



wwPDB EM Validation Summary Report ⓘ

Feb 24, 2024 – 01:49 PM EST

PDB ID : 7LFX
EMDB ID : EMD-23308
Title : Cryo-EM structure of human cGMP-bound open CNGA1 channel in Na⁺/Ca²⁺
Authors : Xue, J.; Han, Y.; Jiang, Y.
Deposited on : 2021-01-19
Resolution : 3.10 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.dev70
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)	:	2.36

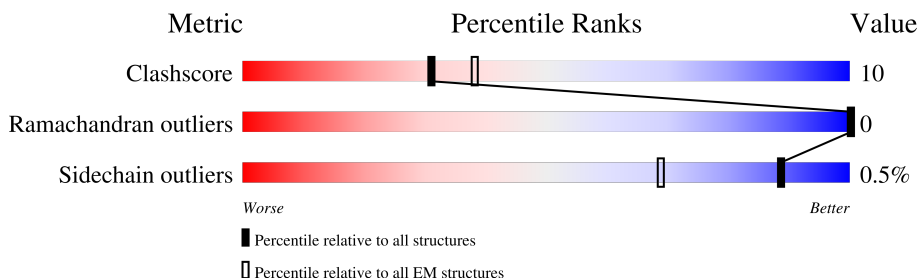
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	560	<div> <div>17%</div> <div>59%</div> <div>21%</div> <div>20%</div> </div>
1	B	560	<div> <div>17%</div> <div>58%</div> <div>22%</div> <div>20%</div> </div>
1	C	560	<div> <div>17%</div> <div>58%</div> <div>22%</div> <div>20%</div> </div>
1	D	560	<div> <div>17%</div> <div>59%</div> <div>21%</div> <div>20%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14846 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 cGMP-gated cation channel alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	450	Total	C	N	O	S	0	0
			3688	2411	594	664	19		
1	B	450	Total	C	N	O	S	0	0
			3688	2411	594	664	19		
1	C	450	Total	C	N	O	S	0	0
			3688	2411	594	664	19		
1	D	450	Total	C	N	O	S	0	0
			3688	2411	594	664	19		

There are 52 discrepancies between the modelled and reference sequences:

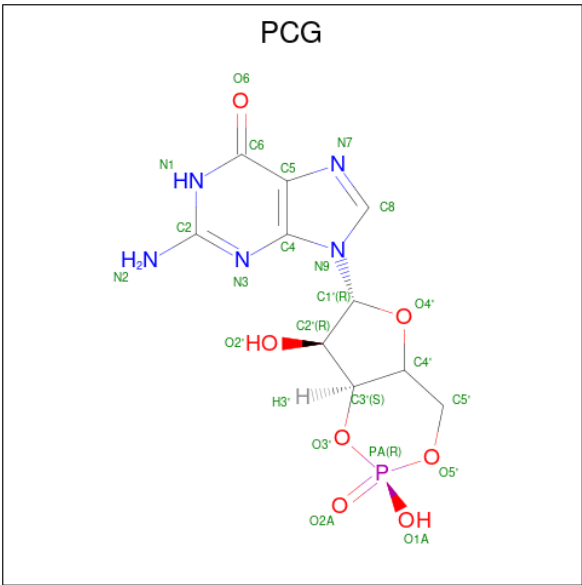
Chain	Residue	Modelled	Actual	Comment	Reference
A	131	MET	-	initiating methionine	UNP P29973
A	132	ASP	-	expression tag	UNP P29973
A	133	TYR	-	expression tag	UNP P29973
A	134	LYS	-	expression tag	UNP P29973
A	135	ASP	-	expression tag	UNP P29973
A	136	ASP	-	expression tag	UNP P29973
A	137	ASP	-	expression tag	UNP P29973
A	138	ASP	-	expression tag	UNP P29973
A	139	LYS	-	expression tag	UNP P29973
A	140	GLY	-	expression tag	UNP P29973
A	141	GLY	-	expression tag	UNP P29973
A	142	SER	-	expression tag	UNP P29973
A	143	ALA	-	expression tag	UNP P29973
B	131	MET	-	initiating methionine	UNP P29973
B	132	ASP	-	expression tag	UNP P29973
B	133	TYR	-	expression tag	UNP P29973
B	134	LYS	-	expression tag	UNP P29973
B	135	ASP	-	expression tag	UNP P29973
B	136	ASP	-	expression tag	UNP P29973
B	137	ASP	-	expression tag	UNP P29973
B	138	ASP	-	expression tag	UNP P29973
B	139	LYS	-	expression tag	UNP P29973

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Chain	Residue	Modelled	Actual	Comment	Reference
B	140	GLY	-	expression tag	UNP P29973
B	141	GLY	-	expression tag	UNP P29973
B	142	SER	-	expression tag	UNP P29973
B	143	ALA	-	expression tag	UNP P29973
C	131	MET	-	initiating methionine	UNP P29973
C	132	ASP	-	expression tag	UNP P29973
C	133	TYR	-	expression tag	UNP P29973
C	134	LYS	-	expression tag	UNP P29973
C	135	ASP	-	expression tag	UNP P29973
C	136	ASP	-	expression tag	UNP P29973
C	137	ASP	-	expression tag	UNP P29973
C	138	ASP	-	expression tag	UNP P29973
C	139	LYS	-	expression tag	UNP P29973
C	140	GLY	-	expression tag	UNP P29973
C	141	GLY	-	expression tag	UNP P29973
C	142	SER	-	expression tag	UNP P29973
C	143	ALA	-	expression tag	UNP P29973
D	131	MET	-	initiating methionine	UNP P29973
D	132	ASP	-	expression tag	UNP P29973
D	133	TYR	-	expression tag	UNP P29973
D	134	LYS	-	expression tag	UNP P29973
D	135	ASP	-	expression tag	UNP P29973
D	136	ASP	-	expression tag	UNP P29973
D	137	ASP	-	expression tag	UNP P29973
D	138	ASP	-	expression tag	UNP P29973
D	139	LYS	-	expression tag	UNP P29973
D	140	GLY	-	expression tag	UNP P29973
D	141	GLY	-	expression tag	UNP P29973
D	142	SER	-	expression tag	UNP P29973
D	143	ALA	-	expression tag	UNP P29973

- Molecule 2 is CYCLIC GUANOSINE MONOPHOSPHATE (three-letter code: PCG) (formula: $C_{10}H_{12}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			23	10	5	7	1	
2	B	1	Total	C	N	O	P	0
			23	10	5	7	1	
2	C	1	Total	C	N	O	P	0
			23	10	5	7	1	
2	D	1	Total	C	N	O	P	0
			23	10	5	7	1	

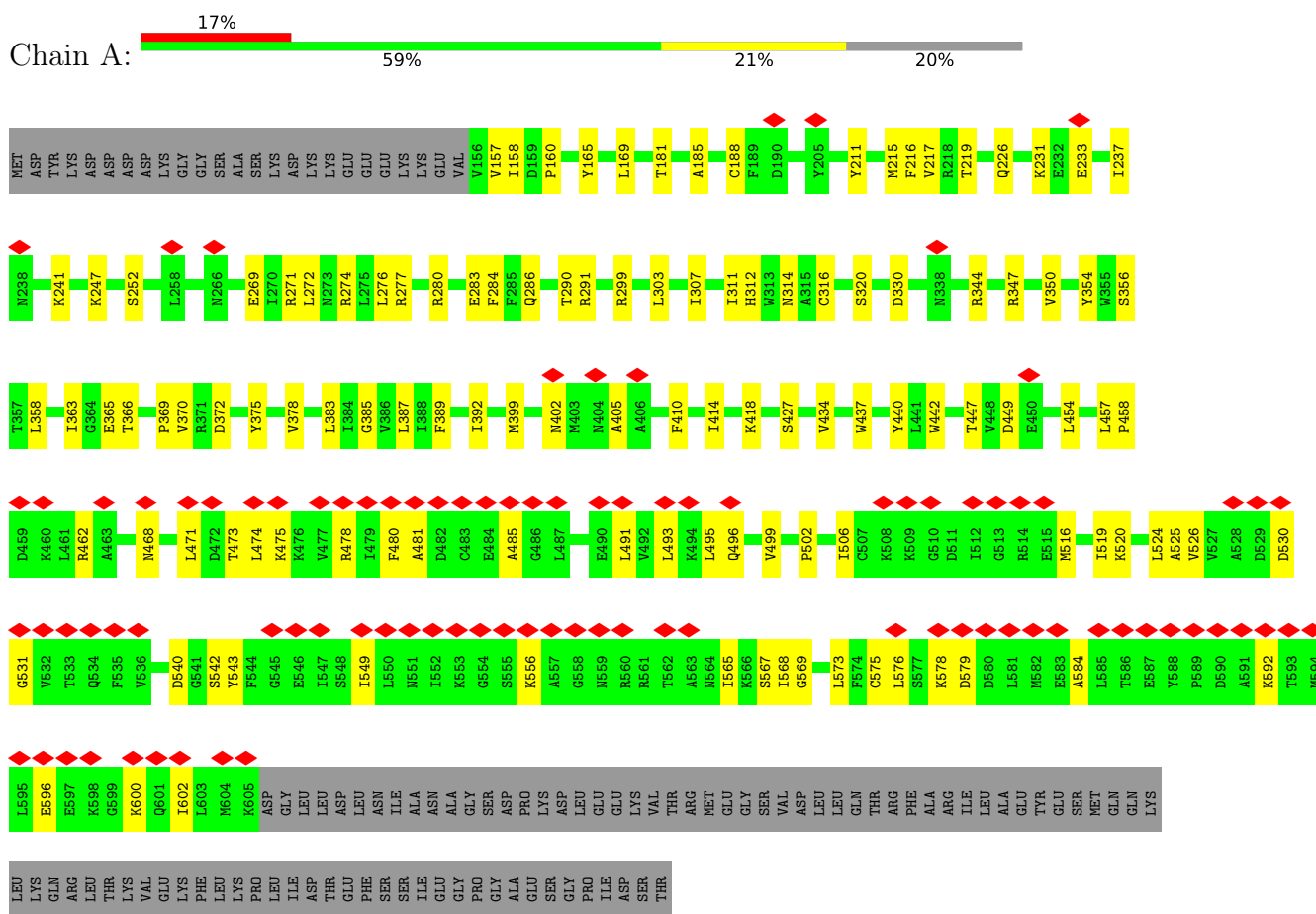
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Ca	0
			2	2	

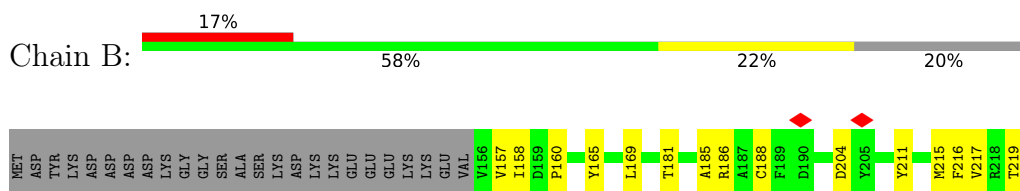
3 Residue-property plots

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: cGMP-gated cation channel alpha-1



• Molecule 1: cGMP-gated cation channel alpha-1





MET	V156	I237	T357	K460	T533	E597	GLN
ASP	V157	N238	L358	L461	Q534	K598	ARG
TYR	I158	K241	I363	R462	F535	G599	LEU
LYS	D159	K247	E364	A463	V536	Q600	THR
ASP	Y165	S252	E365	N468	D540	I601	VAL
ASP	L169	D257	T366	L471	G541	I602	GLU
ASP	T131	L258	P369	D472	S542	L603	LYS
LYS	A185	R266	V370	L473	Y543	M604	PHE
LYS	R186	E269	R371	L474	F544	K605	LEU
GLU	C188	I270	D372	K475	G545	ASP	PRO
GLU	F189	R271	Y375	K476	E546	GLY	LEU
LYS	D190	L272	V378	V477	I547	LEU	LEU
GLU	Y204	R273	I383	R478	E548	ASP	THR
LYS	Y205	R274	I384	I479	I549	LEU	GLU
GLU	Y211	R275	G385	F480	L550	ASN	PHE
LYS	Y216	L276	V386	A481	N551	ILE	SER
LYS	Y217	R277	L387	D482	I552	ALA	SER
LYS	R218	I277	I388	C483	K553	ALA	ILE
LYS	T219	R278	F389	E484	G554	GLY	GLU
LYS	Q226	R279	I392	E485	S555	ASP	PRO
LYS	K231	R280	M399	G486	K556	PRO	GLY
LYS	E232	E283	N402	L487	A557	LYS	ALA
LYS	E233	F284	M403	E490	G558	ASP	GLU
		Q286	N404	L491	N559	LEU	SER
		T290	A405	V492	R560	GLU	GLY
		R291	A406	K493	T562	LYS	VAL
		R299	F410	L495	A563	THR	THR
		L303	I414	K494	N564	ARG	ARG
		I307	K418	L495	I565	MET	GLY
		I311	S427	Q496	K566	GLY	GLY
		H312	V434	V499	S567	SER	VAL
		H313	W437	P502	I568	VAL	ASP
		N314	Y440	I506	G569	LEU	LEU
		A315	W442	C607	L573	GLN	GLN
		C316	T447	K508	F574	THR	THR
		S320	E450	G509	C575	ARG	ARG
		D330	L454	G510	L576	PHE	ALA
		N338	P458	D511	S577	ALA	ILE
		R344	D459	I512	K578	ARG	LEU
		R347	L457	G513	D579	ILE	LEU
		V350	P458	R514	D580	ALA	ALA
		S356	D459	E515	L581	GLU	GLU
				I519	M582	TYR	TYR
				K620	E583	GLY	SER
				L524	A584	SER	SER
				A525	L585	MET	MET
				V526	T586	GLN	GLN
				V527	E587	LYS	LYS
				A528	Y588	LEU	LEU
				D529	P589	LYS	LYS
				G530	D590	LEU	LEU
				G531	A591	LYS	LYS
				V532	K592	LYS	LYS
					T593		
					M594		
					L595		
					E596		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76571	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.107	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.021	Depositor
Map size (\AA)	231.84, 231.84, 231.84	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.805, 0.805, 0.805	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: PCG, CA

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	0.28	0/3773	0.41	0/5111
1	B	0.28	0/3773	0.41	0/5111
1	C	0.28	0/3773	0.41	0/5111
1	D	0.28	0/3773	0.41	0/5111
All	All	0.28	0/15092	0.41	0/20444

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	3688	0	3737	82	0
1	B	3688	0	3737	86	0
1	C	3688	0	3737	84	0
1	D	3688	0	3737	80	0
2	A	23	0	11	1	0
2	B	23	0	11	1	0
2	C	23	0	11	1	0
2	D	23	0	11	1	0
3	A	2	0	0	0	0
All	All	14846	0	14992	288	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 288 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:481:ALA:HA	1:A:485:ALA:HA	1.83	0.60
1:C:385:GLY:O	1:C:389:PHE:HB2	2.02	0.60
1:D:481:ALA:HA	1:D:485:ALA:HA	1.84	0.60
1:C:481:ALA:HA	1:C:485:ALA:HA	1.84	0.59
1:B:481:ALA:HA	1:B:485:ALA:HA	1.83	0.59

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	448/560 (80%)	437 (98%)	11 (2%)	0	100	100
1	B	448/560 (80%)	438 (98%)	10 (2%)	0	100	100
1	C	448/560 (80%)	438 (98%)	10 (2%)	0	100	100
1	D	448/560 (80%)	438 (98%)	10 (2%)	0	100	100
All	All	1792/2240 (80%)	1751 (98%)	41 (2%)	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	405/502 (81%)	403 (100%)	2 (0%)	88	94
1	B	405/502 (81%)	403 (100%)	2 (0%)	88	94
1	C	405/502 (81%)	403 (100%)	2 (0%)	88	94
1	D	405/502 (81%)	403 (100%)	2 (0%)	88	94
All	All	1620/2008 (81%)	1612 (100%)	8 (0%)	89	94

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	556	LYS
1	D	291	ARG
1	C	291	ARG
1	B	556	LYS
1	C	556	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	402	ASN
1	C	468	ASN
1	C	411	GLN
1	C	534	GLN
1	B	302	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
2	PCG	C	701	-	22,26,26	2.15	5 (22%)	25,41,41	1.91	7 (28%)
2	PCG	A	701	-	22,26,26	2.15	5 (22%)	25,41,41	1.90	7 (28%)
2	PCG	D	701	-	22,26,26	2.16	5 (22%)	25,41,41	1.91	8 (32%)
2	PCG	B	701	-	22,26,26	2.15	5 (22%)	25,41,41	1.90	7 (28%)

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
2	PCG	C	701	-	-	0/0/31/31	0/4/4/4
2	PCG	A	701	-	-	0/0/31/31	0/4/4/4
2	PCG	D	701	-	-	0/0/31/31	0/4/4/4
2	PCG	B	701	-	-	0/0/31/31	0/4/4/4

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	PCG	PA-O5'	5.45	1.63	1.57
2	A	701	PCG	PA-O5'	5.43	1.63	1.57
2	B	701	PCG	PA-O5'	5.41	1.63	1.57
2	C	701	PCG	PA-O5'	5.41	1.63	1.57
2	B	701	PCG	O4'-C1'	5.10	1.48	1.41

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	PCG	O3'-C3'-C4'	-4.57	107.26	110.71
2	D	701	PCG	O3'-C3'-C4'	-4.53	107.29	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	PCG	O3'-C3'-C4'	-4.51	107.31	110.71
2	A	701	PCG	O3'-C3'-C4'	-4.49	107.32	110.71
2	B	701	PCG	O1A-PA-O2A	3.13	118.54	108.73

There are no chirality outliers.

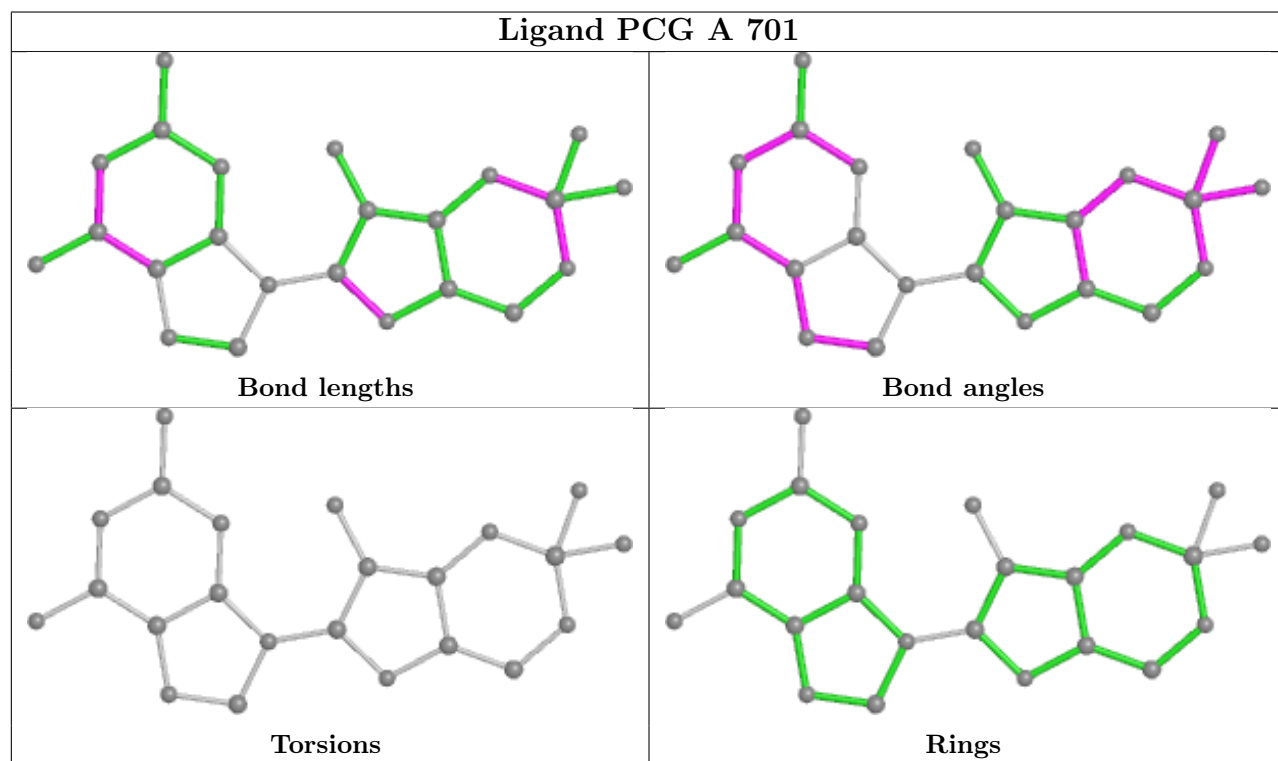
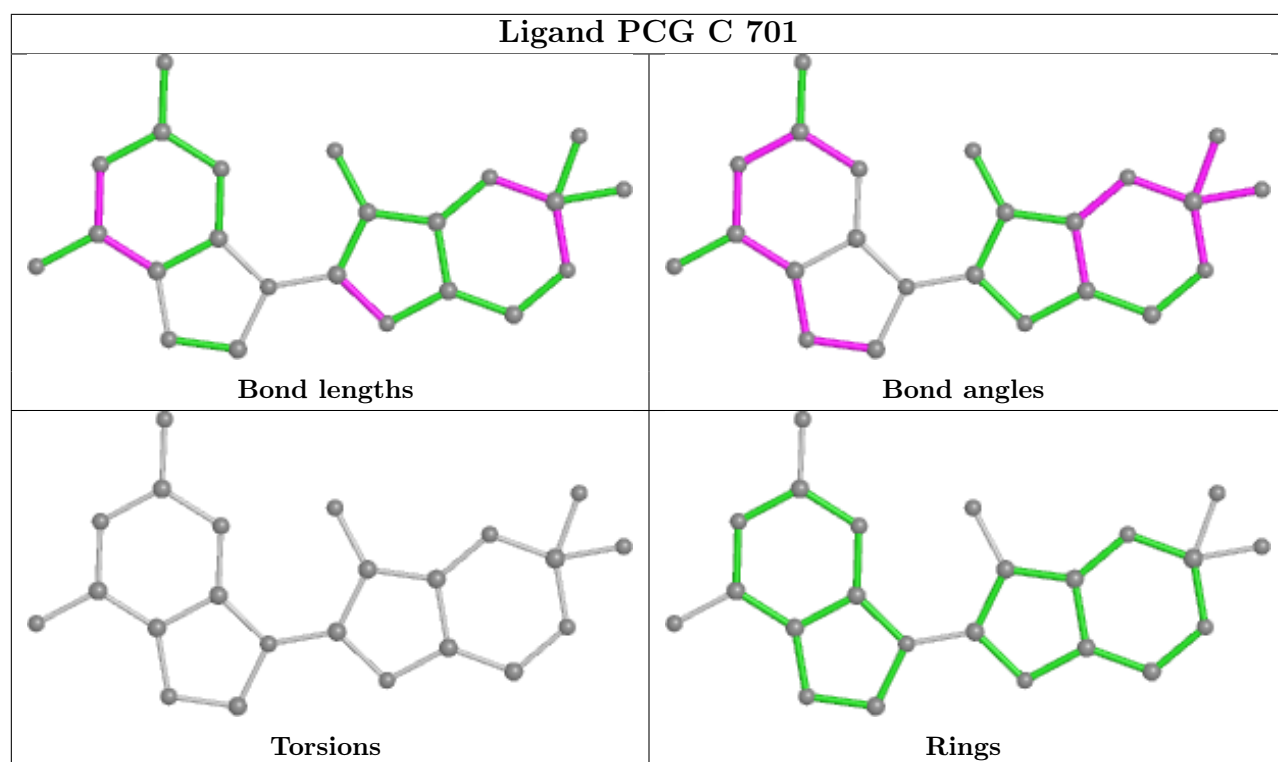
There are no torsion outliers.

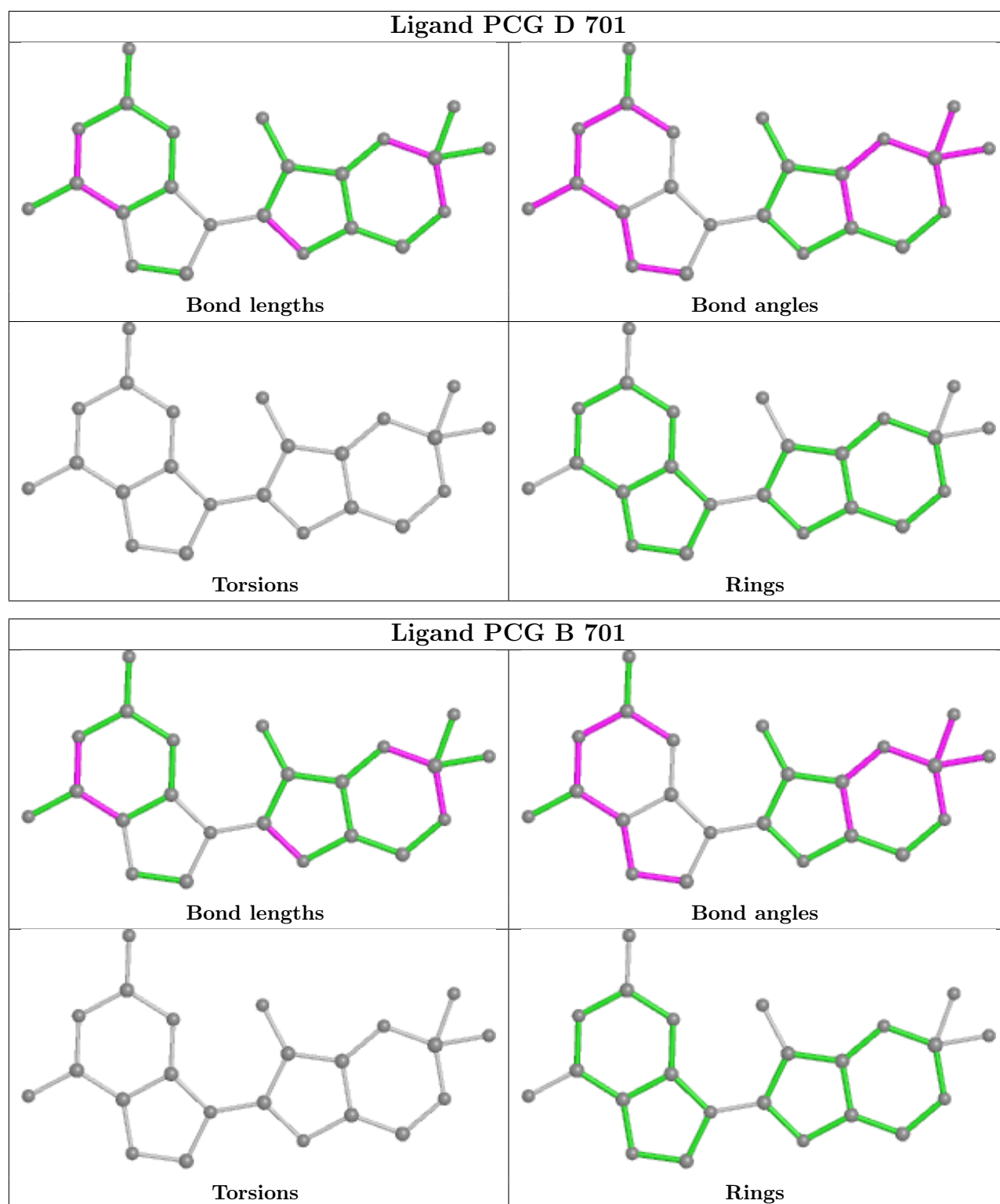
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	PCG	1	0
2	A	701	PCG	1	0
2	D	701	PCG	1	0
2	B	701	PCG	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

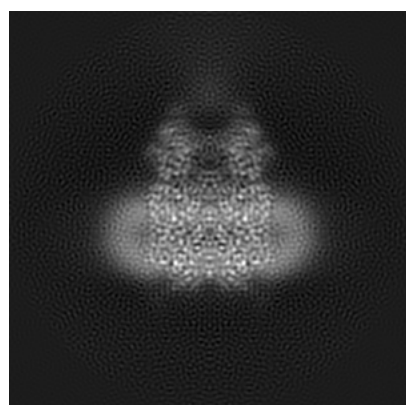
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23308. These allow visual inspection of the internal detail of the map and identification of artifacts.

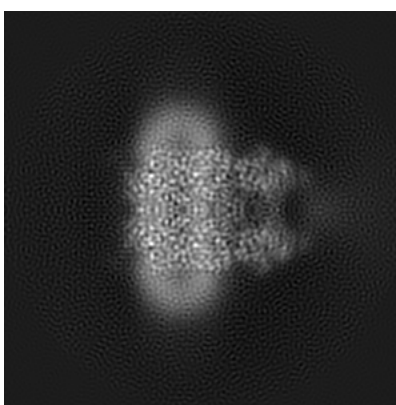
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

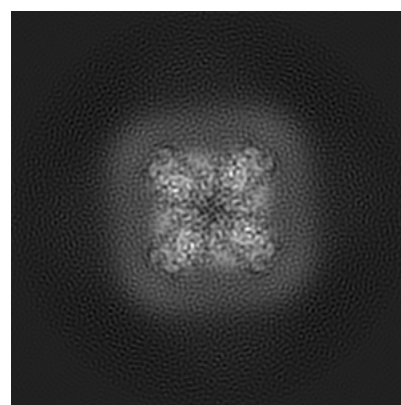
6.1.1 Primary map



X



Y

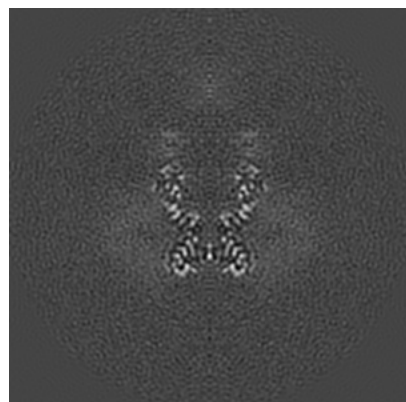


Z

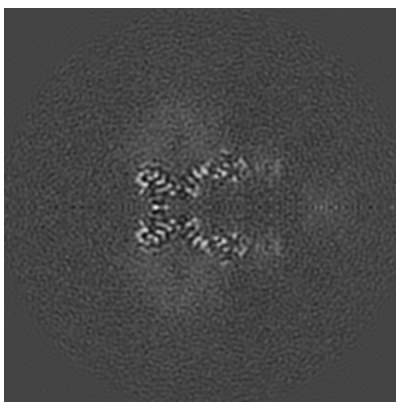
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

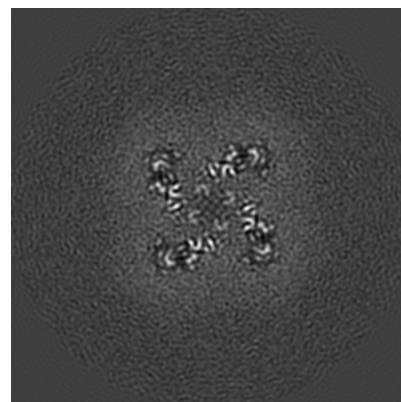
6.2.1 Primary map



X Index: 144



Y Index: 144

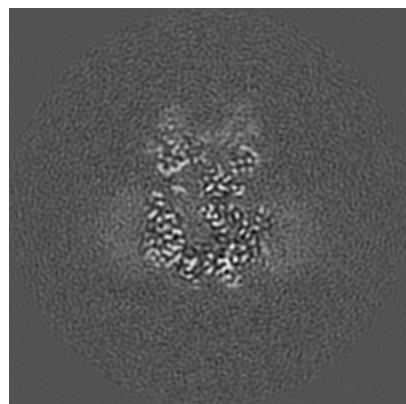


Z Index: 144

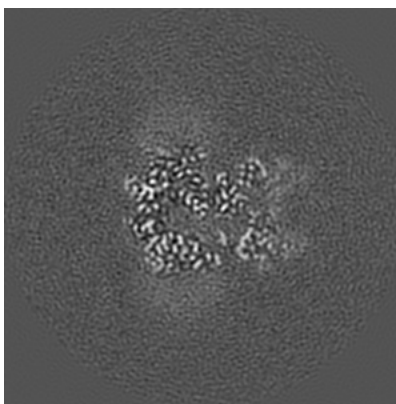
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

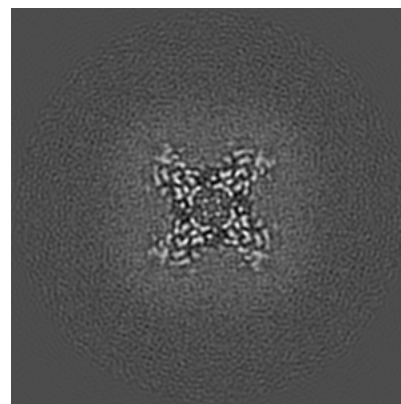
6.3.1 Primary map



X Index: 120



Y Index: 168

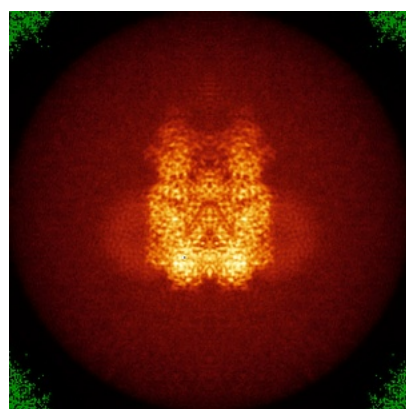


Z Index: 106

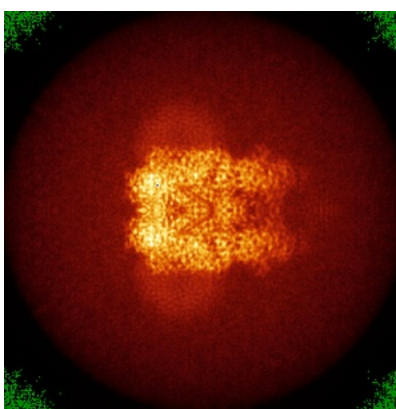
The images above show the largest variance slices of the map in three orthogonal directions.

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

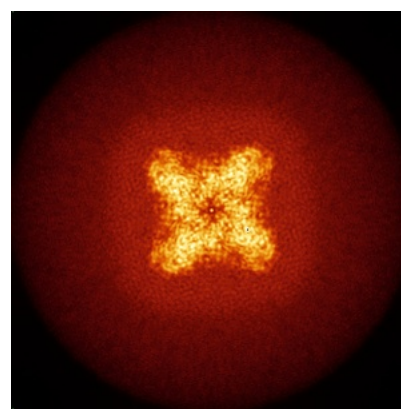
6.4.1 Primary map



X



Y

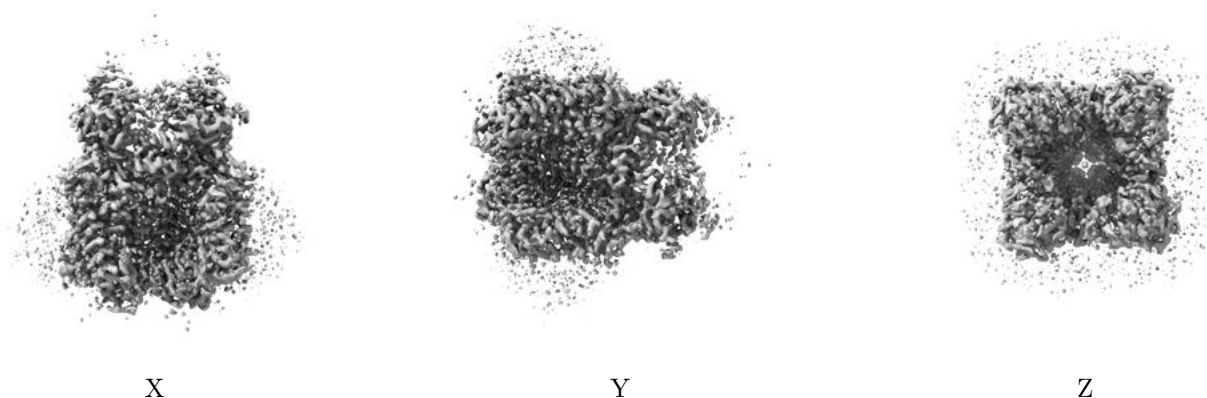


Z

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 0.021. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

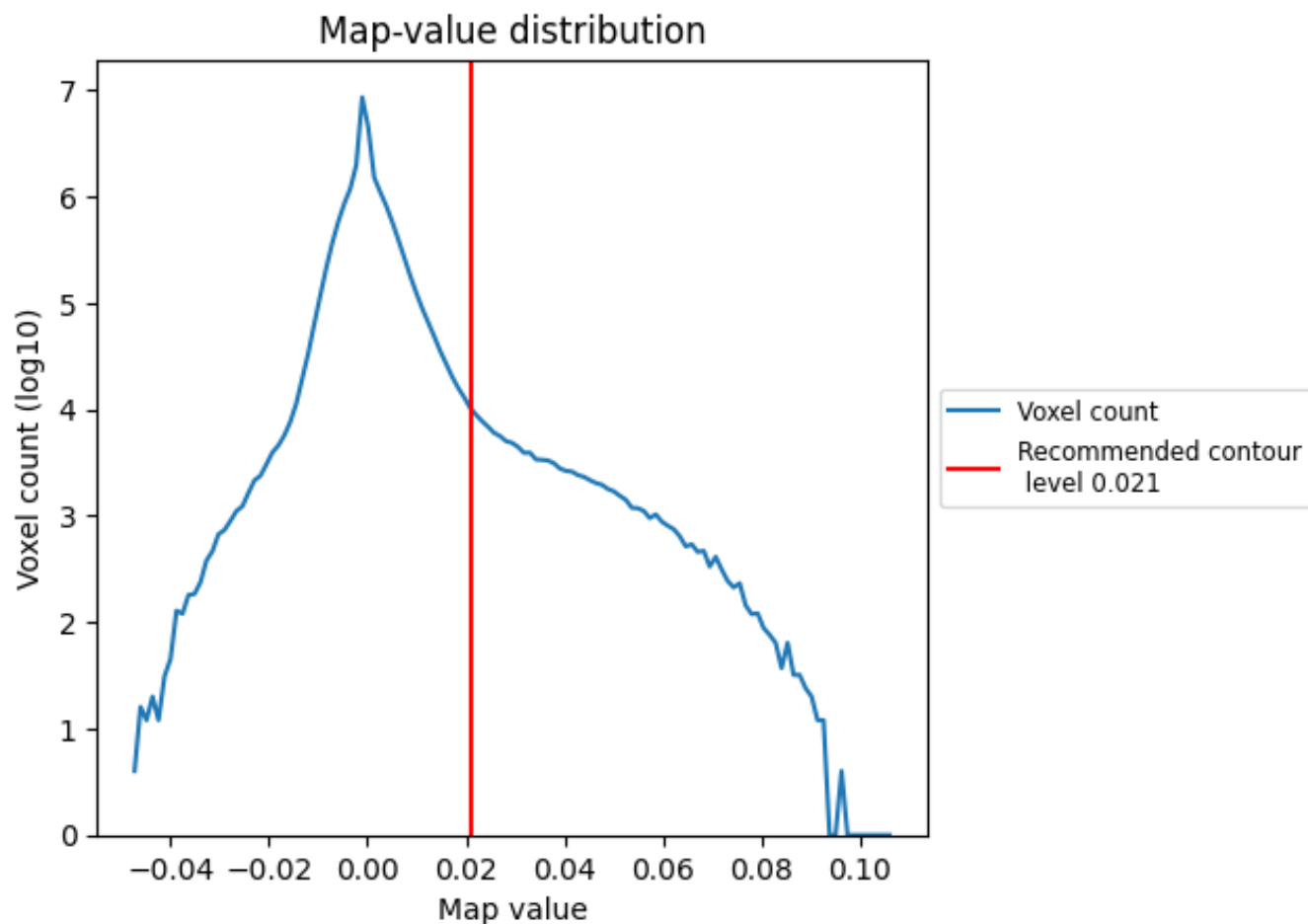
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

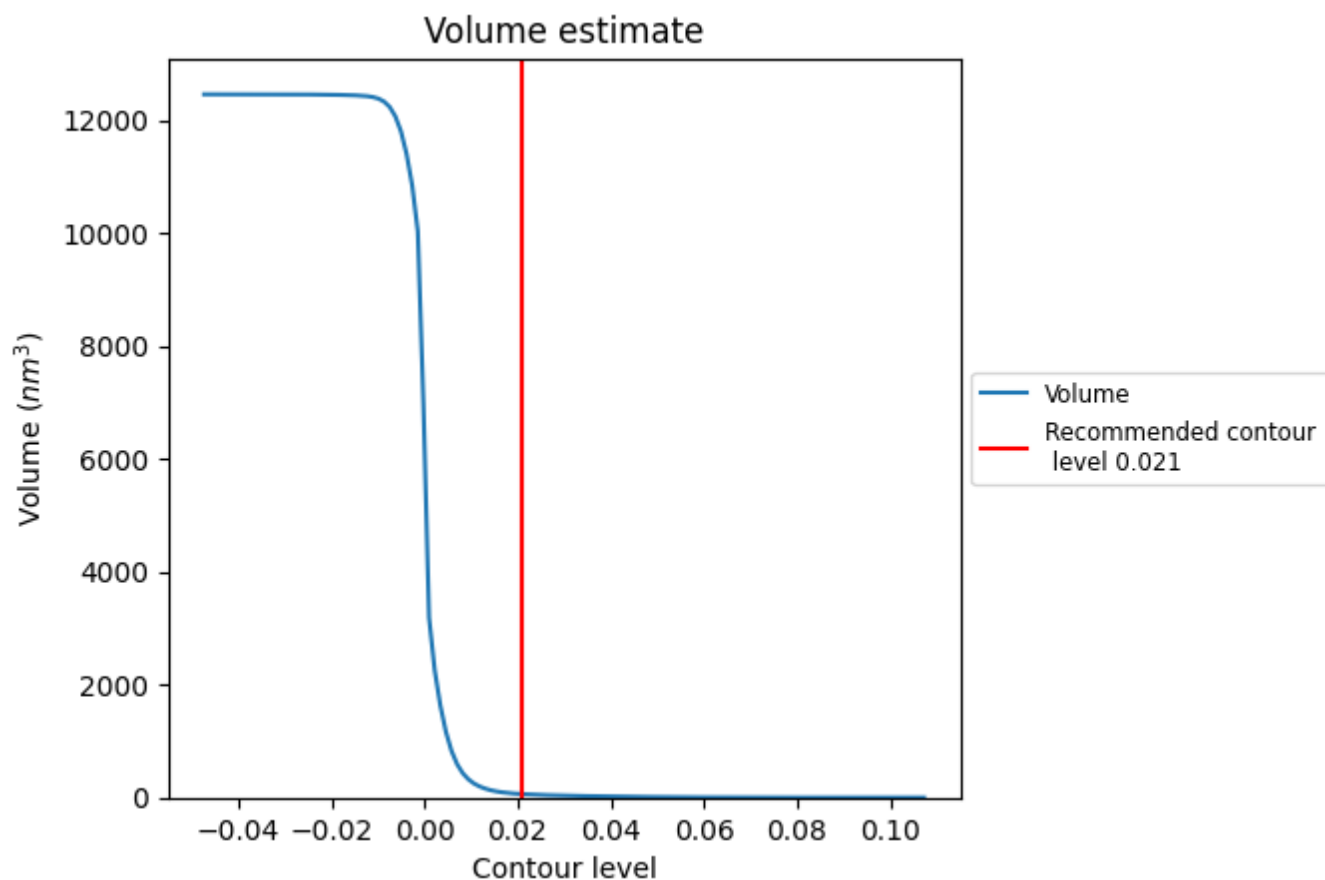
This section contains the results of statistical analysis of the map.

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.

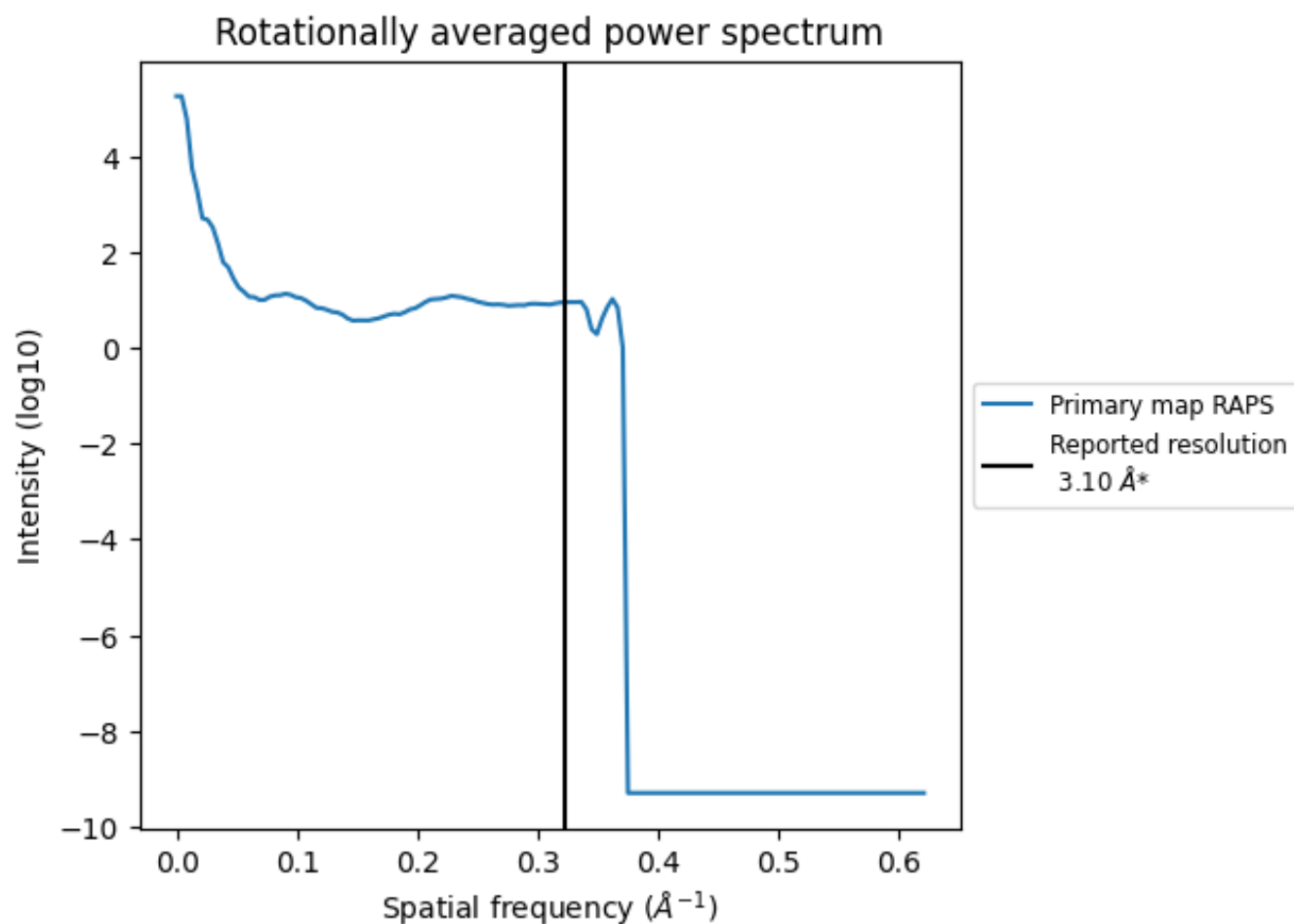
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 62 nm³; this corresponds to an approximate mass of 56 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 ⓘ

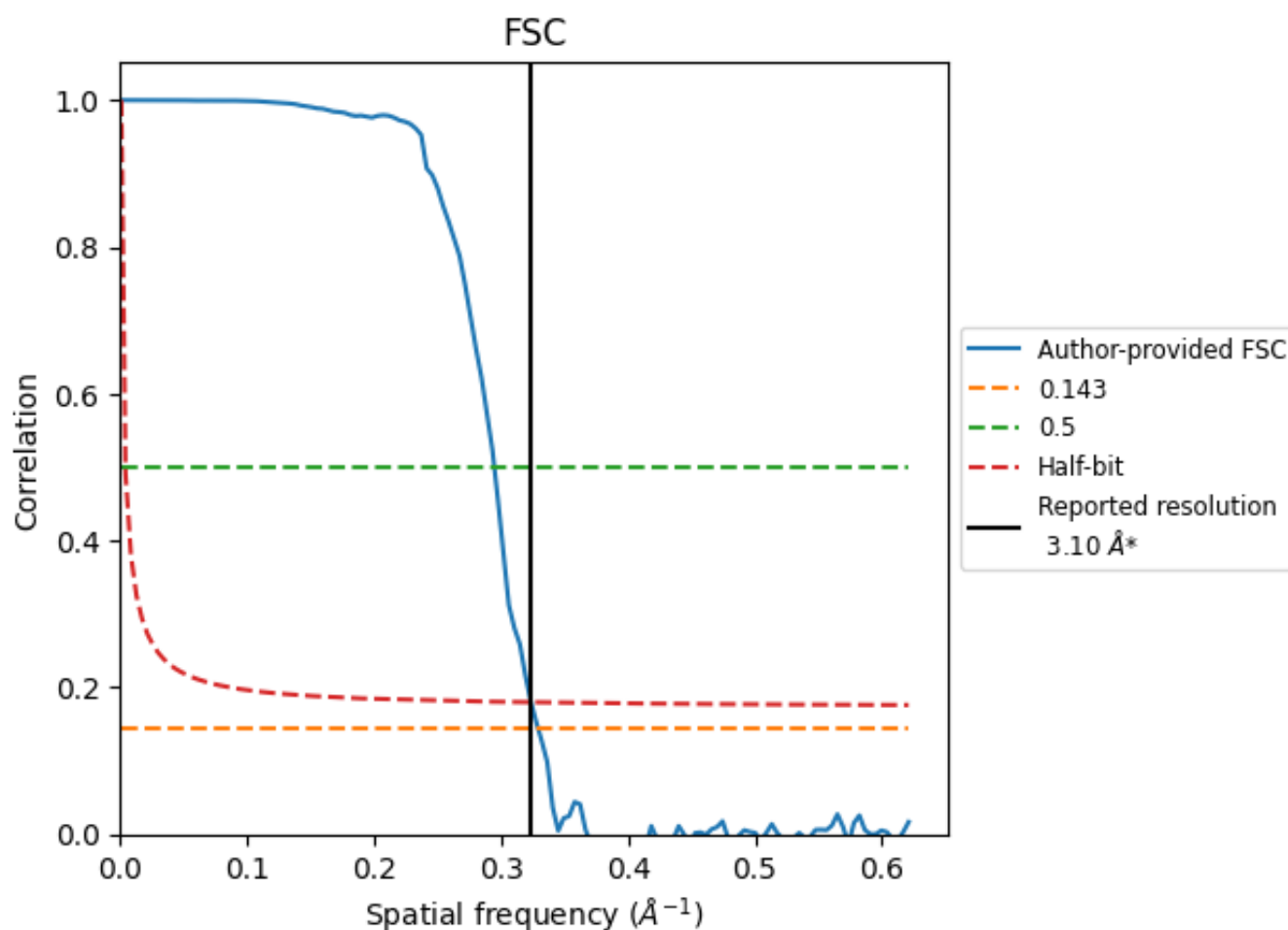


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

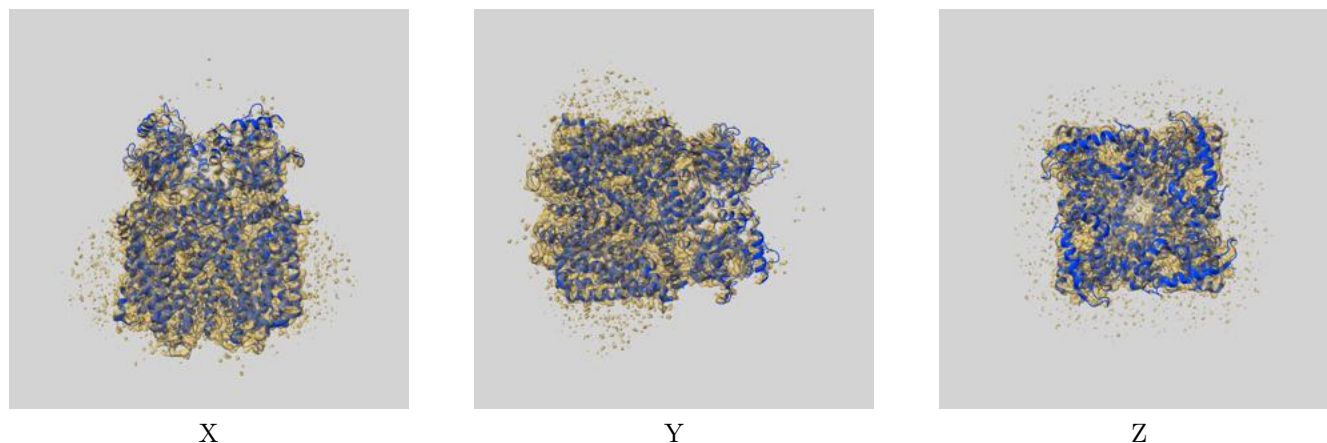
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.04	3.39	3.09
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

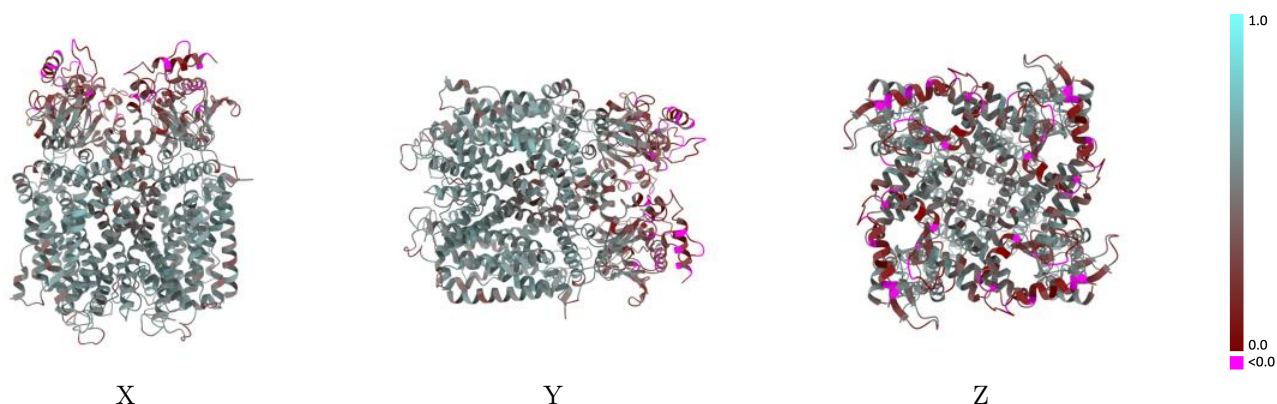
This section contains information regarding the fit between EMDB map EMD-23308 and PDB model 7LFX. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



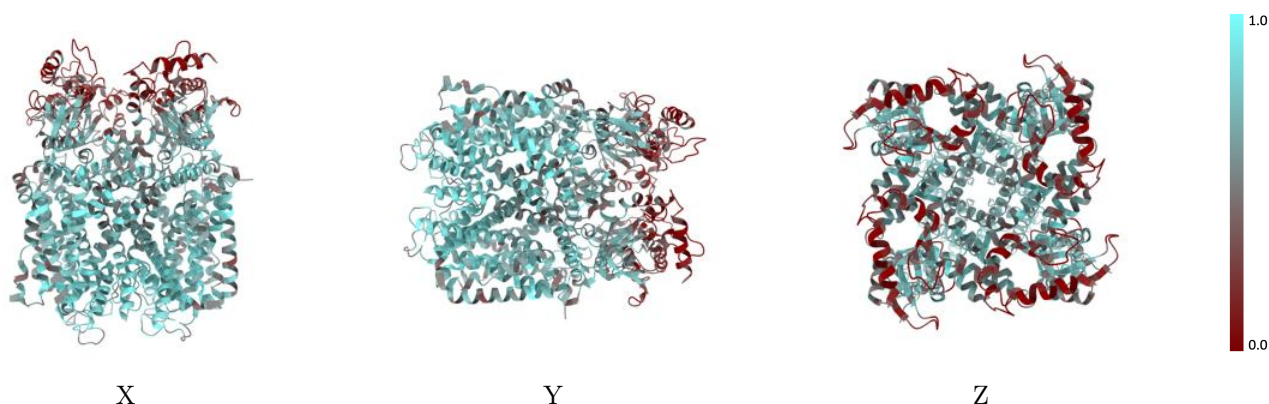
The images above show the 3D surface view of the map at the recommended contour level 0.021 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



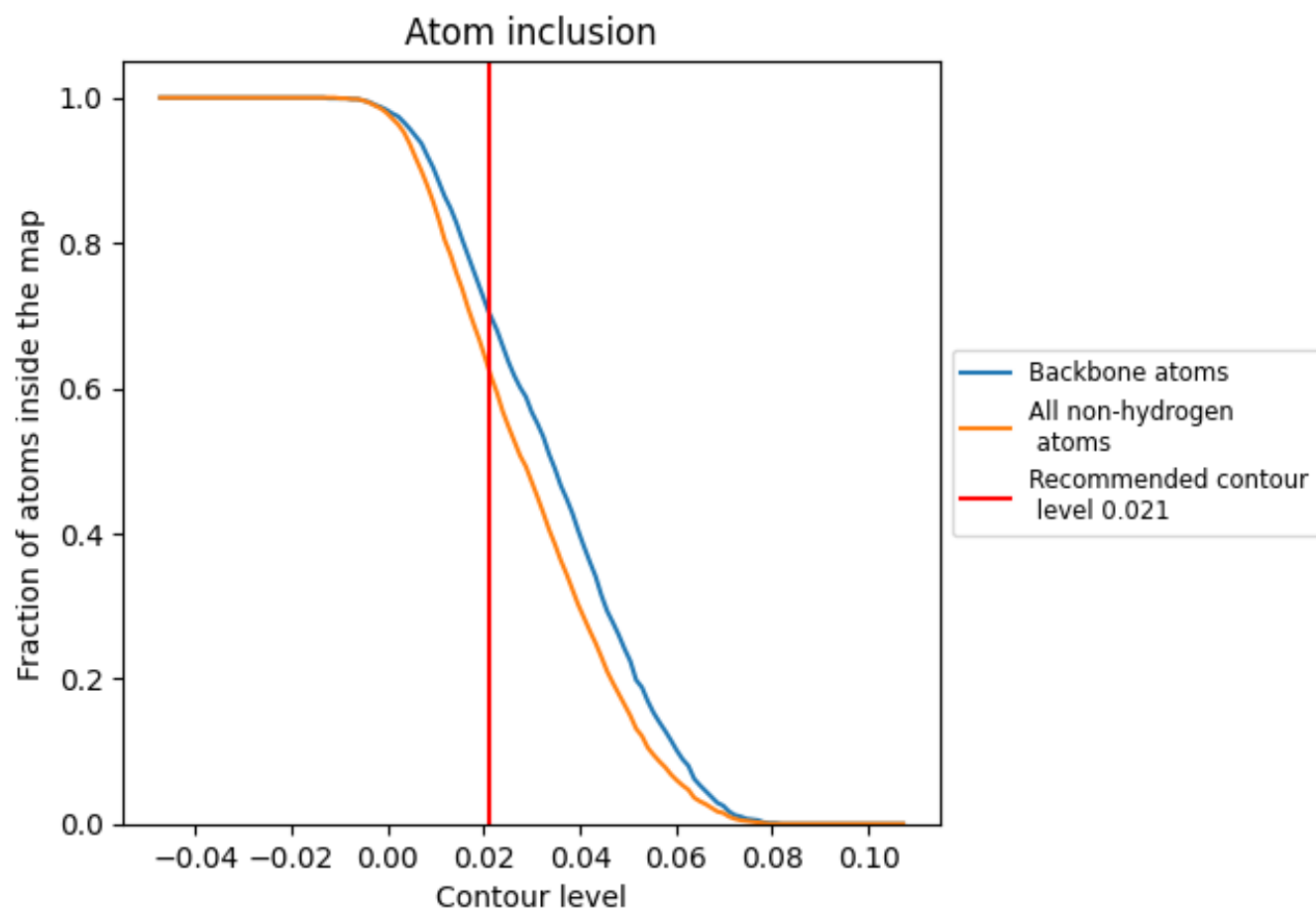
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.021).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 63% 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 (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6270	<div></div> 0.4580
A	<div></div> 0.6270	<div></div> 0.4580
B	<div></div> 0.6270	<div></div> 0.4580
C	<div></div> 0.6270	<div></div> 0.4580
D	<div></div> 0.6260	<div></div> 0.4580

