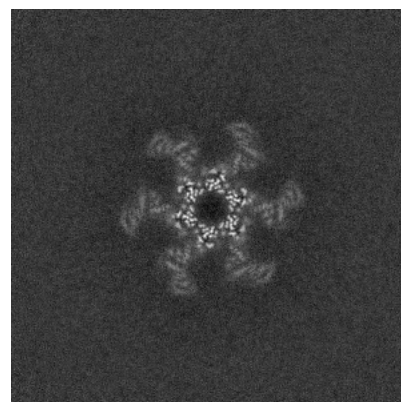
### 6.2.2 Raw map



X Index: 220



Y Index: 220

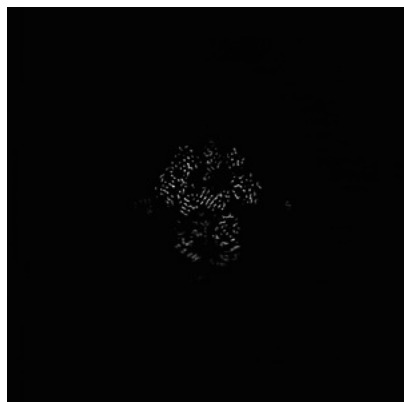


Z Index: 220

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

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

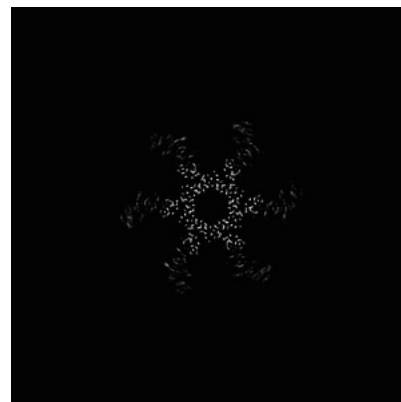
### 6.3.1 Primary map



X Index: 241

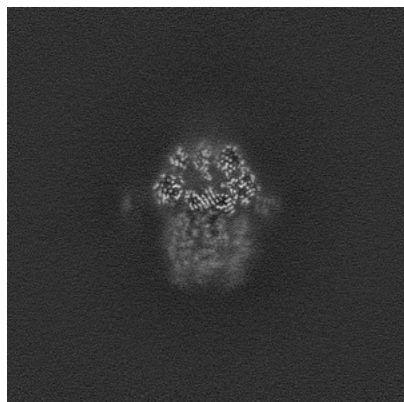


Y Index: 250

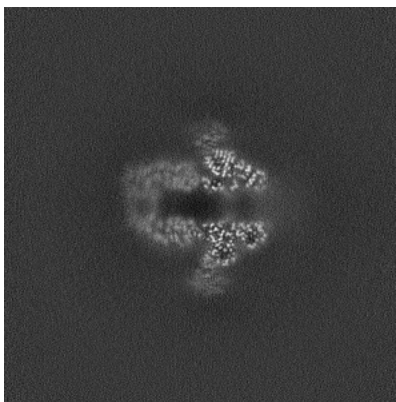


Z Index: 231

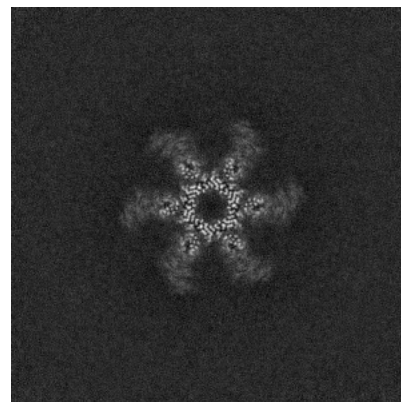
### 6.3.2 Raw map



X Index: 199



Y Index: 218

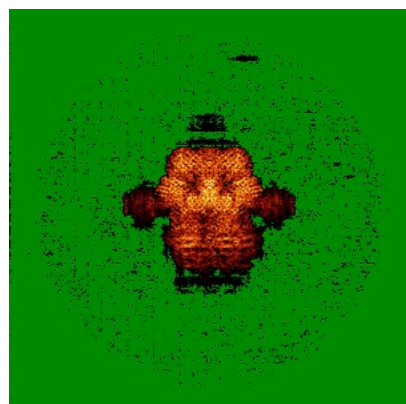


Z Index: 232

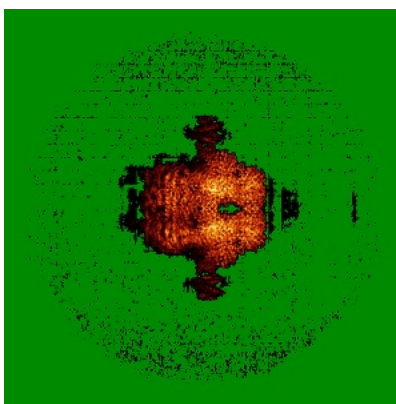
The images above show the largest variance slices of the map in three orthogonal directions.

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

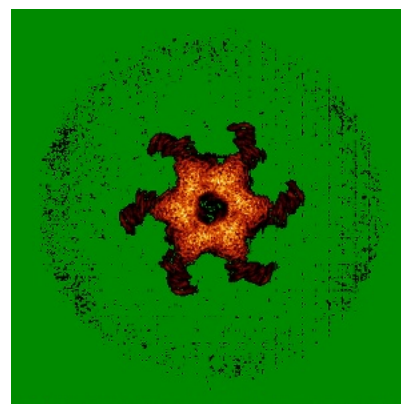
### 6.4.1 Primary map



X

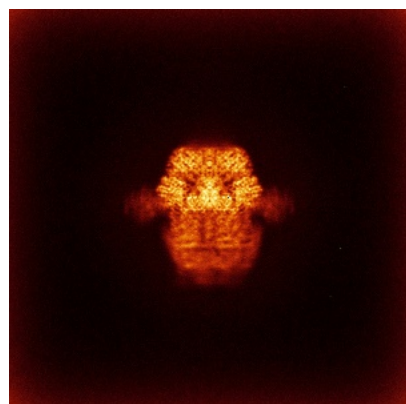


Y

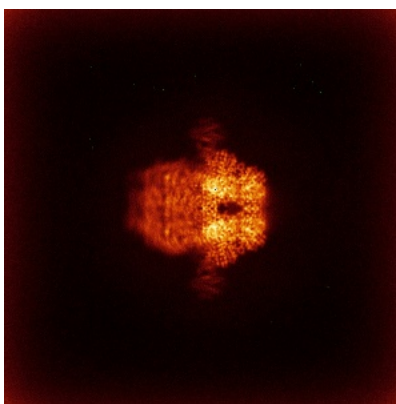


Z

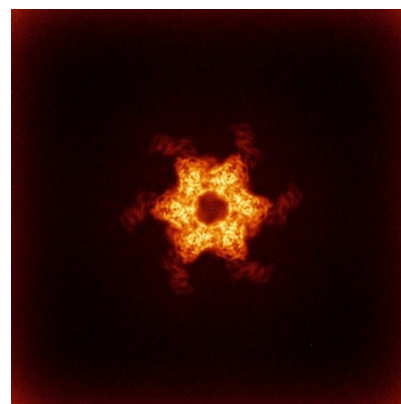
### 6.4.2 Raw map



X



Y

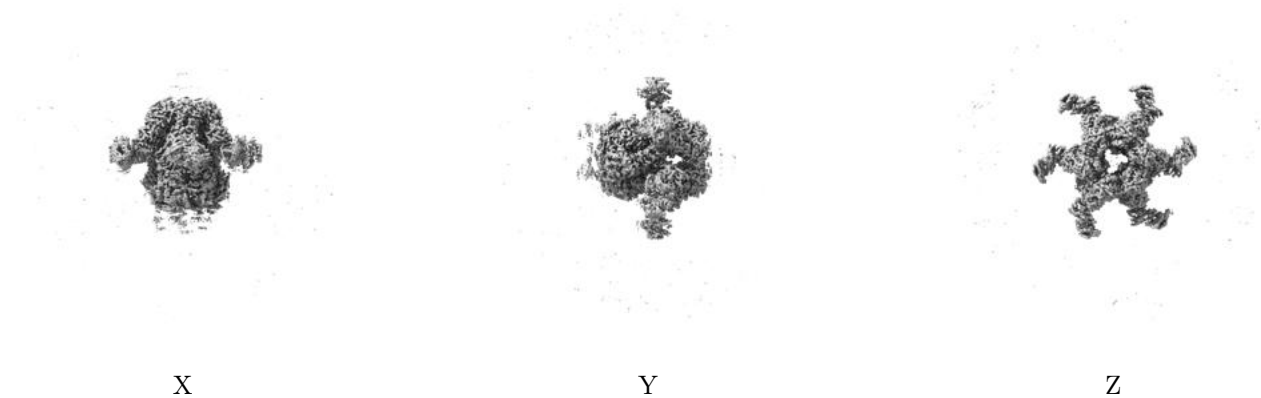


Z

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.

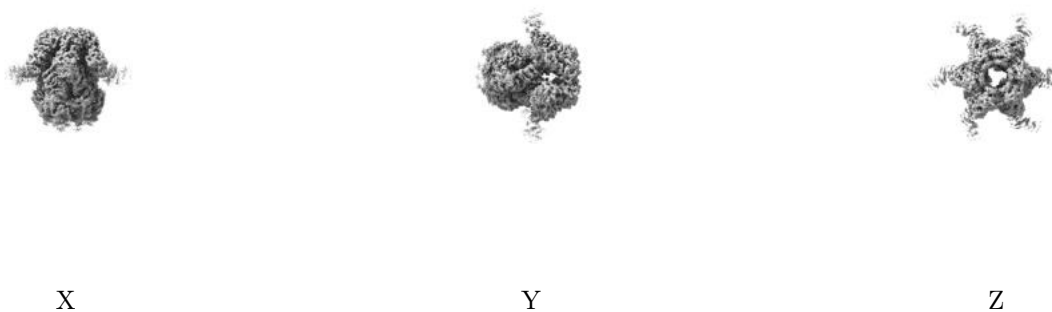
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

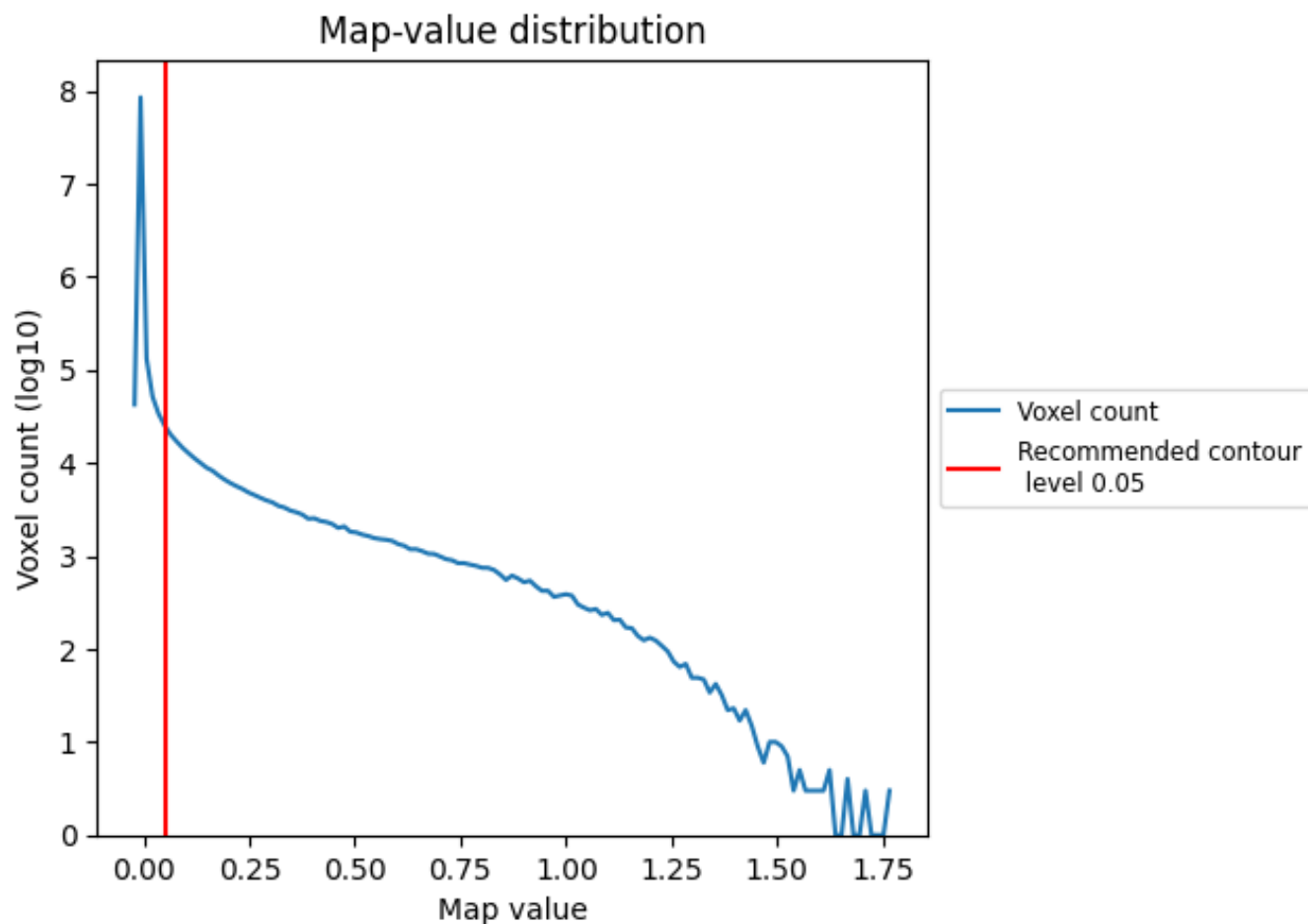
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

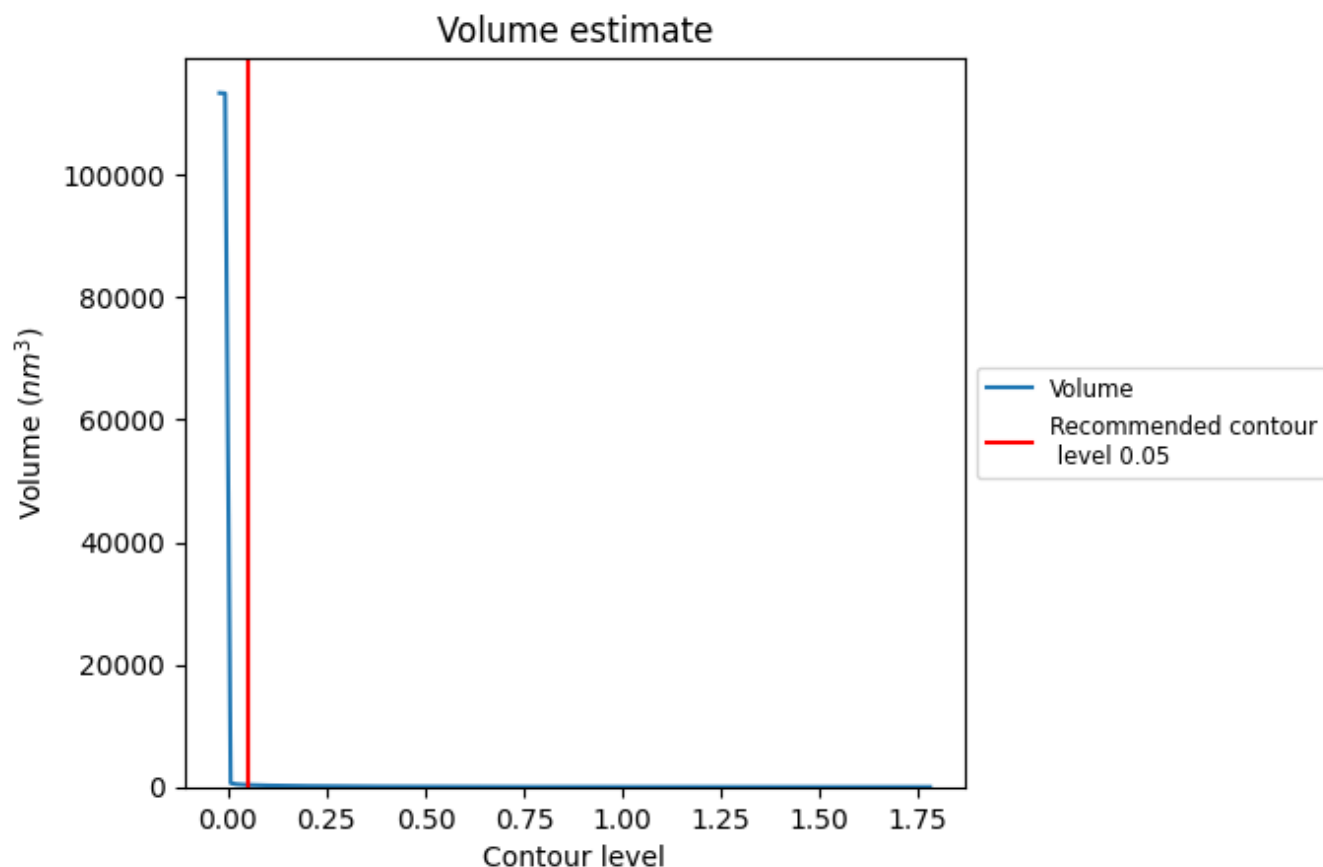
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)

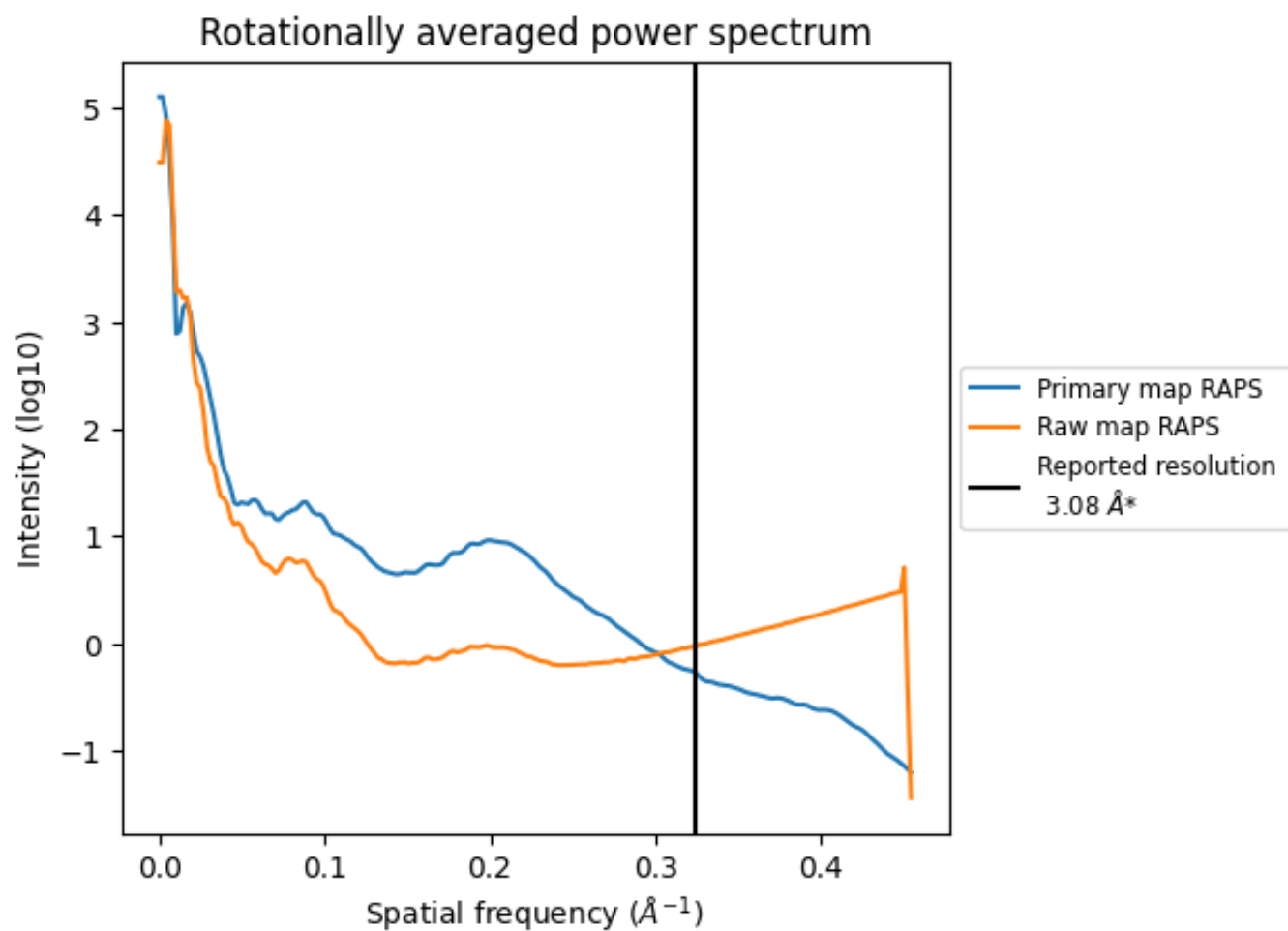


The volume at the recommended contour level is 332  $\text{nm}^3$ ; this corresponds to an approximate mass of 300 kDa.

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 ⓘ



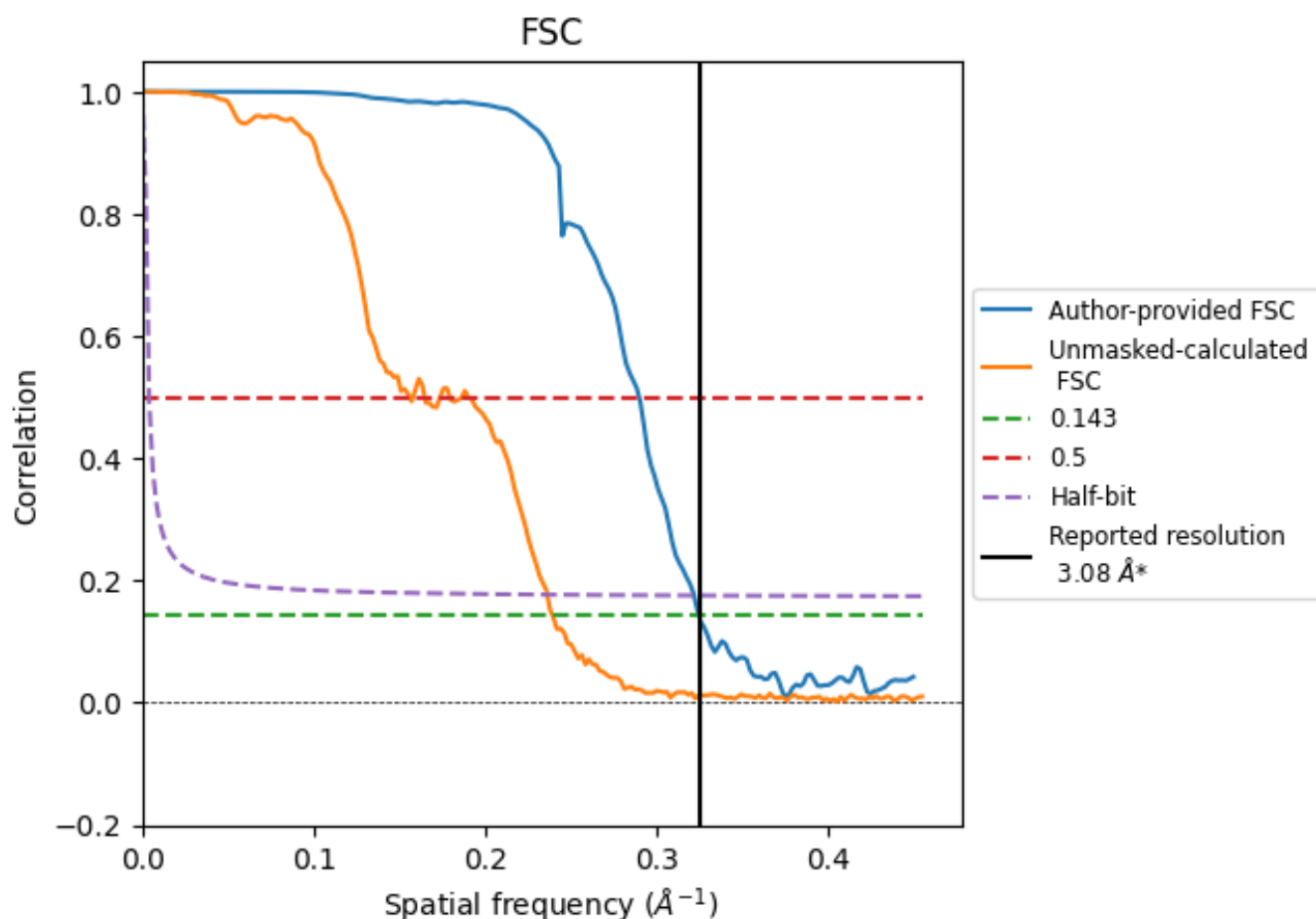
\*Reported resolution corresponds to spatial frequency of  $0.325 \text{ \AA}^{-1}$



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

## 8.2 Resolution estimates [i](#)

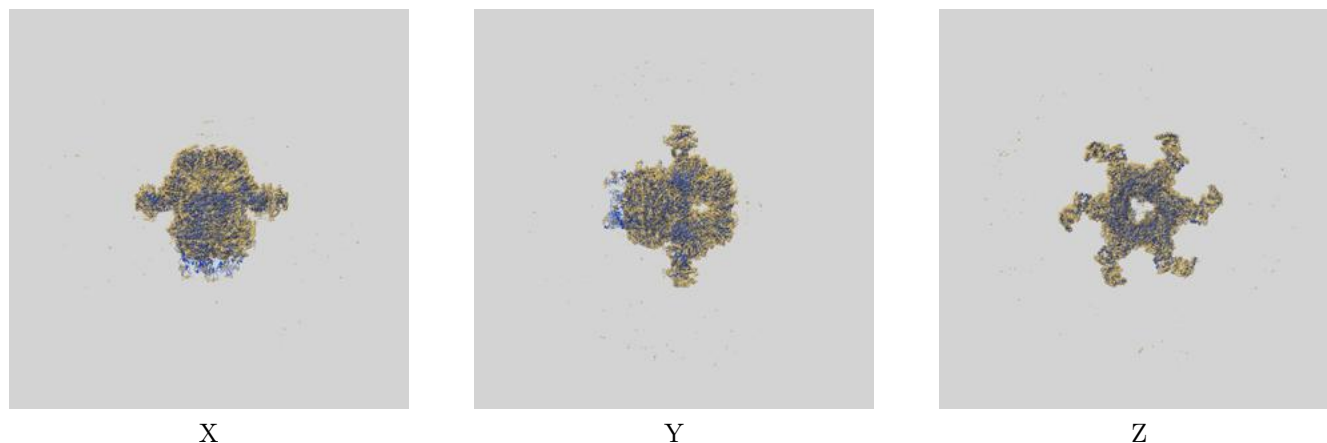
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	3.08	3.45	3.11
Unmasked-calculated*	4.18	6.42	4.24

\*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 4.18 differs from the reported value 3.08 by more than 10 %

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

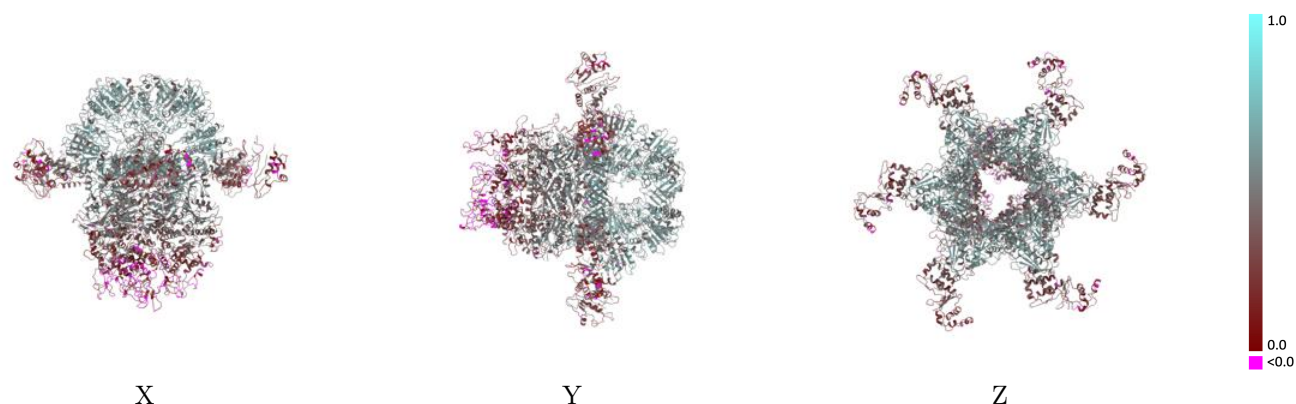
This section contains information regarding the fit between EMDB map EMD-60127 and PDB model 8ZIR. Per-residue inclusion information can be found in section [3](#) on page [6](#).

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



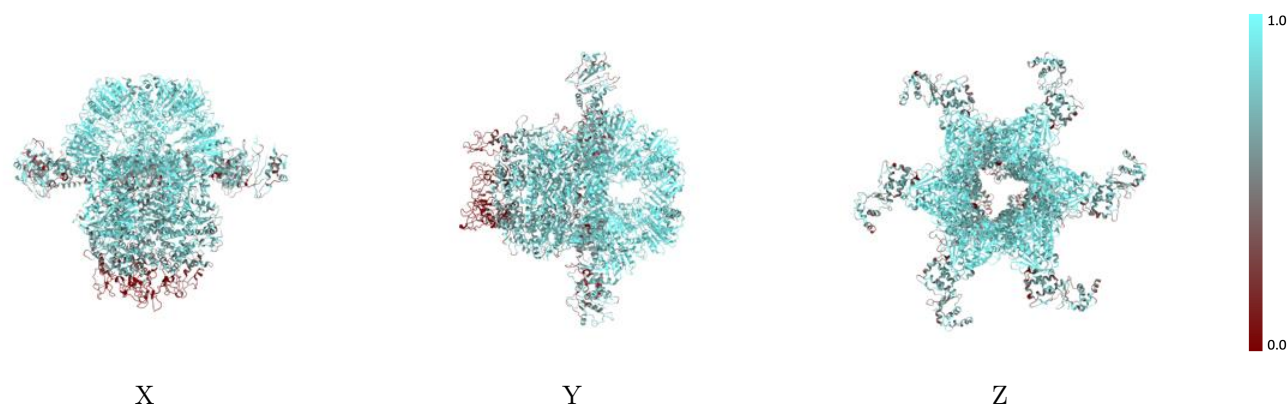
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



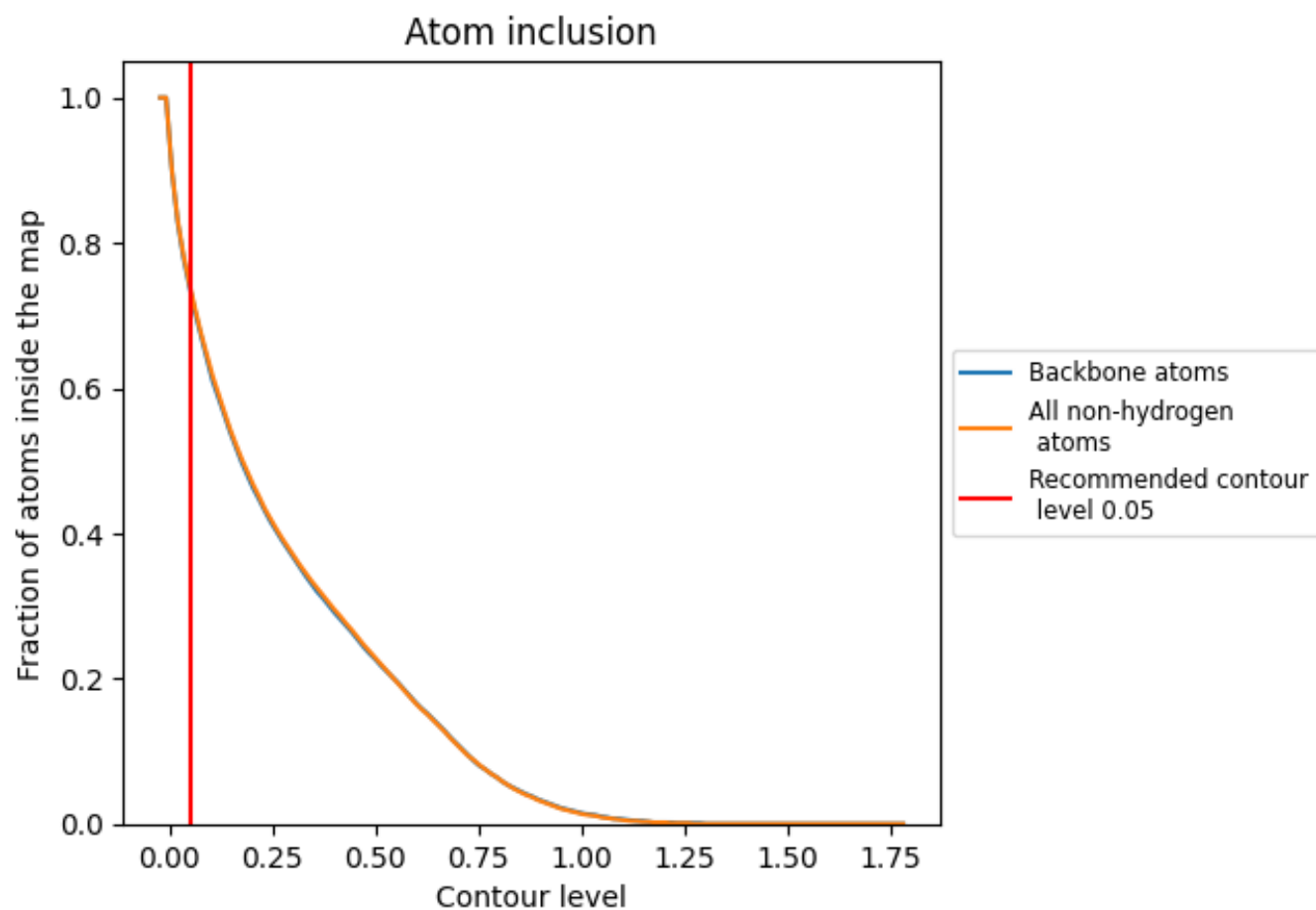
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 74% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7410	 0.4110
A	 0.7450	 0.4090
B	 0.8950	 0.5380
C	 0.7570	 0.4100
D	 0.8940	 0.5360
E	 0.7430	 0.4090
F	 0.8890	 0.5340
G	 0.7530	 0.4150
H	 0.9010	 0.5390
I	 0.7450	 0.4040
J	 0.8850	 0.5250
K	 0.7340	 0.4060
L	 0.8920	 0.5290
M	 0.7590	 0.3960
N	 0.6770	 0.3560
O	 0.7590	 0.3930
P	 0.6490	 0.3480
Q	 0.7470	 0.3850
R	 0.6710	 0.3530

