



wwPDB EM Validation Summary Report ⓘ

Aug 17, 2024 – 05:36 PM EDT

PDB ID : 8V48
EMDB ID : EMD-42968
Title : CryoEM structure of AriA-AriB complex (Form III)
Authors : Deep, A.; Corbett, K.D.
Deposited on : 2023-11-28
Resolution : 3.68 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:

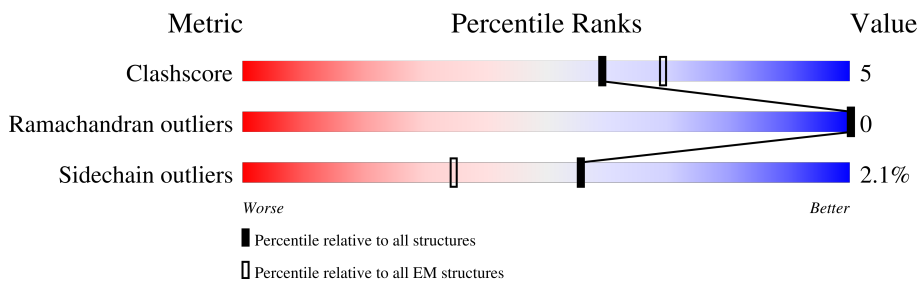
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

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 3.68 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	464	81% 8% 11%
1	B	464	78% 8% 14%
1	C	464	76% 12% 12%
1	F	464	74% 14% 12%
1	H	464	45% 17% 36%
1	K	464	49% 14% 36%
2	D	308	91% 8%
2	G	308	89% 10%

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Mol	Chain	Length	Quality of chain
2	J	308	 <p>85% 90% 9%</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 25334 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 AriA antitoxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	412	3320	2117	561	630	12	0	0
1	B	400	3218	2056	539	611	12	0	0
1	C	410	3301	2102	559	628	12	0	0
1	F	410	3301	2102	559	628	12	0	0
1	H	297	2371	1519	395	446	11	0	0
1	K	297	2371	1519	395	446	11	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	-	expression tag	UNP D6IC77
A	393	GLN	GLU	engineered mutation	UNP D6IC77
B	1	VAL	-	expression tag	UNP D6IC77
B	393	GLN	GLU	engineered mutation	UNP D6IC77
C	1	VAL	-	expression tag	UNP D6IC77
C	393	GLN	GLU	engineered mutation	UNP D6IC77
F	1	VAL	-	expression tag	UNP D6IC77
F	393	GLN	GLU	engineered mutation	UNP D6IC77
H	1	VAL	-	expression tag	UNP D6IC77
H	393	GLN	GLU	engineered mutation	UNP D6IC77
K	1	VAL	-	expression tag	UNP D6IC77
K	393	GLN	GLU	engineered mutation	UNP D6IC77

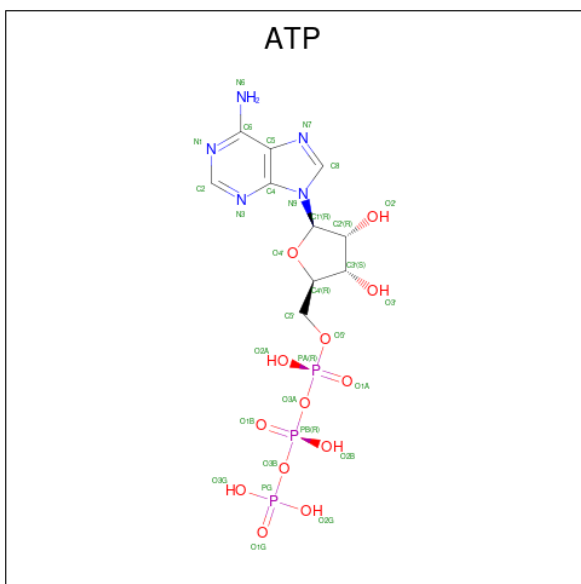
- Molecule 2 is a protein called AriB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	305	Total	C	N	O	S	0	0
			2422	1553	399	461	9		
2	G	305	Total	C	N	O	S	0	0
			2422	1553	399	461	9		
2	J	305	Total	C	N	O	S	0	0
			2422	1553	399	461	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	90	ALA	GLU	engineered mutation	UNP D6IC76
G	90	ALA	GLU	engineered mutation	UNP D6IC76
J	90	ALA	GLU	engineered mutation	UNP D6IC76

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

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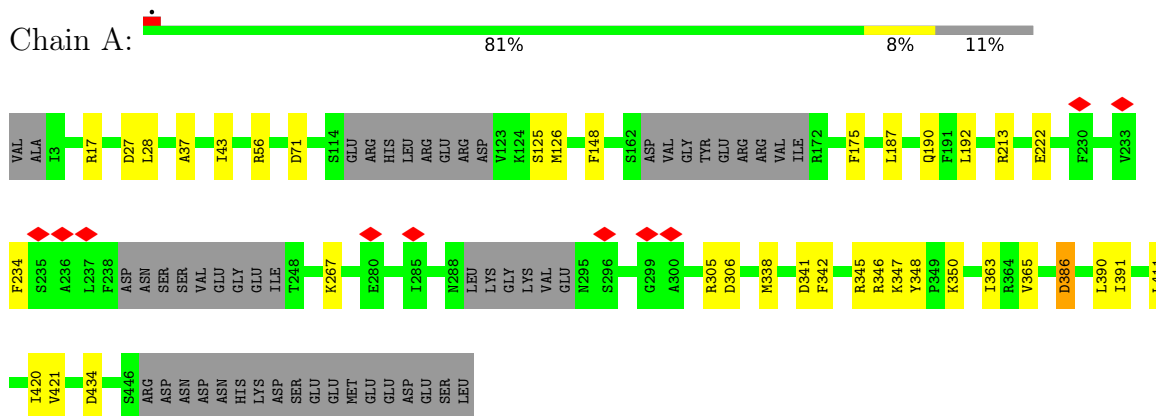
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	K	1	31	10	5	13	3	0

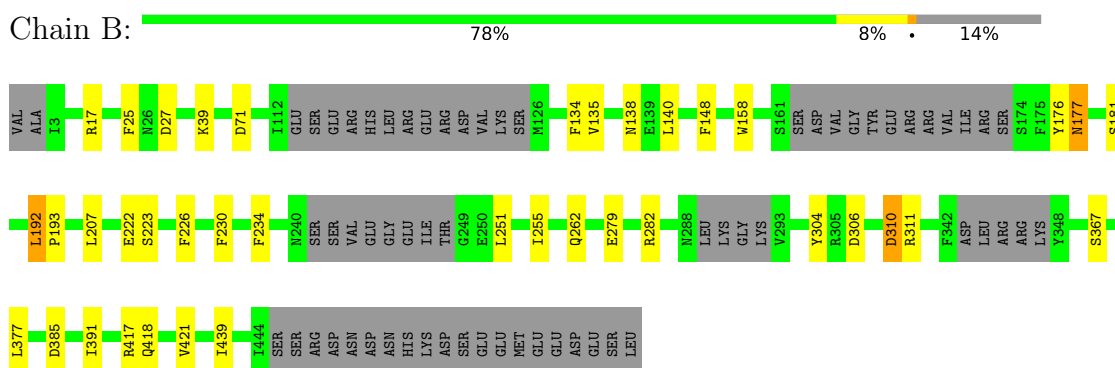
3 Residue-property plots

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

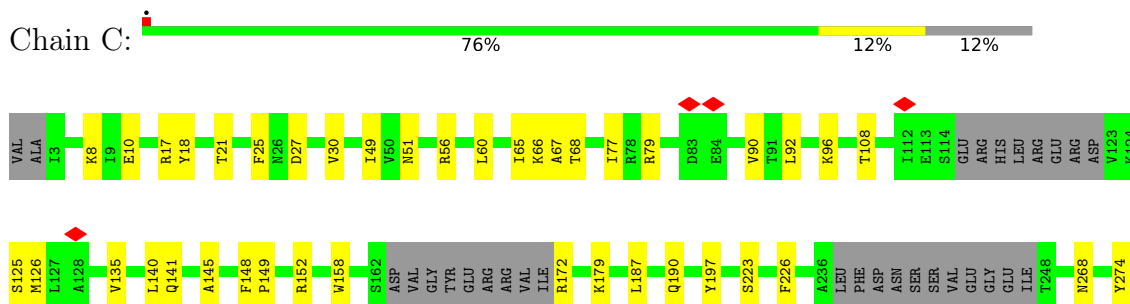
- Molecule 1: AriA antitoxin

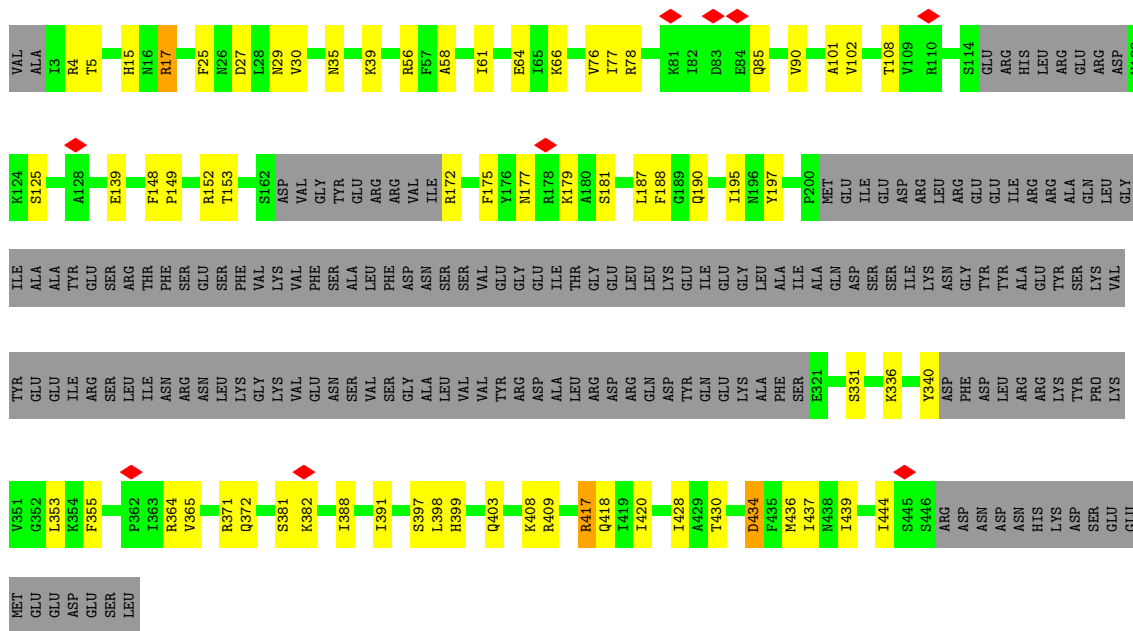


- Molecule 1: AriA antitoxin

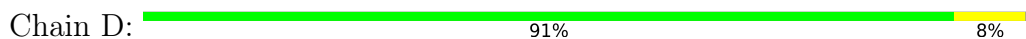


- Molecule 1: AriA antitoxin

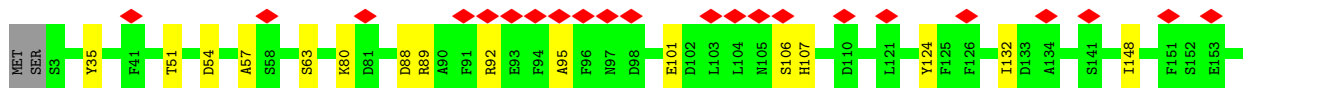
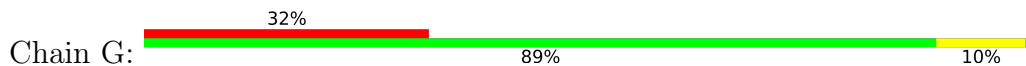




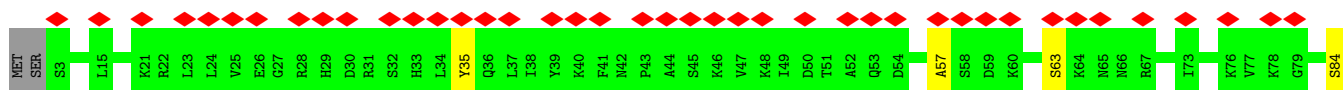
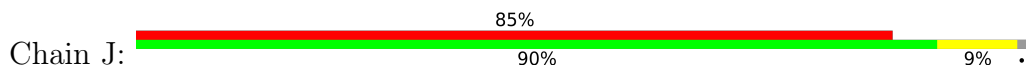
• Molecule 2: AriB



• Molecule 2: AriB



• Molecule 2: AriB



F85	L86	C87	D88	R89	A90	F91	R92	E93	F94	A95	F96	N97	D98	Q99	I100	E101	D102	L103	L104	M105	S106	H107	Y108	C109	D110	D111	S112	L113	Y114	W115	T116	L117	G118	H119	S120	L121	E122	M123	Y124	F125	F126	N127	P128	S129	I130	I131	I132	D133	A134	F135	Q136	F137	L138	S139	P140	S141	E142	Y143	K144
Y145	K146	A147	I148	E149	L150	F151	S152	E153	L154	I155	S156	S157	S158	F159	A160	V161	L162	A163	A164	V165	S166	L167	A168	A169	K170	D171	I172	D173	K174	A175	G176	L177	P178	A179	A180	L181	I182	D183	W184	K185	D186	I187	V188	I189	M190	D191	G192	T193	I194	K195	L196	I197	R198	R199	D200	S201	Y202	D203	I204
D205	S206	A207	C208	V209	D210	S211	F212	F213	N214	A215	F216	D217	A218	V219	L220	P221	R222	V223	I224	A225	S226	D227	V228	G229	I230	C231	S232	R233	V234	V235	R236	G237	H238	T239	G240	I241	L242	L243	L244	Q245	K246	L247	F248	S249	A250	C251	L252	Y253	Y254	V255	G256	R257	E258	D259	D260	A261	L262	Q263	A264
D265	S266	S267	A268	N269	Y270	F271	C272	N273	L274	S275	E276	L277	S278	L279	T280	T281	A282	L283	A284	E285	S286	W287	V288	R289	K290	I291	G292	V293	L294	E295	D296	V297	Y298	F299	P300	D301	S302	L303	L304	K305	N306	I307	GLU																

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24138	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.556	Depositor
Minimum map value	-0.250	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.06	Depositor
Map size (\AA)	359.04, 359.04, 359.04	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.935, 0.935, 0.935	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: ATP

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	0.44	0/3379	0.56	0/4543
1	B	0.45	0/3273	0.55	0/4403
1	C	0.32	0/3359	0.53	0/4516
1	F	0.28	0/3359	0.50	0/4516
1	H	0.28	0/2415	0.49	0/3250
1	K	0.27	0/2415	0.49	0/3250
2	D	0.38	0/2470	0.56	0/3342
2	G	0.29	0/2470	0.54	0/3342
2	J	0.28	0/2470	0.54	0/3342
All	All	0.35	0/25610	0.53	0/34504

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3320	0	3306	19	0
1	B	3218	0	3186	23	0
1	C	3301	0	3286	35	0
1	F	3301	0	3286	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2371	0	2369	51	0
1	K	2371	0	2369	41	0
2	D	2422	0	2412	13	0
2	G	2422	0	2412	17	0
2	J	2422	0	2412	14	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
3	C	31	0	12	0	0
3	F	31	0	12	0	0
3	H	31	0	12	1	0
3	K	31	0	12	2	0
All	All	25334	0	25110	244	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 5.

The worst 5 of 244 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)
2:D:95:ALA:HB3	2:D:101:GLU:HB3	1.73	0.71
1:C:10:GLU:HB2	1:C:66:LYS:HB2	1.78	0.66
1:K:148:PHE:HB2	1:K:391:ILE:HA	1.78	0.65
1:F:8:LYS:HB3	1:F:68:THR:HB	1.78	0.65
1:F:145:ALA:HA	1:F:388:ILE:H	1.63	0.63

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	402/464 (87%)	395 (98%)	7 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	388/464 (84%)	383 (99%)	5 (1%)	0	100	100
1	C	400/464 (86%)	393 (98%)	7 (2%)	0	100	100
1	F	400/464 (86%)	394 (98%)	6 (2%)	0	100	100
1	H	287/464 (62%)	273 (95%)	14 (5%)	0	100	100
1	K	287/464 (62%)	273 (95%)	14 (5%)	0	100	100
2	D	303/308 (98%)	293 (97%)	10 (3%)	0	100	100
2	G	303/308 (98%)	293 (97%)	10 (3%)	0	100	100
2	J	303/308 (98%)	294 (97%)	9 (3%)	0	100	100
All	All	3073/3708 (83%)	2991 (97%)	82 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	364/412 (88%)	354 (97%)	10 (3%)	44	68
1	B	350/412 (85%)	342 (98%)	8 (2%)	50	71
1	C	362/412 (88%)	358 (99%)	4 (1%)	73	85
1	F	362/412 (88%)	358 (99%)	4 (1%)	73	85
1	H	264/412 (64%)	248 (94%)	16 (6%)	18	50
1	K	264/412 (64%)	253 (96%)	11 (4%)	30	59
2	D	268/271 (99%)	266 (99%)	2 (1%)	84	91
2	G	268/271 (99%)	266 (99%)	2 (1%)	84	91
2	J	268/271 (99%)	266 (99%)	2 (1%)	84	91
All	All	2770/3285 (84%)	2711 (98%)	59 (2%)	56	73

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	22	VAL
1	K	434	ASP
1	H	323	ASP
1	K	430	THR
1	K	340	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	85	GLN
1	K	399	HIS
2	J	306	ASN
2	J	29	HIS
1	K	372	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	C	501	-	26,33,33	0.62	0	31,52,52	0.76	1 (3%)
3	ATP	F	501	-	26,33,33	0.60	0	31,52,52	0.75	2 (6%)
3	ATP	B	501	-	26,33,33	0.70	0	31,52,52	0.79	1 (3%)
3	ATP	H	501	-	26,33,33	0.63	0	31,52,52	0.77	1 (3%)
3	ATP	K	501	-	26,33,33	0.62	0	31,52,52	0.74	2 (6%)
3	ATP	A	501	-	26,33,33	0.74	0	31,52,52	0.76	1 (3%)

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	C	501	-	-	3/18/38/38	0/3/3/3
3	ATP	F	501	-	-	5/18/38/38	0/3/3/3
3	ATP	B	501	-	-	1/18/38/38	0/3/3/3
3	ATP	H	501	-	-	5/18/38/38	0/3/3/3
3	ATP	K	501	-	-	2/18/38/38	0/3/3/3
3	ATP	A	501	-	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	ATP	C5-C6-N6	2.33	123.89	120.35
3	H	501	ATP	C5-C6-N6	2.30	123.85	120.35
3	C	501	ATP	C5-C6-N6	2.30	123.84	120.35
3	K	501	ATP	C5-C6-N6	2.30	123.84	120.35
3	F	501	ATP	C5-C6-N6	2.28	123.82	120.35

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

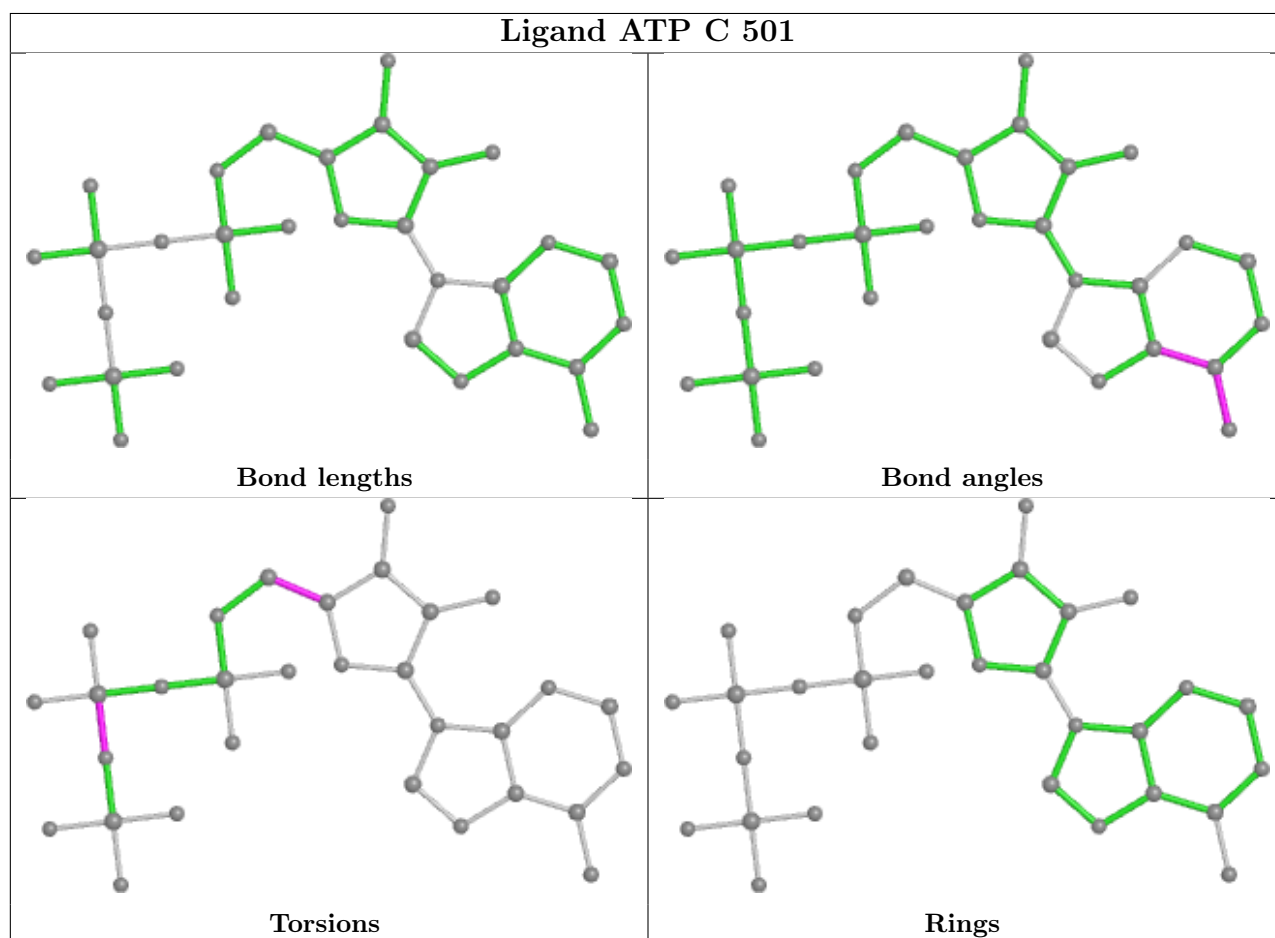
Mol	Chain	Res	Type	Atoms
3	A	501	ATP	PB-O3B-PG-O3G
3	F	501	ATP	C5'-O5'-PA-O1A
3	F	501	ATP	C5'-O5'-PA-O2A
3	H	501	ATP	O4'-C4'-C5'-O5'
3	H	501	ATP	C3'-C4'-C5'-O5'

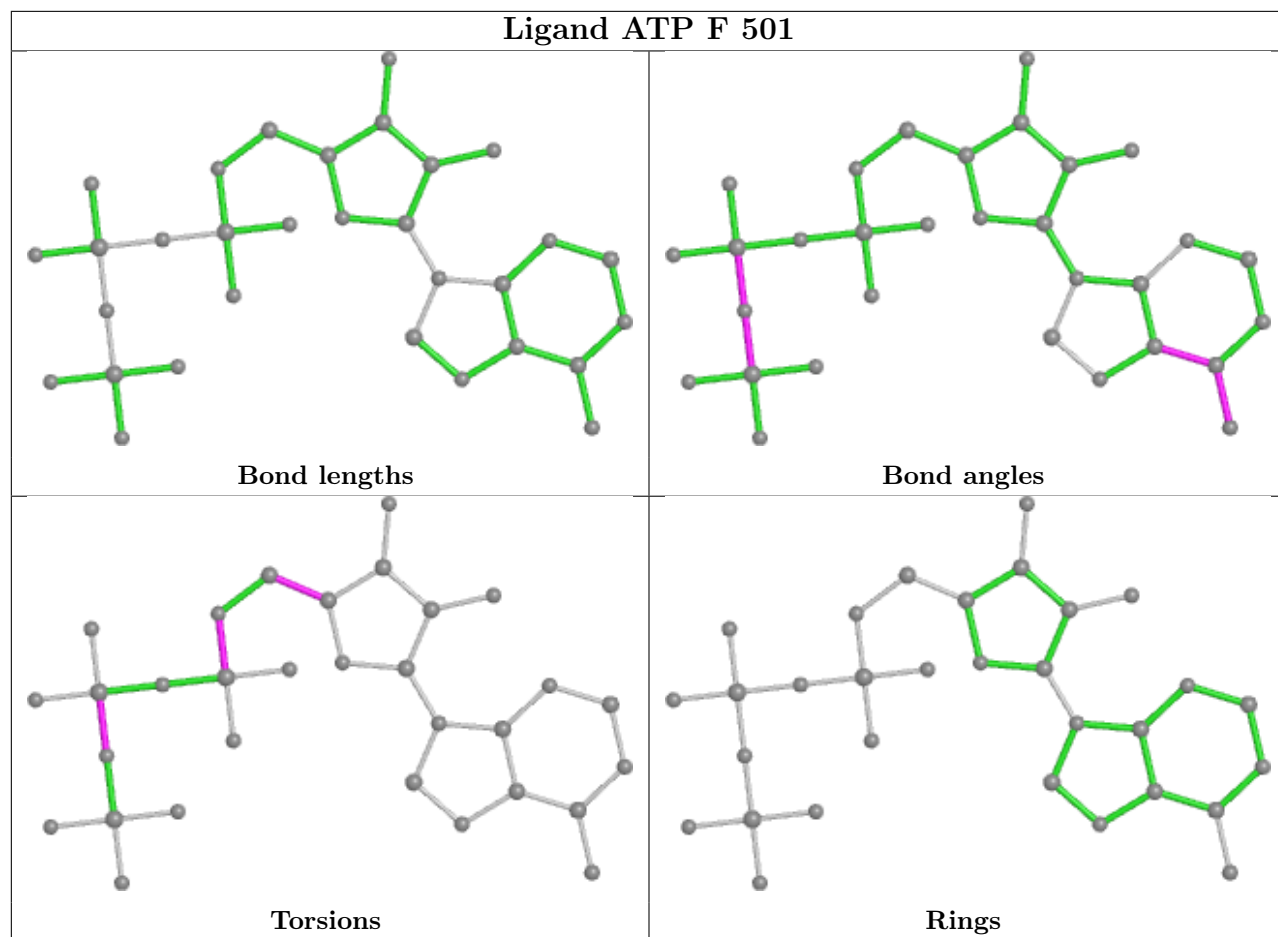
There are no ring outliers.

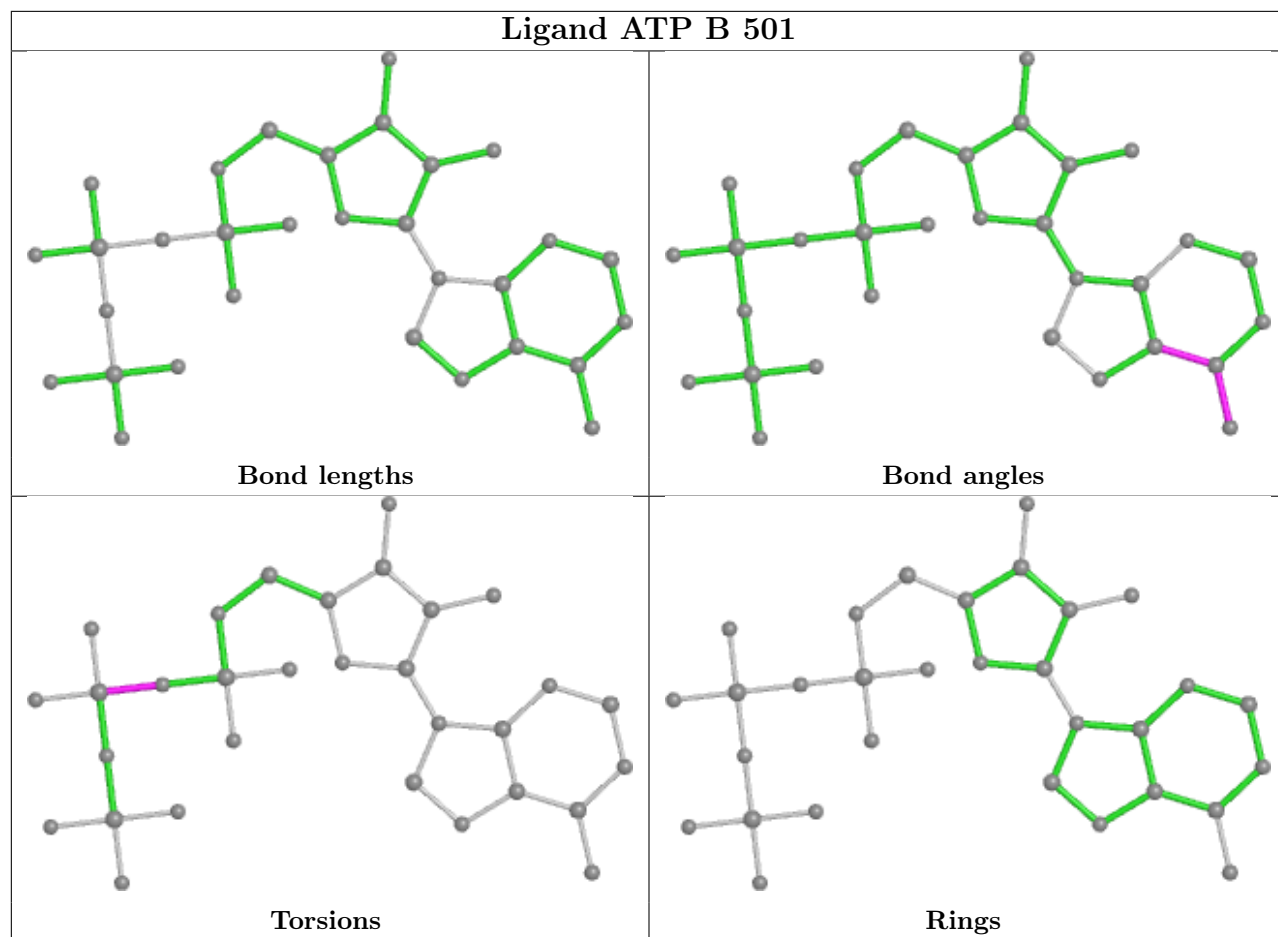
4 monomers are involved in 5 short contacts:

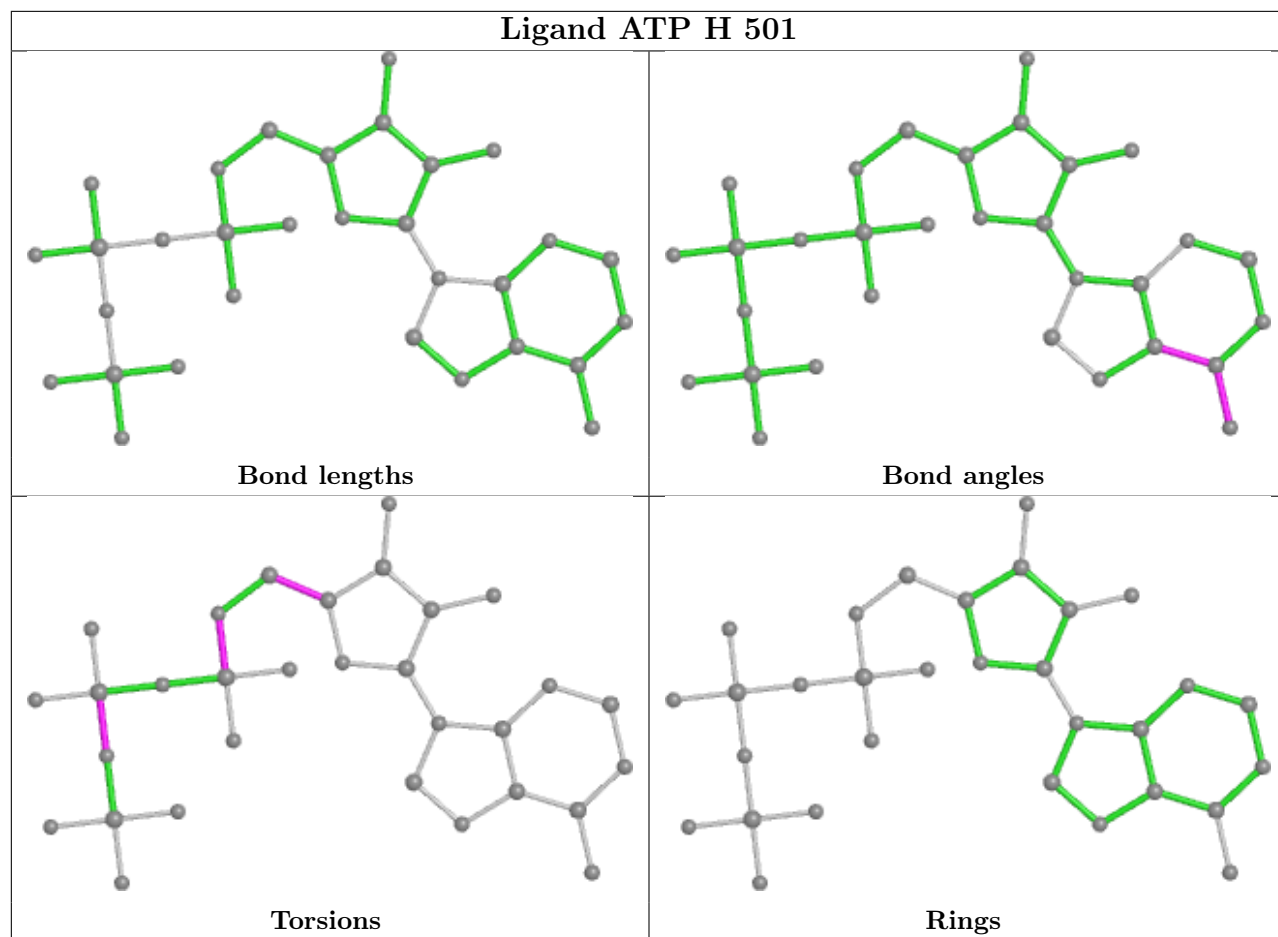
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	ATP	1	0
3	H	501	ATP	1	0
3	K	501	ATP	2	0
3	A	501	ATP	1	0

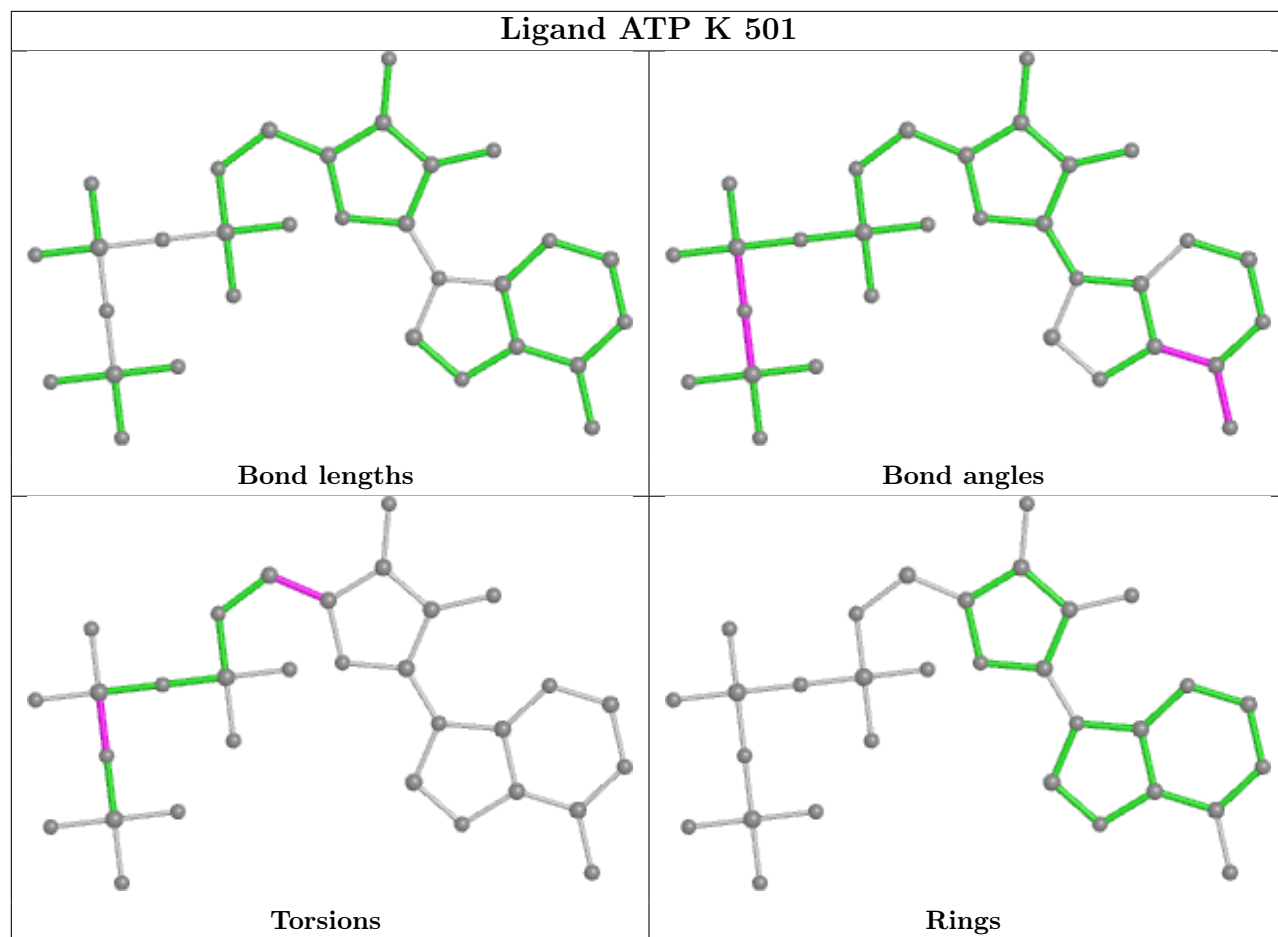
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

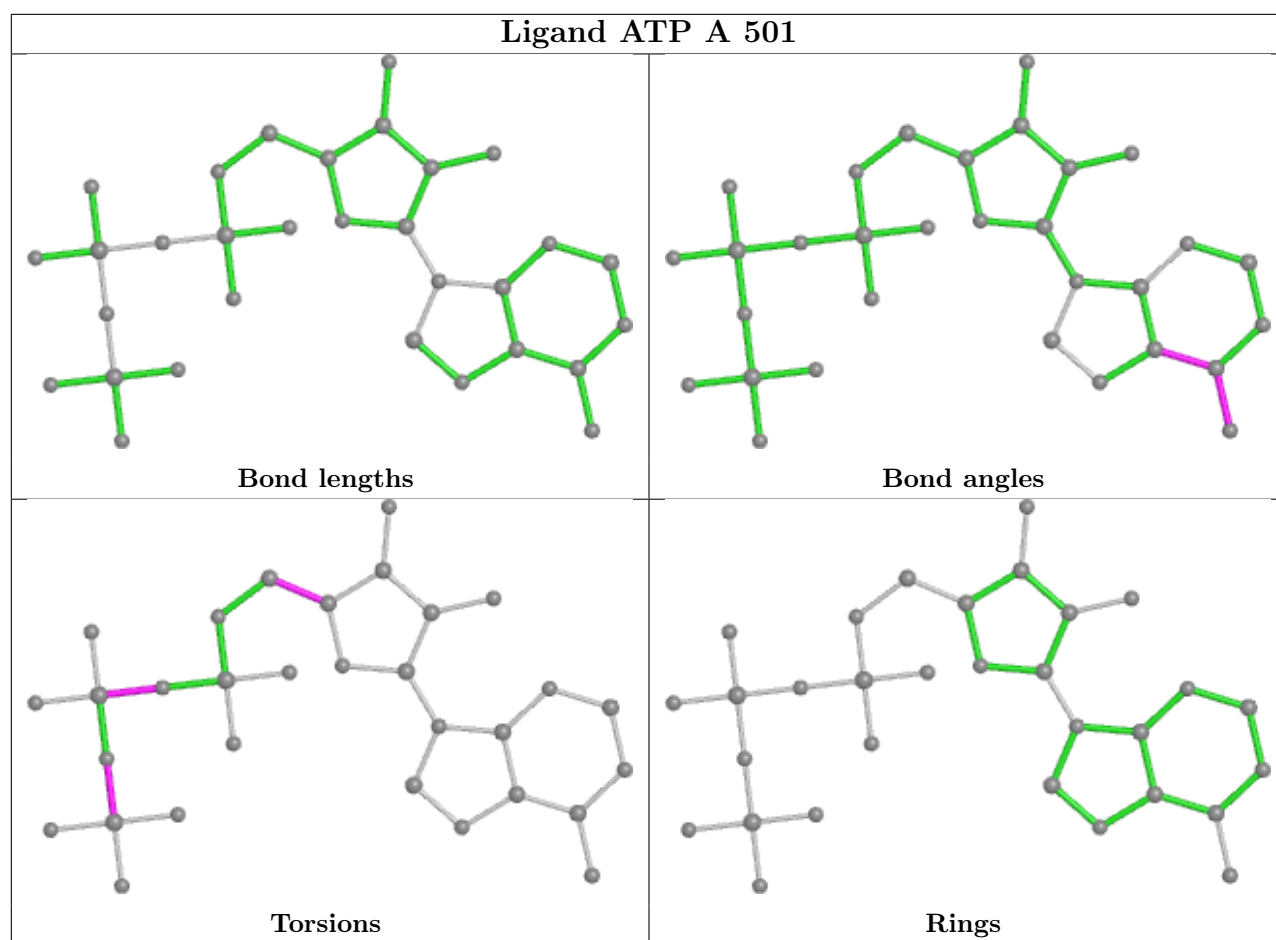












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

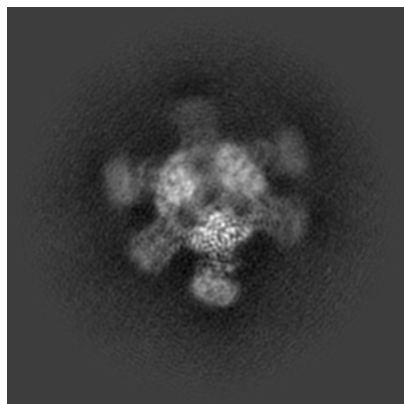
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42968. These allow visual inspection of the internal detail of the map and identification of artifacts.

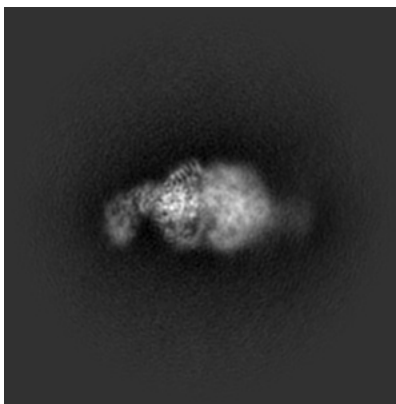
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

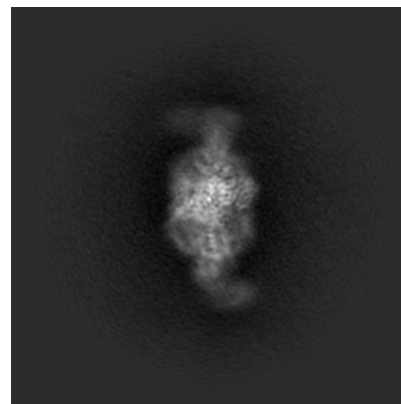
6.1.1 Primary map



X

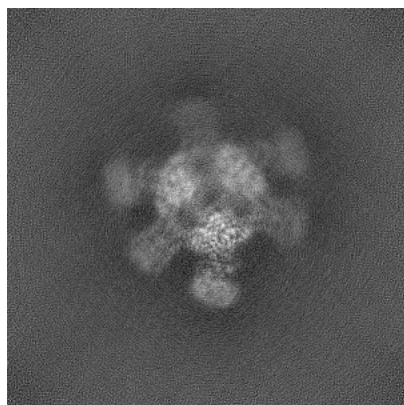


Y

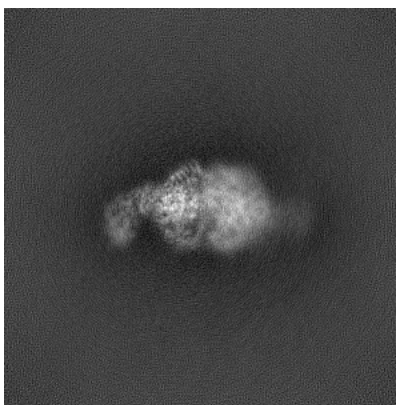


Z

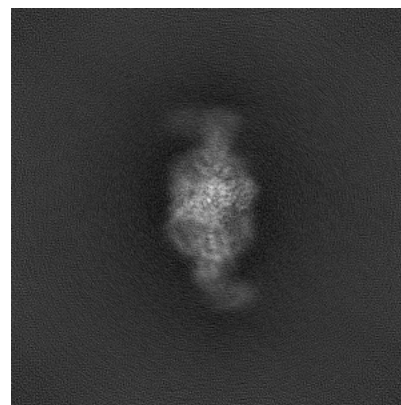
6.1.2 Raw map



X



Y

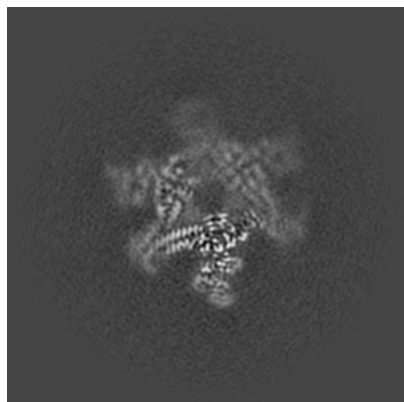


Z

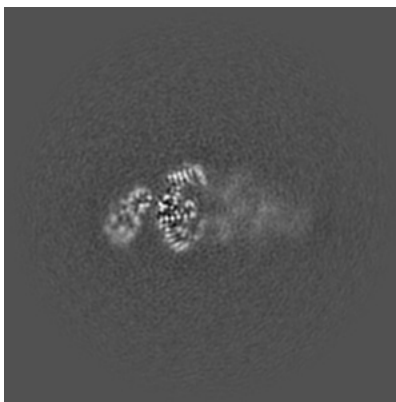
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

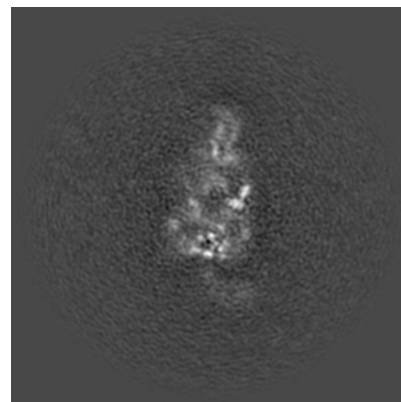
6.2.1 Primary map



X Index: 192

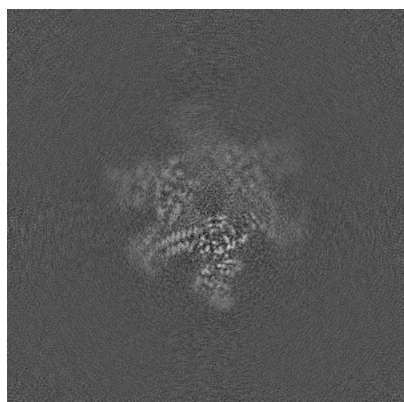


Y Index: 192

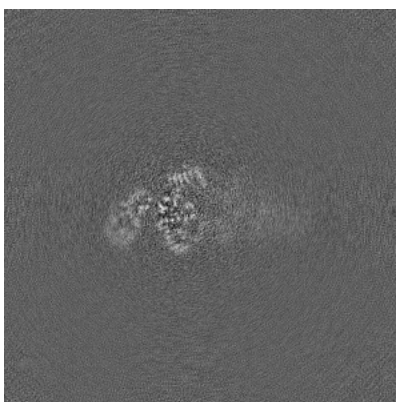


Z Index: 192

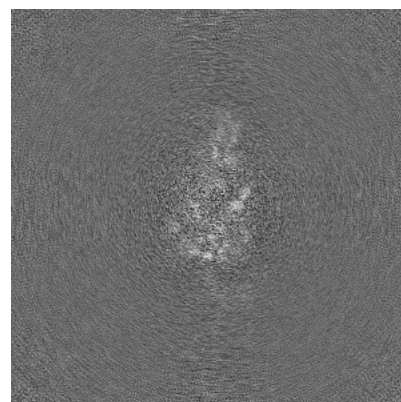
6.2.2 Raw map



X Index: 192



Y Index: 192

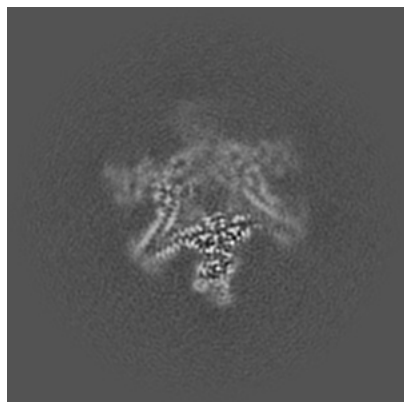


Z Index: 192

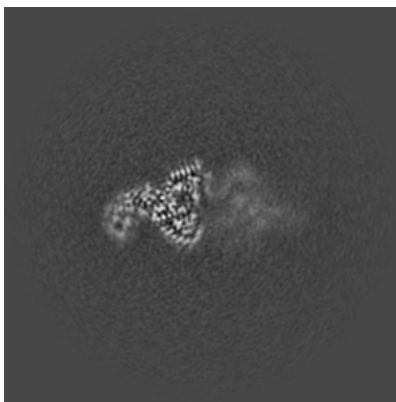
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

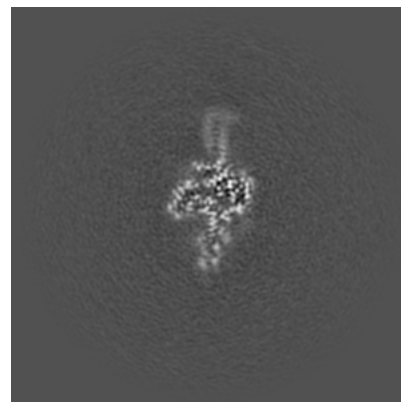
6.3.1 Primary map



X Index: 195



Y Index: 200

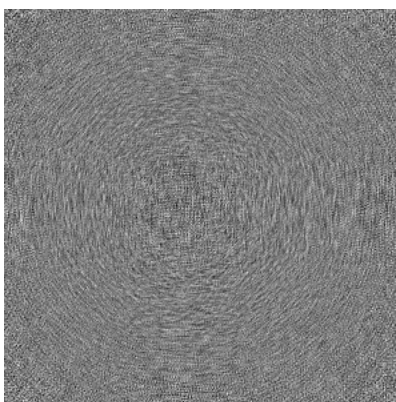


Z Index: 170

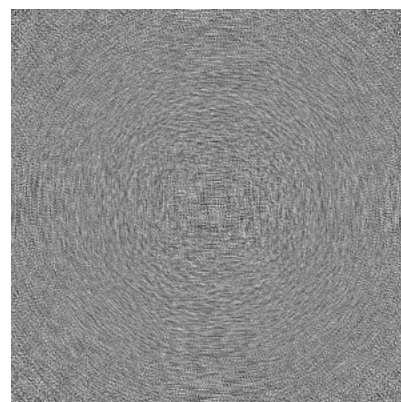
6.3.2 Raw map



X Index: 195



Y Index: 0

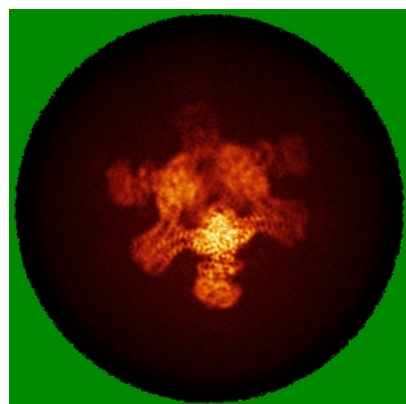


Z Index: 0

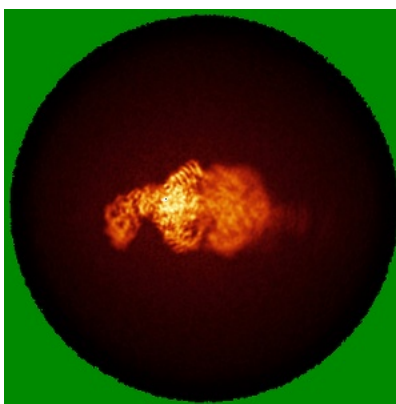
The images above show the largest variance slices of the map in three orthogonal directions.

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

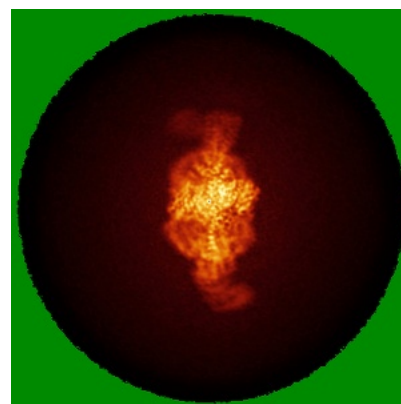
6.4.1 Primary map



X

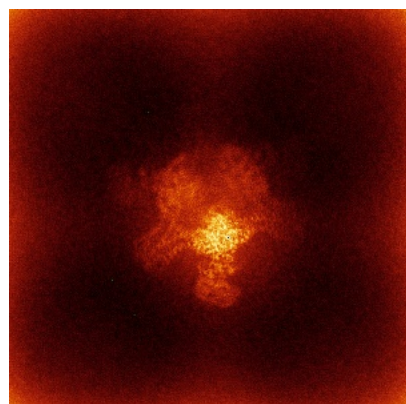


Y

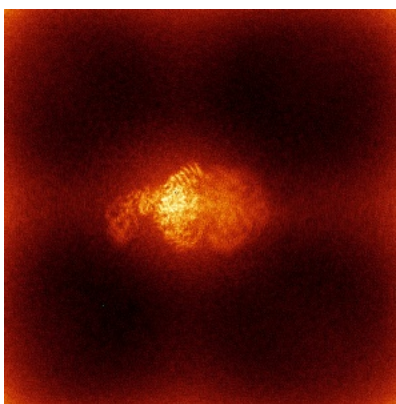


Z

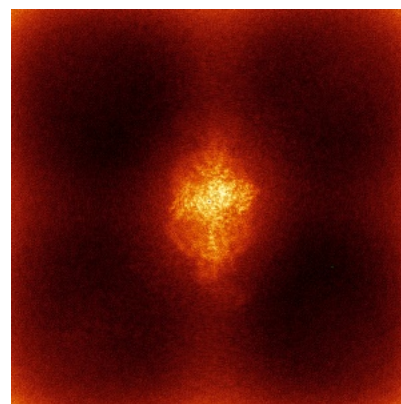
6.4.2 Raw map



X



Y

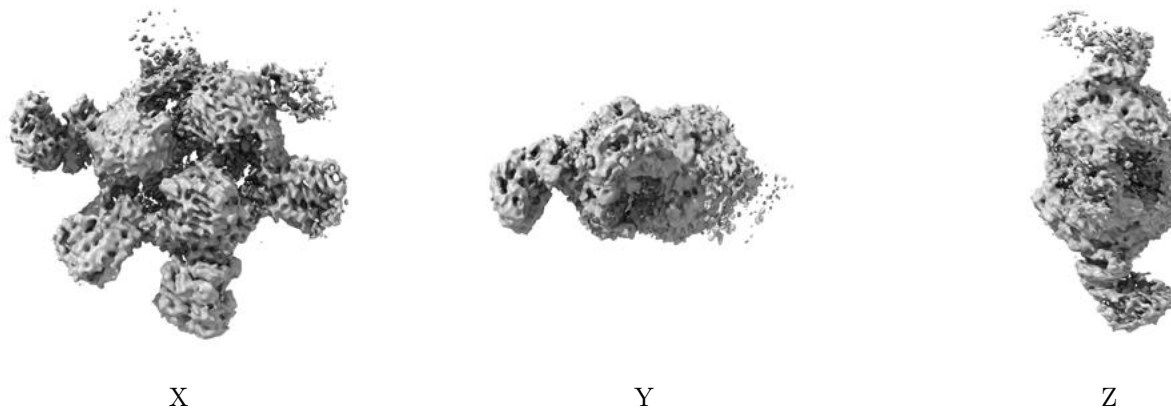


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

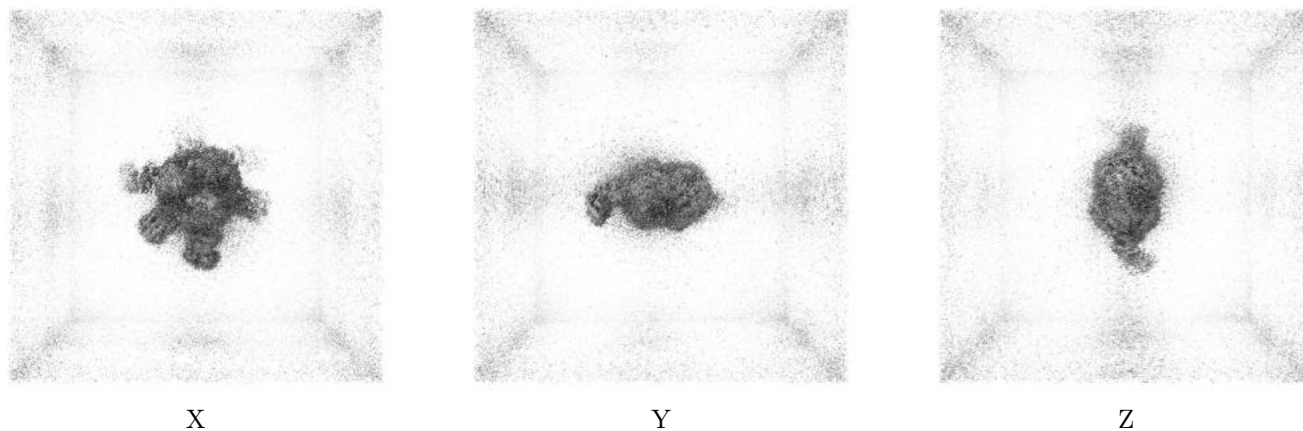
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

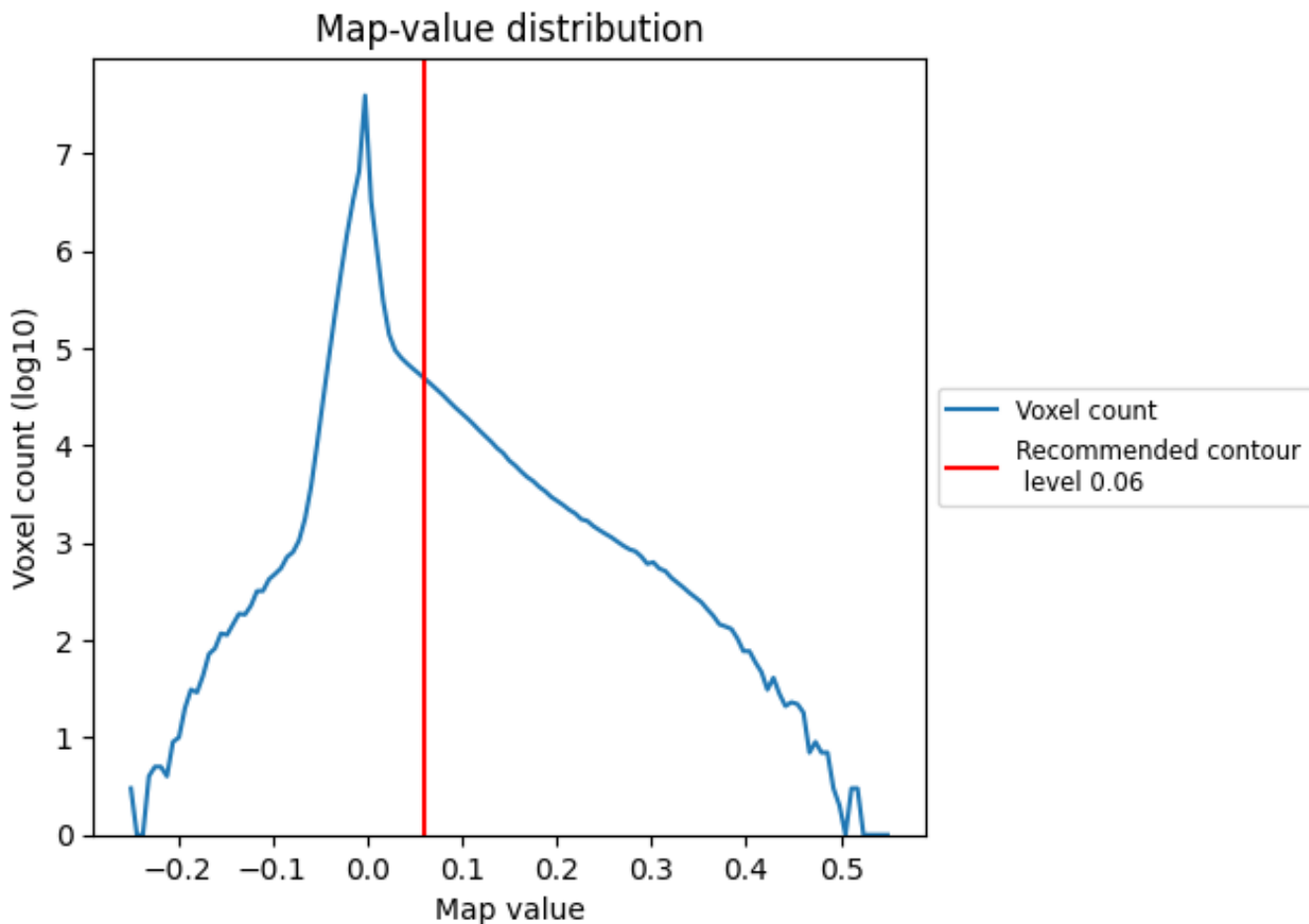
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

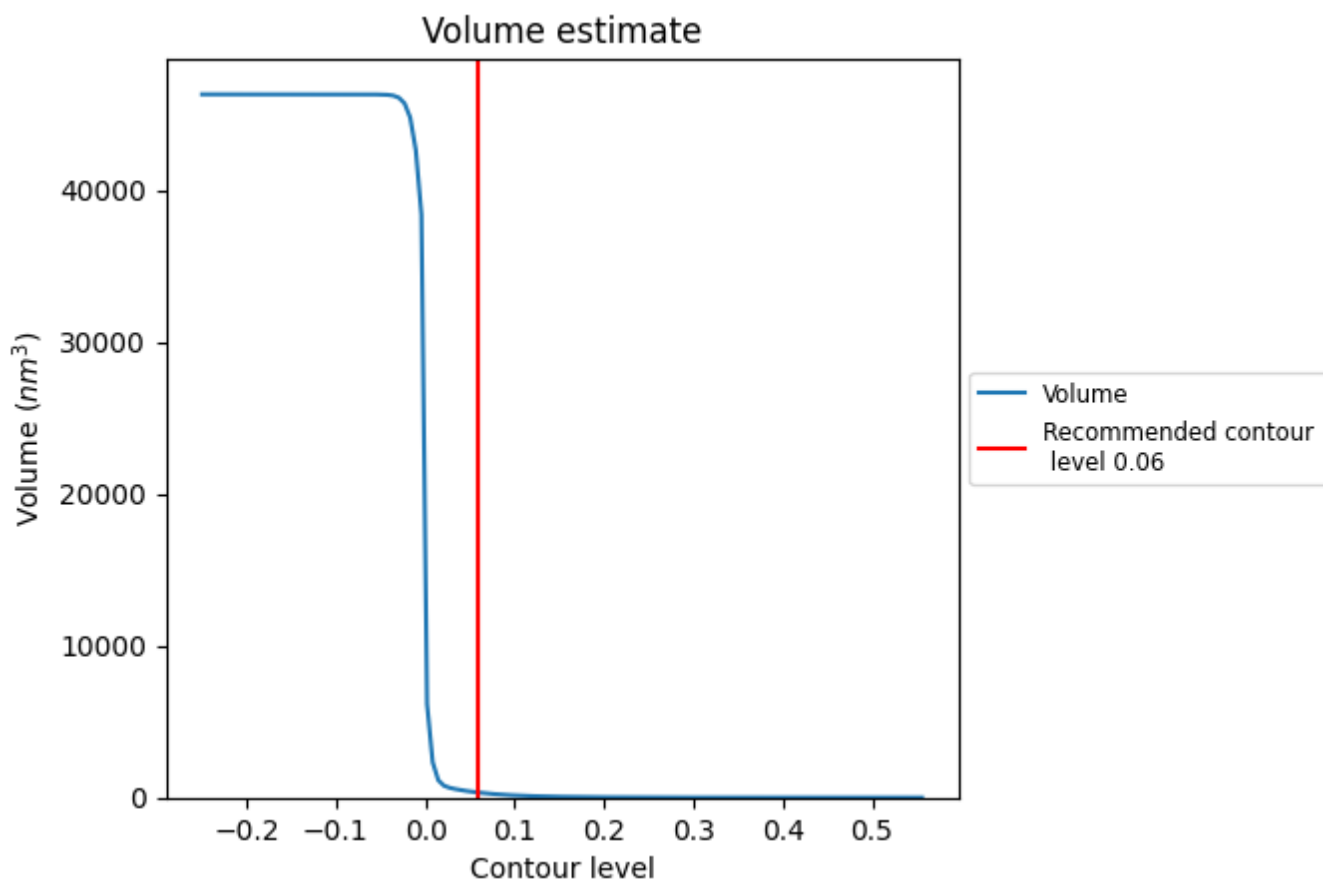
This section contains the results of statistical analysis of the map.

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.

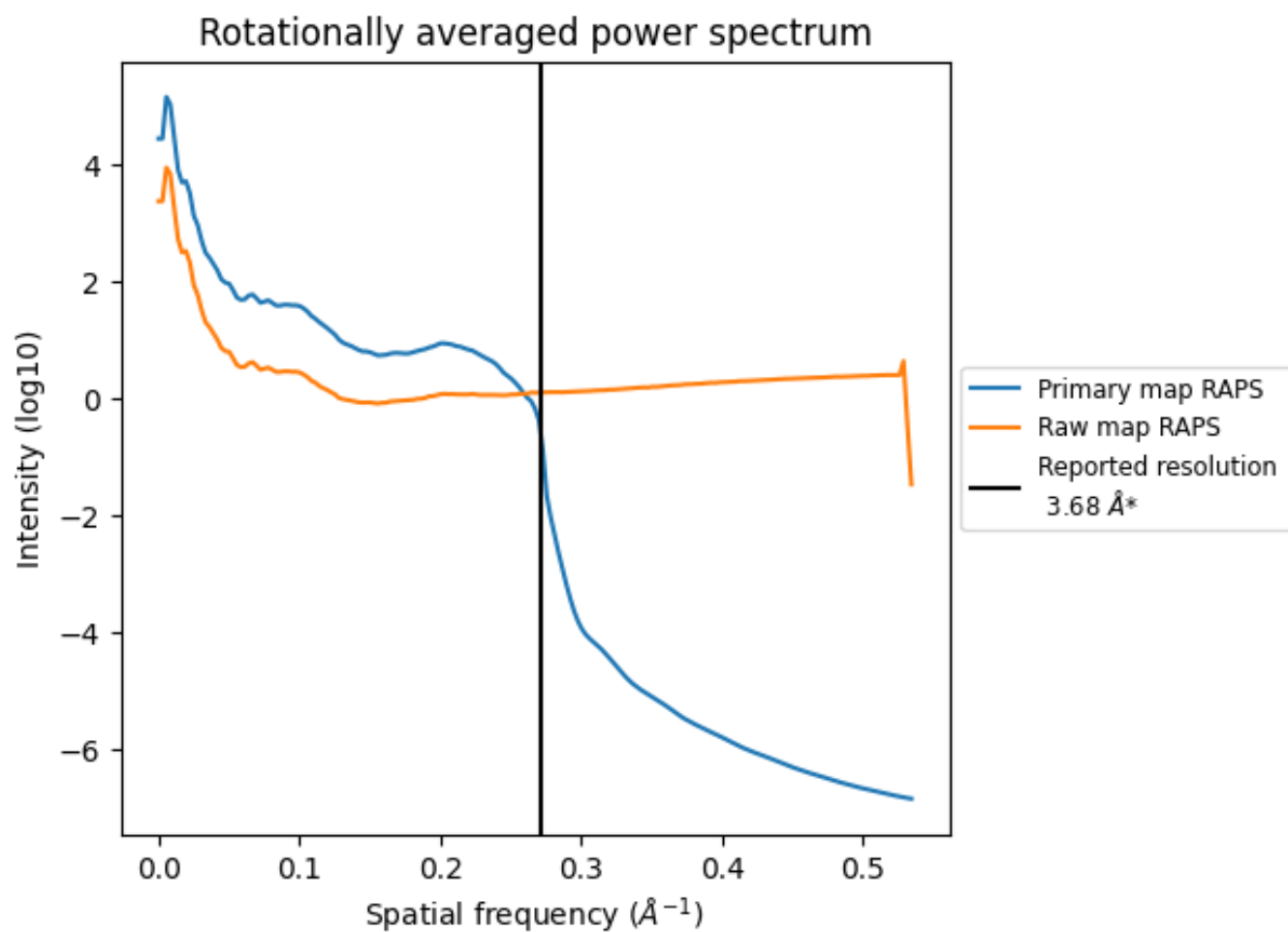
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 327 nm³; this corresponds to an approximate mass of 296 kDa.

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

7.3 Rotationally averaged power spectrum i

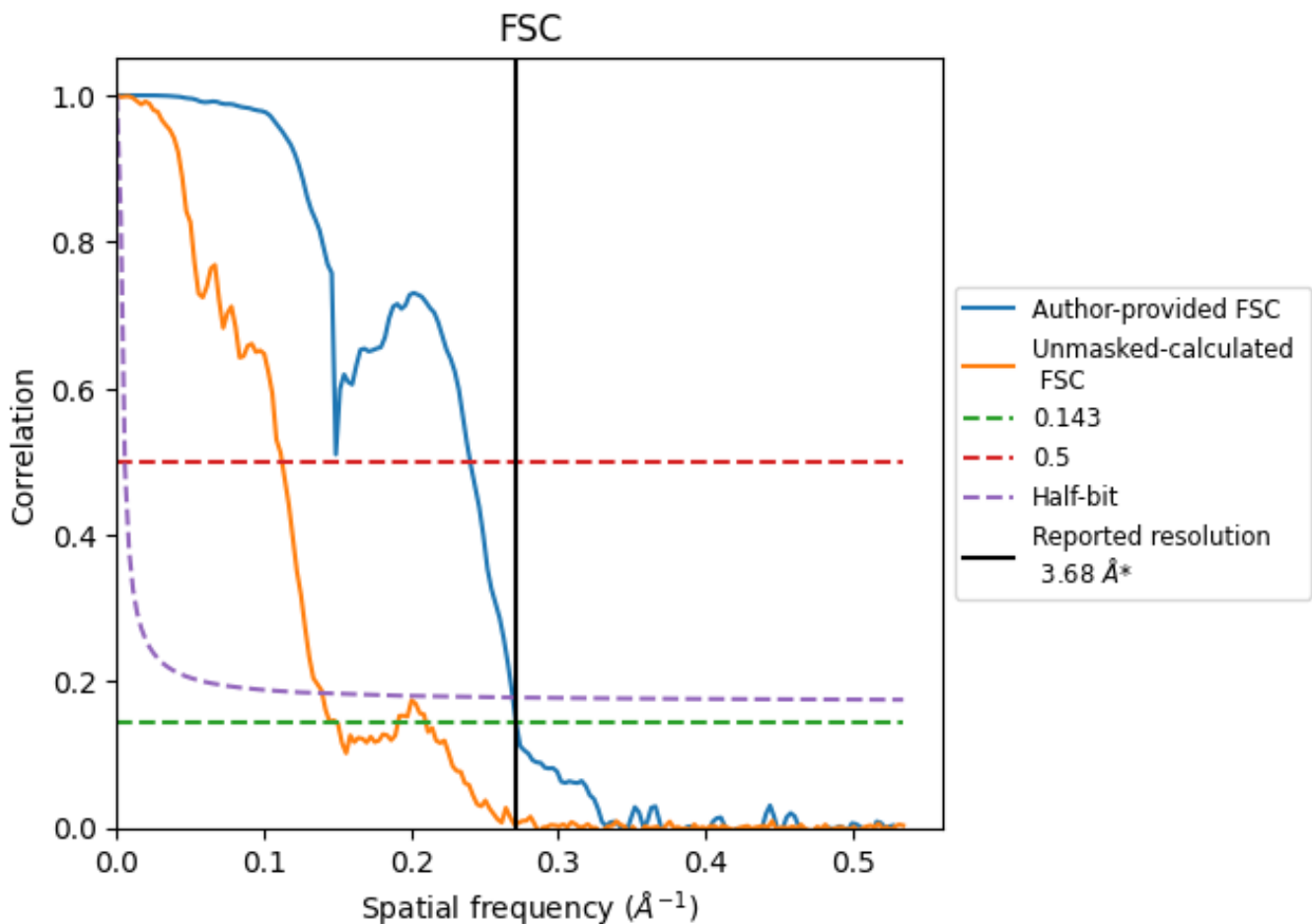


*Reported resolution corresponds to spatial frequency of 0.272 Å⁻¹

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 0.272 Å⁻¹

8.2 Resolution estimates [i](#)

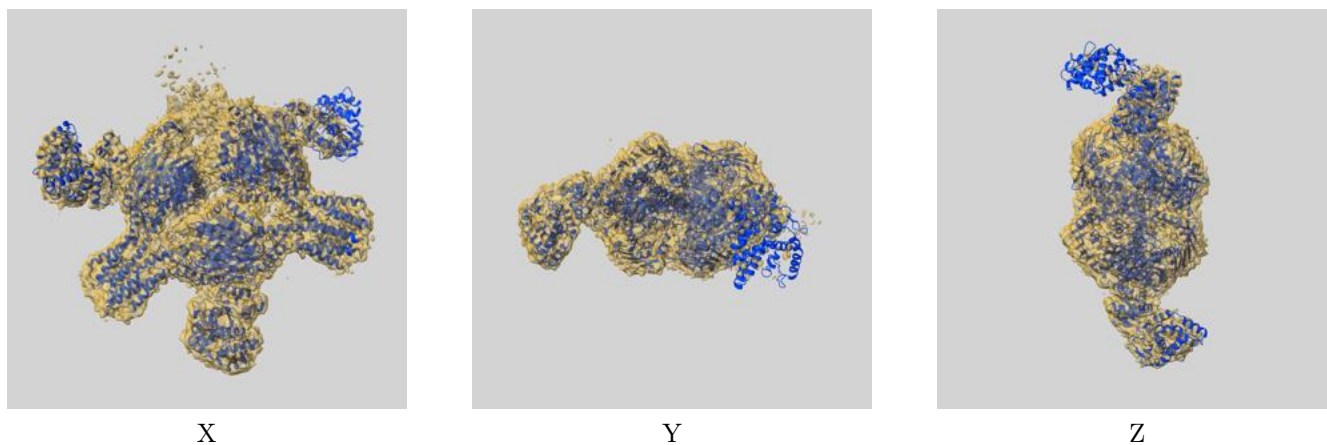
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.68	-	-
Author-provided FSC curve	3.68	4.16	3.71
Unmasked-calculated*	6.68	8.90	7.16

*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 6.68 differs from the reported value 3.68 by more than 10 %

9 Map-model fit [i](#)

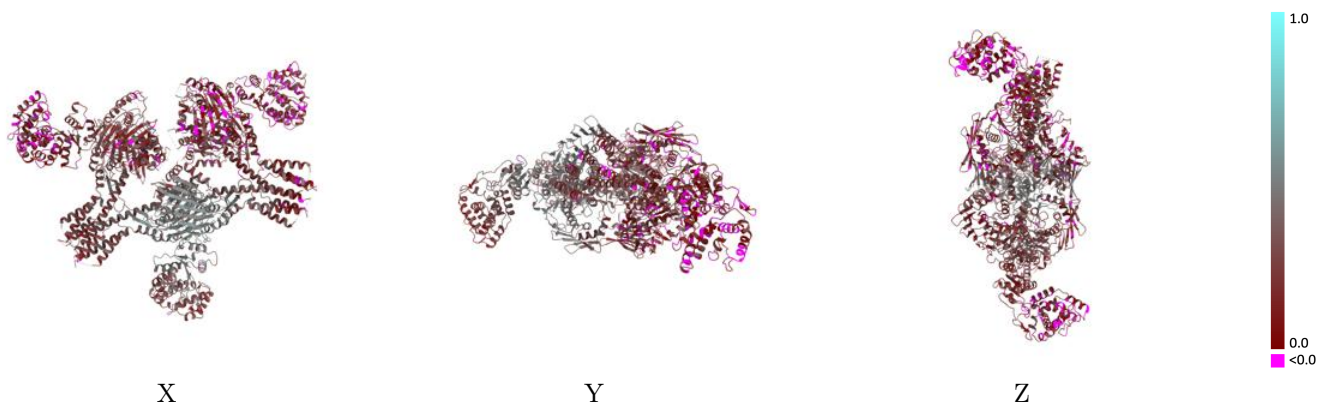
This section contains information regarding the fit between EMDB map EMD-42968 and PDB model 8V48. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



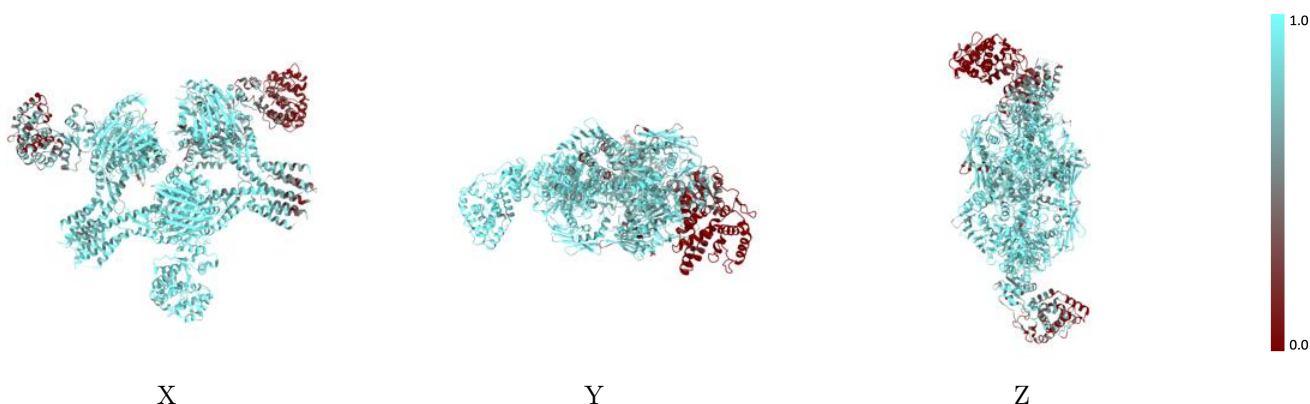
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



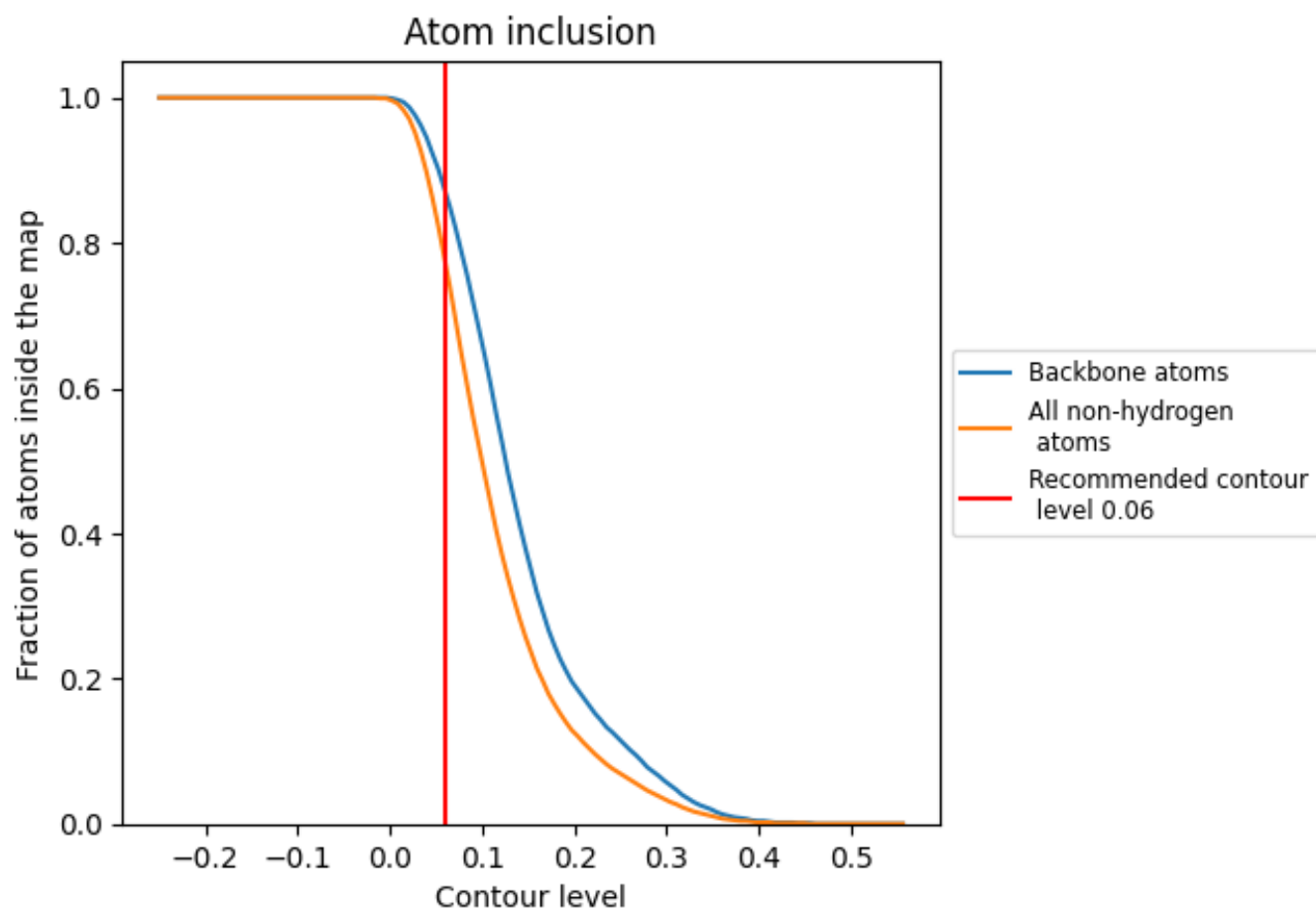
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).





















9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 77% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7730	 0.2570
A	 0.8840	 0.3960
B	 0.9250	 0.4020
C	 0.8710	 0.2710
D	 0.9250	 0.3260
F	 0.7900	 0.1810
G	 0.5520	 0.1400
H	 0.8780	 0.2350
J	 0.1470	 0.0900
K	 0.8540	 0.1950

