



## Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 04:26 PM JST

PDB ID : 7CAL / pdb\_00007cal  
EMDB ID : EMD-30334  
Title : Cryo-EM Structure of the Hyperpolarization-Activated Inwardly Rectifying Potassium Channel KAT1 from Arabidopsis  
Authors : Li, S.Y.; Yang, F.; Sun, D.M.; Zhang, Y.; Zhang, M.G.; Zhou, P.; Liu, S.L.; Zhang, Y.N.; Zhang, L.H.; Tian, C.L.  
Deposited on : 2020-06-09  
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

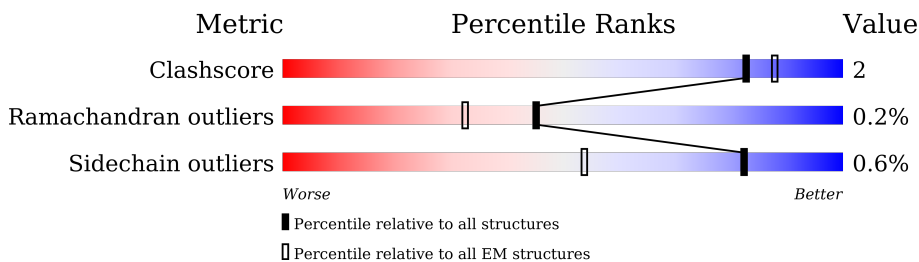
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	677	 61% 34%
1	B	677	 62% 34%
1	C	677	 62% 34%
1	D	677	 61% 34%

## 2 Entry composition [i](#)

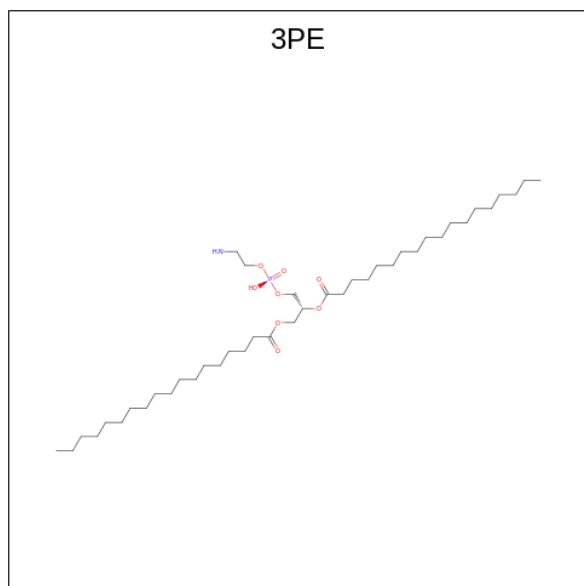
There are 2 unique types of molecules in this entry. The entry contains 14064 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 channel KAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	444	Total	C	N	O	S	0	0
			3465	2282	571	596	16		
1	B	444	Total	C	N	O	S	0	0
			3465	2282	571	596	16		
1	C	444	Total	C	N	O	S	0	0
			3465	2282	571	596	16		
1	D	444	Total	C	N	O	S	0	0
			3465	2282	571	596	16		

- Molecule 2 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
2	B	1	Total	C	N	O	P	0
			51	41	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			51	41	1	8	1	
2	D	1	Total	C	N	O	P	0
			51	41	1	8	1	



LYS	LEU	SER	ILE	LEU	SER	TRP	PRO	SER	SER	ILE	GLU	LEU	ARG	LEU	ALA	GLU	SER	GLY	LYS	PHE	GLY	GLY	CYS	ASN	PHE	THR	LYS	THR	ASN	ALA	ASP	ASN	ALA	GLU	ILE	ASP	ASP	LEU	ASP	VAL	ILE	TRP	ASP	GLY	ASP	HIS	LEU	TYR	PHE	SER	ASN
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● Molecule 1: Potassium channel KAT1



SER	GLU	VAL	GLY	G159	GLY	MET
GLU	LYS	LYS	GLN	L162	GLN	SER
SER	LYS	ILE	SER	L162	ILE	THR
ASN	LYS	LEU	ILE	R165	ALA	ARG
GLY	GLY	GLY	ILE	R174	ILE	ASN
LEU	LEU	GLN	ASP	E186	ASP	PHE
ILE	LEU	LYS	ASP	E186	SER	PHE
LEU	LEU	ILE	SER	E186	ASN	GLU
PRO	ARG	GLU	THR	E240	THR	ARG
SER	ALA	ARG	SER	R246	GLY	PHE
SER	LYS	LYS	GLY	R246	SER	CYS
ILE	VAL	VAL	HIS	Y252	HIS	VAL
GLU	GLU	GLU	GLU	Y252	GLU	GLU
GLU	ARG	ARG	ASN	T256	ASN	GLU
LEU	SER	SER	ASP	T256	ASP	TYR
LEU	SER	SER	ASP	D265	ASP	ASN
ARG	SER	SER	PHE	D265	PHE	ASN
LEU	ARG	GLU	LYS	R310	LYS	ILE
ALA	THR	THR	SER	R310	SER	THR
SER	SER	ALA	MET	D311	MET	ILE
GLY	GLY	GLY	TRP	R314	TRP	LYS
ARG	ARG	ARG	GLY	R314	GLY	GLN
LYS	LYS	LYS	ARG	P411	SER	SER
THR	THR	SER	SER	P411	SER	ALA
LYS	LYS	SER	ARG	T412	ARG	ALA
ILE	LYS	LYS	LYS	D413	LYS	LEU
THR	THR	THR	ASP	D413	ASP	LEU
ILE	LYS	LYS	ASP	F424	GLY	PRO
ASN	ASN	PRO	TYR	T425	TYR	SER
ALA	ALA	TYR	GLY	V426	GLY	LEU
ASP	ASP	CYS	LEU	Y427	LEU	GLY
ASN	ASN	SER	ASP	G430	ASP	ALA
ALA	ALA	SER	VAL	G430	VAL	ARG
GLU	GLU	SER	THR	H431	THR	ILE
ILE	ILE	ASN	ASN	D432	ASN	ASN
ASP	ASP	GLN	PRO	F444	PRO	GLN
ASP	ILE	ILE	THR	F444	THR	SER
LEU	ILE	LYS	SER	L450	SER	THR
ASP	LYS	LYS	ASP	L450	ASP	LYS
VAL	PRO	PRO	THR	Y451	THR	LEU
ILE	ILE	CYS	ALA	Y452	ALA	LEU
TRP	TRP	LYS	LEU	Y452	LEU	ARG
GLY	ASP	ARG	MET	I470	ASP	K49
ASP	GLY	GLU	MET	I470	MET	T85
ASP	ASP	GLU	ALA	S474	ALA	T85
HIS	LYS	LYS	ILE	L475	ILE	T85
LEU	ARG	ARG	HIS	L475	HIS	T85
TYR	THR	THR	GLY	H492	GLY	K87
PHE	THR	THR	LEU	H492	LEU	K87
SER	ILE	ILE	ASP	PHE	ASP	S144
SER	THR	THR	THR	PHE	THR	S144
ASN	MET	MET	GLU	LYS	GLU	S152
			MET	LYS	LYS	S152
			MET	LEU	ARG	N156
			MET	ARG	ARG	N156

● Molecule 1: Potassium channel KAT1



TYR PHE SER SER ASN	VAL	THR	ILE	HIS	MET	SER	GLU	SER	LYS	LYS	ILE	ASN	GLY	LEU	LEU	ILE	LEU	PRO	SER	SER	ILE	SER	LEU	ALA	SER	THR	LYS	ILE	THR	ASN	ASN	CYS	ALA	ASP	ALA	ASN	GLU	ILE	ASP	ASP	ASP	LEU	VAL	VAL	ILE	TRP	ASP	GLY	ASP	LEU
	LYS	GLU	ASP	THR	GLU	VAL	LYS	LYS	ILE	LEU	GLN	LYS	ILE	GLU	ARG	ALA	LYS	VAL	GLU	ARG	LEU	ARG	THR	GLY	ALA	ASN	ASP	THR	ALA	ASN	GLN	ILE	ILE	LYS	PRO	LYS	CYS	ARG	GLU	LYS	ARG	GLU	LYS	LEU						
	LEU	THR	THR	MET	MET	SER	VAL	LYS	LYS	ILE	GLN	LYS	ILE	GLU	ARG	ALA	LYS	VAL	GLU	ARG	LEU	SER	THR	GLY	ALA	ASN	ASP	THR	ALA	ASN	GLN	ILE	ILE	LYS	PRO	LYS	CYS	ARG	GLU	LYS	ARG	GLU	LYS	LEU						
	ASP	THR	THR	THR	ARG	ASN	PHE	ASN	PHE	PHE	GLN	ASP	SER	ASN	THR	SER	GLY	HIS	GLU	ASN	ASP	PHE	LYS	SER	GLY	THR	GLY	THR	VAL	ASN	PRO	THR	SER	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR				
	S144	N156	G159	L162	R165	R174	L181	E186	E240	R246	D265	M282	G286	R310	D311	R314	P356	F387	P411	T412	D413	F424	T425	V426	Y427	G430	H431	D432	F444	L450	Y451	Y452	I470	S474	L475	N492														
	LEU	PHE	MET	LYS	GLN	GLN	SER	ASN	THR	GLY	HIS	GLU	ASN	ASP	THR	THR	GLU	THR	ASP	SER	ARG	LYS	GLY	THR	GLY	LEU	ASP	VAL	THR	ASN	PRO	THR	SER	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR				
	LYS	GLU	LEU	GLY	SER	ILE	ASN	ASP	ASN	GLY	LYS	GLU	LYS	GLY	THR	THR	GLU	THR	ASP	SER	ARG	LYS	GLY	THR	GLY	LEU	ASP	VAL	THR	ASN	PRO	THR	SER	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR				
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	111658	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 ( $e^-/\text{\AA}^2$ )	57.6	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	0.124	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	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: 3PE

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	0.37	0/3568	0.57	0/4876
1	B	0.37	0/3568	0.57	0/4876
1	C	0.37	0/3568	0.57	0/4876
1	D	0.37	0/3568	0.57	0/4876
All	All	0.37	0/14272	0.57	0/19504

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	3465	0	3294	16	0
1	B	3465	0	3294	14	0
1	C	3465	0	3294	16	0
1	D	3465	0	3294	19	0
2	A	51	0	79	1	0
2	B	51	0	79	1	0
2	C	51	0	82	1	0
2	D	51	0	80	2	0
All	All	14064	0	13496	62	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 2.

All (62) 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:D:413:ASP:N	1:D:413:ASP:OD1	2.36	0.58
1:B:413:ASP:OD1	1:B:413:ASP:N	2.36	0.57
1:B:411:PRO:HB2	1:B:444:PHE:HB2	1.88	0.56
1:C:411:PRO:HB2	1:C:444:PHE:HB2	1.88	0.56
1:C:413:ASP:N	1:C:413:ASP:OD1	2.36	0.56
1:A:411:PRO:HB2	1:A:444:PHE:HB2	1.88	0.55
1:A:413:ASP:OD1	1:A:413:ASP:N	2.36	0.55
1:D:411:PRO:HB2	1:D:444:PHE:HB2	1.88	0.55
1:C:186:GLU:O	1:D:310:ARG:NH1	2.41	0.53
1:A:186:GLU:O	1:B:310:ARG:NH1	2.41	0.53
1:B:470:ILE:HA	1:B:474:SER:HB3	1.91	0.52
1:A:470:ILE:HA	1:A:474:SER:HB3	1.91	0.52
1:C:470:ILE:HA	1:C:474:SER:HB3	1.92	0.52
1:D:470:ILE:HA	1:D:474:SER:HB3	1.92	0.52
1:A:310:ARG:NH1	1:D:186:GLU:O	2.42	0.52
1:B:186:GLU:O	1:C:310:ARG:NH1	2.43	0.52
1:B:286:GLY:HA3	2:B:701:3PE:H281	1.92	0.51
1:D:286:GLY:HA3	2:D:701:3PE:H281	1.93	0.49
1:A:246:ARG:HA	1:A:246:ARG:HD2	1.72	0.47
1:B:85:THR:HA	1:B:165:ARG:HH22	1.80	0.47
1:C:252:TYR:O	1:C:256:THR:OG1	2.26	0.46
1:C:85:THR:HA	1:C:165:ARG:HH22	1.80	0.46
1:A:85:THR:HA	1:A:165:ARG:HH22	1.80	0.46
1:D:144:SER:O	1:D:174:ARG:NH2	2.45	0.46
1:A:252:TYR:O	1:A:256:THR:OG1	2.26	0.46
1:D:85:THR:HA	1:D:165:ARG:HH22	1.80	0.46
1:D:311:ASP:OD1	1:D:314:ARG:NH2	2.50	0.45
1:D:475:LEU:HD12	1:D:475:LEU:HA	1.80	0.45
1:A:311:ASP:OD1	1:A:314:ARG:NH2	2.50	0.45
1:D:426:VAL:HG23	1:D:430:GLY:HA3	1.99	0.45
1:B:311:ASP:OD1	1:B:314:ARG:NH2	2.50	0.45
1:C:246:ARG:HA	1:C:246:ARG:HD2	1.73	0.45
1:C:426:VAL:HG23	1:C:430:GLY:HA3	1.99	0.45
1:D:246:ARG:HD2	1:D:246:ARG:HA	1.72	0.45
1:A:426:VAL:HG23	1:A:430:GLY:HA3	1.99	0.45
1:B:426:VAL:HG23	1:B:430:GLY:HA3	1.99	0.45
1:C:311:ASP:OD1	1:C:314:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:MET:HB2	1:D:282:MET:HE2	1.72	0.44
1:B:144:SER:O	1:B:174:ARG:NH2	2.45	0.44
1:C:144:SER:O	1:C:174:ARG:NH2	2.45	0.44
1:D:424:PHE:HB2	1:D:432:ASP:HB2	2.00	0.43
1:A:424:PHE:HB2	1:A:432:ASP:HB2	2.00	0.43
1:B:424:PHE:HB2	1:B:432:ASP:HB2	2.00	0.43
1:C:424:PHE:HB2	1:C:432:ASP:HB2	2.00	0.43
2:C:701:3PE:H372	2:C:701:3PE:H341	1.92	0.42
1:A:62:TRP:NE1	1:A:105:ASP:OD2	2.45	0.42
1:B:426:VAL:HG12	1:B:427:TYR:H	1.85	0.42
1:A:265:ASP:N	1:A:265:ASP:OD1	2.53	0.42
1:D:426:VAL:HG12	1:D:427:TYR:H	1.85	0.42
1:A:426:VAL:HG12	1:A:427:TYR:H	1.85	0.42
1:C:426:VAL:HG12	1:C:427:TYR:H	1.85	0.41
1:B:265:ASP:OD1	1:B:265:ASP:N	2.53	0.41
1:C:152:SER:O	1:C:152:SER:OG	2.35	0.41
1:C:475:LEU:HA	1:C:475:LEU:HD12	1.79	0.41
1:A:203:SER:HB3	2:A:701:3PE:H371	2.03	0.41
1:C:265:ASP:OD1	1:C:265:ASP:N	2.53	0.41
1:D:67:VAL:HG21	1:D:181:LEU:HD13	2.03	0.41
1:D:73:SER:O	1:D:73:SER:OG	2.39	0.41
1:A:144:SER:O	1:A:174:ARG:NH2	2.45	0.41
1:B:475:LEU:HD12	1:B:475:LEU:HA	1.79	0.41
1:D:75:TRP:CD1	2:D:701:3PE:H3E2	2.56	0.40
1:D:265:ASP:N	1:D:265:ASP:OD1	2.53	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	442/677 (65%)	379 (86%)	62 (14%)	1 (0%)	44	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	442/677 (65%)	379 (86%)	62 (14%)	1 (0%)	44	75
1	C	442/677 (65%)	379 (86%)	62 (14%)	1 (0%)	44	75
1	D	442/677 (65%)	379 (86%)	62 (14%)	1 (0%)	44	75
All	All	1768/2708 (65%)	1516 (86%)	248 (14%)	4 (0%)	45	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	356	PRO
1	B	356	PRO
1	C	356	PRO
1	D	356	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	349/607 (58%)	347 (99%)	2 (1%)	84	92
1	B	349/607 (58%)	347 (99%)	2 (1%)	84	92
1	C	349/607 (58%)	347 (99%)	2 (1%)	84	92
1	D	349/607 (58%)	347 (99%)	2 (1%)	84	92
All	All	1396/2428 (58%)	1388 (99%)	8 (1%)	82	92

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	387	PHE
1	A	452	TYR
1	B	387	PHE
1	B	452	TYR
1	C	387	PHE
1	C	452	TYR
1	D	387	PHE

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Mol	Chain	Res	Type
1	D	452	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	ASN
1	A	348	GLN
1	A	365	ASN
1	A	491	ASN
1	B	294	ASN
1	B	348	GLN
1	B	365	ASN
1	B	491	ASN
1	C	294	ASN
1	C	348	GLN
1	C	365	ASN
1	C	491	ASN
1	D	294	ASN
1	D	348	GLN
1	D	365	ASN
1	D	491	ASN

### 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	$\# Z  > 2$
2	3PE	C	701	1	50,50,50	0.94	2 (4%)	53,55,55	0.88	1 (1%)
2	3PE	B	701	1	50,50,50	0.94	2 (4%)	53,55,55	0.92	1 (1%)
2	3PE	A	701	1	50,50,50	0.97	2 (4%)	53,55,55	0.89	1 (1%)
2	3PE	D	701	1	50,50,50	0.94	2 (4%)	53,55,55	0.93	1 (1%)

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	3PE	C	701	1	-	14/54/54/54	-
2	3PE	B	701	1	-	20/54/54/54	-
2	3PE	A	701	1	-	24/54/54/54	-
2	3PE	D	701	1	-	19/54/54/54	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	3PE	P-O13	4.01	1.75	1.59
2	D	701	3PE	P-O13	4.00	1.75	1.59
2	C	701	3PE	P-O13	4.00	1.75	1.59
2	B	701	3PE	P-O13	3.99	1.75	1.59
2	A	701	3PE	P-O11	2.66	1.70	1.59
2	C	701	3PE	P-O11	2.60	1.69	1.59
2	D	701	3PE	P-O11	2.53	1.69	1.59
2	B	701	3PE	P-O11	2.52	1.69	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	3PE	O12-P-O14	4.78	135.86	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	3PE	O12-P-O14	4.77	135.84	112.24
2	C	701	3PE	O12-P-O14	4.76	135.77	112.24
2	A	701	3PE	O12-P-O14	4.73	135.63	112.24

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	3PE	C1-O11-P-O12
2	A	701	3PE	C11-O13-P-O14
2	B	701	3PE	C1-O11-P-O12
2	B	701	3PE	C11-O13-P-O14
2	C	701	3PE	C1-O11-P-O12
2	C	701	3PE	C11-O13-P-O14
2	D	701	3PE	C1-O11-P-O12
2	C	701	3PE	C21-C22-C23-C24
2	B	701	3PE	C22-C21-O21-C2
2	A	701	3PE	C21-C22-C23-C24
2	A	701	3PE	C31-C32-C33-C34
2	D	701	3PE	C22-C21-O21-C2
2	B	701	3PE	O22-C21-O21-C2
2	D	701	3PE	O22-C21-O21-C2
2	A	701	3PE	C25-C26-C27-C28
2	A	701	3PE	C38-C39-C3A-C3B
2	B	701	3PE	C22-C23-C24-C25
2	B	701	3PE	C2E-C2F-C2G-C2H
2	C	701	3PE	C28-C29-C2A-C2B
2	D	701	3PE	C22-C23-C24-C25
2	A	701	3PE	C3B-C3C-C3D-C3E
2	D	701	3PE	C36-C37-C38-C39
2	A	701	3PE	C37-C38-C39-C3A
2	C	701	3PE	C23-C24-C25-C26
2	A	701	3PE	C26-C27-C28-C29
2	B	701	3PE	C36-C37-C38-C39
2	A	701	3PE	C2E-C2F-C2G-C2H
2	A	701	3PE	C33-C34-C35-C36
2	A	701	3PE	C22-C23-C24-C25
2	A	701	3PE	C3A-C3B-C3C-C3D
2	C	701	3PE	C33-C34-C35-C36
2	D	701	3PE	O11-C1-C2-C3
2	C	701	3PE	C1-C2-C3-O31
2	D	701	3PE	C2D-C2E-C2F-C2G

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Mol	Chain	Res	Type	Atoms
2	B	701	3PE	C32-C31-O31-C3
2	D	701	3PE	C32-C31-O31-C3
2	A	701	3PE	C23-C24-C25-C26
2	B	701	3PE	C2F-C2G-C2H-C2I
2	C	701	3PE	C27-C28-C29-C2A
2	B	701	3PE	O32-C31-O31-C3
2	D	701	3PE	O32-C31-O31-C3
2	B	701	3PE	C1-C2-C3-O31
2	D	701	3PE	C1-C2-C3-O31
2	C	701	3PE	C31-C32-C33-C34
2	B	701	3PE	O11-C1-C2-C3
2	B	701	3PE	C32-C33-C34-C35
2	A	701	3PE	C2-C1-O11-P
2	A	701	3PE	C1-C2-C3-O31
2	C	701	3PE	O21-C2-C3-O31
2	C	701	3PE	C11-O13-P-O11
2	B	701	3PE	C2-C1-O11-P
2	C	701	3PE	C2-C1-O11-P
2	D	701	3PE	C2-C1-O11-P
2	D	701	3PE	C32-C33-C34-C35
2	D	701	3PE	C2F-C2G-C2H-C2I
2	C	701	3PE	C2D-C2E-C2F-C2G
2	A	701	3PE	C2C-C2D-C2E-C2F
2	B	701	3PE	O11-C1-C2-O21
2	D	701	3PE	O11-C1-C2-O21
2	A	701	3PE	O21-C2-C3-O31
2	B	701	3PE	C34-C35-C36-C37
2	D	701	3PE	C34-C35-C36-C37
2	D	701	3PE	C3F-C3G-C3H-C3I
2	C	701	3PE	C26-C27-C28-C29
2	A	701	3PE	C11-O13-P-O11
2	B	701	3PE	C11-O13-P-O11
2	D	701	3PE	C11-O13-P-O11
2	A	701	3PE	C39-C3A-C3B-C3C
2	A	701	3PE	C32-C33-C34-C35
2	A	701	3PE	O22-C21-O21-C2
2	A	701	3PE	C27-C28-C29-C2A
2	A	701	3PE	C22-C21-O21-C2
2	B	701	3PE	O21-C2-C3-O31
2	D	701	3PE	O21-C2-C3-O31
2	B	701	3PE	C3F-C3G-C3H-C3I
2	D	701	3PE	C11-O13-P-O14

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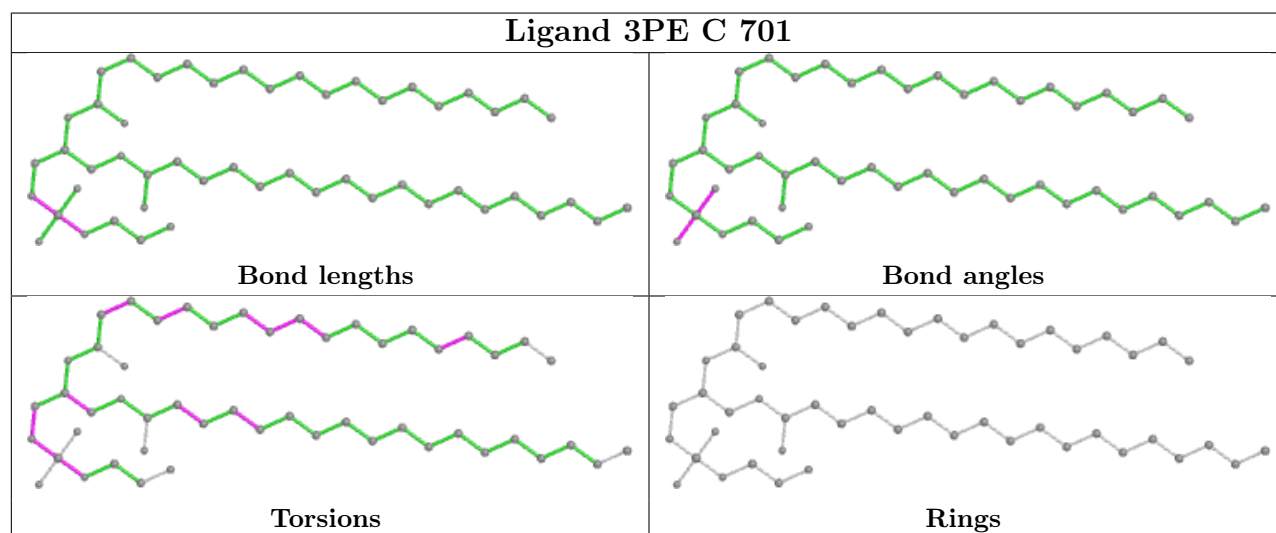
Mol	Chain	Res	Type	Atoms
2	B	701	3PE	C3C-C3D-C3E-C3F

There are no ring outliers.

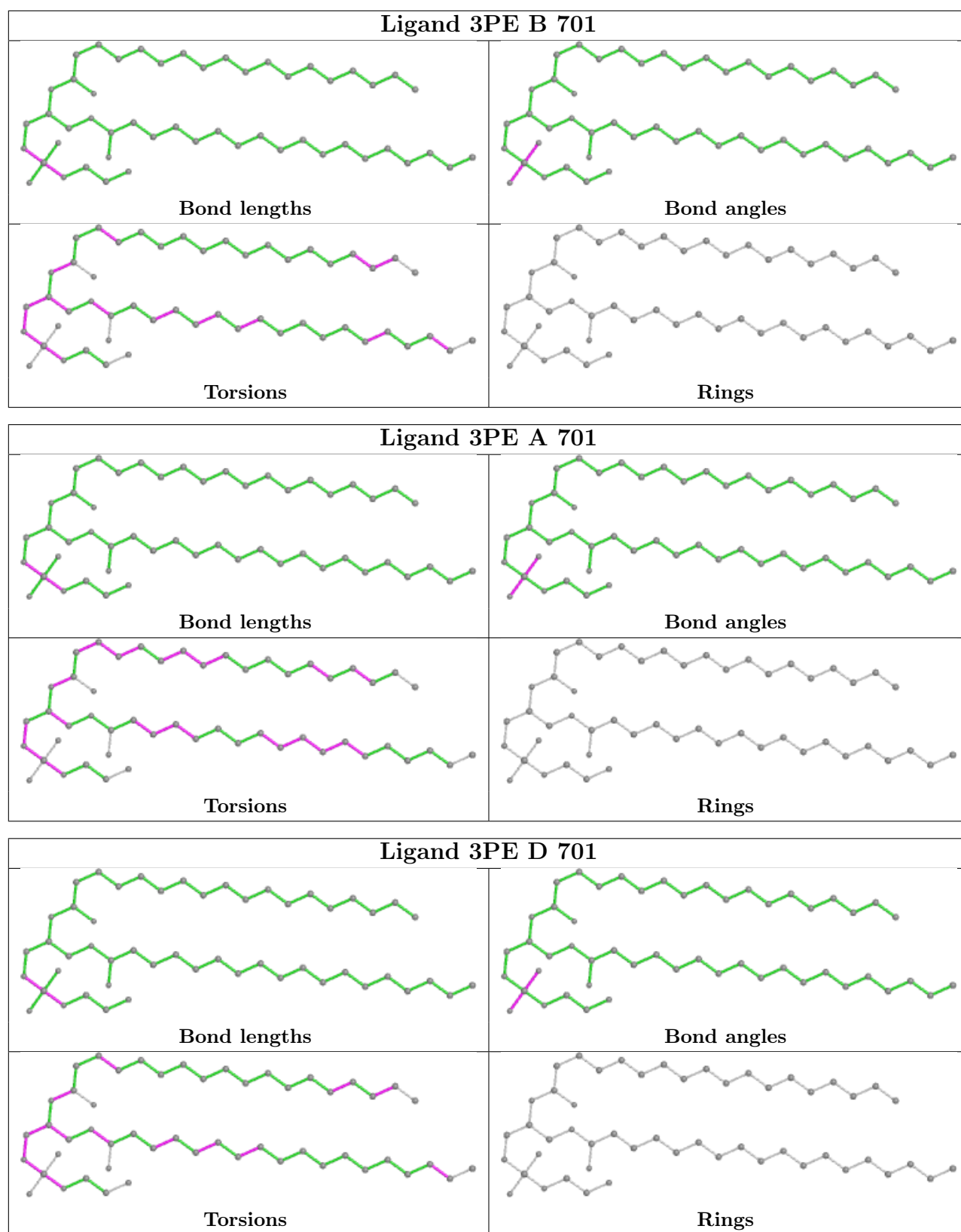
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	3PE	1	0
2	B	701	3PE	1	0
2	A	701	3PE	1	0
2	D	701	3PE	2	0

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







## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

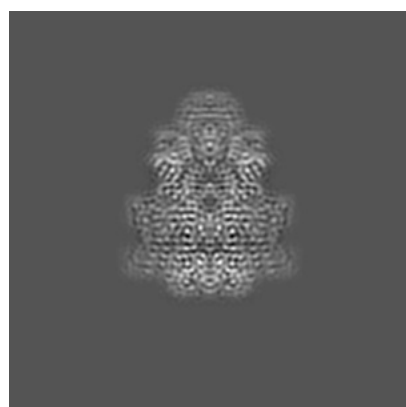
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30334. These allow visual inspection of the internal detail of the map and identification of artifacts.

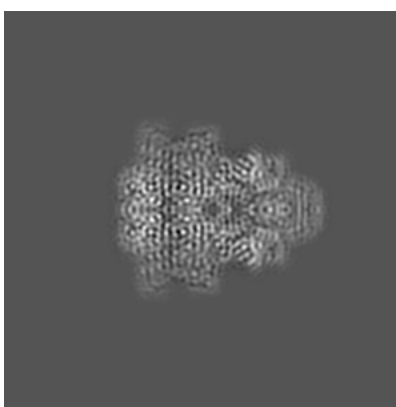
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

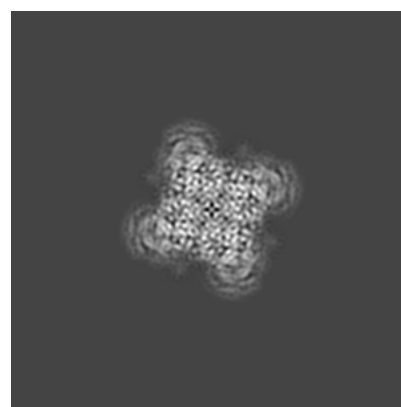
#### 6.1.1 Primary map



X



Y



Z

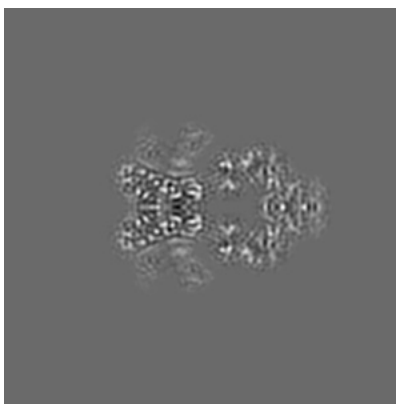
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

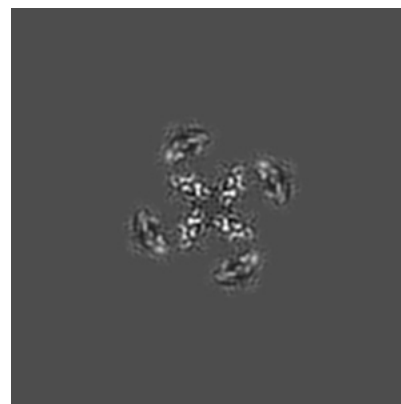
#### 6.2.1 Primary map



X Index: 120



Y Index: 120



Z Index: 120

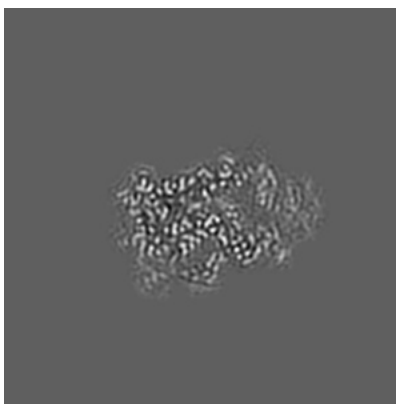
The images above show central slices of the map in three orthogonal directions.

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

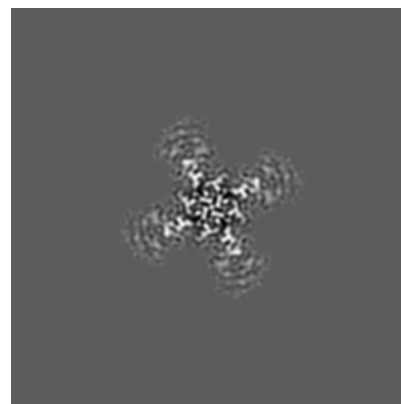
### 6.3.1 Primary map



X Index: 107



Y Index: 107

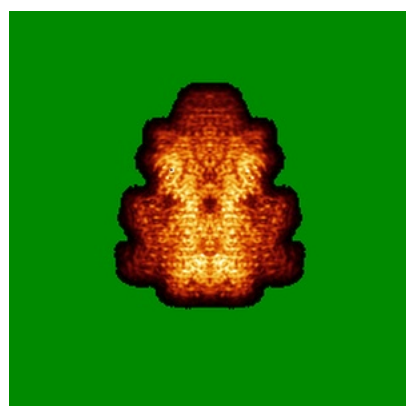


Z Index: 92

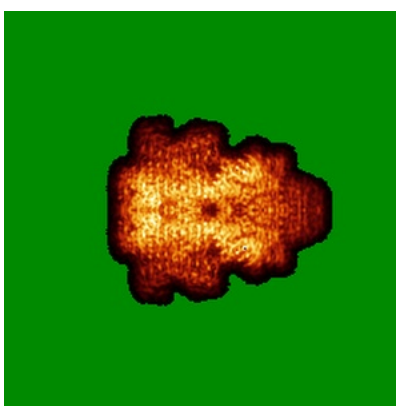
The images above show the largest variance slices of the map in three orthogonal directions.

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

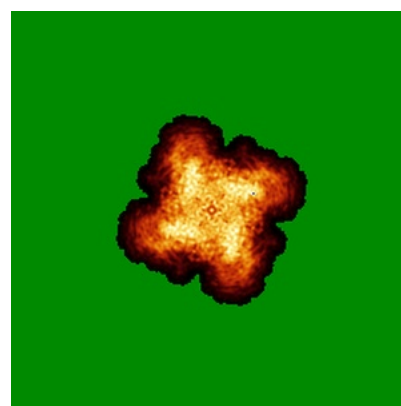
### 6.4.1 Primary map



X



Y

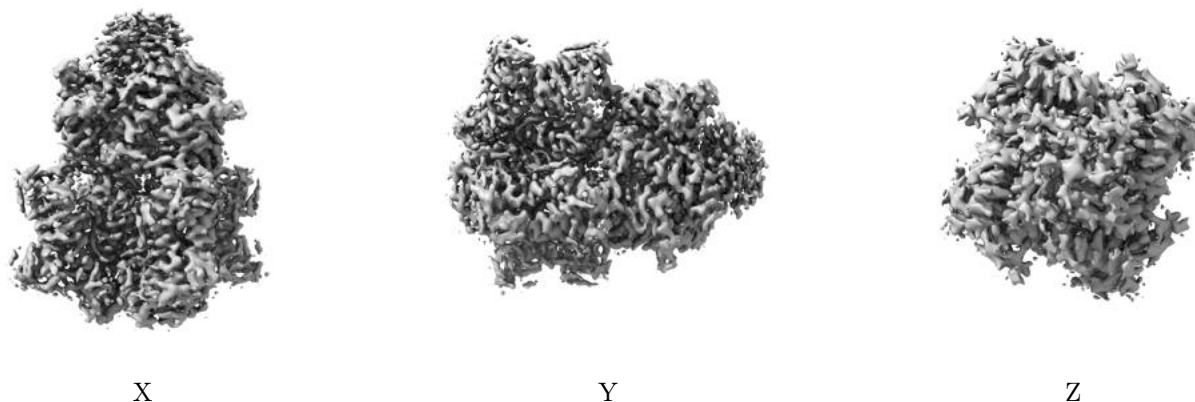


Z

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

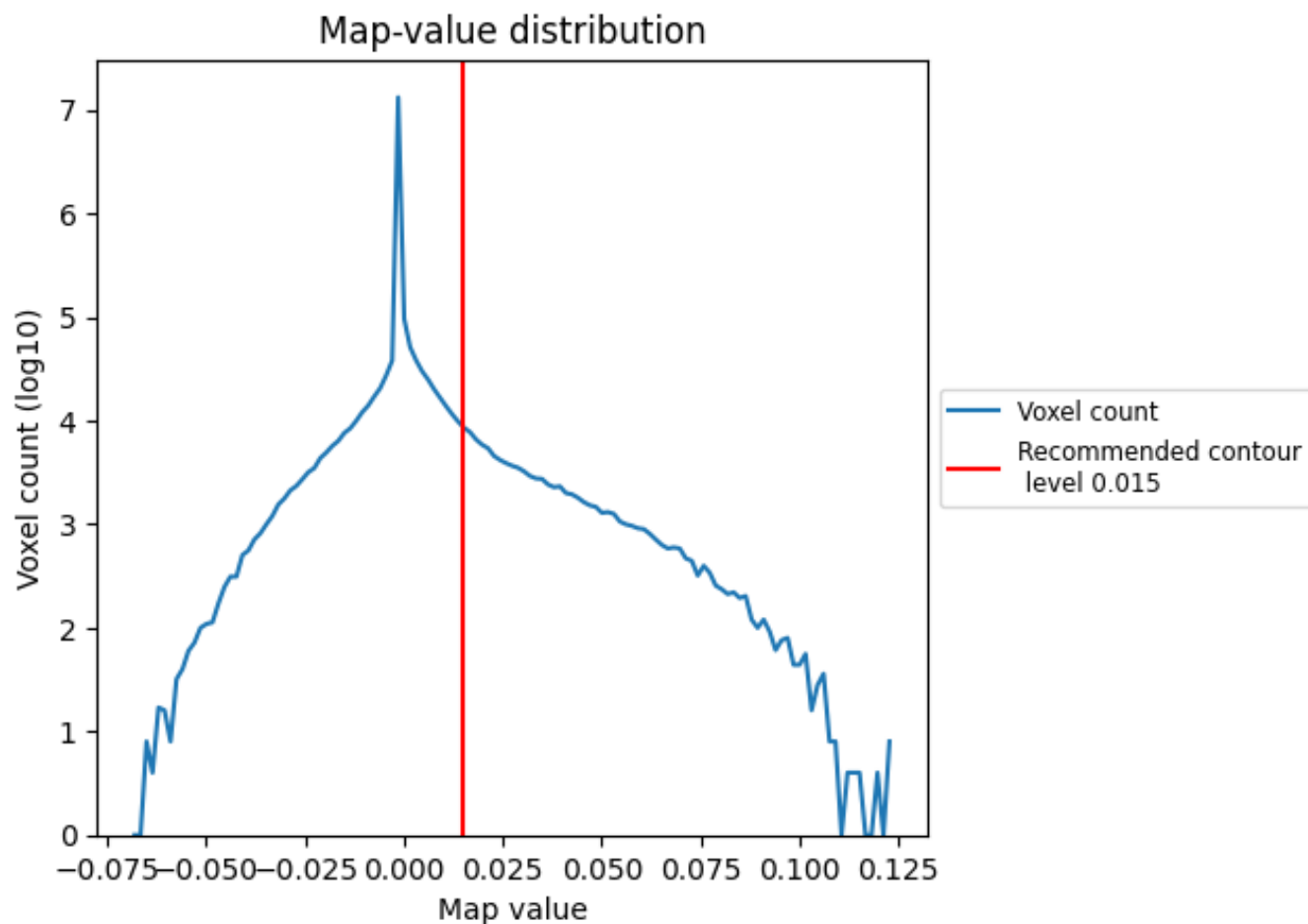
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

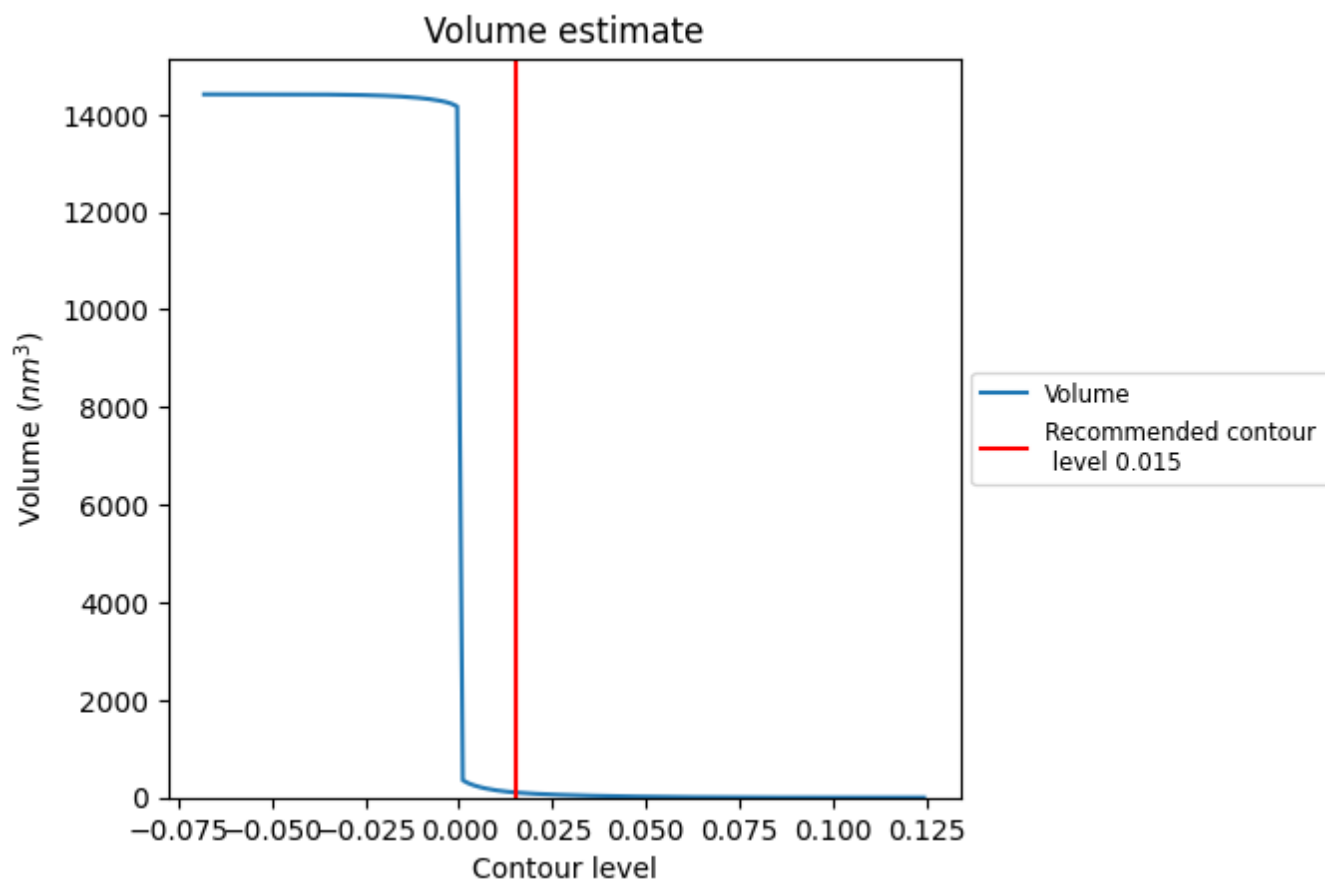
This section contains the results of statistical analysis of the map.

### 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.

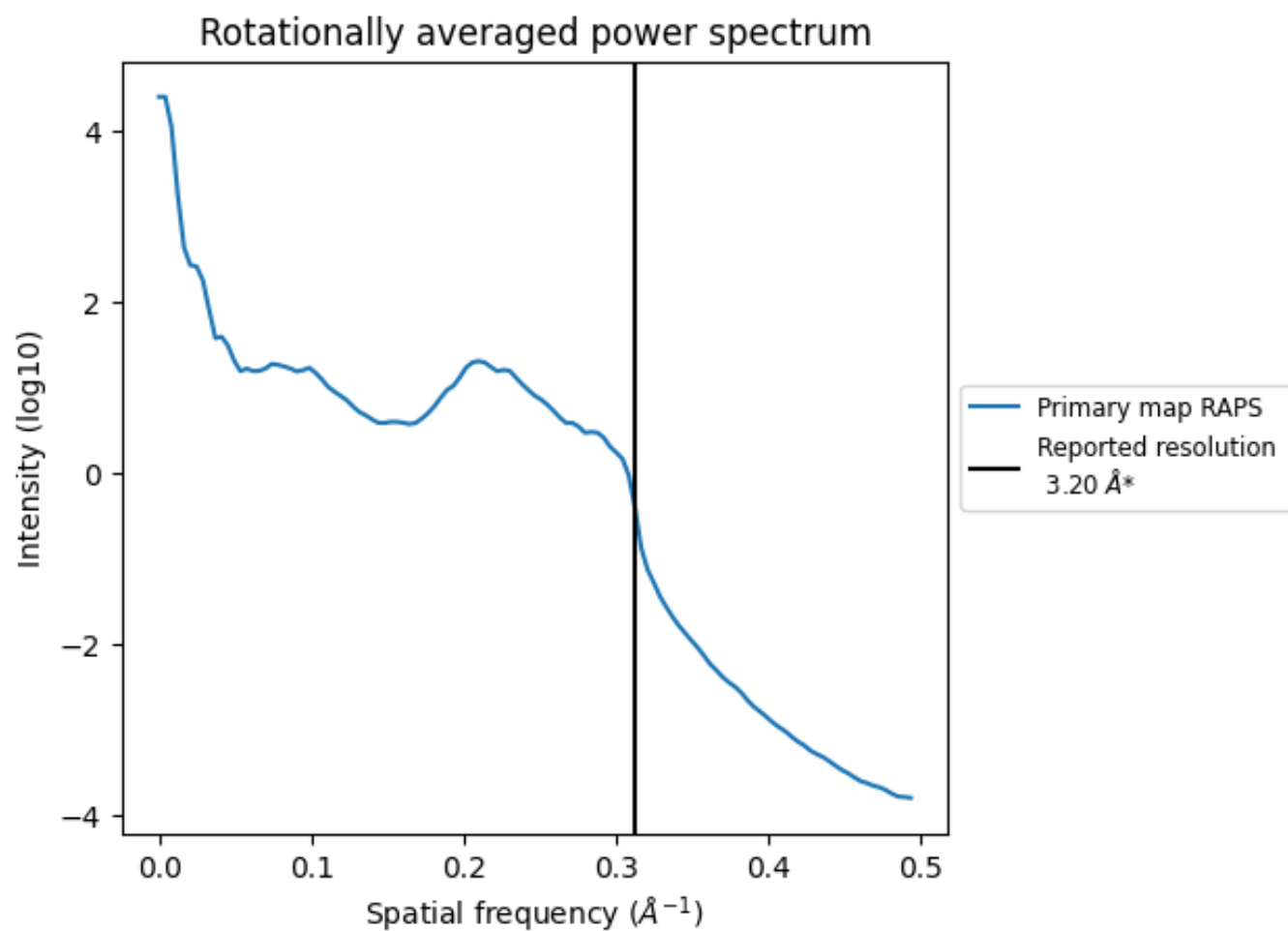
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105  $\text{nm}^3$ ; this corresponds to an approximate mass of 95 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 0.312 Å<sup>-1</sup>



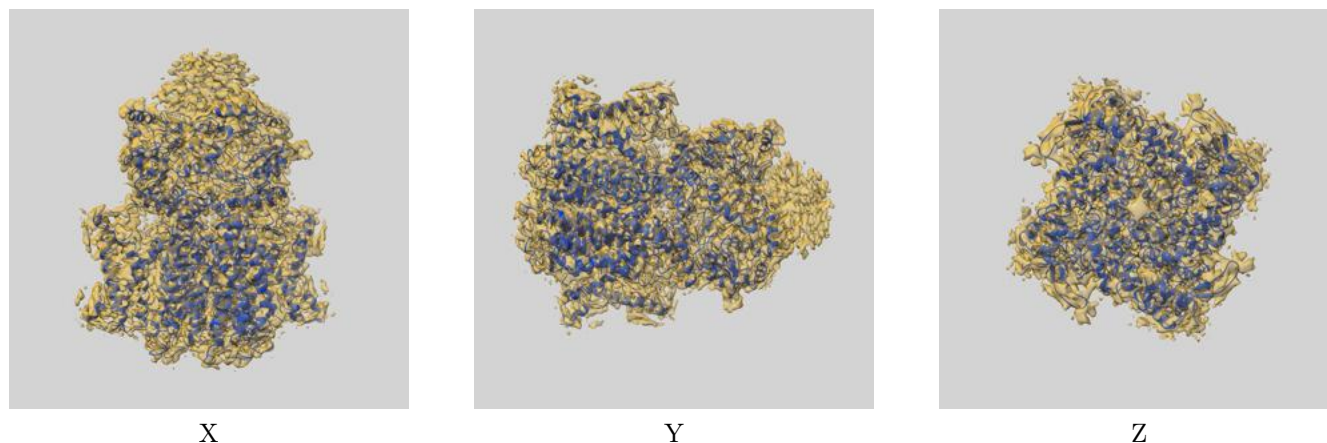
## 8 Fourier-Shell correlation

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

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

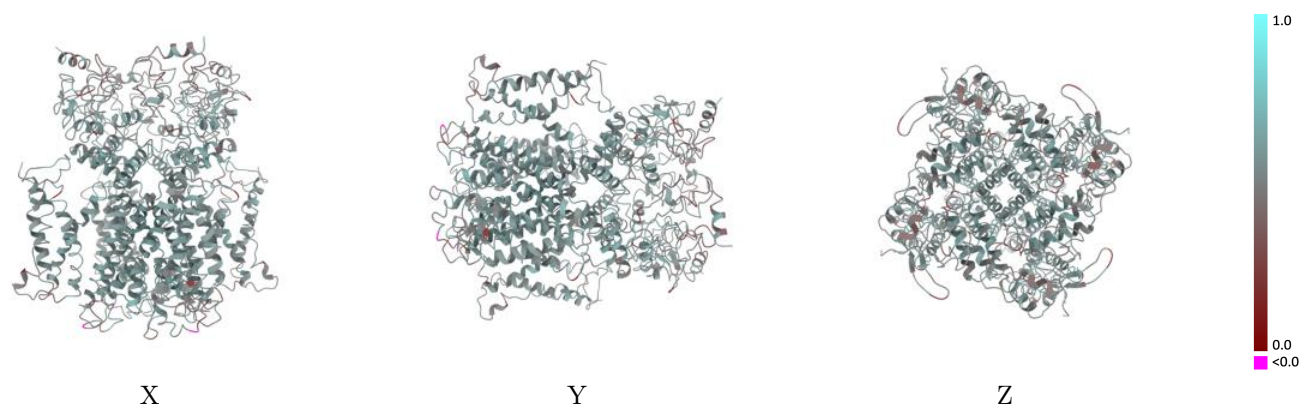
This section contains information regarding the fit between EMDB map EMD-30334 and PDB model 7CAL. Per-residue inclusion information can be found in section [3](#) on page [5](#).

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



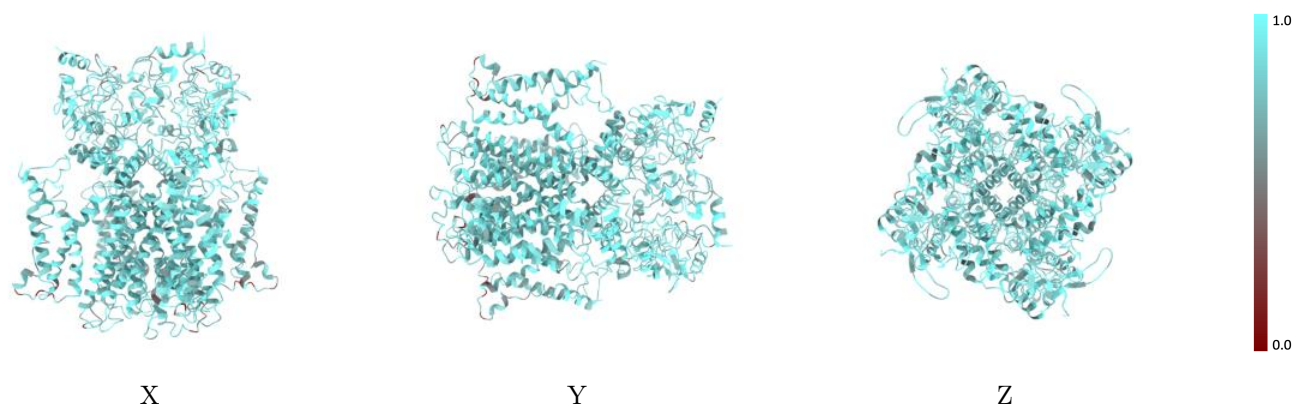
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



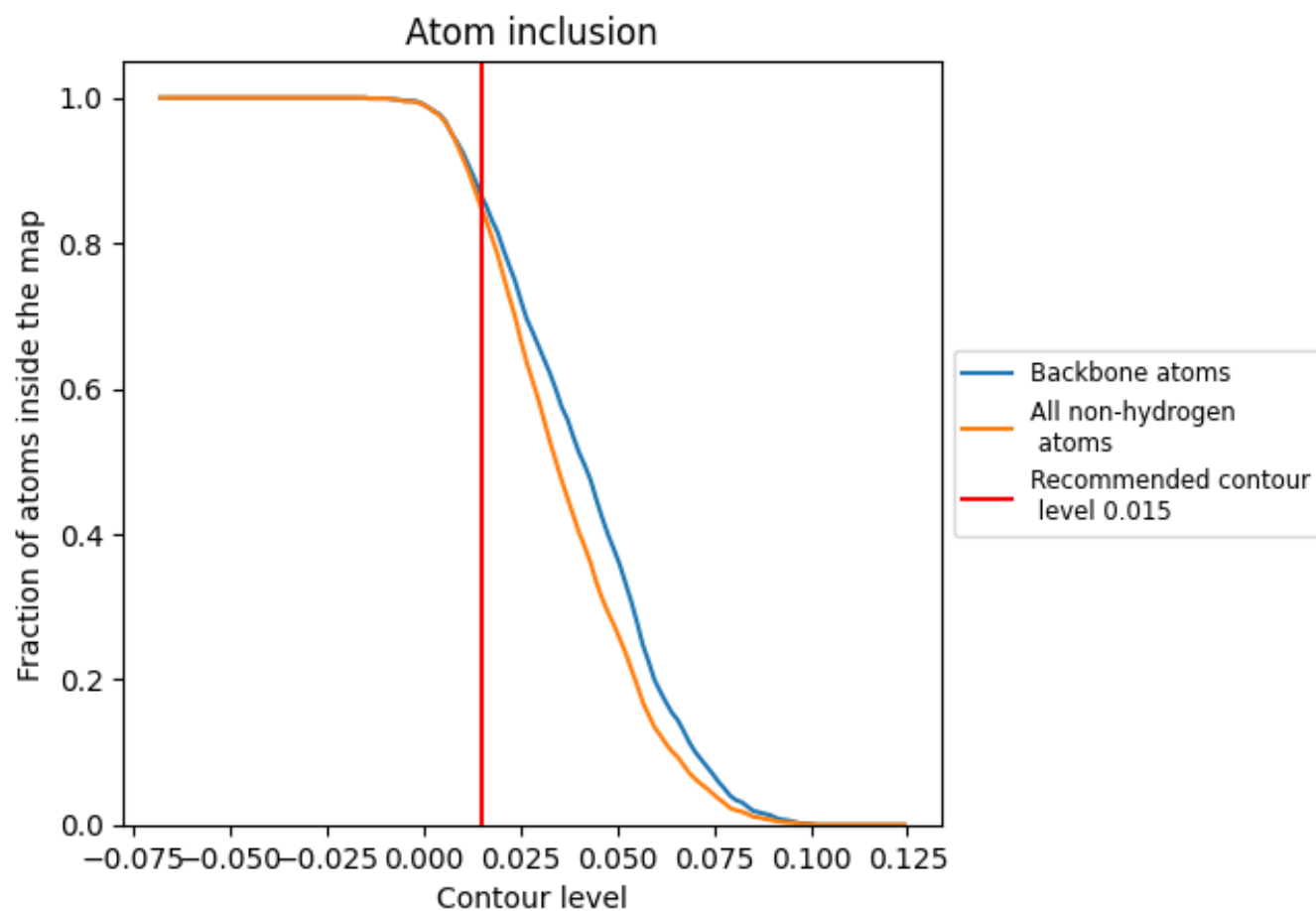
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 85% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8460	<div></div> 0.5320
A	<div></div> 0.8470	<div></div> 0.5310
B	<div></div> 0.8460	<div></div> 0.5320
C	<div></div> 0.8460	<div></div> 0.5340
D	<div></div> 0.8460	<div></div> 0.5320

