



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 08:44 PM UTC

PDB ID : 7CR4 / pdb_00007cr4
EMDB ID : EMD-30447
Title : human KCNQ2-CaM in complex with ztz240
Authors : Li, X.; Lv, D.; Wang, J.; Ye, S.; Guo, J.
Deposited on : 2020-08-12
Resolution : 3.90 Å(reported)

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

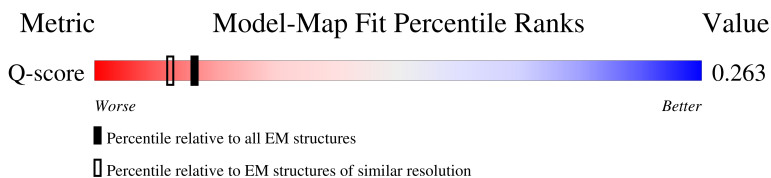
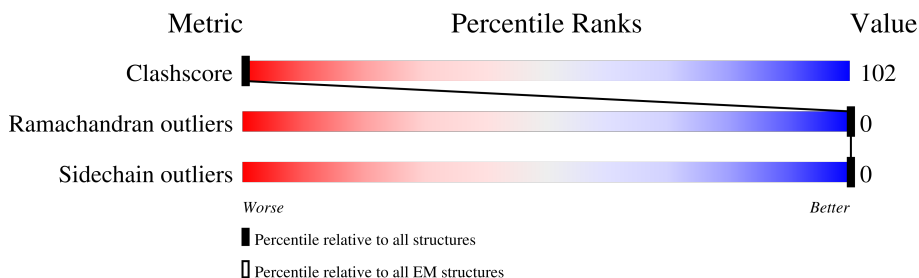
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	656	11% 11% 42% 47%
1	B	656	11% 11% 43% 47%
1	D	656	11% 11% 43% 47%
1	F	656	11% 11% 43% 47%

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Mol	Chain	Length	Quality of chain
2	C	149	
2	E	149	
2	G	149	
2	H	149	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GB9	A	1001	-	X	X	-
3	GB9	B	1001	-	X	X	-
3	GB9	D	1001	-	X	X	-
3	GB9	F	1001	-	X	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16020 atoms, of which 32 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 Potassium voltage-gated channel subfamily KQT member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	349	Total	C	N	O	S	0	0
			2855	1870	498	474	13		
1	B	349	Total	C	N	O	S	0	0
			2855	1870	498	474	13		
1	D	349	Total	C	N	O	S	0	0
			2855	1870	498	474	13		
1	F	349	Total	C	N	O	S	0	0
			2855	1870	498	474	13		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	MET	-	initiating methionine	UNP O43526
A	703	VAL	-	expression tag	UNP O43526
A	704	GLU	-	expression tag	UNP O43526
A	705	GLY	-	expression tag	UNP O43526
A	706	GLY	-	expression tag	UNP O43526
A	707	SER	-	expression tag	UNP O43526
A	708	SER	-	expression tag	UNP O43526
A	709	GLY	-	expression tag	UNP O43526
A	710	GLY	-	expression tag	UNP O43526
A	711	TRP	-	expression tag	UNP O43526
A	712	SER	-	expression tag	UNP O43526
A	713	HIS	-	expression tag	UNP O43526
A	714	PRO	-	expression tag	UNP O43526
A	715	GLN	-	expression tag	UNP O43526
A	716	PHE	-	expression tag	UNP O43526
A	717	GLU	-	expression tag	UNP O43526
A	718	LYS	-	expression tag	UNP O43526
B	63	MET	-	initiating methionine	UNP O43526
B	703	VAL	-	expression tag	UNP O43526
B	704	GLU	-	expression tag	UNP O43526
B	705	GLY	-	expression tag	UNP O43526
B	706	GLY	-	expression tag	UNP O43526

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Chain	Residue	Modelled	Actual	Comment	Reference
B	707	SER	-	expression tag	UNP O43526
B	708	SER	-	expression tag	UNP O43526
B	709	GLY	-	expression tag	UNP O43526
B	710	GLY	-	expression tag	UNP O43526
B	711	TRP	-	expression tag	UNP O43526
B	712	SER	-	expression tag	UNP O43526
B	713	HIS	-	expression tag	UNP O43526
B	714	PRO	-	expression tag	UNP O43526
B	715	GLN	-	expression tag	UNP O43526
B	716	PHE	-	expression tag	UNP O43526
B	717	GLU	-	expression tag	UNP O43526
B	718	LYS	-	expression tag	UNP O43526
D	63	MET	-	initiating methionine	UNP O43526
D	703	VAL	-	expression tag	UNP O43526
D	704	GLU	-	expression tag	UNP O43526
D	705	GLY	-	expression tag	UNP O43526
D	706	GLY	-	expression tag	UNP O43526
D	707	SER	-	expression tag	UNP O43526
D	708	SER	-	expression tag	UNP O43526
D	709	GLY	-	expression tag	UNP O43526
D	710	GLY	-	expression tag	UNP O43526
D	711	TRP	-	expression tag	UNP O43526
D	712	SER	-	expression tag	UNP O43526
D	713	HIS	-	expression tag	UNP O43526
D	714	PRO	-	expression tag	UNP O43526
D	715	GLN	-	expression tag	UNP O43526
D	716	PHE	-	expression tag	UNP O43526
D	717	GLU	-	expression tag	UNP O43526
D	718	LYS	-	expression tag	UNP O43526
F	63	MET	-	initiating methionine	UNP O43526
F	703	VAL	-	expression tag	UNP O43526
F	704	GLU	-	expression tag	UNP O43526
F	705	GLY	-	expression tag	UNP O43526
F	706	GLY	-	expression tag	UNP O43526
F	707	SER	-	expression tag	UNP O43526
F	708	SER	-	expression tag	UNP O43526
F	709	GLY	-	expression tag	UNP O43526
F	710	GLY	-	expression tag	UNP O43526
F	711	TRP	-	expression tag	UNP O43526
F	712	SER	-	expression tag	UNP O43526
F	713	HIS	-	expression tag	UNP O43526
F	714	PRO	-	expression tag	UNP O43526

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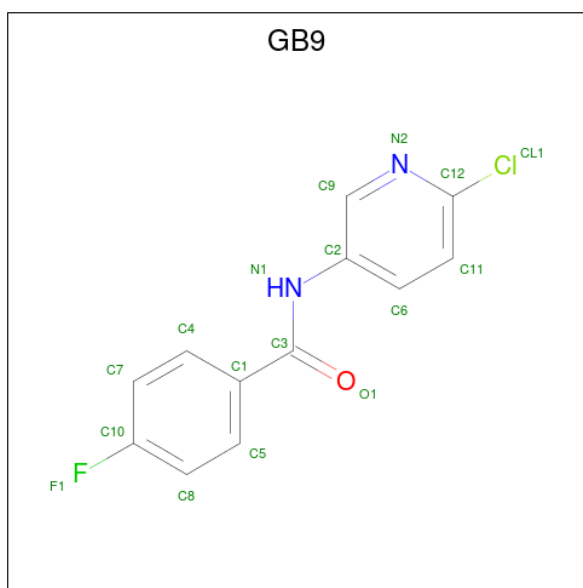
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Chain	Residue	Modelled	Actual	Comment	Reference
F	715	GLN	-	expression tag	UNP O43526
F	716	PHE	-	expression tag	UNP O43526
F	717	GLU	-	expression tag	UNP O43526
F	718	LYS	-	expression tag	UNP O43526

- Molecule 2 is a protein called Calmodulin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	143	Total	C	N	O	S	0	0
			1125	690	181	245	9		
2	C	143	Total	C	N	O	S	0	0
			1125	690	181	245	9		
2	E	143	Total	C	N	O	S	0	0
			1125	690	181	245	9		
2	G	143	Total	C	N	O	S	0	0
			1125	690	181	245	9		

- Molecule 3 is N-(6-chloranilpyridin-3-yl)-4-fluoranyl-benzamide (CCD ID: GB9) (formula: C₁₂H₈ClFN₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
3	A	1	Total	C	Cl	F	H	N	O	0
			25	12	1	1	8	2	1	
3	B	1	Total	C	Cl	F	H	N	O	0
			25	12	1	1	8	2	1	
3	D	1	Total	C	Cl	F	H	N	O	0
			25	12	1	1	8	2	1	

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Mol	Chain	Residues	Atoms							AltConf
			Total	C	Cl	F	H	N	O	
3	F	1	25	12	1	1	8	2	1	0

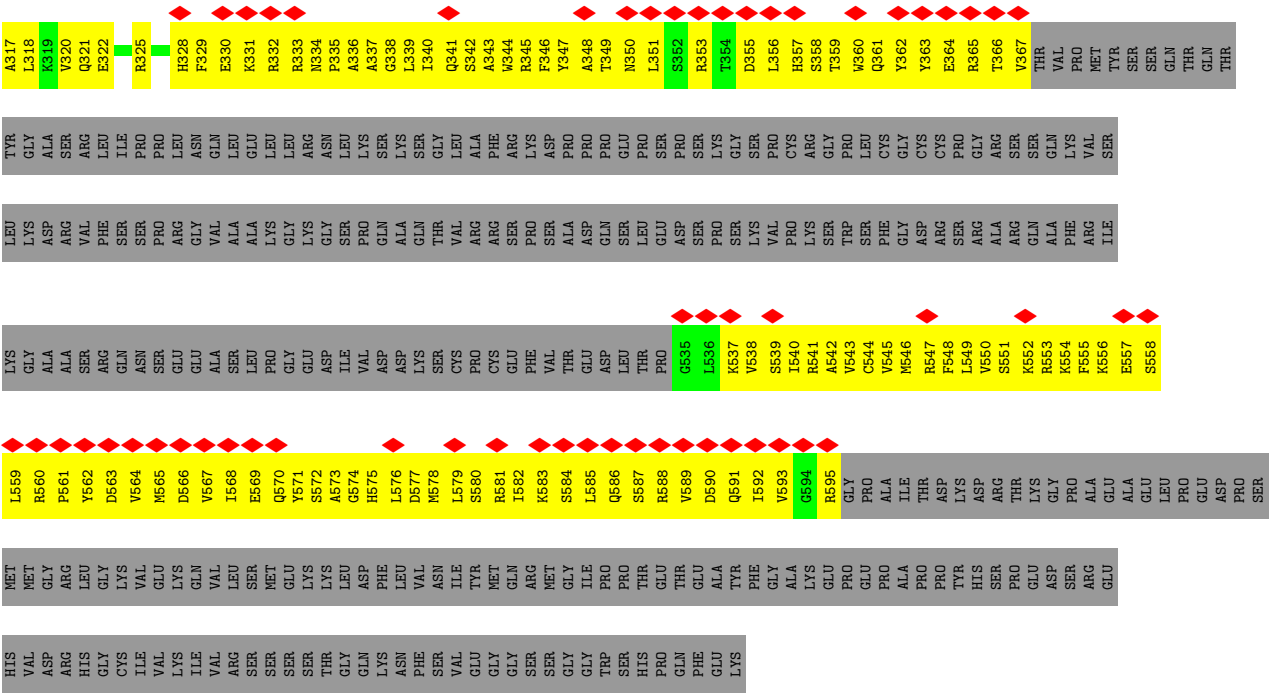
[illegible]

L126	L127	L128	L129	E130	I131	V132	T133	I134	V135	V136	F137	G138	V139	E140	Y141	F142	V143	R144	I145	V146	A147	A148	G149	C150	C151	C152	R153	Y154	R155	R158	G159	R160	L161	K162	F163	A164	R165	K166	P167	F168	C169	V170	I171	D172	I173	V174	V175	L176	I177	A178	S179	I180	A181	V182	L183	A184	ALA	GLY
SER	GLN	GLY	ASN	VAL	PHE	ALA	THR	S196	A196	L197	R198	S199	L200	F201	R202	L203	Q204	I205	L206	R207	M208	I209	R210	M211	D212	R213	R214	T217	W218	K219	L220	L221	G222	S223	N289	V224	V225	Y226	A227	H228	S229	K230	E231	L232	V233	T234	A235	I238	G239	F240	L241	C242	I243	L244	L245	A246	S247	F248
L249	V250	Y251	L252	A253	E254	K255	G256	E257	N258	D259	H260	F261	D262	T263	Y264	A265	D266	A267	W268	L268	L269	L272	I273	T276	T277	I278	D282	K283	Y284	P285	Q286	W288	G290	R291	L292	L293	A294	A295	T296	F297	T298	L299	V302	S303	F304	F305	A306	L307	P308	I311	L312	G313						
F316	A317	L318	K319	V320	Q321	E322	R325	H328	F329	E330	K331	R332	R333	R334	P335	A336	A337	G338	L339	I340	S341	Q342	A343	W344	R345	F346	Y347	A348	PRO	GLN	N350	L351	R352	R353	T354	D355	L356	H357	S358	T359	W360	Q361	Y362	Y363	E364	R365	L366	T367	THR	VAL	PRO	MET	TYR	SER	SER	GLN	THR	GLN
THR	TYR	GLY	ALA	SER	ARG	LEU	ILE	SER	PRO	PRO	ASN	GLN	LEU	ALA	GLY	LEU	GLY	ASN	LEU	SER	LEU	LEU	ALA	ALA	PHE	ARG	LYS	ASP	PRO	ALA	PRO	GLU	GLY	SER	LYS	GLY	SER	GLY	PRO	LEU	CYS	CYS	CYS	CYS	PRO	GLY	ARG	SER	ARG	SER	GLN	GLN	GLY	VAL				
SER	LEU	LYS	ASP	ARG	VAL	PHE	SER	ASN	PRO	PRO	GLY	VAL	ALA	ALA	LYS	GLY	LYS	SER	PRO	GLN	GLN	THR	VAL	ARG	ARG	PRO	LYS	ASP	GLY	VAL	GLN	LEU	ASP	PRO	SER	PRO	SER	LYS	VAL	VAL	VAL	VAL	PHE	ASP	TRP	SER	PHE	GLY	ARG									
ILE	GLY	GLY	ALA	ALA	SER	ARG	GLN	ASN	SER	GLY	ALA	SER	SER	PRO	PRO	GLY	ASP	ILE	VAL	ASP	ASP	LYS	SER	CYS	PRO	CYS	THR	GLY	THR	GLU	LEU	THR	PRO	G335	L336	K337	V338	S339	R340	A341	V342	V343	C344	V345	M346	F347	L348	V349	V350	S351	K352	R353	F354	F355	K356	E357		
S558	L559	R560	P561	Y562	D563	V564	M565	D566	V567	I568	E569	Q570	Y571	S572	G573	G574	H575	L576	D577	M578	L579	S580	R581	I582	K583	S584	L585	Q586	S587	R588	V589	D590	Q591	I592	V593	G594	R595	GLY	PRO	ALA	ILE	THR	PRO	ASP	LYS	ASP	ARG	THR	LYS	GLY	ALA	GLU	PRO	GLU	ASP	PRO		
SER	MET	GLY	ARG	LEU	GLY	LYS	VAL	GLN	VAL	LEU	SER	SER	GLU	LYS	LYS	THR	GLY	ASP	PHE	VAL	ASN	ILE	TYR	GLY	GLY	GLY	ILE	TRP	PRO	PRO	THR	GLU	THR	ALA	PHE	GLY	ALA	LYS	GLU	PRO	PRO	PRO	ALA	ALA	PRO	TYR	TYR	HIS	SER	PRO	GLU	ASP	SER	ARG				
GLU	HIS	VAL	ASP	ARG	HIS	GLY	CYS	ILE	VAL	VAL	SER	SER	SER	SER	THR	GLY	GLN	ASN	PHE	SER	VAL	VAL	GLU	GLY	GLY	GLY	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS	THR	GLY	ALA	LYS	GLU	PRO	PRO	PRO	ALA	ALA	PRO	TYR	TYR	HIS	SER	PRO	GLU	ASP	SER	ARG				

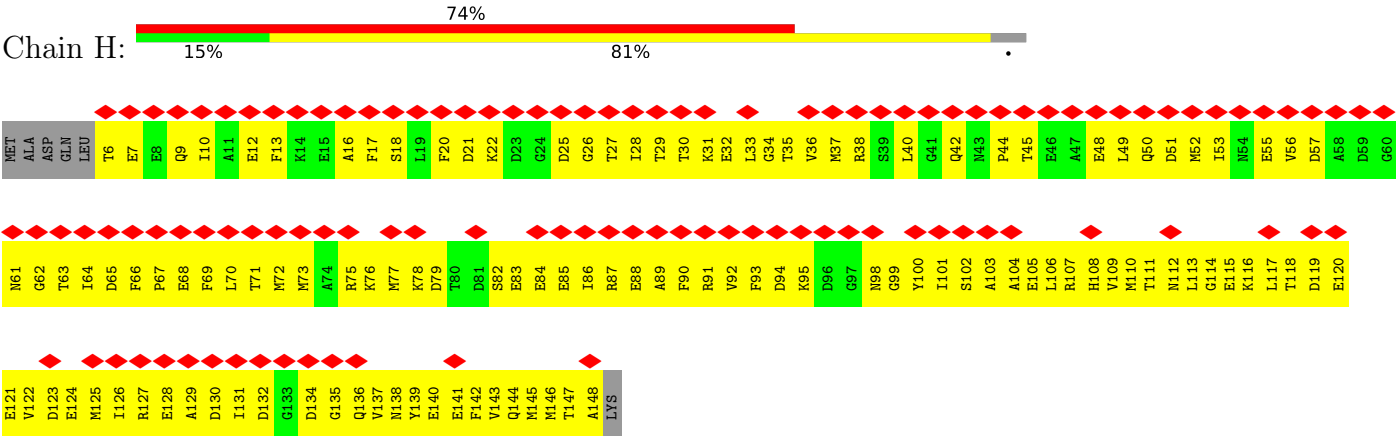
• Molecule 1: Potassium voltage-gated channel subfamily KQT member 2



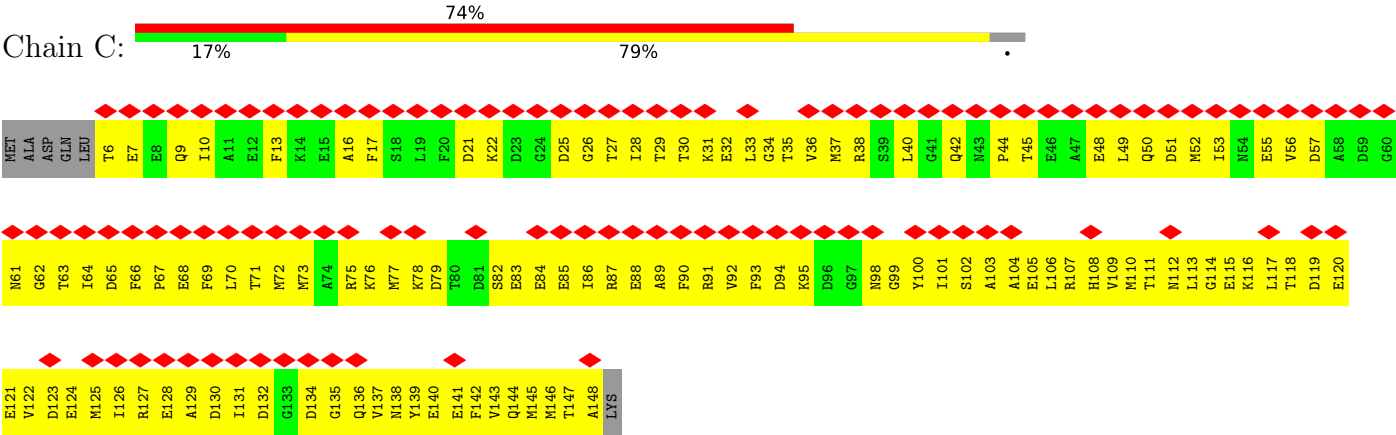
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GLY	ASN	VAL	PHE	ALA	THR	S196	A196	L197	R198	S199	L200	R201	F202	L203	Q204	I205	L206	R207	M208	I209	R210	M211	D212	R213	R214	T217	W218	K219	L220	L221	G222	S223	V224	V225	Y226	A227	H228	S229	K230	E231	L232	F233	T234	A235	I238	G239	F240	L241	C242	L243	I244	L245	A246	S247	F248	L249	V250
L126	Y127	I128	L129	E130	I131	V132	T133	I134	V135	V136	F137	G138	V139	E140	Y141	F142	V143	R144	I145	W146	A147	A148	G149	C150	C151	C152	R153	Y154	R155	R158	G159	R160	L161	K162	F163	A164	R165	K166	P167	F168	C169	V170	I173	L176	I177	A178	S179	I180	A181	V182	L183	A184	ALA	GLY	SER	GLN	
MET	ALA	GLY	LYS	P80	P80	LYS	R70	N71	A72	F73	Y74	R75	K76	L77	Q78	N79	F80	L81	Y82	N83	W84	L85	E86	R87	P88	R89	A92	F93	I94	Y95	H96	A97	Y98	V99	F100	L101	L102	V103	F104	S106	C106	L107	V108	L109	S110	V111	F112	S113	T114	I115	K116	E119	S122	E123	G124	A125	



• Molecule 2: Calmodulin-3



• Molecule 2: Calmodulin-3



• Molecule 2: Calmodulin-3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86371	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.556	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.039	Depositor
Minimum map value	-0.024	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	243.36002, 243.36002, 243.36002	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	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: GB9

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	0.26	0/2926	0.43	0/3953
1	B	0.26	0/2926	0.43	0/3953
1	D	0.26	0/2926	0.42	0/3953
1	F	0.26	0/2926	0.43	0/3953
2	C	0.13	0/1137	0.33	0/1526
2	E	0.13	0/1137	0.33	0/1526
2	G	0.13	0/1137	0.33	0/1526
2	H	0.13	0/1137	0.33	0/1526
All	All	0.23	0/16252	0.40	0/21916

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	2855	0	2911	616	0
1	B	2855	0	2911	656	0
1	D	2855	0	2911	579	0
1	F	2855	0	2911	629	0
2	C	1125	0	1051	304	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1125	0	1051	309	0
2	G	1125	0	1051	300	0
2	H	1125	0	1051	331	0
3	A	17	8	0	13	0
3	B	17	8	0	13	0
3	D	17	8	0	13	0
3	F	17	8	0	13	0
All	All	15988	32	15848	3262	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 102.

The worst 5 of 3262 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:202:PHE:HA	1:A:205:ILE:HD12	1.19	1.15
1:D:202:PHE:HA	1:D:205:ILE:HD12	1.19	1.14
1:F:543:VAL:HA	1:F:546:MET:HE2	1.29	1.14
1:B:543:VAL:HA	1:B:546:MET:HE2	1.29	1.13
1:A:543:VAL:HA	1:A:546:MET:HE2	1.29	1.12

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	343/656 (52%)	323 (94%)	20 (6%)	0	100	100
1	B	343/656 (52%)	322 (94%)	21 (6%)	0	100	100
1	D	343/656 (52%)	323 (94%)	20 (6%)	0	100	100
1	F	343/656 (52%)	322 (94%)	21 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
2	E	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
2	G	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
2	H	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
All	All	1936/3220 (60%)	1846 (95%)	90 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	298/558 (53%)	298 (100%)	0	100	100
1	B	298/558 (53%)	298 (100%)	0	100	100
1	D	298/558 (53%)	298 (100%)	0	100	100
1	F	298/558 (53%)	298 (100%)	0	100	100
2	C	122/127 (96%)	122 (100%)	0	100	100
2	E	122/127 (96%)	122 (100%)	0	100	100
2	G	122/127 (96%)	122 (100%)	0	100	100
2	H	122/127 (96%)	122 (100%)	0	100	100
All	All	1680/2740 (61%)	1680 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	324	HIS
2	G	61	ASN
1	F	328	HIS
1	F	570	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	357	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	GB9	D	1001	-	18,18,18	5.34	16 (88%)	24,24,24	1.87	7 (29%)
3	GB9	B	1001	-	18,18,18	5.35	16 (88%)	24,24,24	1.86	7 (29%)
3	GB9	F	1001	-	18,18,18	5.35	16 (88%)	24,24,24	1.86	7 (29%)
3	GB9	A	1001	-	18,18,18	5.35	16 (88%)	24,24,24	1.87	7 (29%)

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	GB9	D	1001	-	-	0/8/8/8	0/2/2/2
3	GB9	B	1001	-	-	0/8/8/8	0/2/2/2
3	GB9	F	1001	-	-	0/8/8/8	0/2/2/2
3	GB9	A	1001	-	-	0/8/8/8	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	GB9	C8-C5	9.00	1.53	1.38
3	D	1001	GB9	C8-C5	8.98	1.53	1.38
3	B	1001	GB9	C8-C5	8.95	1.53	1.38
3	F	1001	GB9	C8-C5	8.95	1.53	1.38
3	B	1001	GB9	C4-C1	8.64	1.52	1.39

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	GB9	C2-C9-N2	-5.03	119.91	124.07
3	D	1001	GB9	C2-C9-N2	-5.00	119.94	124.07
3	B	1001	GB9	C2-C9-N2	-4.97	119.96	124.07
3	F	1001	GB9	C2-C9-N2	-4.97	119.96	124.07
3	D	1001	GB9	C11-C12-N2	-3.14	120.32	124.87

There are no chirality outliers.

There are no torsion outliers.

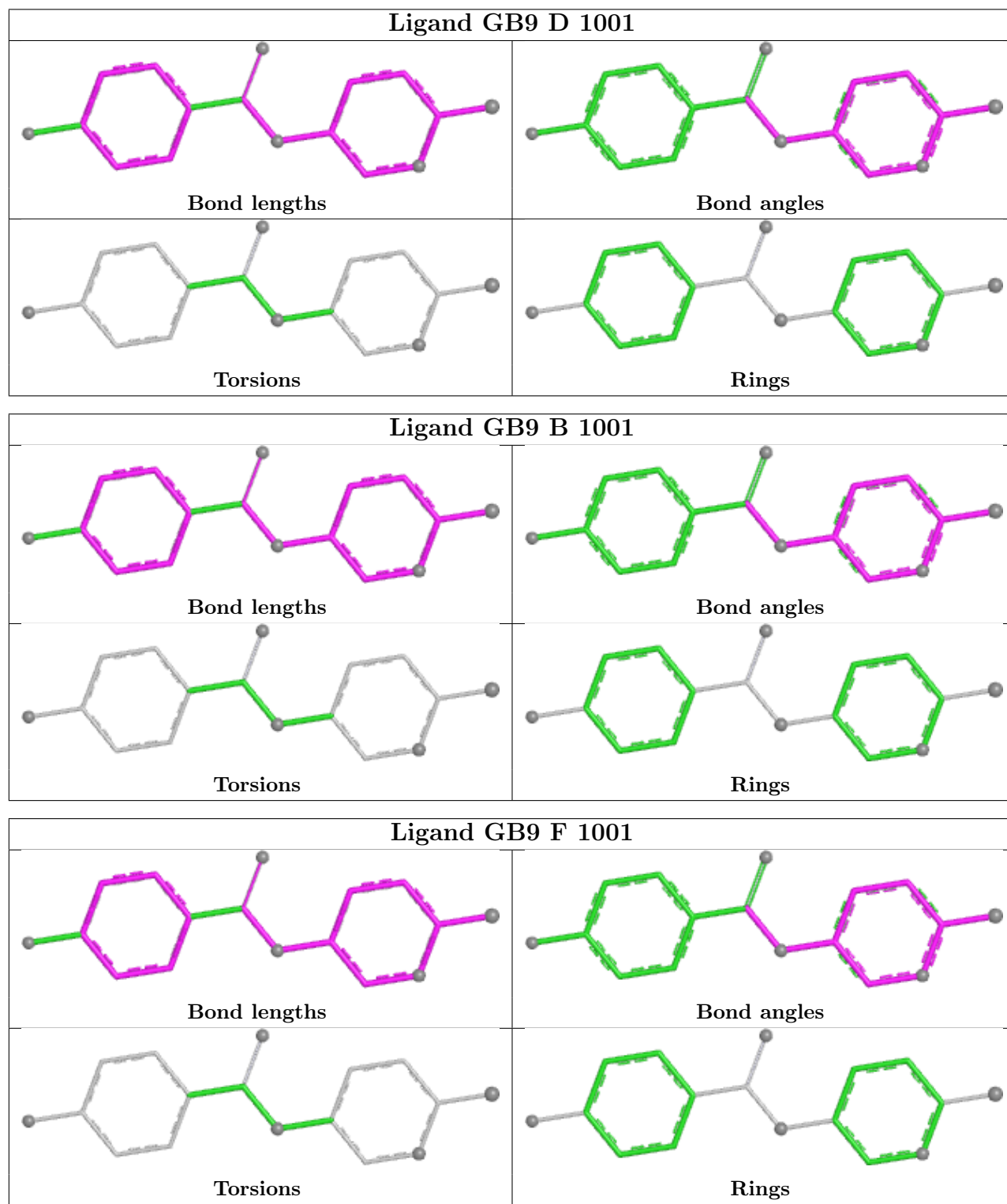
There are no ring outliers.

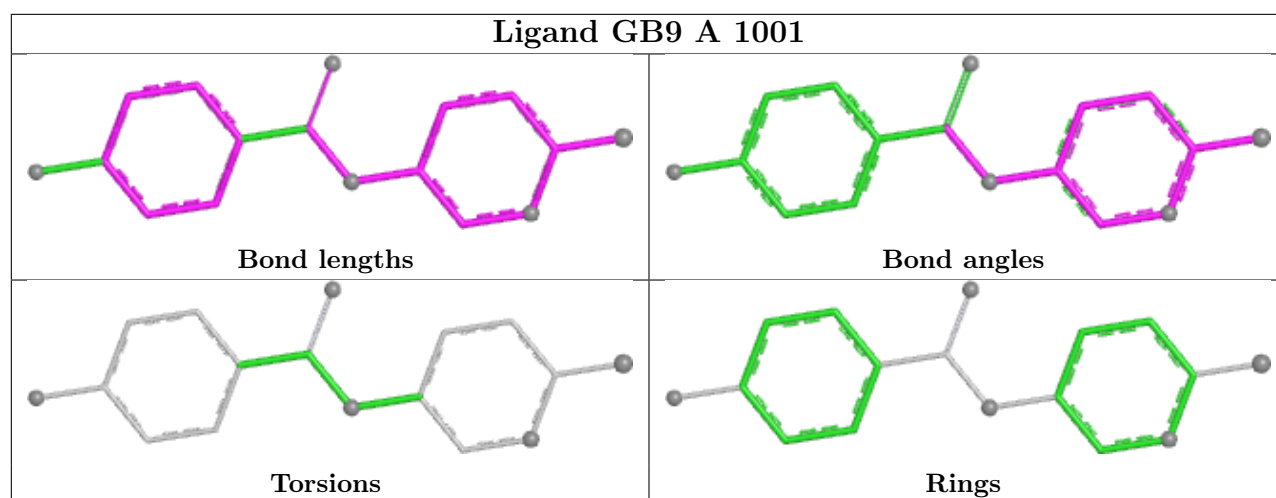
4 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1001	GB9	13	0
3	B	1001	GB9	13	0
3	F	1001	GB9	13	0
3	A	1001	GB9	13	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.

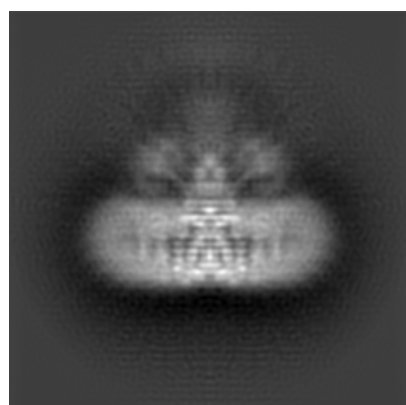
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30447. These allow visual inspection of the internal detail of the map and identification of artifacts.

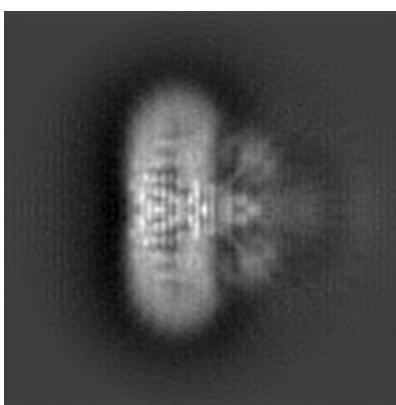
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

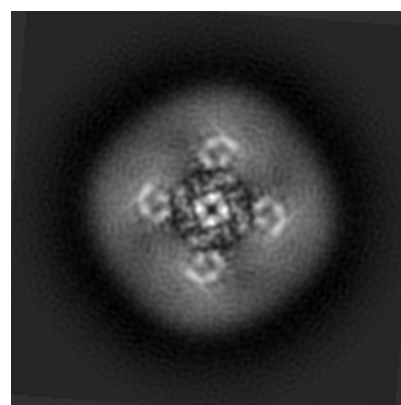
6.1.1 Primary map



X



Y

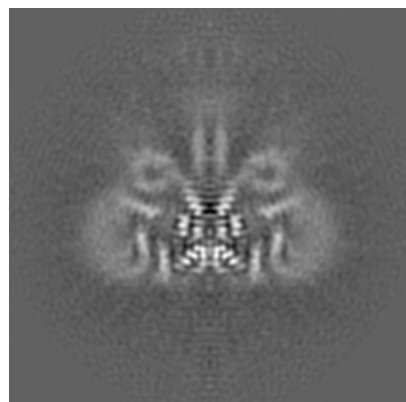


Z

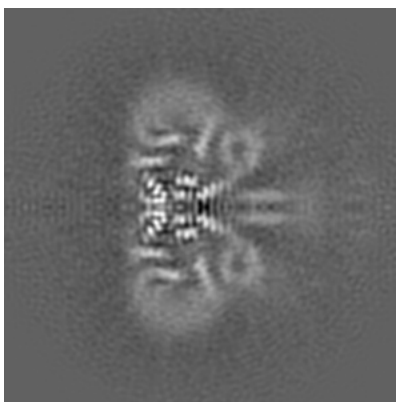
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

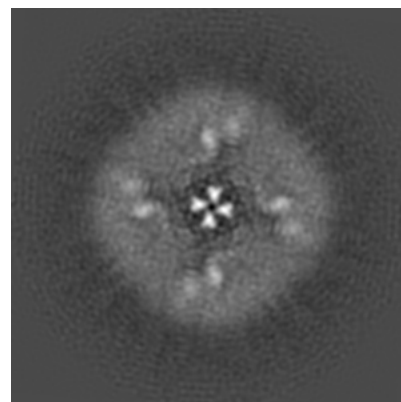
6.2.1 Primary map



X Index: 120



Y Index: 120

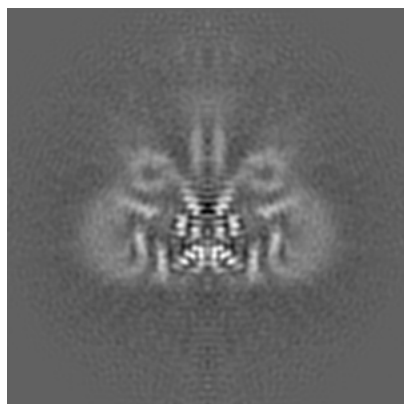


Z Index: 120

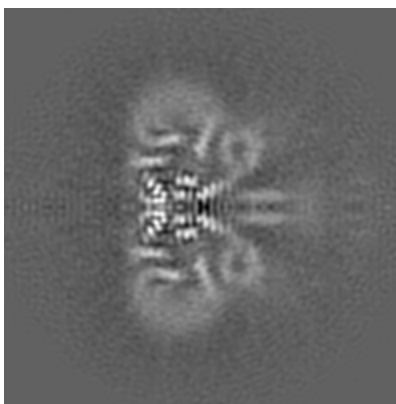
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

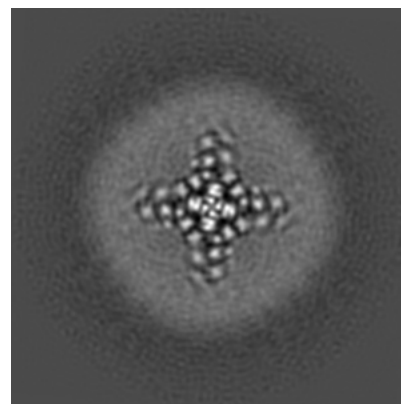
6.3.1 Primary map



X Index: 120



Y Index: 120

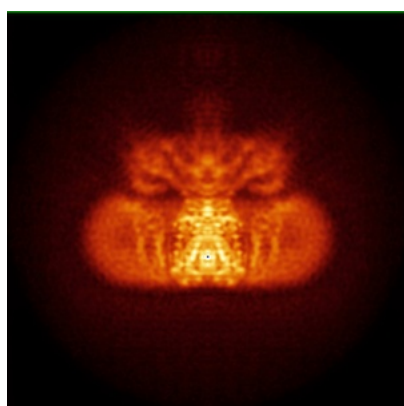


Z Index: 91

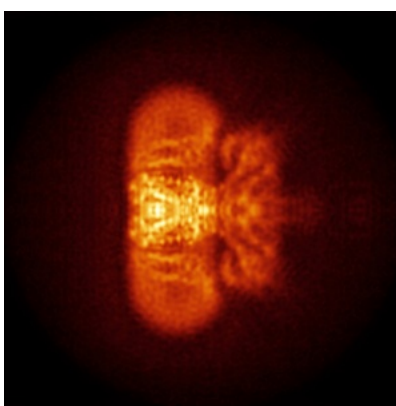
The images above show the largest variance slices of the map in three orthogonal directions.

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

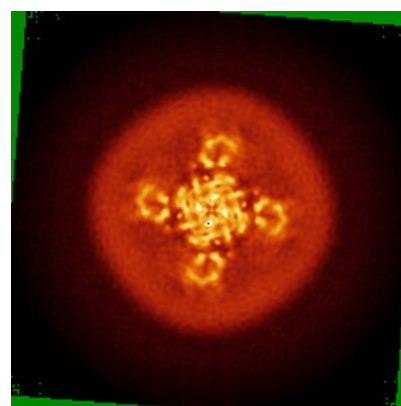
6.4.1 Primary map



X



Y

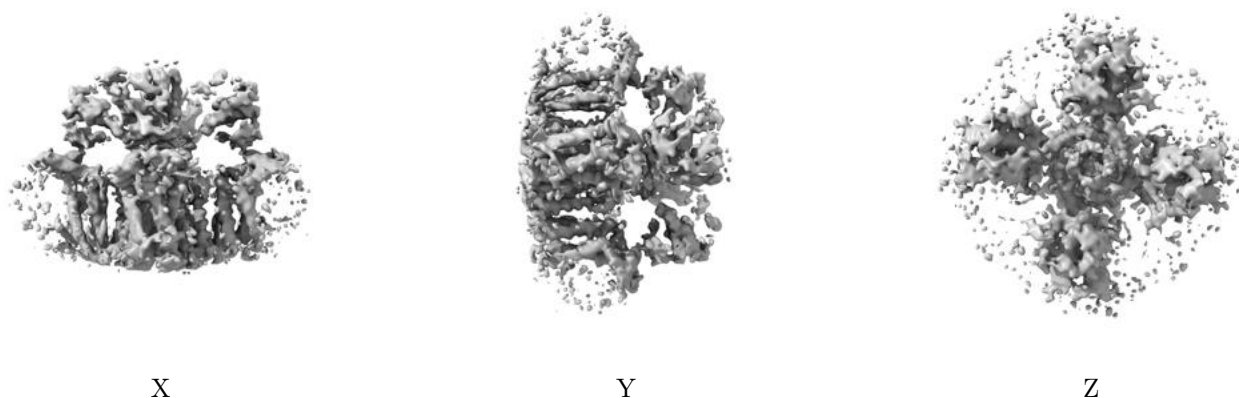


Z

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

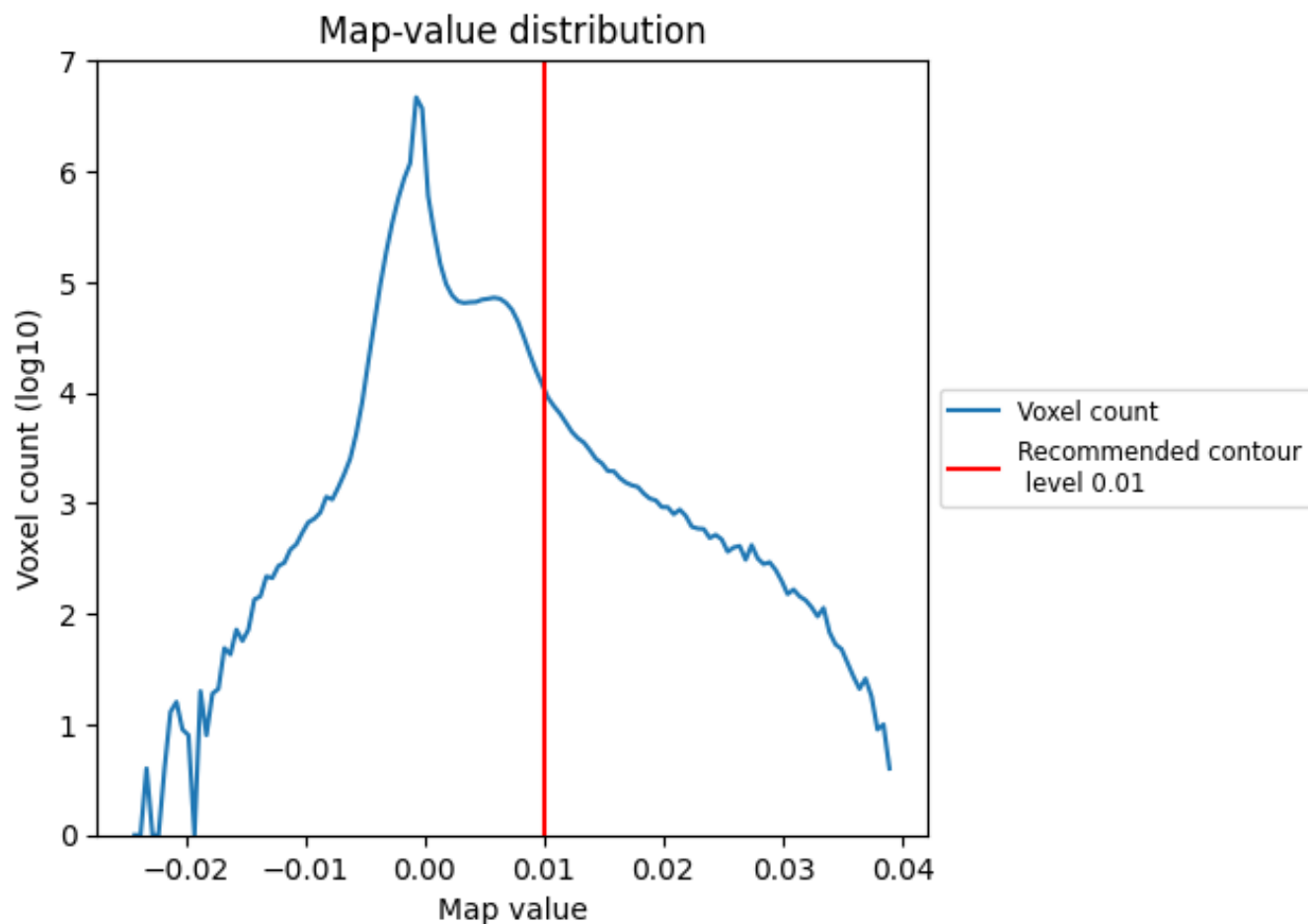
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

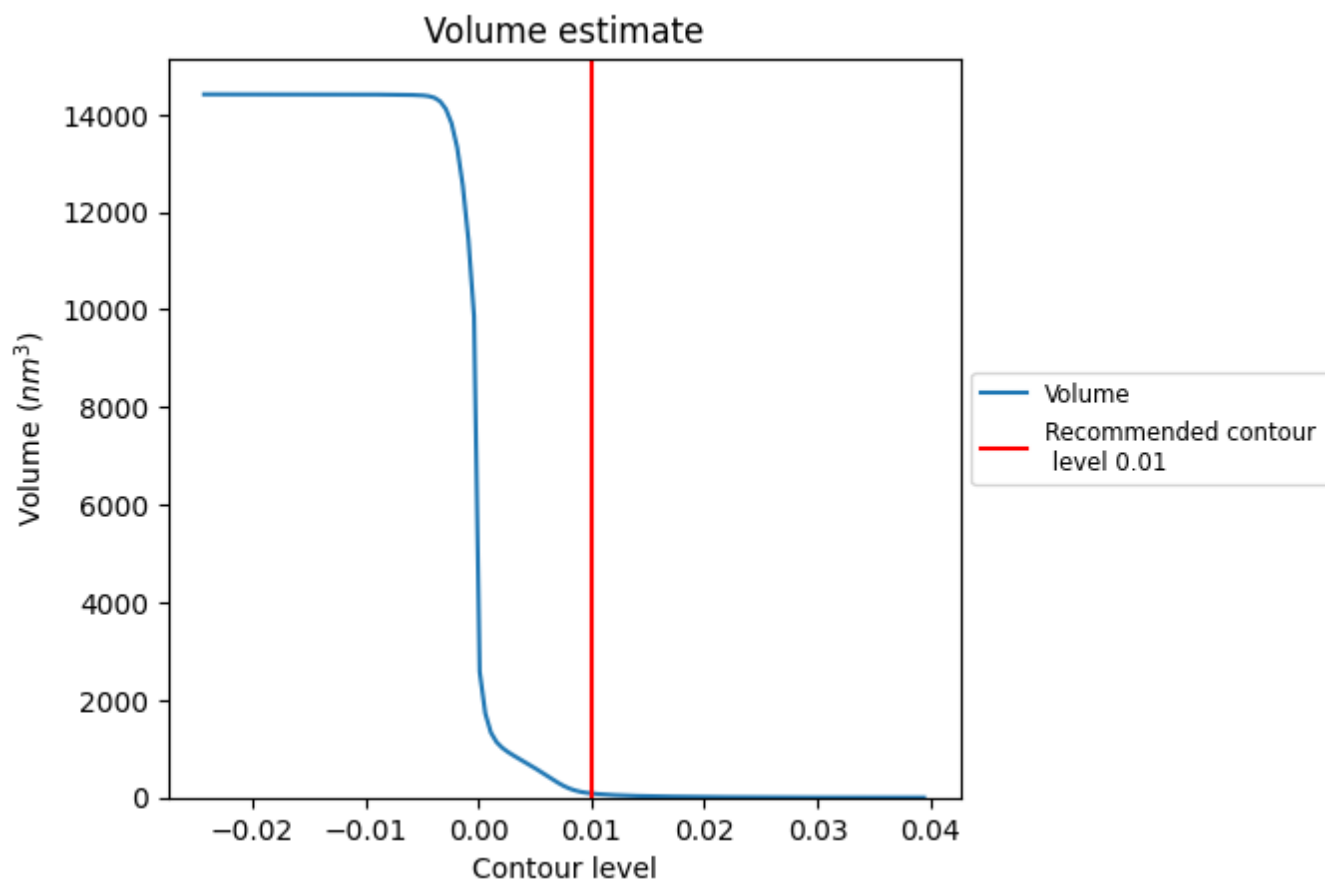
This section contains the results of statistical analysis of the map.

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.

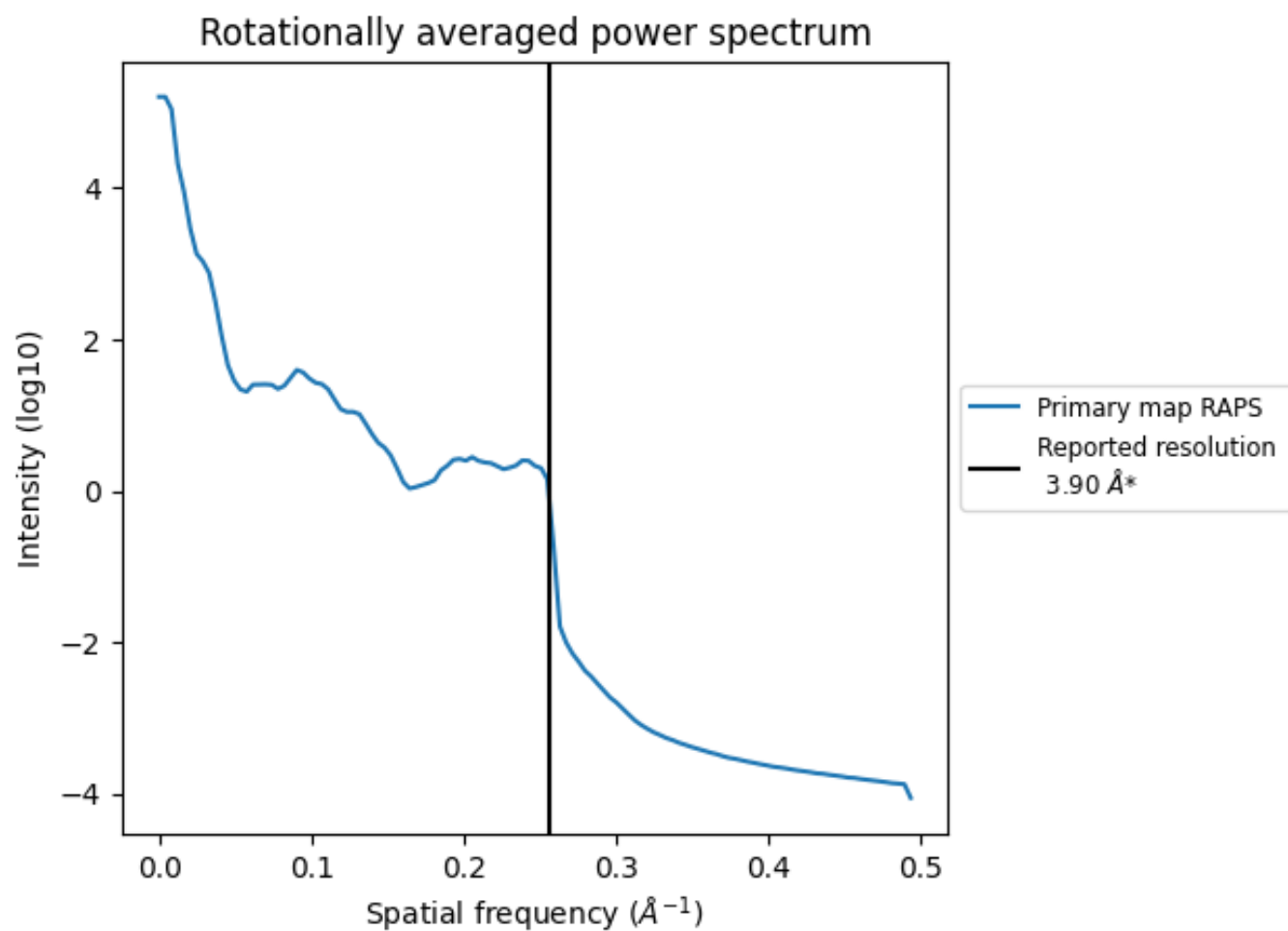
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 85 nm³; this corresponds to an approximate mass of 77 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 0.256 Å⁻¹

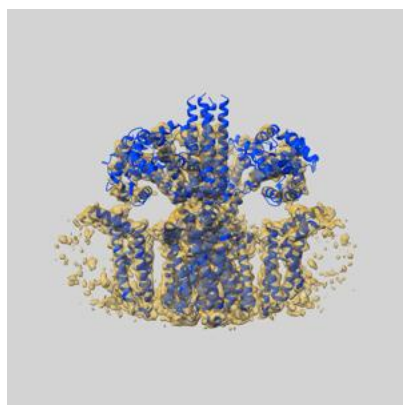
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

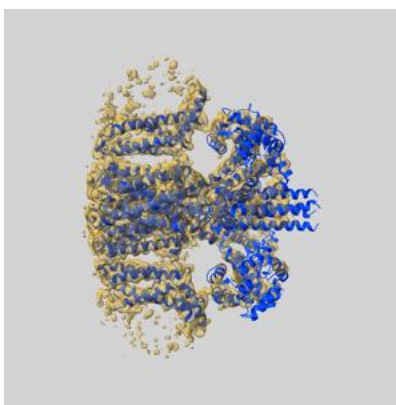
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30447 and PDB model 7CR4. Per-residue inclusion information can be found in section [3](#) on page [8](#).

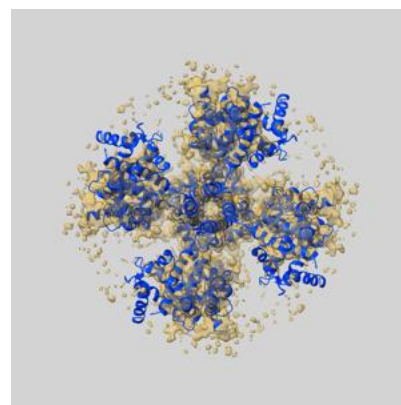
9.1 Map-model overlay [i](#)



X



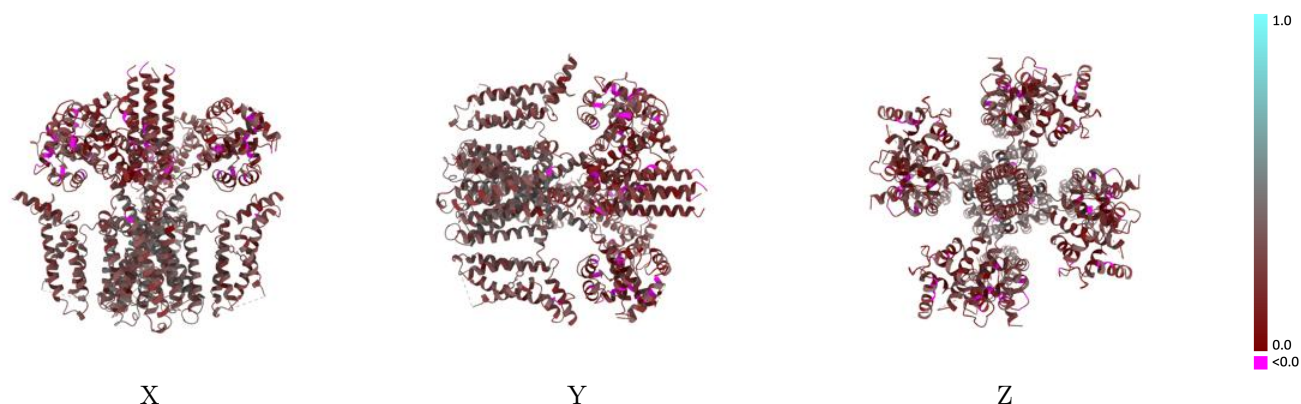
Y



Z

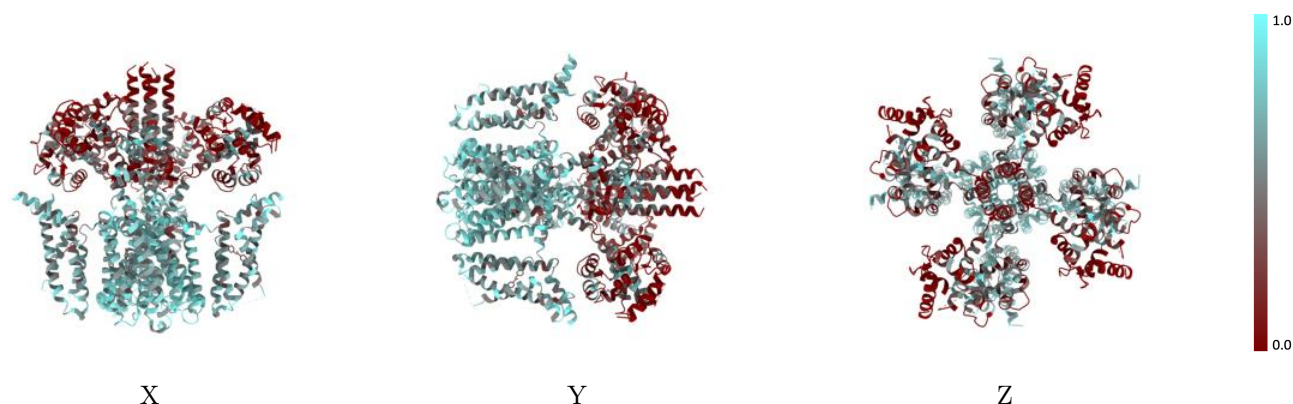
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



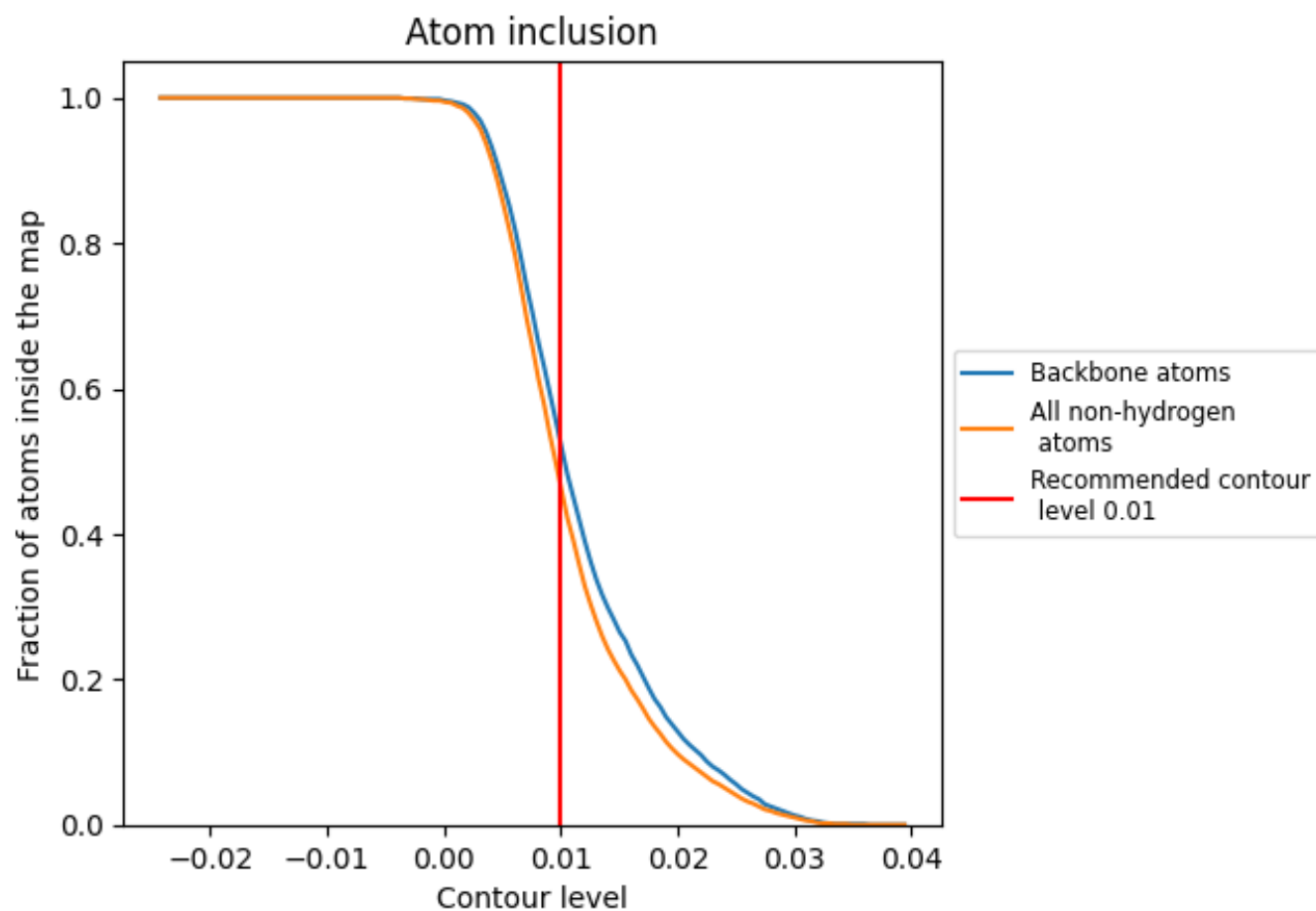
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 47% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	0.4660	0.2630
A	0.5810	0.2880
B	0.5780	0.2900
C	0.1960	0.1920
D	0.5790	0.2900
E	0.2020	0.1960
F	0.5780	0.2910
G	0.2050	0.1980
H	0.1930	0.1920

1.0

0.0

<0.0