



wwPDB EM Validation Summary Report ⓘ

Aug 4, 2026 – 02:40 AM JST

PDB ID : 24VN / pdb_000024vn
EMDB ID : EMD-69845
Title : Cryo-EM structure of the human wild-type KCNQ2/KCNQ3 heterotetramer (2:2 stoichiometry) in apo state (M2323 WT, without symmetry expansion)
Authors : Wang, Y.F.; Yang, H.; Qu, Y.N.; Shen, H.Z.
Deposited on : 2026-03-22
Resolution : 3.58 Å(reported)

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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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

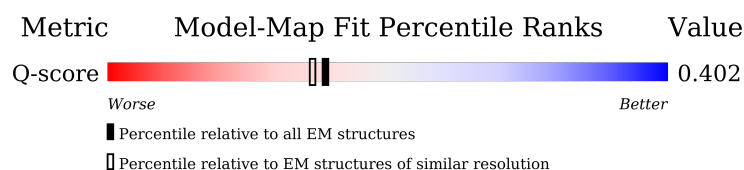
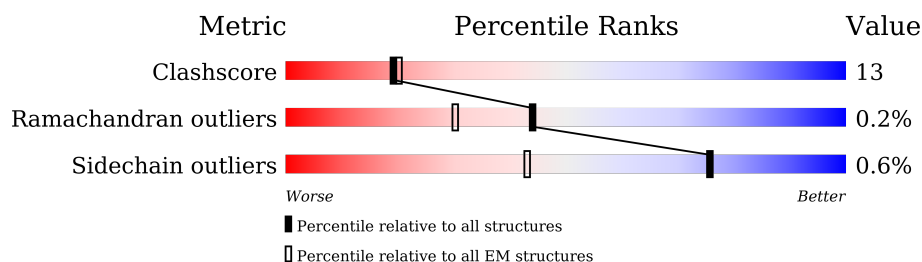
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.58 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	12629 (3.08 - 4.08)

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	892	
1	C	892	
2	B	1142	
2	D	1142	

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
4	YJ0	B	901	X	-	-	-
4	YJ0	D	901	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8056 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 Potassium voltage-gated channel subfamily KQT member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	239	Total	C	N	O	S	0	0
			1913	1269	313	321	10		
1	C	239	Total	C	N	O	S	0	0
			1913	1269	313	321	10		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP O43525
A	-18	ALA	-	expression tag	UNP O43525
A	-17	SER	-	expression tag	UNP O43525
A	-16	ASP	-	expression tag	UNP O43525
A	-15	TYR	-	expression tag	UNP O43525
A	-14	LYS	-	expression tag	UNP O43525
A	-13	ASP	-	expression tag	UNP O43525
A	-12	HIS	-	expression tag	UNP O43525
A	-11	ASP	-	expression tag	UNP O43525
A	-10	ILE	-	expression tag	UNP O43525
A	-9	ASP	-	expression tag	UNP O43525
A	-8	TYR	-	expression tag	UNP O43525
A	-7	LYS	-	expression tag	UNP O43525
A	-6	ASP	-	expression tag	UNP O43525
A	-5	ASP	-	expression tag	UNP O43525
A	-4	ASP	-	expression tag	UNP O43525
A	-3	ASP	-	expression tag	UNP O43525
A	-2	LYS	-	expression tag	UNP O43525
A	-1	GLY	-	expression tag	UNP O43525
A	0	THR	-	expression tag	UNP O43525
C	-19	MET	-	initiating methionine	UNP O43525
C	-18	ALA	-	expression tag	UNP O43525
C	-17	SER	-	expression tag	UNP O43525
C	-16	ASP	-	expression tag	UNP O43525
C	-15	TYR	-	expression tag	UNP O43525
C	-14	LYS	-	expression tag	UNP O43525

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	ASP	-	expression tag	UNP O43525
C	-12	HIS	-	expression tag	UNP O43525
C	-11	ASP	-	expression tag	UNP O43525
C	-10	ILE	-	expression tag	UNP O43525
C	-9	ASP	-	expression tag	UNP O43525
C	-8	TYR	-	expression tag	UNP O43525
C	-7	LYS	-	expression tag	UNP O43525
C	-6	ASP	-	expression tag	UNP O43525
C	-5	ASP	-	expression tag	UNP O43525
C	-4	ASP	-	expression tag	UNP O43525
C	-3	ASP	-	expression tag	UNP O43525
C	-2	LYS	-	expression tag	UNP O43525
C	-1	GLY	-	expression tag	UNP O43525
C	0	THR	-	expression tag	UNP O43525

- Molecule 2 is a protein called Green fluorescent protein,Potassium voltage-gated channel subfamily KQT member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	243	Total	C	N	O	S	0	0
			1982	1318	332	323	9		
2	D	247	Total	C	N	O	S	0	0
			2006	1333	336	328	9		

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-270	MET	-	initiating methionine	UNP P42212
B	-269	ALA	-	expression tag	UNP P42212
B	-268	MET	-	expression tag	UNP P42212
B	-267	HIS	-	expression tag	UNP P42212
B	-266	HIS	-	expression tag	UNP P42212
B	-265	HIS	-	expression tag	UNP P42212
B	-264	HIS	-	expression tag	UNP P42212
B	-263	HIS	-	expression tag	UNP P42212
B	-262	HIS	-	expression tag	UNP P42212
B	-261	HIS	-	expression tag	UNP P42212
B	-260	HIS	-	expression tag	UNP P42212
B	-259	GLY	-	expression tag	UNP P42212
B	-258	GLY	-	expression tag	UNP P42212
B	-257	SER	-	expression tag	UNP P42212
B	-256	MET	-	expression tag	UNP P42212

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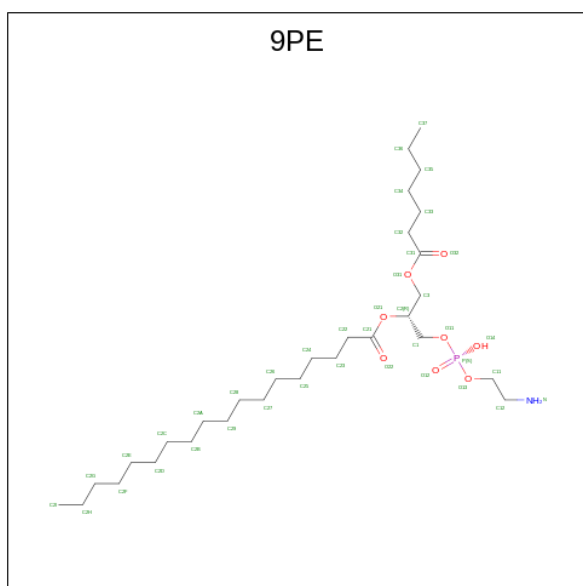
Chain	Residue	Modelled	Actual	Comment	Reference
B	-255	VAL	-	expression tag	UNP P42212
B	-192	LEU	PHE	conflict	UNP P42212
B	-191	THR	SER	conflict	UNP P42212
B	-149	THR	LYS	conflict	UNP P42212
B	-50	LYS	ALA	conflict	UNP P42212
B	-25	LEU	HIS	conflict	UNP P42212
B	-17	SER	-	linker	UNP P42212
B	-16	GLY	-	linker	UNP P42212
B	-15	LEU	-	linker	UNP P42212
B	-14	ARG	-	linker	UNP P42212
B	-13	SER	-	linker	UNP P42212
B	-12	GLY	-	linker	UNP P42212
B	-11	LEU	-	linker	UNP P42212
B	-10	GLU	-	linker	UNP P42212
B	-9	VAL	-	linker	UNP P42212
B	-8	LEU	-	linker	UNP P42212
B	-7	PHE	-	linker	UNP P42212
B	-6	GLN	-	linker	UNP P42212
B	-5	GLY	-	linker	UNP P42212
B	-4	PRO	-	linker	UNP P42212
B	-3	GLY	-	linker	UNP P42212
B	-2	GLY	-	linker	UNP P42212
B	-1	ARG	-	linker	UNP P42212
D	-270	MET	-	initiating methionine	UNP P42212
D	-269	ALA	-	expression tag	UNP P42212
D	-268	MET	-	expression tag	UNP P42212
D	-267	HIS	-	expression tag	UNP P42212
D	-266	HIS	-	expression tag	UNP P42212
D	-265	HIS	-	expression tag	UNP P42212
D	-264	HIS	-	expression tag	UNP P42212
D	-263	HIS	-	expression tag	UNP P42212
D	-262	HIS	-	expression tag	UNP P42212
D	-261	HIS	-	expression tag	UNP P42212
D	-260	HIS	-	expression tag	UNP P42212
D	-259	GLY	-	expression tag	UNP P42212
D	-258	GLY	-	expression tag	UNP P42212
D	-257	SER	-	expression tag	UNP P42212
D	-256	MET	-	expression tag	UNP P42212
D	-255	VAL	-	expression tag	UNP P42212
D	-192	LEU	PHE	conflict	UNP P42212
D	-191	THR	SER	conflict	UNP P42212
D	-149	THR	LYS	conflict	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-50	LYS	ALA	conflict	UNP P42212
D	-25	LEU	HIS	conflict	UNP P42212
D	-17	SER	-	linker	UNP P42212
D	-16	GLY	-	linker	UNP P42212
D	-15	LEU	-	linker	UNP P42212
D	-14	ARG	-	linker	UNP P42212
D	-13	SER	-	linker	UNP P42212
D	-12	GLY	-	linker	UNP P42212
D	-11	LEU	-	linker	UNP P42212
D	-10	GLU	-	linker	UNP P42212
D	-9	VAL	-	linker	UNP P42212
D	-8	LEU	-	linker	UNP P42212
D	-7	PHE	-	linker	UNP P42212
D	-6	GLN	-	linker	UNP P42212
D	-5	GLY	-	linker	UNP P42212
D	-4	PRO	-	linker	UNP P42212
D	-3	GLY	-	linker	UNP P42212
D	-2	GLY	-	linker	UNP P42212
D	-1	ARG	-	linker	UNP P42212

- Molecule 3 is (1R)-2-[[[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy]-1-[(heptanoyloxy)methyl]ethyl octadecanoate (CCD ID: 9PE) (formula: C₃₀H₆₀NO₈P) (labeled as "Ligand of Interest" by depositor).



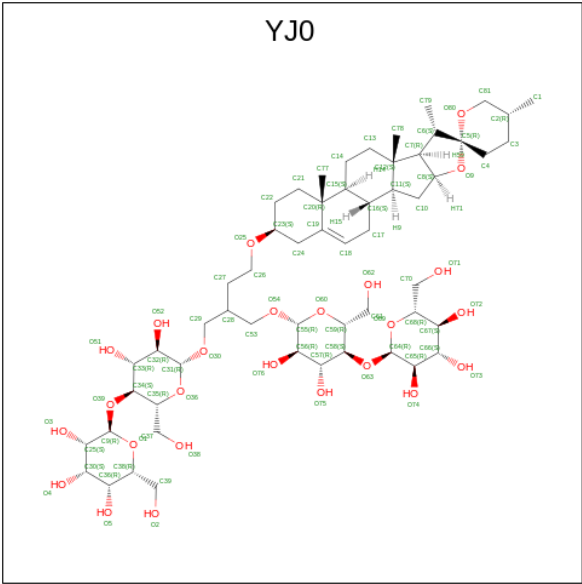
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	P
			40	30	1	8	1
							0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	C	1	40	30	1	8	1	0

- Molecule 4 is (2R)-2-{[(4-O-hexopyranosyl-beta-D-glucopyranosyl)oxy]methyl}-4-{[(25R)-5beta,14beta,17beta-spirostan-3beta-yl]oxy}butyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside (CCD ID: YJ0) (formula: C₅₆H₉₂O₂₅) (labeled as "Ligand of Interest" by depositor).

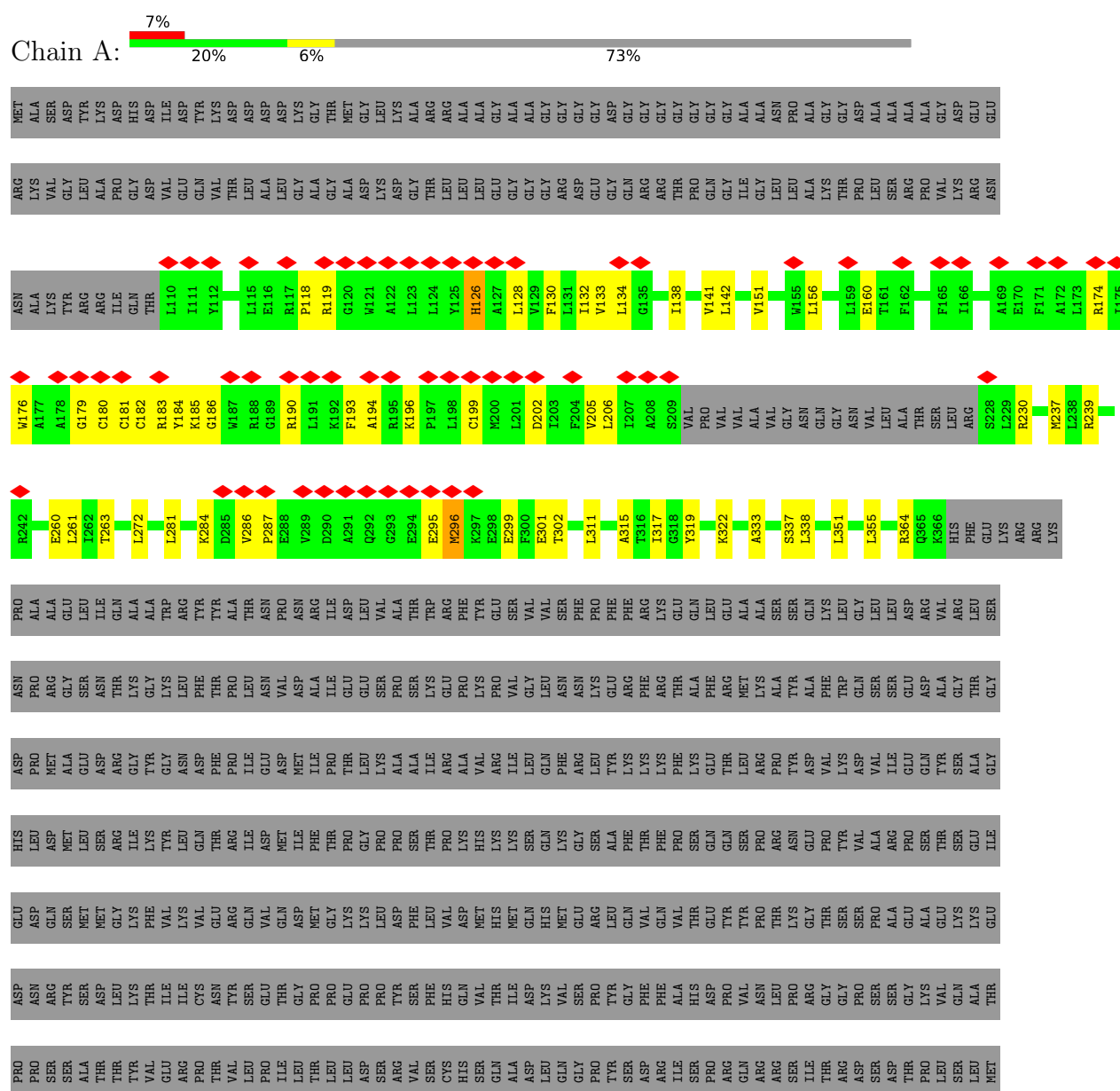


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
4	B	1	81	56	25	0
4	D	1	81	56	25	0

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: Potassium voltage-gated channel subfamily KQT member 3



SER
SER
THR
GLY
ASP
GLY
ILE
SER
ASP
SER
VAL
TRP
THR
PRO
SER
ASN
LYS
PRO
ILE

- Molecule 1: Potassium voltage-gated channel subfamily KQT member 3



ARG LYS VAL GLY LEU ALA PRO GLY ASP VAL GLU GLN VAL THR LEU ALA ALA LYS ASP GLY THR LEU LEU GLU GLY GLY GLY ARG ARG PRO GLN GLY ILE GLY LEU LEU ALA LYS THR PRO VAL LYS ARG ASN

ASN	ASN
L173	L110
R174	I111
I175	Y112
W176	D113
A177	A114
A178	E115
G179	R116
C180	R117
C181	P118
C182	G120
R183	W121
Y184	A122
W187	L124
R188	Y125
G189	H126
R190	A127
L191	L128
K192	F129
A194	V130
R195	V133
K196	L134
P197	G135
L198	A140
C199	T143
M200	T144
L201	F145
D202	K146
E203	E149
F204	D154
V205	W155
L206	L156
I207	L159
A208	E160
S209	F162
VAL	F165
PRO	I166
VAL	A169
VAL	E170
VAL	F171
ALA	A172
VAL	
GLY	
ASN	
GLN	
VAL	
ALA	
THR	
SER	
LEU	
ARG	
S228	
L229	
R230	
Q233	

R236	M237	L238	R239	M240	K259	E260	T263	E283	K284	D285	V286	P287	E288	V289	D290	A291	G293	E294	E295	M296	K297	E298	E299	L311	A315	T316	I317	G318	Y319	G320	K321	K322	T326	A333	S337	L338	L355	R364	Q365	K366	HIS	PHE	GLU	LVS	ARG	ARG	LVS
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ALA	ALA	GLU	LEU	ILE	GLN	ALA	ALA	TRP	TRP	TYR	TYR	ALA	ALA	ASN	ASN	ARG	ASP	LEU	VAL	ALA	THR	TRP	ARG	PHE	TYR	GLY	SER	VAL	VAL	SER	PHE	PHE	PHE	ARG	LYS	GLU	GLN	LEU	GLU	ALA	ALA	LEU	GLY	SER	SER	SER	GLN	LYS	LEU	LEU	LEU	ASP	ARG	VAL	ARG	LEU	ALA	ARG	SER	ASN
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PRO	ARG	GLY	SER	ASN	THR	LYS	GLY	LEU	PHE	THR	PRO	PRO	LEU	ASN	VAL	ASP	ALA	ILE	GLU	GLU	SER	SER	PRO	PRO	LYS	GLY	LEU	ASN	ASN	GLY	LYS	VAL	GLY	ARG	PHE	ARG	THR	ALA	PHE	ARG	MET	LYS	ALA	ALA	TYR	THR	GLU	ASP	ALA	GLY	GLY	ASP
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PRO MET ALA ALA GLU ASP ARG GLY TYR GLY ASN ASP PHE PRO ILE GLU ASP MET ILE THR PRO ARG ALA VAL ILE LEU GLN PHE ARG ARG ILE LEU LEU TYR LYS LYS LYS PHE PHE LYS GLU THR LEU LEU ARG PRO TYR ASP VAL LYS ASP ASP VAL ILE GLU GLN TYR SER ALA ALA GLY HIS

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

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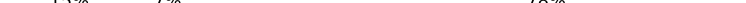
PRO	SER	SER	SER	ALA	THR	THR	TYR	VAL	VAL	GLU	ARG	PRO	THR	VAL	VAL	LEU	LEU	PRO	PRO	ILE	ILE	LEU	THR	THR	LEU	LEU	ASP	ASP	SER	SER	ARG	ARG	VAL	VAL	SER	SER	CYS	HIS	HIS	SER	SER	GLN	GLN	ALA	ALA	ASP	ASP	LEU	LEU	GLN	GLN	GLY	GLY	PRO	PRO	TYR	TYR	SER	SER	SER	ASP	ASP	ARG	ARG	ILE	ILE	ILE	ILE	SER	SER	PRO	PRO	ARG	ARG	GLN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

● Molecule 2: Green fluorescent protein, Potassium voltage-gated channel subfamily KQT member 2



- Chain D:  15% 7% 78%



SER
ALA
THR
GLY
GLU
GLY
PRO
PHE
GLY
ASP
VAL
GLY
TRP
ALA
GLY
PRO
ARG
LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50903	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.965	Depositor
Minimum map value	-2.457	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.086	Depositor
Recommended contour level	0.494	Depositor
Map size ($\text{\AA}$)	260.88, 260.88, 260.88	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	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: 9PE, YJ0

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	0.16	0/1960	0.45	0/2653
1	C	0.15	0/1960	0.46	0/2653
2	B	0.22	0/2036	0.40	0/2757
2	D	0.16	0/2060	0.41	0/2790
All	All	0.17	0/8016	0.43	0/10853

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	1913	0	1970	47	0
1	C	1913	0	1970	48	0
2	B	1982	0	2020	61	0
2	D	2006	0	2046	63	0
3	A	40	0	59	1	0
3	C	40	0	59	1	0
4	B	81	0	0	1	0
4	D	81	0	0	0	0
All	All	8056	0	8124	205	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 13.

The worst 5 of 205 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:182:CYS:SG	1:A:183:ARG:N	2.56	0.78
1:C:182:CYS:SG	1:C:183:ARG:N	2.55	0.78
2:D:144:ILE:HG22	2:D:159:ARG:HD3	1.68	0.74
1:A:193:PHE:O	1:A:196:LYS:NZ	2.21	0.74
2:B:259:HIS:HB3	2:B:282:LYS:HG2	1.70	0.72

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	235/892 (26%)	215 (92%)	19 (8%)	1 (0%)	30	60
1	C	235/892 (26%)	214 (91%)	21 (9%)	0	100	100
2	B	239/1142 (21%)	223 (93%)	15 (6%)	1 (0%)	30	60
2	D	243/1142 (21%)	228 (94%)	15 (6%)	0	100	100
All	All	952/4068 (23%)	880 (92%)	70 (7%)	2 (0%)	44	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	156	TRP
1	A	296	MET

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	196/743 (26%)	193 (98%)	3 (2%)	57	70
1	C	196/743 (26%)	196 (100%)	0	100	100
2	B	204/961 (21%)	202 (99%)	2 (1%)	68	75
2	D	206/961 (21%)	206 (100%)	0	100	100
All	All	802/3408 (24%)	797 (99%)	5 (1%)	76	79

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	151	VAL
1	A	272	LEU
2	B	167	PHE
2	B	205	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	78	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 [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	9PE	C	1001	-	39,39,39	0.97	4 (10%)	42,44,44	0.94	2 (4%)
3	9PE	A	1001	-	39,39,39	0.97	4 (10%)	42,44,44	0.96	2 (4%)
4	YJ0	B	901	-	90,90,90	0.30	0	136,138,138	1.01	9 (6%)
4	YJ0	D	901	-	90,90,90	0.20	0	136,138,138	0.53	1 (0%)

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	9PE	C	1001	-	-	15/43/43/43	-
3	9PE	A	1001	-	-	25/43/43/43	-
4	YJ0	B	901	-	14/14/33/34	15/32/200/200	1/10/10/10
4	YJ0	D	901	-	9/9/33/34	11/32/200/200	1/10/10/10

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1001	9PE	O21-C2	-2.52	1.40	1.46
3	A	1001	9PE	O21-C2	-2.49	1.40	1.46
3	C	1001	9PE	O31-C31	2.42	1.40	1.33
3	A	1001	9PE	O31-C31	2.40	1.40	1.33
3	A	1001	9PE	O21-C21	2.14	1.40	1.34

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	901	YJ0	C12-C7-C8	-5.15	97.90	104.13
3	A	1001	9PE	O21-C21-C22	4.03	120.19	111.50
3	C	1001	9PE	O21-C21-C22	3.99	120.09	111.50
4	B	901	YJ0	C10-C8-C7	-3.53	100.16	107.52
4	B	901	YJ0	O9-C8-C7	-3.37	100.10	105.07

5 of 23 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	901	YJ0	C16
4	B	901	YJ0	C5
4	B	901	YJ0	C55
4	B	901	YJ0	C59
4	B	901	YJ0	C34

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	9PE	C1-O11-P-O12
3	A	1001	9PE	C11-O13-P-O14
3	A	1001	9PE	O13-C11-C12-N
3	A	1001	9PE	C22-C21-O21-C2
3	C	1001	9PE	C11-O13-P-O12

All (2) ring outliers are listed below:

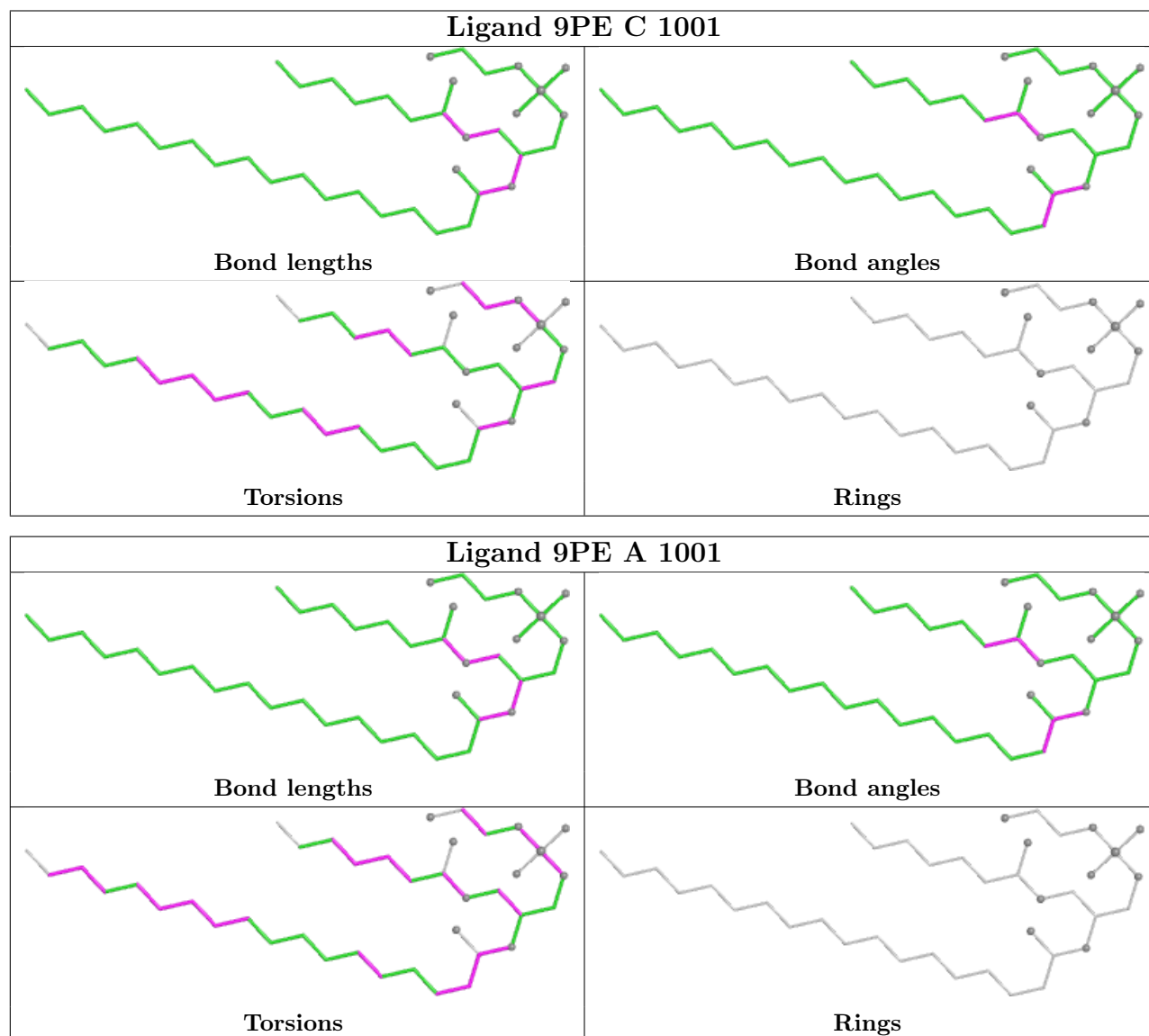
Mol	Chain	Res	Type	Atoms
4	D	901	YJ0	C2-C3-C4-C5-C81-O80
4	B	901	YJ0	C2-C3-C4-C5-C81-O80

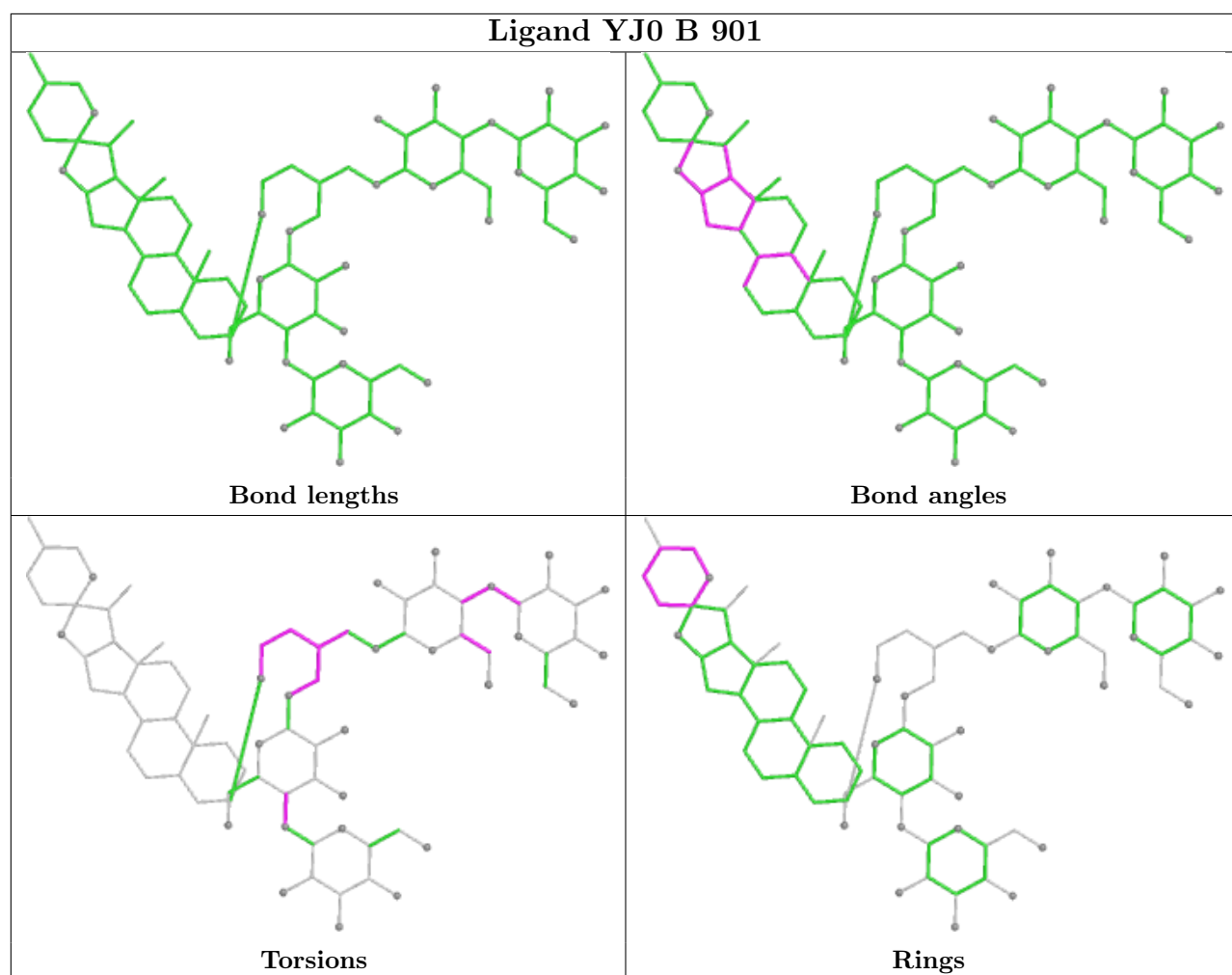
3 monomers are involved in 3 short contacts:

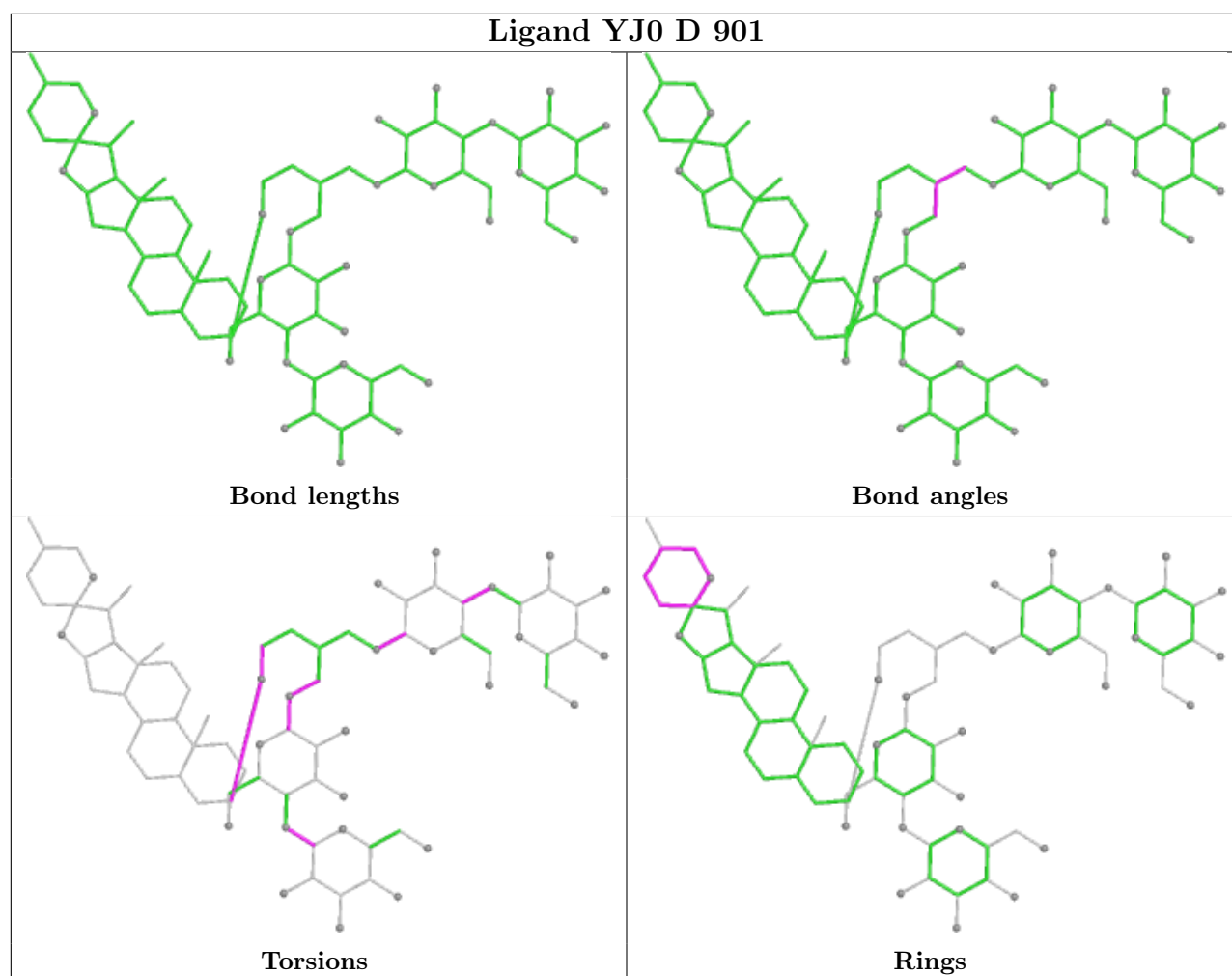
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1001	9PE	1	0
3	A	1001	9PE	1	0
4	B	901	YJ0	1	0

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.

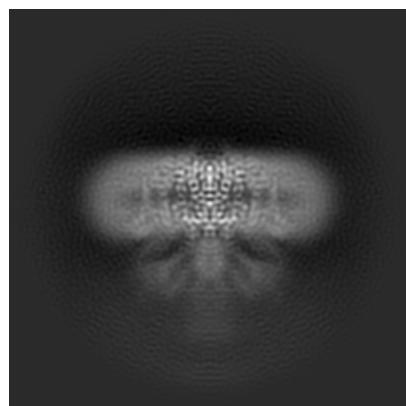
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-69845. These allow visual inspection of the internal detail of the map and identification of artifacts.

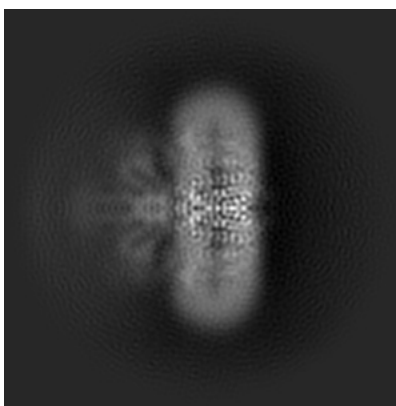
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

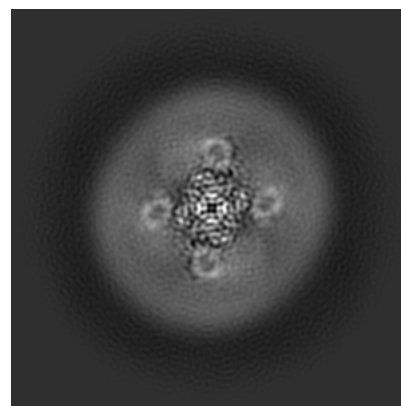
6.1.1 Primary map



X

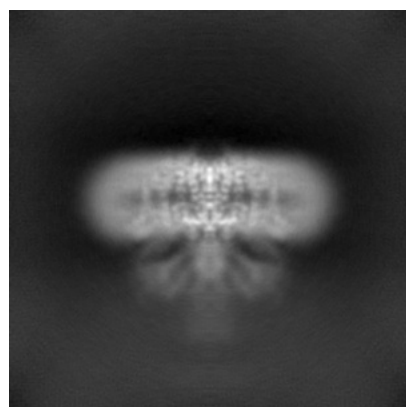


Y

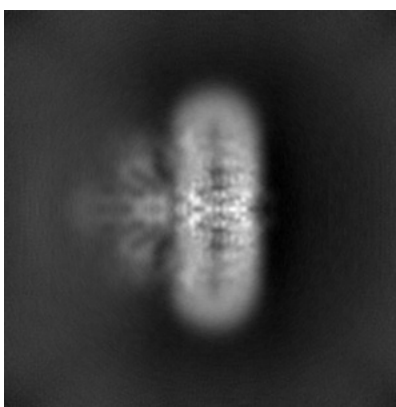


Z

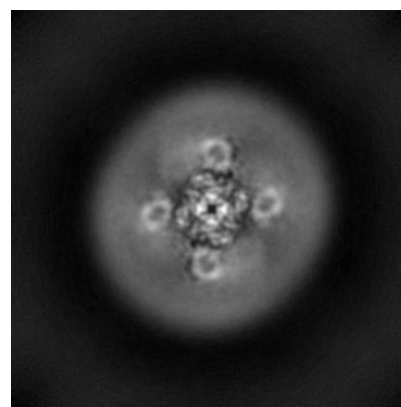
6.1.2 Raw map



X



Y

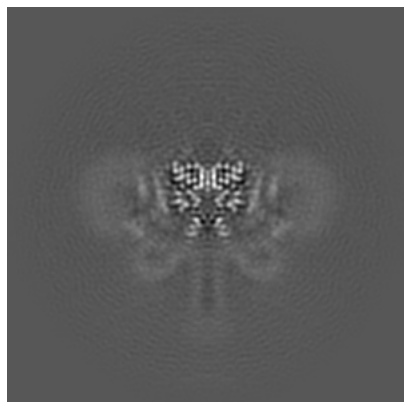


Z

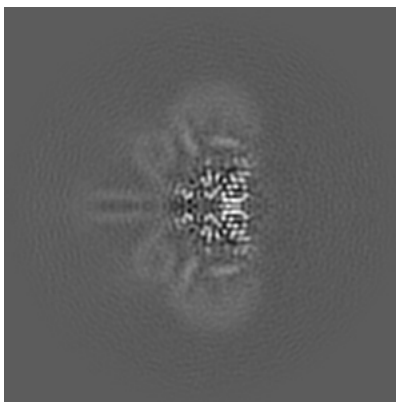
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

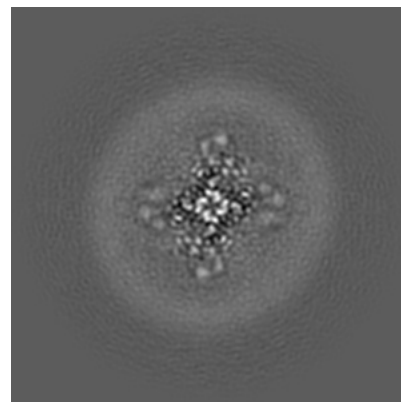
6.2.1 Primary map



X Index: 120

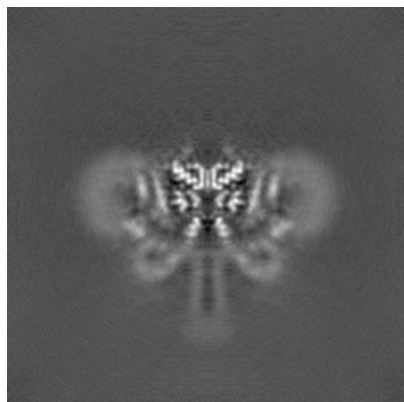


Y Index: 120

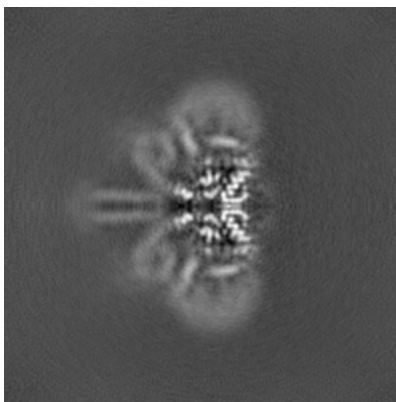


Z Index: 120

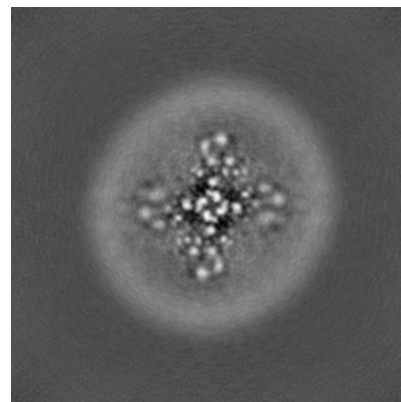
6.2.2 Raw map



X Index: 120



Y Index: 120

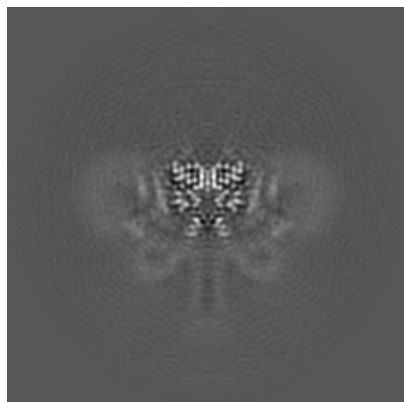


Z Index: 120

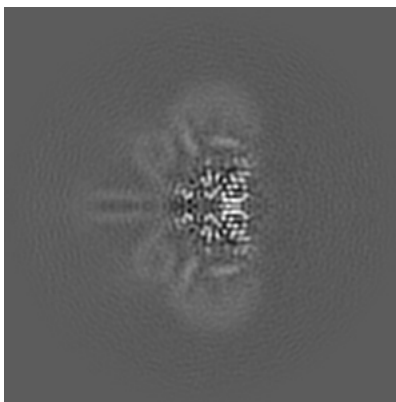
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

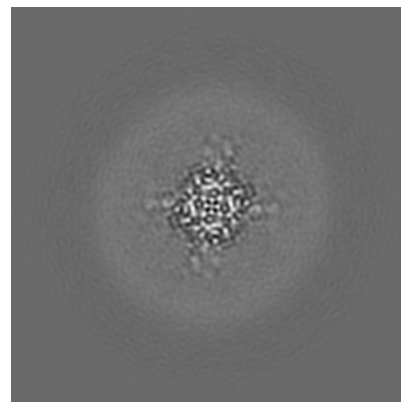
6.3.1 Primary map



X Index: 120

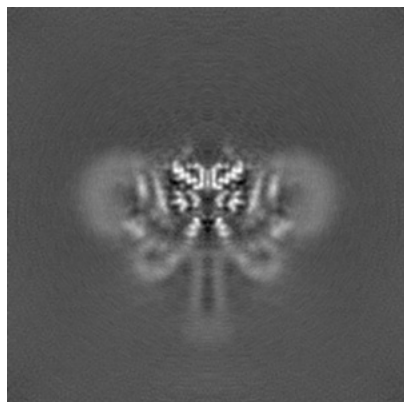


Y Index: 120

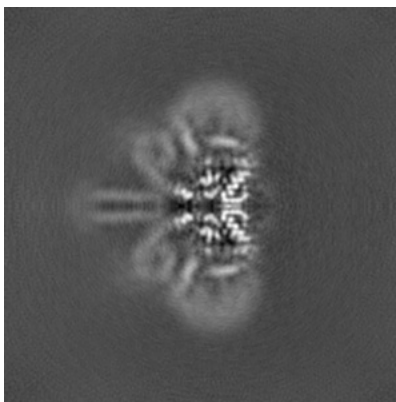


Z Index: 139

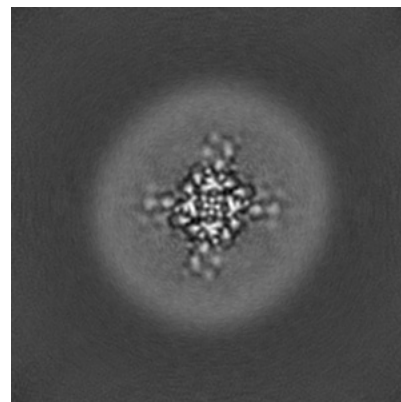
6.3.2 Raw map



X Index: 120



Y Index: 120

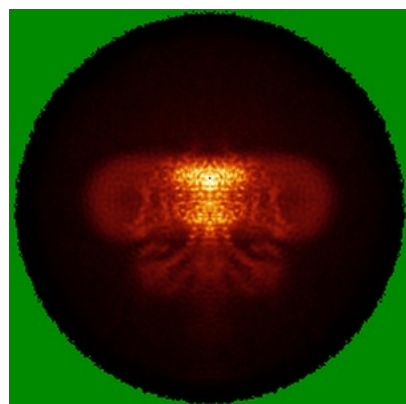


Z Index: 139

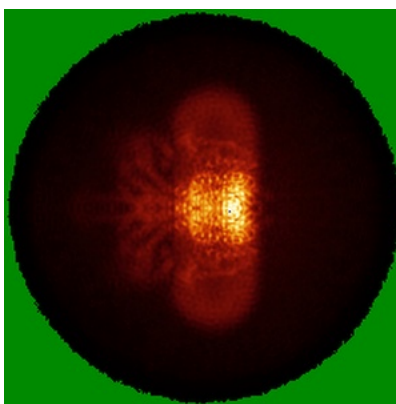
The images above show the largest variance slices of the map in three orthogonal directions.

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

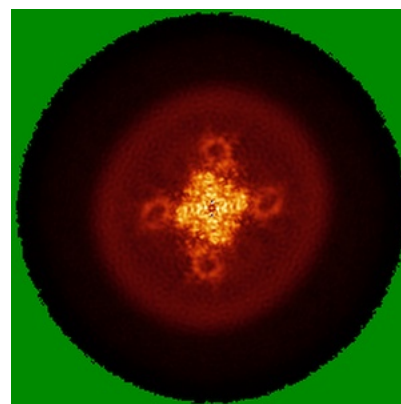
6.4.1 Primary map



X

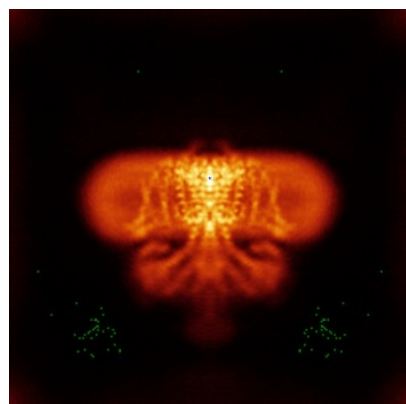


Y

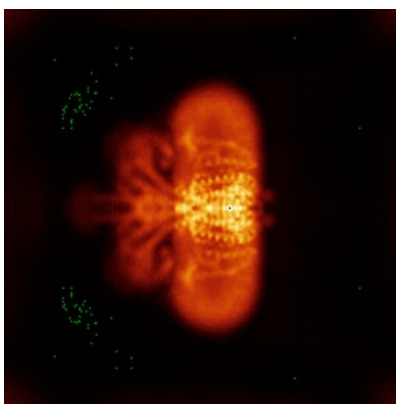


Z

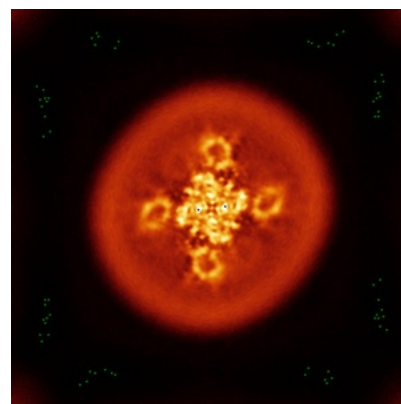
6.4.2 Raw map



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.

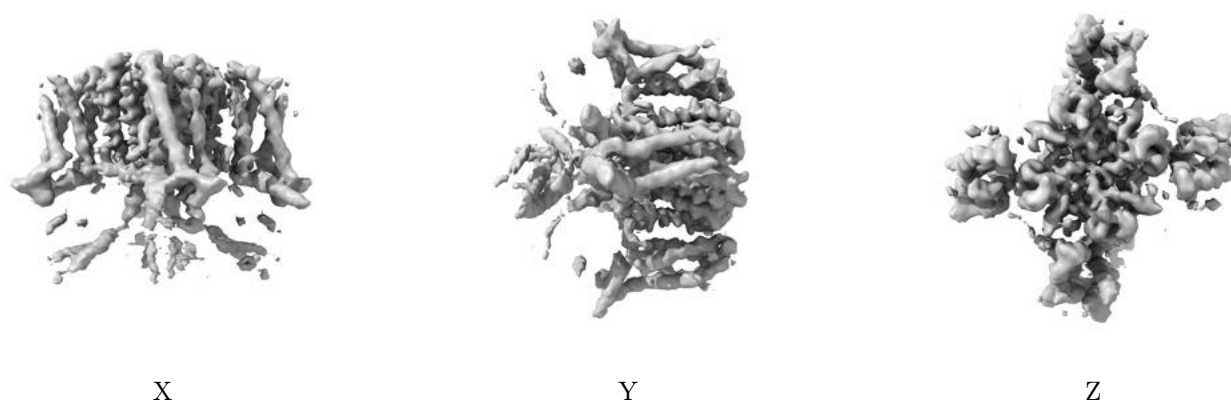
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.494. 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.

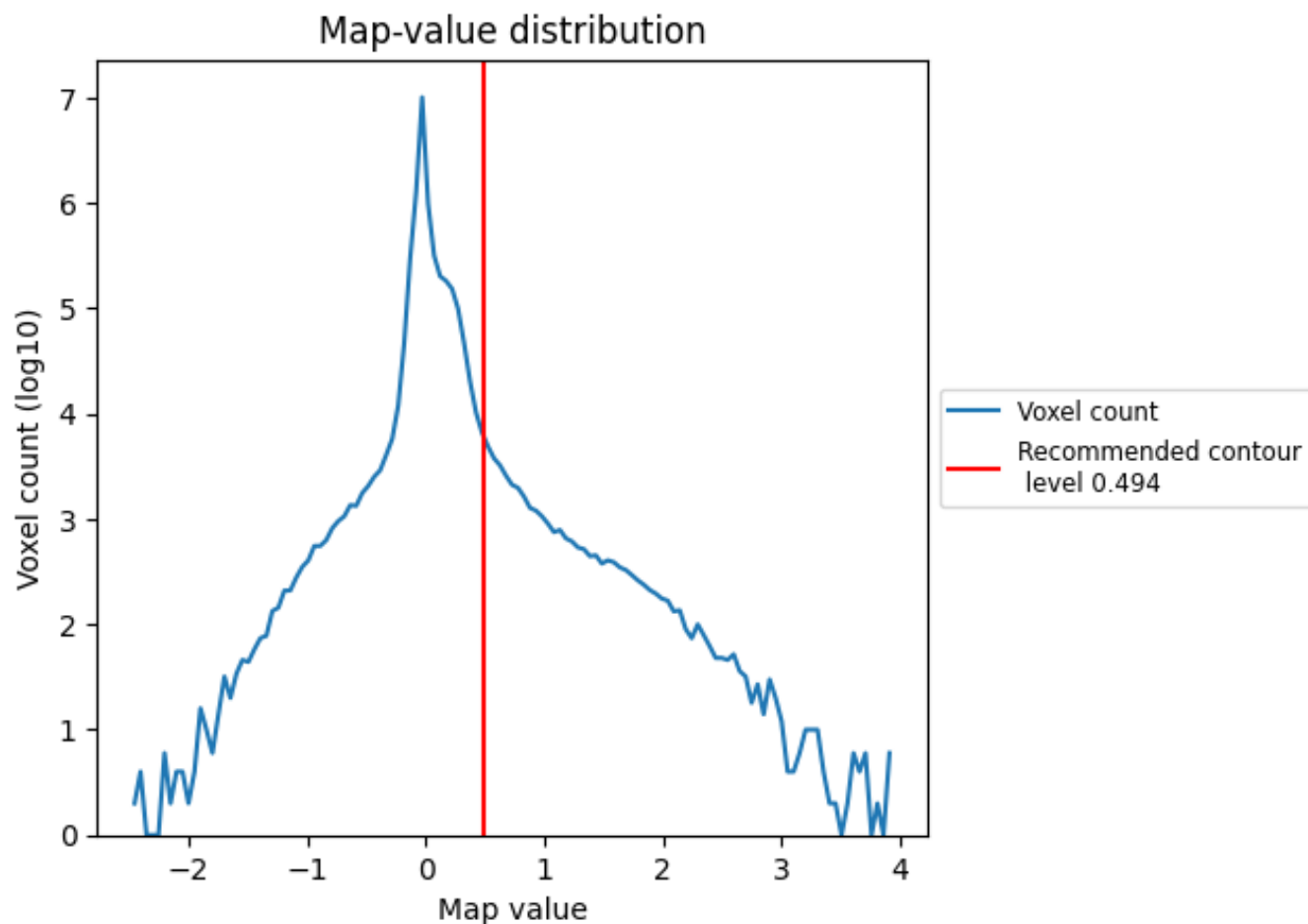
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

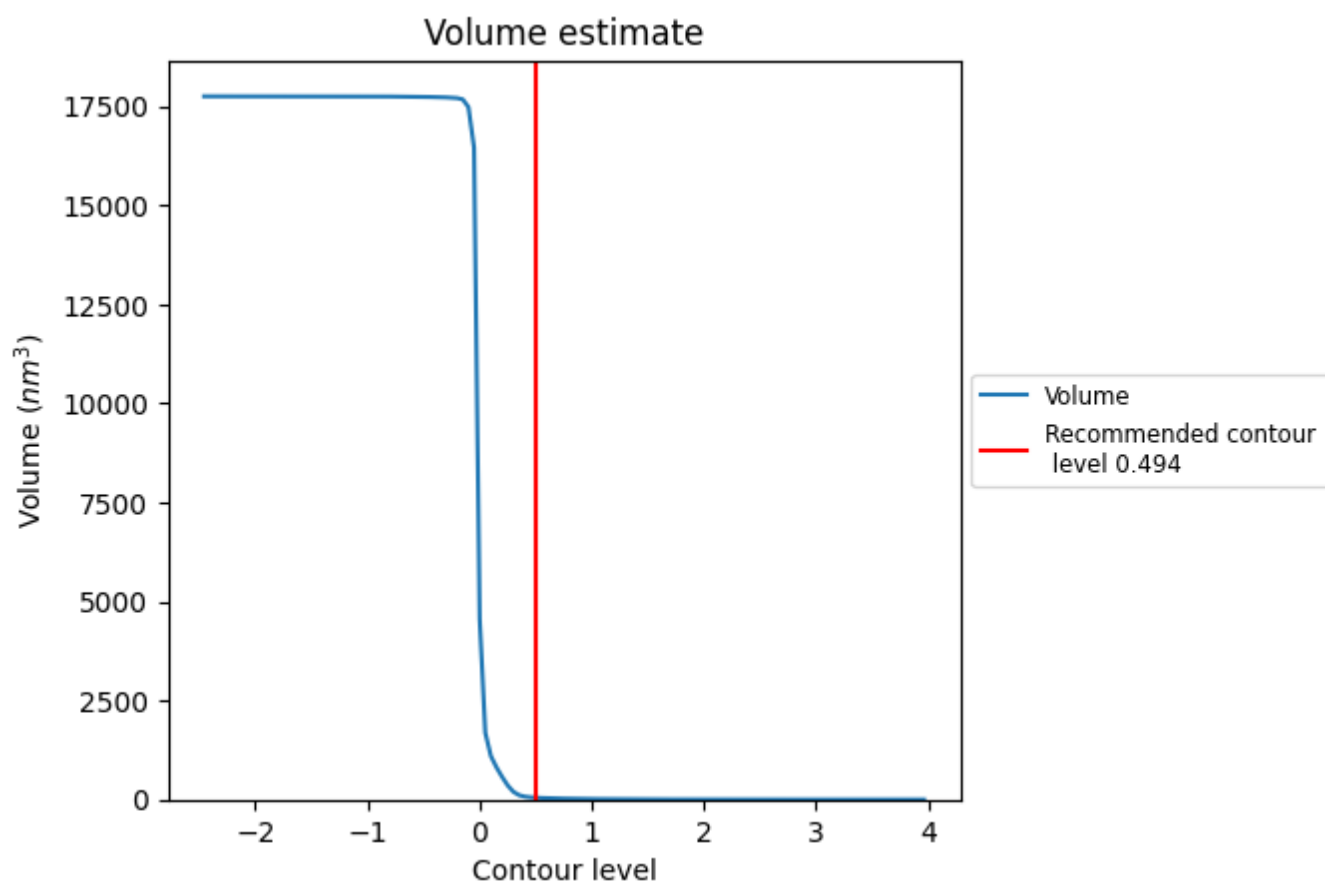
This section contains the results of statistical analysis of the map.

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.

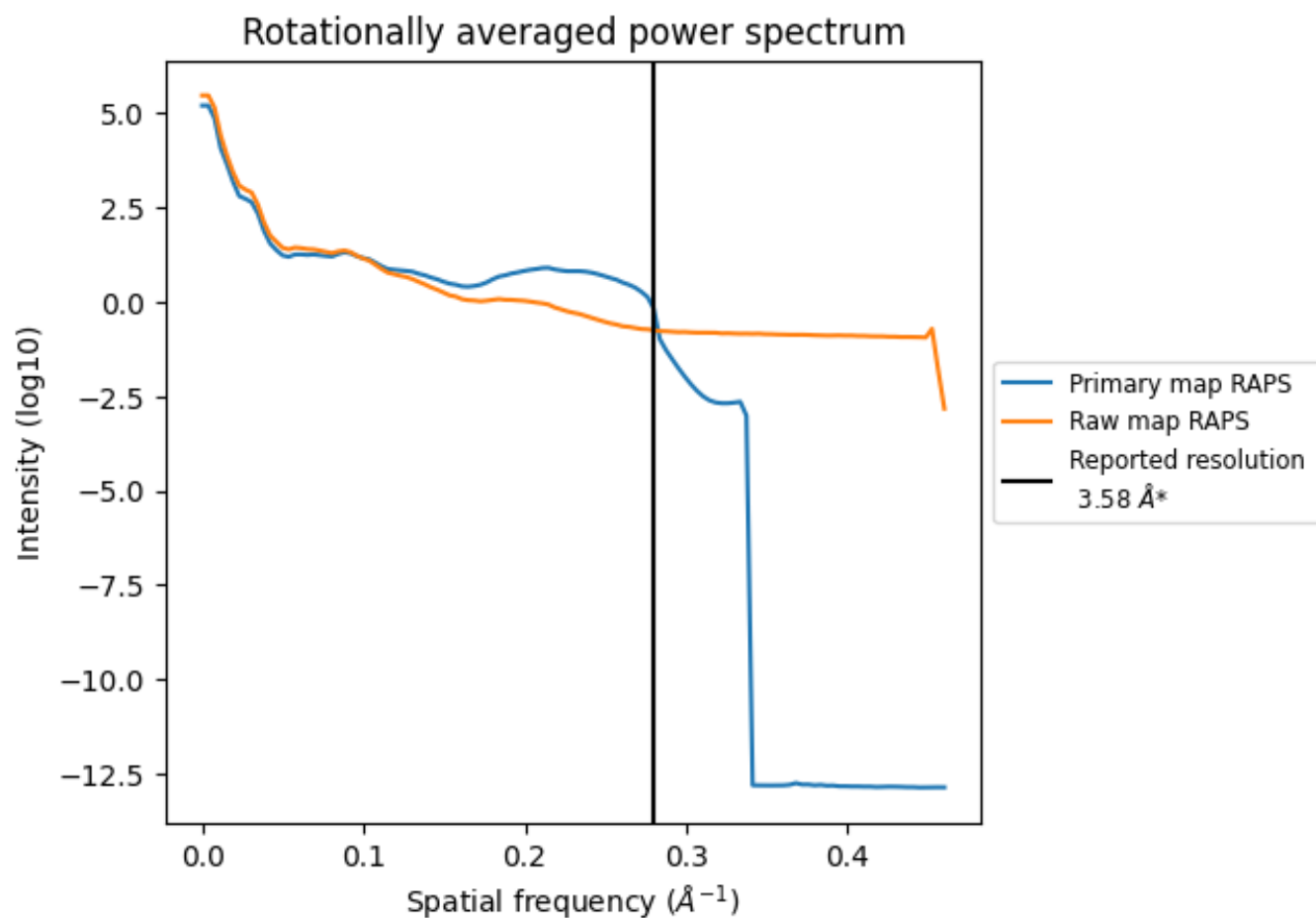
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 49 nm³; this corresponds to an approximate mass of 44 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 ⓘ

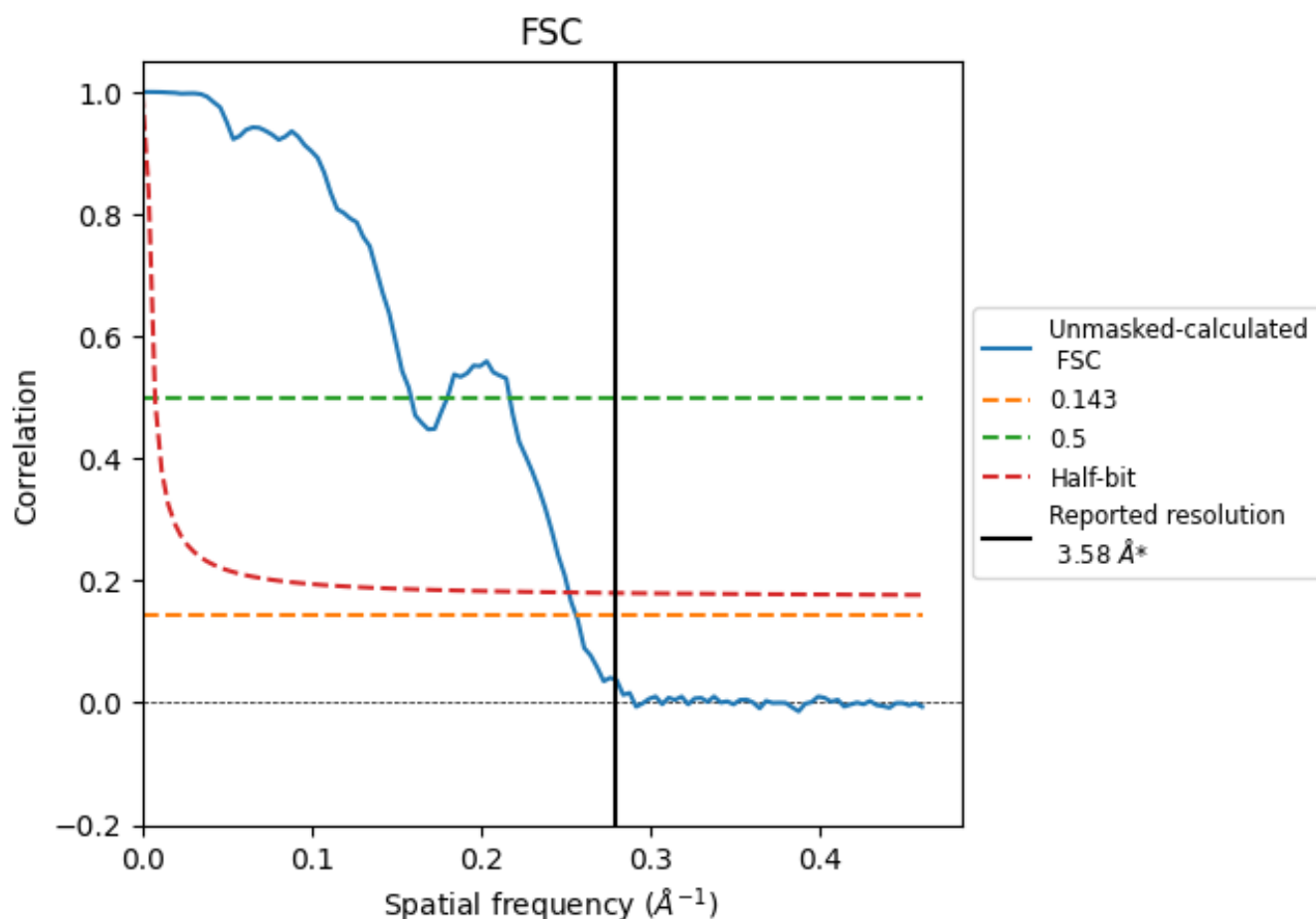


*Reported resolution corresponds to spatial frequency of 0.279 Å⁻¹

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 0.279 Å⁻¹

8.2 Resolution estimates [i](#)

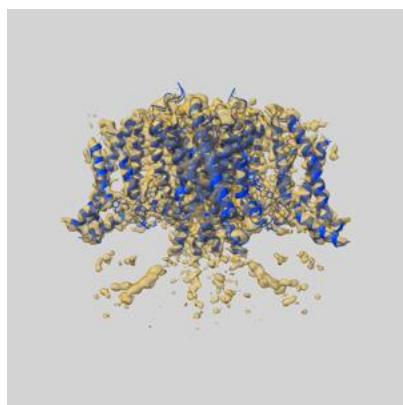
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.58	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.91	6.31	3.97

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

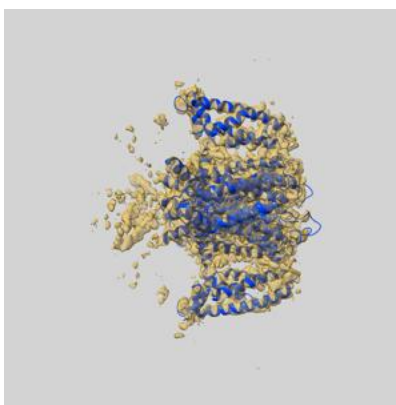
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-69845 and PDB model 24VN. Per-residue inclusion information can be found in section [3](#) on page [9](#).

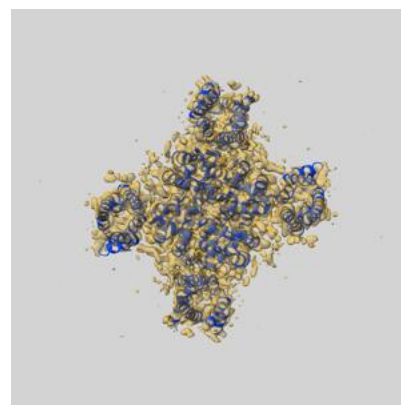
9.1 Map-model overlay [i](#)



X



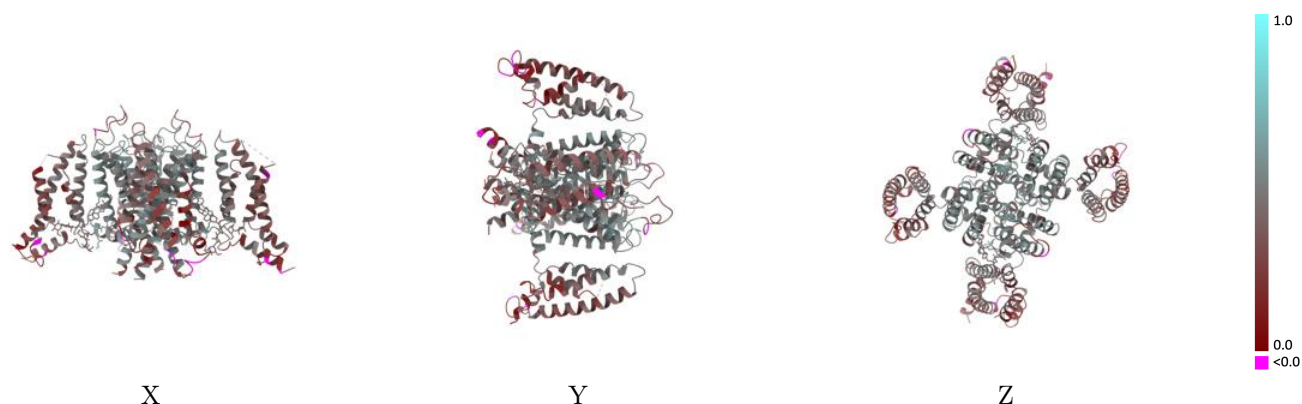
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.494 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](#)



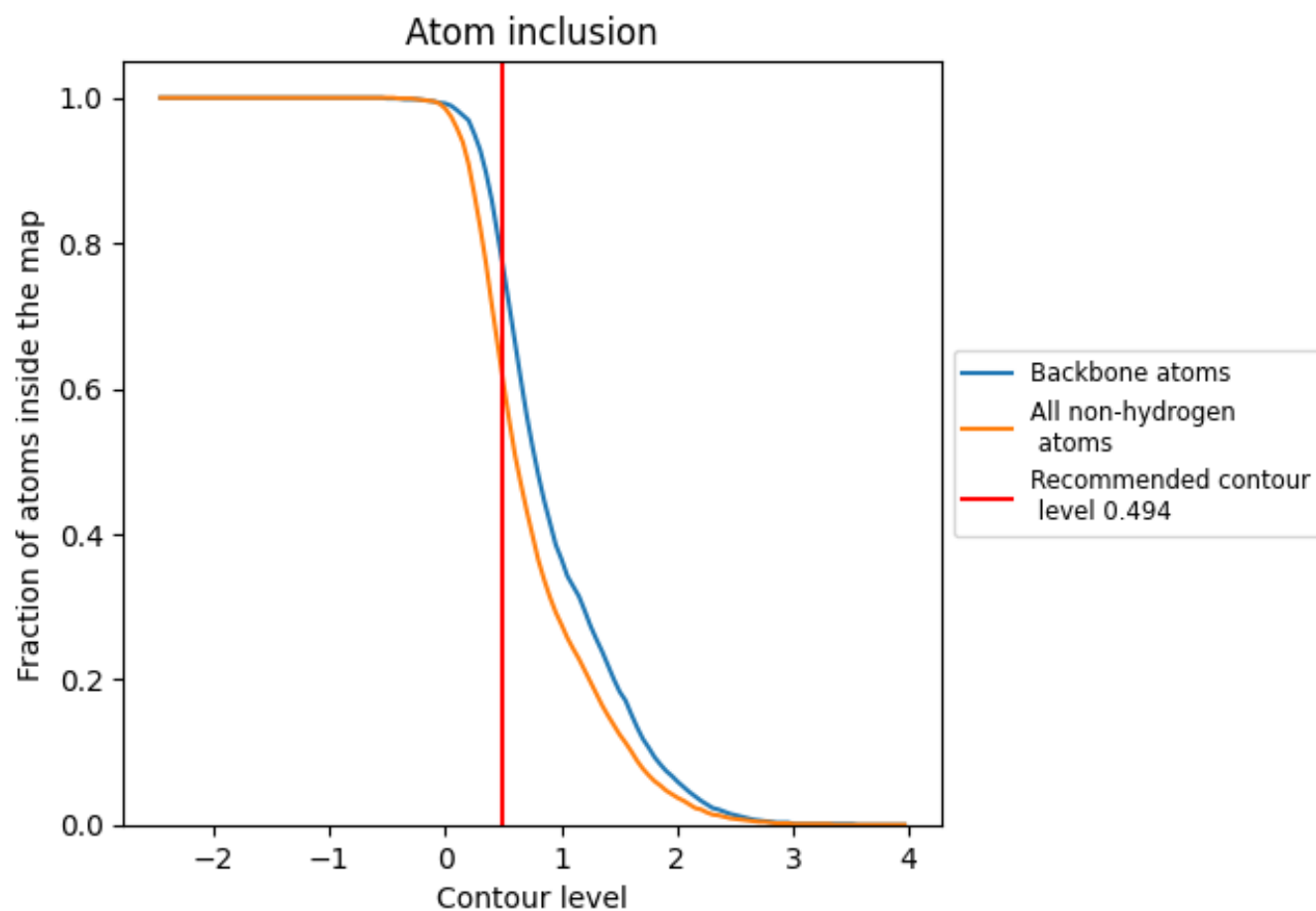
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.494).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 62% 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 (0.494) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6160	0.4020
A	0.5870	0.3900
B	0.6480	0.4140
C	0.5910	0.3900
D	0.6370	0.4110

